# NANGE AND NANOTECHNICICON CONFERENCE

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# Book of Abstracts





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NanoTR-16 Book of Abstract

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# Preface

There is no doubt this century has revealed significant changes in the field of nanotechnology. Since the 1st conference in 2005, annual Nanoscience and Nanotechnology Conference (NanoTR) series have been one of the most important and prestigious nanotechnology meetings of Turkey. It did welcome not only Turkish researchers but also international researchers from all over the world with expertises in materials science, life sciences, basic sciences and engineering. In this context, NanoTR-16 brought approximately 500 researchers, scientists and experts together from academia, institutions and companies to highlight their current studies and share their latest knowledge. Within the remarkable advancements in the research field, NanoTR-16 provided an inspring program on the topics, including as diverse as nanofabrication, photonics, electronics, nanosensors and nanoactuators, nanorobotics, nanodevices, energy, polymer technology, electrochemistry, bioengineering, medicine, modeling and simulation. The conference had 4 plenary talks, 20 invited talks, 187 oral presentations, and 154 poster presentations. We are happy to share that all participants had the opportunity to meet well-known and eligible scientists working in different disciplines. Therefore, the conference had a great impact on encouraging young researchers, particularly postdoctoral researchers, graduate and undergraduate students, to present and discuss their work and ideas. Moreover, NanoTR-16 offered great opportunity for nanotech companies to meet with their community.

The conference has started with the Opening Speech of Prof. Dr. Hasan Mandal, President of The Scientific and Technological Research Council of Türkiye and continued in 3 parallel sessions for 4 days. We would like to thank our Plenary Speakers, Invited Speakers, participants, and all sponsors for the valuable contributions to NanoTR-16. We would like to thank Prof. Dr. Oğuz Gülseren, the chair of NanoTR-15 for his valuable support and mentoring. Our thanks and appreciations also go to the Organization Committee Members and Scientific Board Members. We would like to thank the Organization Office, Arber Kongre for their hard work.

We once again thank all the NanoTR-16 community who made this meeting a truly successful one.

With best regards,

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# **Opening Speech**



Hasan Mandal President of TÜBİTAK

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Nader Engheta University of Pennsylvania USA



Hong Jin Fan Nanyang Technological University Singapore



Arben Merkoçi Catalan Institute of Nanoscience and Nanotechnology ICN2 Spain



**Joseph Wang** University of California, San Diego USA

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# **Oral Presentations**

ID: 380

#### **Metaphotonics for Structuring Light**

#### Nader Engheta

H. Nedwill Ramsey Professor, University of Pennsylvania, Philadelphia, United States

In this talk, I will present an overview of some of our ongoing research programs on metaphotonics, in which we explore how metamaterials and metasurfaces can provide exciting possibilities for light-matter interaction with useful functionalities. As one scenario, I will discuss how metamaterials can be designed to perform analog computation with waves, effectively working as metamaterial computing machines, solving equations and inverting matrices with waves. As the second case, I will discuss our work on near-zero-index photonics and its roles on extreme wave physics and quantum phenomena. If time permits, I will also present some of our results on four-dimensional (4D) metastructures, in which the materials parameters can rapidly change with time, in addition to the spatial inhomogeneities, offering novel phenomena in light-matter interaction. I will also discuss some of the possible future research directions in these areas.

## Ubiquitous Nanobiosensors Technologies for REASSURED Diagnostics Applications

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There is a need for new, innovative and overall cost/efficient diagnostic devices especially in low-resource settings. The need for such diagnostic tools is raising not only in health area but also in other fields such as environment, safety and security industries. COVID19 has overall heightened the need the society has for such kind of devices known also as biosensors. Their development is strongly related to new materials and technologies being nanomaterials and nanotechnology of special role. We study how new nanomaterials such as nanoparticles or graphene can be integrated into simple biosensing platforms like paper thanks to their advantageous properties. Chemical and mechanical properties of cellulose in both micro and nanofiberbased networks combined with their abundance in nature or easy to prepare and control procedures are making these materials of great interest while looking for cost-efficient and green alternatives for device production technologies. These devices should be REASSURED: Real-time connectivity, Ease of specimen collection, Affordable, Sensitive, Specific, User-friendly, Rapid, Robust, Equipment-free, Delivered to those who need it. How to design simple paper-based biosensor architectures including wearables through printing or stamping? How to fabricate these devices in a fast, efficient and overall reasonable cost? How to tune their analytical performance upon demand? How one can couple nanomaterials with paper and what is the benefit? Which are the perspectives to link these simple platforms and detection technologies with mobile communication? I will try to give responses to these questions through various interesting applications related to protein, DNA and even bacteria and viruses with extreme interest for clinical emergency applications. Various biosensing technologies ranging from screen and inkjet printing, stamping including its combination with laser scribing technique will be given. The developed platforms and related technologies are related to ubiquitous methods that would be quite important for democratising diagnosis and improving healthcare coverage.

### Wearable Electrochemical Sensors: Towards Labs on the Skin and on the Mouth

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Wearable sensors have received a major recent attention owing to their considerable promise for monitoring the wearer's health and wellness [1,2]. The medical interest for wearable systems arises from the need for monitoring patients over long periods of time. These devices have the potential to continuously collect vital health information from a person's body and provide this information to them or their healthcare provider in a timely fashion. Such sensing platforms provide new avenues to continuously and non-invasively monitor individuals and can thus tender crucial real-time information regarding a wearer's health. This presentation will discuss recent developments in the field of wearable electrochemical sensors integrated directly on the epidermis, under the skin, or within the mouth for various non-invasive and minimally-invasive biomedical monitoring applications [3-6]. Particular attention will be given to non-invasive monitoring of metabolites and electrolytes using flexible electrochemical sensors, to multiplexed microneedle sensor arrays, along with related materials, energy and integration considerations. The preparation and characterization of such wearable electrochemical sensors will be described, along with their current status and future prospects and challenges.

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### **Zn-Based Batteries: Opportunities and Challenges**

#### <u>Hong Jin Fan</u>

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Rechargeable aqueous Zn batteries (AZB) are being widely and extensively studied. In recent years, there has been tremendous progress in fundamental understanding, battery performance by rational design of electrode materials and electrolytes as well as their interface, and device architectures. So far, the energy density of AZB is still not competitive compared to Li-ion batteries. Among most cathode materials, manganese oxide and related compounds are being mostly investigated. However, the reaction mechanism has been complicated and varies from one report to another report. On the Zn anode side, bare Zn is unstable in a wide pH range. The Zn anode suffers from a few issues, including dendrite growth due to inhomogeneous nucleation and growth, corrosion due to hydrogen evolution reaction, and passivation due to side reactions.

Our group has been actively working in designing nanostructured electrode materials for secondary batteries and recently focus on rechargeable AZB. This seminar will give a complete story about the evolution of  $Zn-MnO_2$  batteries with a focus on the understanding of charge storage mechanism in sulfate electrolytes. It will elaborate some typical strategies for Zn anode stabilization with a focus on mechanistic understanding rather than materials engineering.

# Group III-V Epilayers Grown by Molecular Beam Epitaxy: Growth and Characterization

### <u>Uğur Serincan</u>

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Nowadays, group III-V based structure are very attractive choice for a wide range of applications. Among those, the most important ones could be listed as light emitting diodes, photodetectors, transistors and high efficiency solar cells. In this study, group III-V semiconductor epilayers were grown using molecular beam epitaxy (MBE) method and investigated using various characterization techniques.

Regarding photodetectors, type II superlattice (T2SL) detectors are received much interest due to their tunable responsivities between 3 and 32  $\mu$ m by varying the thickness of epilayers in T2SL periods. Considering the lattice match case between epilayers and substrate, T2SL structures are commonly grown on GaSb substrates. On the other hand, GaSb is quite expensive compared to GaAs and Si substrates. Recently, in order to fabricate cost effective T2SL detectors they are grown on GaAs and Si substrates by developing new approaches to overcome the difficulties because of the lattice mismatch between the epilayers and substrates. In this study, T2SL detectors grown on GaSb, GaAs and Si substrates are presented by comparing their structural and optoelectronic properties [1-3].

The other group of materials are high efficient solar cells. There is an increasing demand for high-efficient GaAs-based group III-V solar cells (SC) in satellite-space, aviation and similar strategic areas. Although the GaAs-based single and multiple junction group III-V SC technologies have records in efficiency, they are mainly used in special applications where the Watt/weight value is a priority rather than the production costs. The largest input with a percentage of 80-85% at this high cost are expensive substrates. Recently, flexible thin film cell technology based on the epitaxial lift-off (ELO) method has attracted attention in order to minimize costs. In this approach, based on the separation of the epilayer from the substrate and transferring it to another platform, the production costs can be reduced at several orders as the substrates can be used multiple times. In addition, the cells produced by this method are much more functional in applications due to the advantages brought by their flexibility, having higher temperature and radiation tolerances and record Watt/weight compared to substrate-based SC. It is important to use much cheaper Si substrates instead of GaAs substrates to further reduce the costs. Hence, to compare the performances, we fabricated high efficient solar cells on GaAs and Si substrates and by using ELO method we manage to transfer those structures on flexible thin films [4-5].

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Keyword: T2SL, solar cell, flexible, photodetector, infrared

# **High-Efficiency Thermoelectric Materials**

#### Umut Aydemir

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Since the discovery of the thermoelectric effects by Seebeck, Peltier, and Thomson in the XIX<sup>th</sup> century, thermoelectricity has attracted attention for both fundamental and industrial reasons. Nowadays, this interest has been rejuvenated by the evergrowing worldwide energy demand and the concomitant environmental concerns. Globally, two-thirds of the energy produced is lost as waste heat. Among renewable energy sources, thermoelectricity stands for a possible alternative that could not only allow for waste-heat energy harvesting but could also replace compression-based refrigerators [1]. This versatile technology directly converts heat into electricity and vice-versa. Being vibration- and noise-free, reliable, scalable, and without hazardous emissions, solid-state thermoelectric generators can be considered as a clean and sustainable energy source. The thermoelectric efficiency of a given material is quantified through the dimensionless thermoelectric figure of merit, zT, defined as  $zT = a^2T / rk$  where T is the absolute temperature, a is the thermopower (or Seebeck coefficient), r is the electrical resistivity and k is the total thermal conductivity which is the sum of the lattice thermal conductivity,  $k_{\rm L}$ , and the electronic thermal conductivity,  $k_{\rm E}$ , in non-magnetic materials. Thus, a good thermoelectric material must strike a balance between a large  $\alpha$ , low  $\rho$ , and low, which is very challenging.

In my talk, I will discuss the fundamentals of thermoelectric theory and devices, the basics of efficiency optimization, and how such devices are used in space and other technological applications. With promising novel structure types and compounds being reported on a frequent basis, Zintl phases as "phonon-glass electron-crystal" materials represent an important and incredibly diverse new class of thermoelectrics. Herein, I will explain why Zintl phases' characteristics make them good thermoelectric materials. I will introduce the crystal structure, tunable electronic transport properties, and glass-like lattice thermal conductivity of n-type Mg<sub>3</sub>Sb<sub>2</sub> as a high-efficiency Sb-based Zintl phase representative. Additionally, I will talk about stress/pressure-stabilized cubic polymorph of Li<sub>3</sub>Sb displaying improved thermoelectric performance.

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Keyword: Thermoelectric, Zintl Phase, Energy

# Engineering Organic Materials for Optoelectronics and Nanotechnology

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The past century has been the era of mastering chemistry to develop modern functional materials.  $\pi$ -conjugated small molecules and polymers have attracted great attention over the last three decades as functional materials. Owing to their unique features over traditional inorganics and metals, they are envisioned as essential components of next-generation optoelectronics and nanotechnology applications. Our research is focused on designing and building state-of-the-art, high-performance organic optoelectronic materials as well as understanding key structure-property-device relationships. Herein, we describe the molecular design, synthesis, characterization, and device performances of novel solution-processable [1]benzothieno[3,2-b][1]benzothiophene (BTBT)- and indenofluorene (IF)-based *n*-type organic semiconductors in organic thin-film transistors (OTFTs), BODIPY-based molecular/polymeric semiconductors for organic surface-enhanced Raman spectroscopy (organic-SERS) platforms, rod-shaped fluorescent molecules with high exciton utilization rates in organic light-emitting diodes (OLEDs), and molecular materials for physically unclonable functions (PUFs).<sup>1-4</sup>

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Keyword: pi-conjugated materials, organic optoelectronics, molecular engineering, synthesis, organic semiconductors

# Universal Dissipative Self-Assembly: From Quantum Dots to Colloids, Microorganisms, and Human Cells

# Serim Ilday

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Self-assembly research has started with a question: *Can we design and build planned structures and functionalities, starting from simple building blocks*? A vast body of work points to the possibility of this approach. However, the demonstrations so far suffer from being extremely specific solutions. Change, e.g., the material or the experimental conditions slightly, and to repeat the same achievement, takes months/years. The question is: *Can self-assembly methodologies transcend the specificity of the systems that are being studied*? In this talk, I will argue that fundamental principles of universal self-assembly lie in the intrinsic physical mechanisms, namely, nonlinearity, fluctuations, and feedback that drive and control self-assembly processes. I will showcase this approach on a diverse spectrum of materials, from simple, passive, identical quantum dots to complex, active, non-identical human cells with sophisticated internal dynamics. Then, I will demonstrate the effectiveness of this approach using completely different experimental settings and materials.

# Use of Surface-Enhanced Raman Scattering (SERS) Probes to Detect Pathogens in a Microfluidic Device

## <u>Uğur Tamer</u>

# Gazi University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Turkey

Accurate and robust detection of important analyte are still challenge in a in complex matrix. This presentation will underline Surface Enhanced Raman Spectroscopy (SERS) based sensitive and selective analytical methodologies regarding the most suitable active surface preparation of SERS techniques. The new labelled and label-free applications of SERS spectroscopy in a complex matrix for the detection of pathogens and especially contributions to microfluidic are the main topics of this presentation. The optimization strategies and the analytical performance of the SERS-based assays in a microfluidic device will be presented.

One of the most encountered proble is a weak Raman signal intensity due to the low cross section of Raman sacttering. Raman signals can be substantially increased using a metallic substrates. Numerous approaches have been suggested for this purpose and multipurpose functionalized hybrid nanoparticles are very promising for the detection of trace amounts of analyte. Simple and fast generation of nanoparticles and modification with appropriate probe provide SERS applications. For SERS to translate to the pathogen detection, there are some obstacle to overcome such as spectral reproducibility and suitable sample preparation. SERS should provide accurate and robust quantitative results. Furthermore, Raman spectrometer should be sensitive and low-cost instrumentation. These constraints can be more pronunced for resource-limited settings. Our research group demonstrated several SERS based applications such as nanoparticle embedded substrates for the fast bacteria detection. As an example, the target malachite green captured by molecularly-imprinted magnetic nanoparticles serves as SERS sensing platform in tap water and carp samples. The disposable SERS substrate was also used to detect the target in food samples, and suitable results were obtained. Besides, the proposed SERS substrate offered a selective, sensitive, reliable and economical method in a less time-consuming way.

# **Materials Design for Energy Storage**

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The global electrochemical energy storage market ranging from electric vehicles and personal electronics to physical grid storage and defense applications demands the development of new classes of materials for fabricating high performance batteries and supercapacitors. I will describe innovative approaches for the design and synthesis of nanostructured materials towards enhanced reversible capacity; superior rate performance and cycling stability; superior gravimetric capacitance; and enhanced energy density and power density. A novel 3D architecture called a pillared graphene nanostructure (PGN) is a combination of two allotropes of carbon, including graphene and carbon nanotubes possessing ultra large surface area, tunability, mechanical durability and high conductivity can be grown on a variety of substrates, which are appealing to diverse energy storage systems. Another type of 3D superporous carbonaceous architecture called chrysanthemum Nanofibers can be grown in roll-to-roll form on commercial nickel foams. Integration of nanostructured pseudocapacitive metal oxides to such 3D templates can provide superior electrochemical performance in supercapacitor applications. PGN templates can also be transformed into cone-shaped clusters decorated with amorphous silicon for advanced lithium ion (Li-ion) battery anodes. Single and multilayer stacked 3D carbonaceous architectures could also be envisioned for future applications in hydrogen storage. Next, I will describe recent advancements in upcycling polyethylene terephthalate (PET) waste and glass waste bottles into active electrode materials for energy storage. An interconnected silicon-network is directly derived from glass-bottles via magnesiothermic-reduction. For PET plastic-waste, materials are dissolved in a mixture of trifluoroacetic acid and dichloromethane, followed by carbonization under an argon/hydrogen atmosphere. Electrodes derived from PET are employed in supercapacitors and Li-ion battery anodes. Glass bottles utilizing magnesiothermic-reduction without pre-leaching offers an environmentally-benign and energy-saving route to prepare silica-source materials, employed in fabricating Li-ion battery anodes. Both conversion processes for plastic and glass waste are highly scalable with environmental and economic advantages, and could provide the means for achieving a circular economy in energy storage technologies. Finally, I will talk about selected metal oxide (M<sub>x</sub>O<sub>y</sub>) thin film barrier layers to mitigate the polysulfide shuttling effects in Li-S batteries, and enhance their performance and cyclic stability. Through analysing the binding energies of Li<sub>2</sub>S<sub>n</sub> adsorbed onto selected M<sub>x</sub>O<sub>y</sub> surfaces via density functional theory (DFT) calculations and Molecular dynamics (MD) simulations, we show that the strong Li-O bonds dominate the interactions between  $Li_2S_n$  and selected  $M_xO_y$  surfaces. Our studies demonstrate that selected  $M_xO_y$ thin film barrier layers could be employed in scaled up manufacturing to enhance Li-S battery performance.

# Graphene for Fuel Cells, Batteries and Hydrogen Production

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Graphene, as a unique, single-atom thick layered structure of carbon, can be utilized for various applications especially for energy including fuel cells, batteries and supercapacitors. The previous reports have revealed that graphene and its derivatives with spectacular theoretical electrical, and mechanical properties could be used as highly efficient electrodes in various energy related applications. Nevertheless, the crucial role of graphene-based materials in providing the reliable solid- state support for fuel cells, Li-air and Li-ion batteries should be explored.

Polymer electrolyte membrane (PEM) fuel cells are attractive for portable, stationary and automotive applications while there are still challenges because of cost and durability issues. Especially, platinum (Pt) nanoparticles, used as catalyst in PEM fuel cells, have high cost, performance and durability problems and low abundance as well. Catalyst support materials are of great importance in regulating the properties of catalyst nanoparticles such as shape, size, and dispersion. Carbon black, the most commonly used commercial catalyst support, has several limitations which cause the degradation of catalyst activity and performance. The use of graphene as the catalyst support due to its high surface area, high conductivity and chemical stability, could lead to an improvement in both catalytic activity and catalyst utilization in PEM fuel cells1. The deposition of metal nanoparticles on graphene layers results in formation of a heterogeneous catalyst system which further leads to decrease in metal catalyst consumption, and leaching, while increasing the catalytic activity via high charge mobility of the graphene-based support. In the present work, graphene nanoplatelets, reduced graphene oxide, functionalized graphenes and various hybrids of graphene have been employed as the catalyst support. Graphene supported Pt nanoparticles were prepared by means of impregnation-reduction, microwave-assisted deposition, photocatalytic deposition, supercritical carbon dioxide deposition, surfactant assisted deposition methods. Highly dispersed and uniformly decorated 2-3 nm Pt nanoparticles were achieved<sup>1,2</sup>. These graphene-based structures are also utilized for PEM electrolyzers for hydrogen production.

Graphene based materials are also promising candidates for energy storage applications such as Li- ion and Li-air batteries, especially when used as a substrate for metal oxides, because of their high theoretical capacities. We aimed to simultaneously enhance the electronic and ionic conductivities of the active material in the anode by adding graphene as a conductive component. For a stronger attachment, titania nanotubes are hydrothermally grown on nitrogen doped graphene oxide (NrGO) sheets in an aqueous medium. This novel 3D architecture resulted in a reduction of conductive additive components, such as carbon black, and enhanced the overall performance of the anode<sup>3</sup>.

Moreover, We have reported the high stability and superior performance of graphene oxide aerogel supported ultrafine  $Fe_3O_4$  particles for Li-ion batteries recently<sup>4</sup>. Cerium oxide-based catalysts were decorated on NrGO in order to achieve structures with stable capacity for Li-air batteries and high performance for fuel cells as well<sup>5</sup>.

Our research group have been focused on various graphene-based materials for energy applications. This talk will provide a profound insight about the use of graphene for PEM fuel cells, Li-ion & Li- air batteries and hydrogen production.

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Keyword: Graphene, Fuel Cell, Hydrogen, Li-ion battery, Li-air battery, Electrolysis

# CVD Grown 2D Materials - TMDs, Graphene and MXene - for Future Devices

#### Nihan Kosku Perkgöz, Feridun Ay

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Following the great interest in graphene, 2D materials have received growing attention in the fields of physics, materials science and optoelectronics due to their outstanding optical and electrical properties. The growth and transfer optimization studies of semiconductor 2D MoS<sub>2</sub>, MoSe<sub>2</sub> and WS<sub>2</sub> as well as graphene and MXene using chemical vapor deposition (CVD) techniques will be summarized aiming for their utilization in different electronic and optoelectronic devices as well as avionic applications. Specifically, the production of  $MoS_{2(1-x)}Se_{2x}$  alloys and their band gap engineering, ALD-supported large-area growth of MoS<sub>2</sub> structures, obtaining glass-supported large-area MoS<sub>2</sub>, WS<sub>2</sub> and MoSe<sub>2</sub> structures, and growth of thin MXene structures by CVD will be discussed [1-3]. Finally, the supercapacitor applications of graphene with MoS<sub>2</sub> phototransistors enhanced with semiconductor quantum wells will be summarized as a device demonstration [4,5]. These studies were supported by TUBITAK projects no. 118E996 and 20AG025 (under 20AG001).

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# **Emerging Two-dimensional Materials for Energy and Electronic Applications**

#### Engin Durgun

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During the last decade, there has been growing interest in two-dimensional (2D) materials due to their unique chemical, mechanical, electronic, and optical properties. Motivated by the synthesis of graphene and its extraordinary properties, researchers have focused on predicting and synthesizing 2D allotropes of other elements and compounds. On the theoretical front, these efforts led to the prediction of 2D allotropes of group-IV elements, group IV-V, III-V, and II-VI compounds, silicon dioxides, transition metal dioxides, dichalcogenides and monochalcogenides, and alkali-earth metal hydroxides. It was shown that these 2D materials display diverse electronic, optical, and magnetic properties for a wide range of technological applications, such as optoelectronics, spintronics, catalysts, chemical and biological sensors, supercapacitors, solar cells, nanotribology, hydrogen production, and alkali-ion batteries. In this respect, the main theme of this talk is to present results on the prediction of new emerging 2D materials by identifying stable atomic structures, investigating fundamental properties, and revealing their potential for advanced applications. Among the variety of possibilities, nanoscale capacitors [1], thermoelectric devices [2], ultra-thin transistors [3], and photocatalytic water-splitting applications [4, 5] based on 2D systems will be discussed. The results obtained by advance computational methods are not only substantial for fundamental understanding but also are helpful for near-future technological advancements.

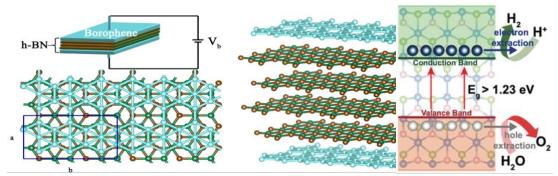


Figure 1

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# **Can We Tune Refractive Index Several Times?**

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It would be great if we could tune refractive index of a material, for instance, by several times. However, the present technology gives us a tuning capability of the index only by a few percent! Fortunately, a new —quantum optics origin— method [1,2] allows the tuning of refractive index by, for instance, 4 or 5 times! The new method does this with a small fingerprint, e.g., without heating the material. In this talk, I will mention about this groundbreaking work, theoretical [1] and experimental [2], and talk about its implementations such as first tunable supreme nuclear particle detector [3] and full-band-gap operating photonic crystal switch [4].

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# Polycationic Cyclodextrin Nanoparticles and Nanoplexes for The Local Chemo-Immunotherapy of Gastrointestinal Tumors

#### Erem Bilensoy

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Cancer is still a leading cause of death worldwide and colorectal cancers are one of the most frequently diagnosed cancer types in both men and women as a result of modern life and nutrition styles. Cancer chemotherapy is almost completely relying on injectable dosage forms and more than 90% of the chemotherapeutics are administered with intravenous infusion. Oral chemotherapy is still very limited due to low oral bioavailability of chemotherapeutics and the stability problems arising from the harsh pH and enzymatic conditions of the gastrointestinal tract. Along with chemotherapeutic agents, combined immunotherapy is the clinical choice currently to boost the immune response of the patient to help fight the tumor. Our group has been working on positively charged nanoparticles based on different cyclodextrin polymers. Nanoparticle formulations with positive charge were able to maintain the stability of the encapsulated chemotherapeutic small molecule in simulated gastrointestinal fluids, with good mucosal penetration, intestinal permeability, anticancer efficacy in cell and 3D tumor culture studies. Animal studies performed on early and late stage colorectal tumor induced mice models revealed a significant antitumoral and antimetastatic effect when compared to free drug solution with favorable biodistribution as seen in Figure 1. Recently, nanoplexes based on the charge interaction of cationic cyclodextrin polymers with immunotherapeutic agent Interleukin-2 were further loaded with 5-fluroouracil and evaluated for anticancer efficacy on colon cancer via oral and parenteral administration.

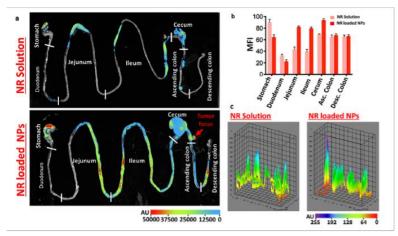


Figure 1: Biodistribution of free and polycationic cyclodextrin nanoparticle bound NR in tumor induced animals after single administration within 24 hours

# Nanocrystalization: Crystal Growth and Polymorphism of Confined Polymers

#### Hatice Duran

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Nanoporous hard templates provide a two-dimensionally confined space in which self-organization processes such as crystallization, protein secondary structure formation, and phase separation can be fundamentally different from those obtained in thin films and in the bulk. Understanding the crystallization, thermodynamics and dynamics of polymers under confinement allow for their rational design as functional devices with tunable mechanical strength, processability, electronic and optical properties. The principal focus of this lecture is finding the basic underlying principles that give rise to nucleation and crystal growth in a range of soft materials (crystallizable polymers, amphiphilic molecules, liquid crystals, low-molecular weight liquids and biopolymers) under hard-confinement.

Bulk crystallization of polymers proceeds usually via heterogeneous nucleation and gives rise to structure over multiple length scales: from the crystalline unit cell (1-2 nm), to alternating crystalline/amorphous lamellae (50-100 nm) and to spherulitic superstructures (>500 nm and up to cm). This is the dominant nucleation mechanism in bulk polymers. Important studies of polymer crystallization confined to droplets and within the spherical nanodomains of block copolymers emphasized the interplay between heterogeneous and homogeneous nucleation and explored the kinetics of homogeneous nucleation observed at high supercooling. Some authors have even reported only homogeneous nucleation under hard confinement typical for AAO: Is the crystallization process always homogeneous within the small AAO nanopores? Do surface effects always dominate? And even more, can hard confinement completely suppress polymer crystallization and if so what is the required size? Providing answers to these questions is of technological relevance for the understanding of nanocomposites containing semi-crystalline polymers. We will try to explore these issues both comparing the recent studies and research activities of our group.

# From the Power of Nano-Structures to the Personalized Diagnostics and Imaging Guided Therapies

# <u>Suna Timur</u>

# Ege University, Science Faculty, Biochemistry Department, İzmir, Turkey

The race in the development of new nanotechnology-based materials has been in constant increase. The applications of nanoparticles and nanocomposites for different applications such as biosensors and drug delivery systems are an important category that needs continuous development. Biosensors have many fields where they shine especially in the development of point of care (POC) tools based on electrochemical or paper-based materials for the detection of small molecules such as illicit drugs or virus particles. On-site detection lowers the burden on test centers due to their selectivity and sensitivity, fast turnaround, low price, and because they don't need trained staff. The development of biosensors is also associated with many tools such as smartphone that can facilitate readout through special applications and color-assisted analysis. These makes the process of using biosensor more accessible to the population. In this presentation, we will share our recent findings in the development of nanoparticles-based biosensors for the detection of biomolecules such as abuse drugs (cocaine, methamphetamine, synthetic cannabinoids), viruses (covid-19), and other target molecules (pesticides, etc.) using paper-based biosensors (lateral flow assays) and electrochemical biosensors. Various nanoparticles (NPs) such as magnetic, gold, silver NPs and polymeric structures loaded with different dyes were used in order to produce satisfying signals and colors that can compete with the traditional known sensing methods. These techniques were combined with smartphones to analyze colors and electrical signals through available and in-house developed applications. Additionally, our team explored the development of various POC model prototypes such as wearable watches for the detection illicit drugs. On the other hand, our advances in the development of drug delivery systems using various types of nanocarriers (liposomes, niosomes, polymersomes) for the detection and treatment of various diseases such as cancer and age-related disorders are presented.

Our findings demonstrate the importance of such structures for the personalized and specific delivery of particular molecules to their targets with lower levels of toxicity and enhanced effect compared to traditional chemotherapy approaches. These nanocarriers provides an important advantage through their flexibility and tunability allowing the preparation of interesting structures that can be used for both therapy and diagnostics (theranostics). The current presentation highlights the importance of nanomaterials development for future applications in the biomedical field.

# Perovskite Solar Cells: The Next Generation of Solar Power Technology or the Perfect Partner for Silicon Photovoltaics?

# <u>E. Görkem Günbaş</u>

ODTÜ-GÜNAM, Emerging PV Division / ODTÜ, Department of Chemistry, Ankara, Turkey

We all witnessed the incredible rise of a new photovoltaics devices, perovskite solar cells (PSCs), in the last decade, with immense improvements in the initial shortcomings of the technology such as efficiency and large area demonstrations. However, PSCs are not, as of now, ready for making their appearance in the commercial market due to two significant issues that yet to be addressed, long-term stability and reproducibility. Significant advancements have already been made, and new approaches to tackle these shortcomings are being utilized in an unforeseen pace. In this talk a general overview of these recent advancements and our contributions along these lines will be highlighted. Finally, once the critical shortcomings surmounted, the possible commercialization applications of this technology and where it will be standing next to the market dominator silicon solar cells will discussed.

# Graphene-Based Stimuli-Responsive Polymer Composites: Turning up the Heat in Drug Delivery

# <u>Amitav Sanyal</u>

Bogazici University, İstanbul, Turkey

Graphene oxide (GO) based drug delivery systems have been extensively studied due to their high drug loading capacity via  $\pi$ - $\pi$  stacking and hydrophobic interactions. Drugs release from graphene oxide could be triggered by various external stimuli such as pH and light. Graphene oxide as a near infrared (NIR) light absorbent can rapidly convert NIR light to heat. This heating ability of graphene oxide is mostly utilized for photo-induced drug release since heat disrupts interactions between graphene oxide and drug molecules allowing the release of drug. As an alternative these photothermal nanomaterials can be integrated with polymeric scaffolds. Several polymeric platforms such as hydrogels, cryogels and Nanofibers containing GO have been developed in our laboratory. The presentation will highlight examples where different strategies have been developed to deliver therapeutic molecules such as enzymes and antibiotics in an on-demand controlled manner.

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# Graphene/SOI Based Photodetector Array Technology

# <u>Cem Çelebi<sup>1</sup>, Alper Yanılmaz<sup>1</sup>, Özhan Ünverdi<sup>2</sup></u>

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Photodetector array is a light sensitive device with multiple semiconductor photodiodes arranged in a single package. These type of optoelectronic devices are formed with close diode-to-diode spacing and minimized cross-talk between diodes in the array by isolating them from one to another with trenches that are formed between the photodiodes in the array. These photodetectors are used in a wide range of applications such as light position detection, position encoders, imaging, X-ray scanners and spectrophotometry.

The photodiodes based on Graphene/Silicon (G/Si) heterojunction have attracted a great deal of attention in the last decade since they exhibit photo-responsivity similar to p-n or p-i-n type Si photodiodes. A rectifying Schottky contact with an energy barrier level of around 0.5-0.8 eV is formed when graphene is laid on the surface of bulk Si substrate. Because of the fact that G/Si heterojunction operates as a Schottky barrier diode which is sensitive to light in the spectral range between 400–1100 nm due to the bandgap of Si. When graphene is employed as an electrode on Si, it does not only act as optically transparent conductive layer, but it functions also as a photon absorbing active material similar to metal silicide electrodes used in conventional metal/Si Schottky barrier photodiodes. Under light illumination, although a large amount of photons is converted into photo-generated charge carriers in Si, the optical absorbance in graphene (~2.3 %) contributes to light detection as well through internal photoemission over the Schottky barrier.

Here we fabricated for the first time a multi-channel Gr/Si Schottky barrier photodiode array (PDA) on Silicon on Insulator (SOI) substrates using standard and conventional microfabrication techniques employed in CMOS technology. In our device design, we used the advantage of the burried oxide (BOX) layer in SOI which acts as a well-defined etch-stop and provides an excellent electrical isolation in between laterally aligned neighboring photoactive Gr/Si elements in the array. In the fabrication process, chemical vapor deposition (CVD) grown single layer graphene is utilized as common electrode on a linear array of multiple n-type Si channels which were lithographically exposed on a single SOI substrate. Current-voltage (I–V) and wavelength resolved photocurrent spectroscopy measurements showed that each Gr/Si element in the PDA operates in self-powered mode and responds to incident light independently of each other. The optoelectronic device parameters including spectral responsivity, specific detectivity, noise equivalent power and response speed of the Gr/Si PDA sample were systematically investigated and reported. Time-dependent photocurrent spectroscopy measurements showed excellent on/off photocurrent reversibility of the PDA device with ~1.36 us and ~1.27 us rise time and decay time, respectively.

The study presented here is expected to offer exciting opportunities for the realization of high-value added technological applications based on motion and position detection, imaging and spectrophotometry in which graphene and SOI technology can be used together.

#### ID: 420

# **Controlling Collective Motions by Speckle Tweezers**

# <u>Ali-Reza Moradi</u>

# Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran

Several fundamental research and applications in biomedicine and microfluidics often require controlled manipulation of collection of suspended micro- and nanoscale particles. Speckle tweezers (ST) by incorporating randomly distributed light fields represents a wider possibility, compared to periodic potentials, to be operated for such tasks on mixture of various types of particles: low and high index dielectric particles and metallic ones. ST can also manipulate the nano-particle loaded vesicles which opens a new window on controlling collective transportation of drug micro-containers along with their wide applications in soft matter.

In this talk we introduce ST and present some of their recent important applications.

# SERS-Based Trace Molecule Detection by Size and Shape Controlled Noble Metal Micro-/Nano-Particles

# Özge Demirtaş<sup>1,2</sup>, Ghazanfar Ali Khan<sup>3</sup>, R. M. Faheem Iftikhar<sup>3</sup>, İ. Murat Öztürk<sup>2,4</sup>, A. Kemal Demir<sup>5</sup>, Waqqar Ahmed<sup>3</sup>, <u>Alpan Bek<sup>1,2,4</sup></u>

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For reproducible surface enhanced Raman spectroscopy (SERS)-based trace molecule detection, we have developed facile synthesis methods of metal nanostructures that ensure highly concentrated hotspots and uniform distribution on the substrate. Firstly, we demonstrated a size-controlled synthesis of multi-spiked gold nanoparticles (MSGNPs) that can be assembled into monolayers over a centimeter length scale simply by drying the suspension on a substrate under ambient conditions [1]. The close-packed assembly of MSGNPs increases the hotspot concentration by generating interparticle hotspots. Furthermore, the calculated experimental enhancement factor is at the order of 10<sup>7</sup>. The SERS platforms fabricated this way reveals that a crystal violet (CV) concentration of as low as 10 fM was measurable. In a second study, the fabrication of Ag nanostructures with worm-like bends and high surface roughness has been demonstrated as highly stable, sensitive, and costeffective (per-substrate material costs = \$0.05) SERS platforms. Surfactant-free and uniformly interconnected branched nanostructure fabrication takes only a few minutes by our method. The limit of detection studies of SERS substrates revealed that they allow detection of concentrations down to 10<sup>-8</sup> M. Furthermore, a linear correlation between the intensity and CV concentration has been observed. The calculations using the linear fit equation show that CV concentrations down to 10<sup>-12</sup> M can be quantitatively detected. The seed-mediated method, in which nucleation and growth are decoupled, is often used for the synthesis of Au nanoparticles [2,3]. However, surprisingly, we have seen in our recent study that a higher initial starting concentration of HAuCl4 and ascorbic acid (AA) in the growth solution, nucleation, and subsequent growth can occur in the absence of seed solution. We demonstrate that the shape and size of the gold microparticles (GMPs) can be tuned simply by changing the concentration of AA and cetrimonium bromide (CTAB) in the growth medium. GMPs were synthesized using a single-step reaction. Finite-element simulations indicate that the most intense electromagnetic enhancement is seen to be at the tips of the branches. The maximum SERS enhancement obtained for this sample was more than 10<sup>9</sup>. The small surface protrusions have shown better enhancement for shorter laser wavelengths, while longer branches exhibit more pronounced enhancement for longer excitation wavelengths. Although the enhancement seems to be different for different excitation wavelengths, due to different concentrations of hotspots for a particular excitation, SERS peak intensities in all cases are substantially strong with a signal-to-noise ratio of at least 25. Therefore, GMPs have great potential to become a universal SERS substrate.

**Keywords:** surface enhanced Raman spectroscopy, gold nanoparticles, gold microparticles, silver nanoparticles, nanostars, nanoworms, enhancement factor, seedless synthesis

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ID: 6 Synthesis and Characterization of Nanomaterials

# Preperation of Carbon Nanotube Substituted Polycaprolactone/ Polyethylene Glycol Composite Fibers by Electrospinning and Investigation of Surface Energies

# Serbülent TÜRK<sup>1</sup>, Mahmut ÖZACAR<sup>2</sup>

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Electrospinning, one of the essential techniques since 1990 [1], has been used in many fields such as fuel cells [2], drug delivery systems and tissue engineering [3]. It is widely used for the production of nanofiber mats with the desired diameter and porosity for the application. In the last decade, researchers have been increasingly interested in using electrospun polymeric structures with the increase in their usage areas. This study was investigated the surface energies of electrospun mats with different contents. Polycaprolactone (PCL), polyethylene glycol (PEG), PCL/PEG, and carbon nanotube (CNT) substituted PCL/PEG-CNT composite fibers were fabricated using an electrospinning assembly consisting of a high-voltage power supply, a syringe with a metallic needle, a syringe pump, and a metallic plate as the collector. Chloroform:ethanol (7:3 v/v) solution was used as an electrospinning solution. Electrospinning solutions were prepared by adding PEG (10 wt%) and CNTs (1 wt%) to the prepared PCL (10% w/v) solution. They were dispersed to obtain a homogeneous mixture before electrospinning. This composite solution (PCL, PEG, PCL/PEG, and PCL/PEGs) was connected to a 10 mL syringe electrospinning system equipped with a 1mm conductive needle. Electrospun mats were produced with a distance of 15 cm between the syringe and the collector, a power supply of 15 kV, and a flow rate of 0.5 mL/h. FTIR analysis of electrospun composite fibers was performed, and their morphology was characterized by scanning electron microscopy. Surface energy measurements of each electrospun mat produced were carried out. As a result of the characterizations, it was observed that the composite fibers were made successfully, and it was observed that the morphologies of the composite fibers differed depending on the electrospun solution.

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Keyword: Electrospinning, Surface energy, Polycaprolactone, PEG

### ID: 8 - Synthesis and Characterization of Nanomaterials

# Atomistic Diffraction Simulations for Advancing Structural Characterization of Nanocrystals

# Hande Öztürk Ozyegin University, İstanbul, Turkey

In this talk. I will present how atomistic diffraction simulations and subsequent numerical analyses can be useful tools to identify problems in applying classical formulations to characterize nanocrystalline materials. Due to their characteristic atomic configurations, nanocrystals diverge significantly from their bulk crystalline counterparts. This difference results from the enhanced ratio of the number of undercoordinated surface atoms with respect to that of core atoms within a nanocrystal. Also known as the surface effect, this phenomenon is also the source of many desirable physical and chemical properties which make nanocrystals popular materials in industry.

Because properties of nanocrystals are closely dependent on the particular way atoms stack themselves in the particle, accurate structural characterization practices are in high demand with as high resolution as possible. In that respect, X-ray diffraction is a key method for both accurate synthesis and optimization of nanocrystalline materials. However, existing analysis algorithms of diffraction data rely on certain fundamental assumptions such as the investigated material being composed of infinitely long stacks of atoms in 3 dimensions. This assumption, unfortunately, is incompatible with the very nature of nanocrystals. Hence one needs to be aware of the potential inaccuracies of analyzing the diffraction data measured from nanocrystalline materials with existing numerical algorithms. However, currently used algorithms provide no such information of expected uncertainties in obtained structural parameters.

One way to address this issue is to resort to atomistic diffraction calculations; in this case, we simulate realistic nanocrystal models and obtain their expected diffraction data without relying on any of the bulk crystalline concepts used in the literature. These data, then, are analyzed by well-known diffraction analysis packages (e.g. Rietveld refinement) used by the community. Finally the obtained structural parameters are compared against those from the nanocrystal model used as input while simulating the diffraction signature. We observe that errors related to structural parameters such as crystallite size, lattice constant etc. can be high and might be very misleading in drawing an accurate picture of the studied nanocrystal.

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Keyword: x-ray diffraction, nanocrystals, structural characterization

#### ID: 15 - Synthesis and Characterization of Nanomaterials

# Straightforward, Size Tunable, Ultra-Small Silver Nanoparticles Synthesis in a Linear Range with Glycerol as a Reducing Solvent Medium

#### Iqra Munir, Gurkan Yesiloz

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Despite all the possibilities available so far for the synthesis of nanoparticles (NPs), synthesizing ultra-small (<10nm) monodispersed particles is still a demand. Getting a particular size with a straightforward recipe is a hit and trial game. To explore this prospective, in the current study, we have introduced a protocol which offers a linearity range to successfully generate the NPs of similar particle size in each synthesis, thus giving an escape from lengthy tentative preparations and/or testing protocols. Since, synthesizing controlled sized nanoparticles in aqueous medium is somewhat difficult as the balance of particle growth and nucleation is challenging to control. Here, we used polyol method with glycerol both as a solvent medium as well as reducing specie for silver nitrate, to click the nanoparticle synthesis. In order to maintain the stability of the synthesized NPs, Polyvinylpyrolidone (PVP) was added as a strong stabilizer. The synthesis, monodispersity, and stability was confirmed using physical techniques like UV-Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR), Dynamic Light Scattering (DLS), and X-ray powder diffraction (XRD), while morphological analysis and ultra-small size validation was conducted using Transmission electron microscopy (TEM), scanning electron microscope (SEM) and Atomic force microscopy (AFM). Interestingly, in various concentrations of glycerol solution used (10%-100%), we have observed linearity range to obtain ultra-small nanoparticles (<10 nm) up to 60% glycerol, while further increasing the glycerol component also increased the size equal to  $\sim 160$  nm, providing tunable properties in the synthesis protocol. Hence, this study provides a pronounced possibility to obtain ultra-small nanoparticles in a single set of experiment for further applications in numerous fields.

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Keyword: Glycerol, Ultra-small nanoparticles., Monodispersity, Reducing solvent, Ambient Temperature

ID: 16 - Synthesis and Characterization of Nanomaterials

# Synthesis of CdTe/ZnS Core/shell QDs with a Photochemical Approach, Investigating Hg2+ Sensitivity in Aqueous Media and Photocatalyst Applications

#### Mehdi Molaei, Farzad Farahmandzadeh

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In this work, CdTe/ZnS high luminescence quantum dots (QDs) were synthesized by a facile, rapid, one-pot and room temperature photochemical method. Thioglycolic acid (TGA) used as both of the capping agent molecule and sulfur source for ZnS shell growth. XRD results confirmed successful formation of CdTe/ZnS core/shell structure. TEM image showed that synthesized QDs are spherical and also formation of ZnS shell around CdTe QDs is observable in this picture. CdTe QDs indicated green emission with PL quantum yield (QY) of 23% which after growth ZnS shell achieved to 51% and also 62 nm red-shift was observed in photo emission and PL peak position. Sensitivity of CdTe/ZnS QDs versus Hg<sup>2+</sup> ions investigated by different concentration of Hg<sup>2+</sup> ions in aqueous media and results showed that PL intensity of CdTe/ZnS QDs was quenched after addition of 1 m molar Hg<sup>2+</sup> and was a good relationship (R<sup>2</sup>=0.9957) between the degree of PL intensity quenching and the Hg<sup>2+</sup> concentration, therefore CdTe/ZnS QDs have potential for use in Hg<sup>2+</sup> sensors. Photocatalyst activity of CdTe/ZnS QDs was investigated by rhodamine b, methylene blue, and methylene orange pollutants under both sun and UV illuminations and results showed that CdTe/ZnS QDs had the best photocatalyst activity for methylene blue degradation under UV irradiation and radical scavenger results indicated that electrons have a main role in photo-degradation of methylene blue dye by CdTe/ZnS QDs under UV irradiation.

Keyword: CdTe/ZnS, Sensitivity, Photocatalyst activity, QDs

#### ID: 18 - Synthesis and Characterization of Nanomaterials

# Synthesis Smart Hybrid Colloidal Particles and Photochromic Properties

# Esma Mutluturk<sup>1</sup>, Tuncer Çaykara<sup>2</sup>

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Hybrid materials which consist of organic and inorganic components play an important role in different applications [1] It is possible to designing these materials using the combination of organic polymers and inorganic particles [2]. In this study, we developed multifunctional photochromic hybrid colloidal nanoparticles. For this purpose, we synthesized the particles into three main step: i) Synthesis of attachment of 3-aminopropylthriethoxysilane (APTES) to silica particles ii)Grafting of 4-cyano-4-[(dodecyl sulfanyl thiocarbonyl) sulfonyl] pentanoic acid (CPAD) on amine ended particles iii) Interface mediated RAFT polymerization of methacrylated-spiropyran monomer. The particles were characterization by GA-FTIR and SEM analysis. Moreover, the polymer was analyzed with H-NMR and GPC spectrums [1]. The molecular weight and polydispersity of poly(methacrylated-spiropyran was determined as 7877 g/mol and 1.16, respectively. The photochromic property of the particles were examined under different wavelength light irradiation. The results showed that Spiropyran (SP) – merocyanin (MC) isomerization of polymer can be controlled using light. Furthermore, the isomerization efficiency of the particles was investigated in different solvents. In this context, photochromic, Si-p(MMASP) hybrid colloids were dispersed in DMF which both SP and MC form were dispersible. In initial stage, the isomerization increased remarkably and the colorless Si-p(MMASP)was turned to purple. Optimum isomerization time from SP to MC form and from MC to SP form was found as 7 min and 9 min, respectively. In conclusion, these hybrid particles exhibited great photochromic properties.

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Keyword: spiropyran, colloidal particles, photochromic materials

# Mesoporous NiO, NiCo<sub>2</sub>O<sub>4</sub> and MnCo<sub>2</sub>O<sub>4</sub> Thin Film Electrodes, Their Electrochromic and Electrocatalytic Behaviors Towards OER

Assel Amirzhanova<sup>1</sup>, Ömer Dağ<sup>2</sup>

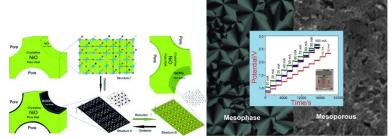
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Mesoporous transition metal oxides and mixed metal oxides thin films having high surface area are essential materials in an electrochemical application, especially in electrochemical water splitting[1,2]. Molten Salt Assisted Self-assembly (MASA)[3] was employed for the synthesis of mesoporous NiO, NiCo<sub>2</sub>O<sub>4</sub> and MnCo<sub>2</sub>O<sub>4</sub> thin films by coating clear ethanol solutions of nickel salt and two surfactants (charged, CTAB and neutral, 10-lauryl ether), nickel/cobalt and manganese/cobalt salts with the same surfactants, respectively, followed by calcination from 250 to 500 °C with 50 °C increment. Calcination of spin-coated thin gel films produces thin mesoporous metal oxide films. The drop-cast-coated ones make thicker metal oxide films or monoliths that crack during calcination[4,5].

The annealed films were characterized by recording x-ray diffraction (XRD), N<sub>2</sub>-adsorption-desorption measurements, imaging (SEM and TEM), and spectroscopy (FTIR, UV-Vis absorption, and XPS) techniques. The N<sub>2</sub> adsorption-desorption isotherms are type IV and characteristic of mesoporous materials. The XRD data show that the crystalline NiO, NiCo<sub>2</sub>O<sub>4</sub> and MnCo<sub>2</sub>O<sub>4</sub> form at around 300 °C, with a pore wall thickness around 3-4 nm. The pore-walls grow with increasing the calcination/annealing temperature up to 20 nm at about 500 °C in the case of nickel oxide and nickel cobaltite. BET surface area decreases with increasing calcination temperature; it is 223 m<sup>2</sup>/g at 300 °C and drops to 20 m<sup>2</sup>/g at 500°C in mesoporous nickel oxide, 223 m<sup>2</sup>/g at 250 °C, and drops to 31 m<sup>2</sup>/g at 500 °C in mesoporous nickel cobaltite. In contrast, the mesoporous manganese cobaltite resists calcination, and even at 500°C, the surface remains relatively high, 83 m<sup>2</sup>/g. The data accords well with XRD diffraction patterns where no visible line sharpening occurs, indicating no significant pore wall growth. The XRD diffraction patterns are indexed to the rock salt cubic structure in NiO and cubic spinel structure in NiCo<sub>2</sub>O<sub>4</sub> and MnCo<sub>2</sub>O<sub>4</sub>. In the case of NiO and NiCo<sub>2</sub>O<sub>4</sub>, the diffraction lines gradually become sharper, indicating crystallization and growth of the pore walls[4,5].

Mesoporous Nickel Oxide electrodes coated over the FTO glass are used as the electrodes for electrochromic applications and electrocatalysis for oxygen evolution reactions (OER) with an overpotential of as low as 0.200 V at 1 mA/cm<sup>2</sup> current density. During CV and CP analysis, the NiO pore walls transform to Ni(OH)<sub>2</sub> species which is highly active in the water-splitting process. Reversibly oxidizing Ni<sup>2+</sup> species can explain the electrochromic behavior of Ni<sup>3+</sup> species. Mesoporous Nickel cobaltite and Manganese cobaltite coated over the FTO glass is stable during electrochemical analysis and display low overpotentials of 0.204 and 0.227 V, respectively at 1 mA/cm<sup>2</sup> current density. Tafel slopes of MnCo<sub>2</sub>O<sub>4</sub> and NiCo<sub>2</sub>O<sub>4</sub> are 60 and 85 mV/dec, respectively, indicating they have different oxygen evolution reaction mechanisms[4,5].



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Electrodes as Electrocatalysts for the Oxygen Evolution Reaction in Alkaline Solutions. ACS Appl. Energy Mater. 2021, 4, 2769–2785.

**Keyword:** mesoporous materials, lyotropic liquid crystals, molten salt assisted self-assembly, soft template, hard template, metal cobaltite, metal oxide, electrocatalysis, oxygen evolution reaction, electrochromism.

ID: 27 - Synthesis and Characterization of Nanomaterials

# Acid-Salt-Surfactant Lyotropic Liquid Crystalline Mesophases: Synthesis and Characterization of Mesoporous M<sub>2</sub>P<sub>2</sub>O<sub>7</sub> (M=Mn(II), Co(II) and Ni(II))

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Energy storage materials have been synthesized using different synthetic approaches by many researchers due to their promising energy applications. [1] Supercapacitors have been noticed as one of the most promising energy storage devices for the fast and highly reversible storage and release of electrical energy. [2] A surfactant assisted approaches by using moltensalt assisted self-assembly (MASA) method [3] for the synthesis of mesoporous M<sub>2</sub>P<sub>2</sub>O<sub>7</sub> would be a good solution since high surface area is crucial for the energy storage materials.

Here, we show the synthesis of mesoporous  $M_2P_2O_7$  particles using related acid; phosphoric acid (H<sub>3</sub>PO<sub>4</sub>) or pyro-phosphoric acid (H<sub>4</sub>P<sub>2</sub>O<sub>7</sub>), salts ([Mn(H<sub>2</sub>O)<sub>4</sub>](NO<sub>3</sub>)<sub>2</sub>, [Co(H<sub>2</sub>O)<sub>6</sub>](NO<sub>3</sub>)<sub>2</sub>, [Ni(H<sub>2</sub>O)<sub>6</sub>](NO<sub>3</sub>)<sub>2</sub>) and surfactant (pluronic, P123 (EO<sub>20</sub>-PO<sub>70</sub>-EO<sub>20</sub>) mesophases. The lyotropic liquid crystalline (LLC) mesophases have been investigated using broad range of ingredients as clear solutions first then as in a gel-phase to determine the stability and flexibility of the synthesis media. The process starts as clear aqueous solutions of the ingredients that can be spin coated or drop-cast coated over glass substrate for the further thermal treatments to synthesize the mesoporous M<sub>2</sub>P<sub>2</sub>O<sub>7</sub> (M = Mn, Co, Ni) particles. The LLC mesophases have been investigated during their aging whereas the mesoporosity and crystallinity have been analyzed by changing the calcination temperature. The samples have been characterized at every stage using XRD, ATR-FTIR, N<sub>2</sub>-adsorption-desorption, and SEM imaging techniques. The LLC mesophases have been also coated on pure graphite rod by dip-coating method and calcined at various temperatures to generate electrodes for electrochemical characterizations. The cyclic voltammograms and galvanostatic charging ad discharging abilities of mesoporous M<sub>2</sub>P<sub>2</sub>O<sub>7</sub> have been collected from prepared electrodes in three electrode systems using alkaline solution as an electrolyte.

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**Keyword:** Supercapacitors, Molten-salt assisted self-assembly (MASA), Lyotropic liquid crystalline (LLC), Mesophase, Mesoporous materials, cyclic voltammogram, galvanostatic charge discharge

ID: 29 - Synthesis and Characterization of Nanomaterials

# Pd-Fe Modified PGE Nanosheets for Formic Acid Oxidation

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Formic acid (FA) is a nonflammable and nontoxic acid having a high energy density. FA with its simple structure (HCOOH) has been served as an intermediate for the oxidation of alcohol molecules. Therefore, the electrochemical oxidation of FA has attracted considerable attention in these days [1] and has replaced the conventional fuel cells and batteries [2]. Among many fuel cells, there is an increasing demand for direct FA fuel cells (DFAFCs) as renewable and clean energy resources gaining advantages such as high power output, low crossover effect, easy storage, portability and environmental friendliness [3]. On such an occasion, anode material for FA oxidation is very important and various nanostructured materials have been developed thanks to their large specific surface areas, improved conductivity properties and wide band gaps. Palladium (Pd) metals are widely applied as anode materials for the electrochemical oxidation of FA [4] and the electrocatalytic activity of Pd-based anodes has been increased by binary metallic materials (Pd-M). Among these Pd-M nanosheets, the presence of iron (Fe) as a second metal has induced the adsorption behavior of the active oxygen, so Pd-Fe anodes have come into prominence. In this work, Pd-Fe nanoparticles were successfully synthesized and they were used to modify pencil graphite electrode (PGE) surfaces. The Pd-Fe modified PGE nanosheets were performed in FA oxidation at +0.26 V vs. silver/silver chloride (Ag/AgCl) electrode. The atomic ratios and compositions of the Pd-Fe nanoparticles were determined by Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) as 1:7, 1:21 and 1:33. The surfaces of Pd-Fe modified PGE nanosheets were characterized by Scanning Electron Microscopy-Energy Dispersive X-Ray (SEM-EDX) analysis. Thus, this work presented an outstanding example of new Pd-Fe modified PGE sensors for FA oxidation.

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Keyword: formic acid oxidation, nanosheets, palladium, iron, pencil graphite electrode

ID: 33 - Synthesis and Characterization of Nanomaterials

# Investigation of the Antibacterial Properties and the Release Behavior of in-situ Synthesized AgNPs on Plasma-treated PCL Scaffolds

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Skin is the largest organ in mammals and acts as a physical barrier between the human body and the external environment. The skin is directly exposed to harmful microbial, thermal, mechanical, and chemical damages. Skin loss can occur for many reasons, such as disorders, burns and chronic wounds. For years autografts and allografts have been used to treat burns or other skin imperfections, yet the inability of damaged skin tissue to heal completely opens up the field of tissue engineering to repair skin-related defects broadly.

In this study, we aimed to synthesize silver nanoparticles (AgNP) in situ on argon plasma-treated polycaprolactone (PCL) scaffolds for use in second or third-stage pressure ulcers, to investigate the antibacterial properties of these scaffolds, and to test AgNP release from these scaffolds. To date, in situ synthesis of AgNP directly on the scaffold by modifying the fabricated PCL scaffolds has not been reported in the literature. AgNP synthesis was carried out by the chemical reduction method using sodium borohydride as a reducing agent and polyvinylpyrrolidone as a stabilizer. For the optimization studies, the concentration and amount of the stabilizer and the concentration of the reducing agent were used as the basic parameters. The electrospun PCL scaffolds were treated with argon plasma to increase the accumulation of AgNPs during in situ synthesis. The basis for this treatment was the theory that the surface of PCL scaffolds treated with argon plasma is positively charged and interacts more strongly with negatively charged AgNPs compared to untreated PCL scaffolds.

As a result of the optimization studies of AgNP synthesis, the silver precursor:reducing agent concentration in the ratio 1:3 showed the best results in the UV-Vis spectrophotometer measurements compared to the ratios 1:1-6. The characteristic absorption peak of AgNPs was observed at a wavelength of 392 nm, which gave a sharp peak. The hydrodynamic size and polydispersity index of the AgNPs prepared at this ratio were measured to be 91.54±7.60 nm and 0.126, respectively, by dynamic light scattering (DLS). The low polydispersity index confirms the monodisperse distribution of the synthesized silver nanoparticles. Scanning electron micrographs (SEM) proved the presence of AgNPs on the plasma-treated PCL scaffolds. Elemental analysis results also confirmed the presence of silver in scaffolds. Energy dispersive X-ray analysis (EDAX) showed that the atomic content of the elements was 72.71% carbon, 25.85% oxygen, and 1.44% silver.

Consequently, In-situ synthesis optimization, AgNP release studies from the scaffolds, and investigation of the antibacterial properties of the scaffolds are still in progress. Additionally, evaluation of antibacterial and antioxidant properties of argon plasma-treated oleuropein-loaded PCL scaffolds to prevent cell damage caused by reactive oxygen species (ROS) that may occur in the wound area are under consideration.

Keyword: AgNPs, in-situ synthesis, antibacterial, plasma-treated PCL scaffold

# Characterization of Mesoporous LiMn<sub>2</sub>O<sub>4</sub> and LiMn<sub>2</sub>-xM'xO<sub>4</sub> (M': Co, Ni) Modified by SILAR Method for Efficient Water Oxidation Electrocatalysis

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Noble transition metal oxides such as IrO<sub>2</sub> and RuO<sub>2</sub> are used as efficient electrocatalysts for oxygen evolution reaction (OER) for many years, however these materials are not abundant on earth and have high costs compared to first row transition metal based oxides (TMOs) [1]. The lithiated first row transition metal oxides (LTMOs) are alternative catalysts for OER due to their higher abundances and lower costs. De-intercalation of lithium ions from LTMOs during electrochemical process produces highly active surface distinct from common TMOs and brings stability and efficiency under harsh catalytic conditions, [2] In this work, we demonstrated a two-step method based on earth abundant manganese to produce mesoporous spinel LiMn<sub>2</sub>-xM'xO<sub>4</sub> (M': Co, Ni) (x = 0-1) thin films having high surface area and modification of the catalytic surface to promote the amount of more active transition metals such as, cobalt and nickel on the electrode surface. Integrating two transition metals into spinel oxide systems amplifies the OER performance through synergistic electronic effects. [3] In the first step, molten salt-assisted self-assembly (MASA) process was utilized to fabricate mesoporous spinel LiMn2-xM x04 thin films. The spinel LiMn2-xCoxO4 electrodes (x=0, 0.5, and 1) were performed as electro-catalysts and displayed Tafel slope values of 130, 67 and 64 mV/dec, respectively. The overpotential also dropped from 491 mV to 304 mV at 1 mA/cm2 going from LiMn<sub>2</sub>O<sub>4</sub> to LiMnCoO<sub>4</sub>. Tafel slope of the spinel LiMn1.5Ni0.5O<sub>4</sub>, is 47 mV/dec with overpotential values of 262 mV at 1 mA/cm2 and 578 mV at 10 mA/cm2. In the second step, the  $LiMn_2-xM'xO_4$  (x = 0–0.5) electrodes were modified by a systematic incorporation of Co(II) or Ni(II) into the structure using successive ionic layer adsorption (SILAR) followed by an annealing process. This modification process could be repeated many times in order to enhance the amount of deposited active species on the surface. Tafel slope of mesoporous LiMn<sub>2</sub>O<sub>4</sub> thin film dropped from 130 to 82 mV/dec by applying the SILAR/annealing process once using cobalt species. Modification of the LiMn<sub>2</sub>O<sub>4</sub> using nickel by once, three, and five times gave Tafel slopes of 44, 37,34 mV/dec, respectively. LiMn<sub>2</sub>O<sub>4</sub> electrode modified by five times nickel showed overpotential values of 268 mV at 1mA/cm2 and 634 mV at 10 mA/cm2 and resulted in high efficiency and catalytic stability in long term OER performance.

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Keyword: lyotropic liquid crystal, molten salt assisted self assembly, mesoporous thin films, SILAR, water oxidation electrocatalyst

# Study of Defect Structure of Zinc Oxide Prepared by PVD

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Zinc Oxide (ZnO) thin films with various thickness (d=100 nm-650 nm) are obtained by firstly deposition of Zn in vacuum ( $\sim$ 10<sup>-6</sup> Torr) onto unheated glass substrate by PVD technique, secondly the as-deposited Zn films were heated under ambient atmosphere at temperature (673K). Optical transmittance, Raman spectroscopy and EPR spectroscopy have been studied to identification of the change of optical and structural properties depending on the defect density and precisely determining which of the defect structure is oxygen vacancy, zinc vacancy, zinc interstitial atom and oxygen interstitial atom defects by evaluating the results of electron paramagnetic resonance EPR.

ZnO is a well-known wide band gap (3.4eV), non-toxic, extremely clean and low-cost metal oxide semiconductor material. Understanding the defects that occur in the growth and synthesis process of ZnO thin films and controlling them is very important in modifications of the optical and electrical properties of ZnO nanomaterial to enhance their performance.

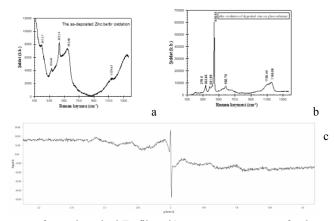


Figure a) Raman spectroscopy for as-deposited Zn films. b) raman spectroscopy after heat treatment. c) The EPR spectroscopy result for ZnO thin film.

Intrinsic defects (oxygen vacancy  $V_0$ , interstitial zinc Zni and so on) in ZnO play important roles on some fundamental properties including photoluminescence [1,2], electrical properties [1] and ferromagnetism [3]. Despite efforts for several decades. ZnO thin films is prepared in two steps, firstly deposition of zinc powder of purity of 99.995% supplied by Sigma Aldrich-324930 on glass substrate by using vacuum chamber unit (PVD-HANDY/25-TE) produced by VAKSIS, then the as-deposited Zn films with different thickness were heated in ambient air using a tube furnace. The heating temperature was 400 °C and the heating time divided to three stages as, annealing for 30 min, annealing for 1h then finally film annealed for 2 h. When the appropriate heating time is finished, the corresponding sample is pulled out quickly from the furnace, between annealing steps the films were left to get cold at room temperature.

We study the optical properties of ZnO thin films and effect of defect on it through Raman, optical transmittance and EPR spectroscopy.

In Figure a & b, the Raman spectrum of two heat treated and untreated thin film samples of zinc deposited under vacuum is given. The intense Raman mode at  $\sim$ 439cm<sup>-1</sup> is due to high frequency oxygen vibration [4, 5, 6]. It is possible that the vibrational mode at 582 cm<sup>-1</sup>, which is not observed in the untreated sample, is seen in the Raman spectrum of the heat-treated sample, possibly due to the oxygen vacancy in the zinc-rich ZnO thin film sample [5]. The electron paramagnetic resonance (EPR) spectroscopy for ZnO thin film is shown in figure c, where it can be observed that there is signal at g factor equal to nearly 2 which is due to the point defects, the EPR signals at g= 2.0048 is attributed to an unpaired electron trapped oxygen vacancy (Vo). [7, 8]

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ID: 92 - Synthesis and Characterization of Nanomaterials

# Experimental and Computational Investigation of Lanthanum Strontium Manganese Synthesis by Flame Spray Pyrolysis

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Flame spray pyrolysis (FSP) is a simple and effective way to synthesize nanoparticles with unique properties [1]. The organic fuel with precursors burns, and the combustion reaction generates enough energy to allow the precursor to decompose and oxidize, resulting in a supersaturated atmosphere of metallic oxide vapor. The atmosphere causes nucleation, resulting in primary particles that grow through agglomeration and sintering processes [2]. Numerous experimental and numerical studies of nanoparticle production by FSP have been carried out, with the main goal of understanding the effects of operational parameters like dispersion gas flow rate, precursor concentration, precursor-solvent combinations, atomization quality, nozzle and reactor configurations [3]. In this study, La<sub>0.8</sub>Sr<sub>0.2</sub>MnO<sub>3</sub> nanoparticles were synthesized. La, Sr and Mn acetate precursors were dissolved in an organic (propionic acid + 1-butanol) solvent, and carried to the center of a  $CH_4/O_2$  premixed flame by using a syringe pump through the capillary tube of two fluid nozzle placed in the center of the burner. Vacuum applied glass fiber filters were used for the collection of the nanoparticles produced in the system. Several characterization methods were used to identify the crystal structure, thermal behavior and morphology of the as prepared products. A simulation study was performed using the commercial ANSYS FLUENT v.19 software coupled with a MATLAB code to predict the multicomponent droplet evaporation, temperature, velocity, gas density and the particle growth in the flame spray pyrolysis process. Experimental and numerical results were compared to validate the model applied in the simulation.

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# Effects of Molecular Forces on the Ultimate Electroactive Smart Behaviour of HNT/GO/SO Suspensions

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Electrorheology (ER) is related to the flow behaviour of electrically polarizable particles in a non-conducting fluid such as silicon oil (SO). Halloysite (HNT), which is tubular alumina silicate clay, is used as ER active particle and it has been reported that the interaction between pure HNT particles is weak and ER activity is low under external electric field strength. Therefore, its composites are prepared to increase ER performance as well as to improve the rheological, thermal and mechanical properties. Graphene oxide (GO) is very advantageous for potential ER applications due to its dielectric nature and functional oxide surface. The aim of this study is to improve the ER activity of HNT tubular particles via introducing GO both non-covalent (HNT/GO) and covalent (HNT-GO) interactions, and to investigate the effects of type of molecular forces on ER properties. Structural characterizations of the synthesized materials are analysed by ATR-FTIR, Raman, XPS spectroscopies. Electrical conductivities are determined with a 4-Point probe conductivity meter. Then, a series of HNT/GO/SO dispersions are prepared and the optimum concentration determined to be 20wt.% according to the dielectric and ER flow curves. The colloidal stabilities, dielectric properties, ER flow curves, and electroactive viscoelastic properties of HNT/GO/SO and (HNT-GO)/SO dispersions are compared in terms of the magnitudes of inner- and inter-molecular forces. As a results of these tests, it was concluded that interfacial type polarization was the driving force for the HNT/GO/SO system. On the other hand, orientational type of polarization was dominant in the (HNT-GO)/SO system. The highest electric field induced yield stress was obtained for the (HNT-GO)/SO system as 92 Pa under E = 1.5 kV/mm condition.

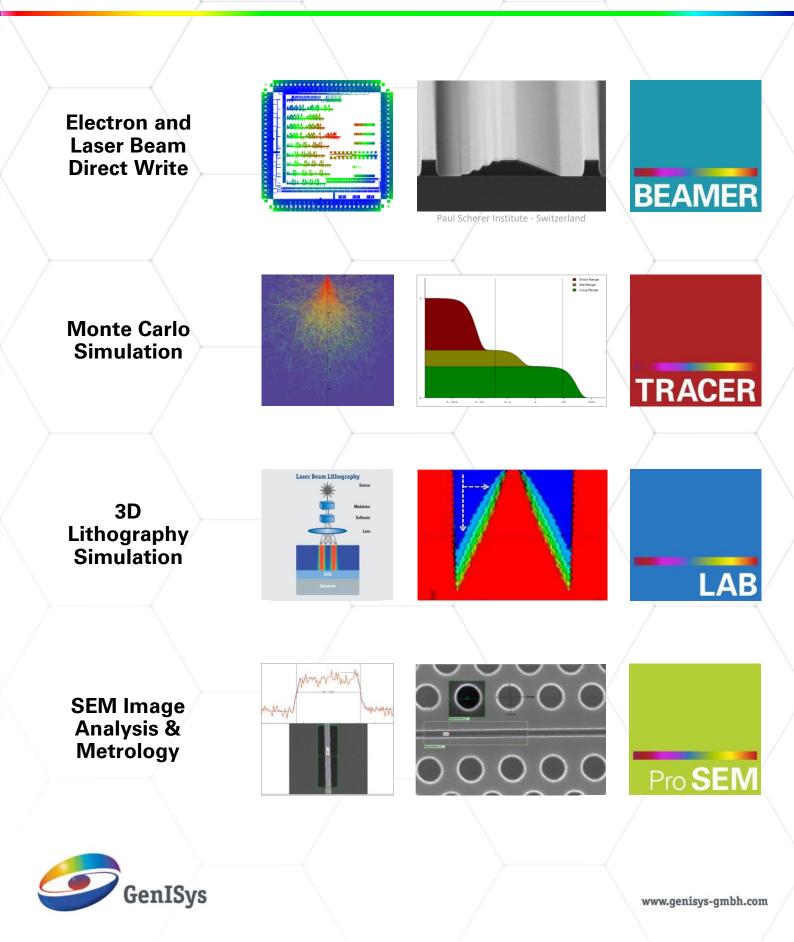
#### Acknowledgement:

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Keyword: electrorheology, dielectric, halloysite, graphene oxide, molecular forces



# Software for Advanced Lithography, Analysis & Metrology



# Photoluminescence Mapping and Lifetime Imaging Microscopy for MoS<sub>2</sub> directly grown on MXene Structures

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Transition metal dichalcogenides (TMDCs), specifically molybdenum disulfide (MoS<sub>2</sub>) structure, have already been extensively investigated for optoelectronic and photonic systems. In particular, the van der Waals (vdW) heterostructures consisting of MoS<sub>2</sub> is looked promising for novel optoelectronic devices because of their high optical quantum yield and strong light-matter interaction. However, few studies are reported for molybdenum carbide (Mo<sub>2</sub>C) - MoS<sub>2</sub> heterostructures where these heterostructures consist of Mo2C structures synthesized from MoS<sub>2</sub> [1], [2]. As an inverse approach to the others, in this study, Mo<sub>2</sub>C - MoS<sub>2</sub> heterostructure was obtained from the chemical vapor deposition (CVD) grown Mo<sub>2</sub>C.

Initially, Mo<sub>2</sub>C, grown by the CVD, was transferred on SiO<sub>2</sub>/Si substrate. Then, the composed structure, Mo<sub>2</sub>C/SiO<sub>2</sub>/Si, was used as a substrate to grow MoS<sub>2</sub> into the CVD furnace. After all, MoS<sub>2</sub>/Mo<sub>2</sub>C/SiO<sub>2</sub>/Si structure was obtained. This new structure was characterized via Raman spectroscopy and atomic force microscopy (AFM).  $\mu$ -photoluminescence (PL) and fluorescence lifetime imaging microscopy (FLIM) were performed to understand the growth of MoS<sub>2</sub> on Mo<sub>2</sub>C.

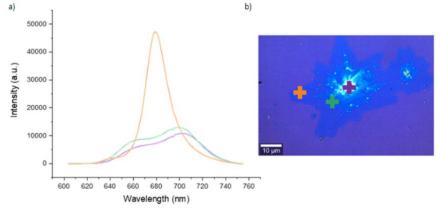


Figure 1: (a) PL intensities at different locations on (b) the new structure.

The quenching or enhancement and the spectral shift of PL were investigated: Shifts of PL bands, A exciton - B exciton - A trion, displayed over the range 610 to 750 nm, as the MoS2 thickness increased due to the reduction of the gap energy in the Brillouin zone at the K-point [3]. Also, as shown in figure 1, PL intensities changed at different locations on the structure. In addition, fluorescence lifetime for a different location on the new structure was observed: Diversity in decay lifetime over the structure was observed due to the change in defect density, crystallinity, and charge carrier density [4]. Ultimately, determining thicknesses, as a result of AFM values and Raman peaks, and their locations on the new structure were described in the sense of PL spectra and fluorescence lifetime. The outcomes of this study give comprehensive information on Mo<sub>2</sub>C - MoS<sub>2</sub> heterostructures for optoelectronics and photonic systems.

# Acknowledgments

This work is supported by the Scientific and Technological Research Council of Turkey under project number 20AG025.

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Keyword: PL, FLIM, Optoelectronic System, Photonic System, Mo2C/MoS2 Heterostructure

# ID: 124 - Synthesis and Characterization of Nanomaterials

# An Alternative In-situ Fluorination Source for Atomic Layer Deposition

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Atomic layer deposition (ALD) is a unique deposition technique that has several benefits such as providing conformal coverage, large-scale production in simple setups and producing highly uniform thin films at low temperatures [1]. In-situ fluorination of semiconductors by ALD has been a challenging process because of the lack of fluorine related metal organic precursor. Only in Park et al.'s studies, fluorine doped zinc oxide (FZO) was produced by using hydrofluoric acid (HF) and DI water [2-4]. However, HF is highly corrosive, so it is necessary to protect the ALD system with a protective coating such as Teflon. On the other hand, ammonium fluoride (NH<sub>4</sub>F) is a much weaker acid than HF and there is no requirement to make any changes in the ALD system for relatively low concentrations. In this study, fluorination of zinc oxide films was demonstrated by using ALD. A new homemade precursor, a mixture of ammonium fluoride (NH<sub>4</sub>F/H2O) solution, was used as a fluorine doping source in ALD for the first time in literature.

To demonstrate fluoriation with NH<sub>4</sub>F, zinc oxide films were chosen. All zinc oxide films were grown over silicon and quartz substrates. Diethyl zinc (DEZ) was used as the zinc source, and a mixture of NH4F/H2O solutions with different concentrations (0.5%-20% NH4F) were used as the oxygen and fluorine source. Pulse time for zinc precursor (diethyl zinc), NH4F/H2O solution were chosen to be 100 ms for surface saturation and nitrogen purge time was chosen as 10 s. The canister that contains NH4F/H2O solution was heated to 50 °C. FZO thin films were grown at temperatures in between 140°C-220°C to determine the effect of growth temperature on fluorine doping.

Samples were characterized with X-ray diffraction (XRD) to determine the presence of crystalline phases and X-ray photoelectron spectroscopy (XPS) for elemental composition determination. The distribution of the fluorine atoms in the film was observed by secondary-ion mass spectrometry (SIMS) analysis. The fluorine content up to 1.15 at. % was achieved.

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Keyword: Atomic Layer Deposition, Fluorine Doping, Zinc Oxide

# Polydopamine Coated Halloysite Nanotubes as Clay-Based Photothermal Agents

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Photothermal nanoparticles, that can convert light to heat can provide vital solutions in many different application areas where light-triggered remote heating is needed. In this study, halloysite nanotubes (HNTs), which are natural clay nanoparticles, were converted into efficient photothermal agents by functionalizing them with polydopamine (PDA), a photothermal agent. HNT-PDA nanohybrids, which contain different amounts of PDA were produced by varying reaction conditions such as the dopamine monomer concentration and reaction time. When irradiated with 808 nm laser light, HNT-PDA nanohybrids presented significant temperature increases, where they reached 250 °C in 2 min. The HNT-PDA nanohybrids were shown to be stable when exposed to multiple laser light activation cycles demonstrating their reusability. Other near-infrared (NIR) light sources such as a solar simulator, an infrared incandescent lamp, and a light-emitting diode (LED) lamp were also demonstrated to activate the HNT-PDA nanohybrids, their light-activated heating. As a demonstration of the potential applications of the photothermal HNT-PDA nanohybrids, their light-activated antibacterial activity on Staphylococcus aureus (*S. aureus*) was investigated. The viability of *S. aureus* that was treated with HNT-PDA decreased by 6.3 log at 5 min of NIR laser irradiation, while bacteria not treated with the nanohybrids remained alive under the same irradiation conditions. The versatile clay-based photothermal agents presented in this study are promising nanoparticles thanks to their natural, non-toxic, biocompatible, and cost-effective properties, and they can be utilized in a variety of photo-driven applications.

Keyword: Photothermal agents, Antibacterial effect, Nanohybrid, Light-to-heat conversion

# Electrospun Nanofibers Containing Photothermal Agents as Light-Activated Antibacterial Nanofibers

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Antibacterial air filter media, that can deactivate the captured bioaerosol particles are needed to prevent bioaerosol-related indoor air pollution. Herein, we present photothermal agent functionalized Nanofibers for use as an effective antibacterial air filter capable of killing bacteria via near-infrared (NIR) activated heat generation. Nanohybrids prepared by coating the halloysite nanotube (HNT) clay nanoparticles with polydopamine (PDA) were utilized as photothermal agents, that can heat up when irradiated with NIR light. Integration of HNT-PDA nanohybrids into polyacrylonitrile (PAN) via the electrospinning method resulted in PAN/HNT-PDA Nanofibers that can heat to 102 °C after 2 min NIR irradiation and kill *Staphylococcus aureus* cells that are in contact with the Nanofibers. While demonstrating 99.972 % filtration efficiency and a quality factor of 0,14 in a simulated air filtration system, photothermal Nanofibers also maintained their light-activated antibacterial properties over multiple exposures to light. The strong potential of the PAN/HNT-PDA Nanofibers as photothermal agents containing light-activated antibacterial air filters will be discussed.

Keyword: Nanofiber, Photothermal agent, Antibacterial

ID: 144- Synthesis and Characterization of Nanomaterials

# Effects of Morphological Changes on Electrical Conductivity of Metal-Containing Carbon Nanofibers

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Electrospinning is the most widely used method for the production of Nanofibers. The working principle of electrospinning is a solution consisting of a polymer, an additive and a solvent, is sprayed on to a collector drum via nozzle under electrical field. Parameters of the electrospinning are voltage, feeding rate, the distance between nozzle and drum, and the rotating speed of drum. The most widely used polymer for the production of carbon Nanofibers is polyacrylonitrile (PAN) which is a carbon precursor material. In this study, PAN-based carbon Nanofibers consisting of micro-sized and nano-sized metal particles were produced by using electrospinning process. Micro-sized and nano-sized metal-containing carbon Nanofibers were processed with various solvents and mechanical methods to obtain different morphological structures such as nanoparticles, nanowires and continuous Nanofibers. The morphological structures of metal-containing carbon Nanofibers were determined with Scanning Electron Microscope (SEM). Metal-containing carbon Nanofibers which have different morphological structures such as nanoparticles, nanowires and continuous Nanofibers and continuous Nanofibers were also investigated in terms of electrical conductivity with 4-point probe method.

## Acknowledgments

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Keyword: Carbon Nanofibers, Electrical conductivity, Morphology, Nanomaterials, Metal additives

#### ID: 145 - Synthesis and Characterization of Nanomaterials

# Effects of Micro and Nano-Sized Metal Particles on Electrical Properties of Carbon Nanofibers

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Among carbon-based nanomaterials, the carbon Nanofibers are good alternative to expensive carbon nanotubes. The carbon Nanofibers have ultralong 1D structure at nanoscale. The network structure of carbon Nanofibers can provide excellent specific stiffness and good electrical conductivity for various nanocomposite applications. For the production of carbon Nanofibers, the electrospinning is fast and cost-effective method. The morphology of carbon Nanofibers can be changed in diameter and length with the electrospinning process parameters, solution viscosity and type of additives. To improve their conductivity, the carbon Nanofibers can be doped with the conductive metal particles. Metal additives can exhibit different properties at nano and micro scale. In this study, the undoped and doped carbon Nanofibers were produced from Polyacrylonitrile (PAN) polymer by using the electrospinning method with constant process parameters. The electrospinning solutions involving different amounts of nano and micro metal particles were prepared to produce the doped PAN nanofibers. After the electrospinning process, stabilization and carbonization as thermal treatments were performed on PAN Nanofibers to obtain carbon Nanofibers and distribution of metal particles on the carbon nanofibers. The electrical conductivities of undoped and metal particles doped carbon Nanofibers were measured by using four-probe-point method. We will present as a comparison study about effects of the nano and micro metal particles on properties of carbon Nanofibers in terms of morphological and electrical conductivity.

## Acknowledgments

This study was supported by the Scientific and Technological Research Council of Turkey (TUBITAK) (Project No: 5210117).

Keyword: carbon nanofibers, metal additives, electrospinning, conductive nanocomposites

# Characterization and Testing of Novel Nano-Inorganic Particles to Enhance Hydrophobicity in Coil Coatings

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Prepainted metals find wide use in domestic and industrial applications as well as high-end appliances in such areas as industrial facilities. Aluminum and hot-dip galvanized (HDG) plates comprise majority of painted metal manufacturing owing to their formability, high surface quality and low cost. These metals, coated and coiled in high-speed lines as flexible sheets, also pose excellent mechanical strength and high chemical resistance. Though strong anticorrosion behavior is also a must for preserving the integrity of the coating, and eventually of the metal substrate, the current state of the art in the industry has still a long way to go towards solving the problem.

A contact between the metal and the aquatic medium is a must for initiating electrochemical reactions, making the contact reduction between the two paramount for corrosion prevention. Though lowering the surface energy of the coating is one way to achieve reduced contact, creating nanoscale roughness on the surface is another. This study aimed creating coil coating surfaces with nanoscale roughness by use of silica nanoparticles. SNPs prepared by Stöber sythesized were blended to the clear and pigmented coating recipes as additives. Hydrophobicity and rheology of the SNP-doped coatings were compared with reference materials already in use in coil coating manufacturing. The coated surfaces were further characterized by SEM, AFM and FTIR analyses as well as mechanical (adhesion, pencil hardness, solvent resistance, impact, and flexibility) testing for strength and durability to meet the universal standards in coil coating industry.

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Keyword: nanosilica, corrosion, hydrophobic coating, surface energy, coil coating

# SiO<sub>2</sub> Nanoparticles: Sol-Gel Synthesis, Characterization, and Hansen Dispersibility Parameters in Various Solvents

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SiO<sub>2</sub> nanoparticles have an attraction in automotive coating applications like increasing the thermal stability and UV resistance[1], being additive as nano lubricants for the applications in the automotive air conditioning (AAC) systems[2], increasing the self-healing properties of the materials[3], enhancing both weathering resistance[4], and the scratch resistance especially for the clearcoats[5], etc. All these enhancements can be achieved via well-dispersible nanoparticles in various systems. That is the reason why it is critical to choose appropriate vehicles for nanoparticle dispersions. Hansen solubility parameters (HSP) may help to determine "good" and "bad" vehicles by subdividing the cohesion energy into three contributions as polar contribution of, dispersive contribution od, and hydrogen bonding contribution oh[6]. Although HSP is the best for the solubility of molecules in the solvent systems, it is also found suitable for dispersion chemicals for the nanoparticles, [7].

In this study, 21 different solvents are used to optimize the sol-gel synthesis of SiO<sub>2</sub> nanoparticles depending on the sedimentation process and Hansen Dispersibility Parameters (HDP). 2 % (by weight) of silica nanoparticles are added to solvents individually under high shear mixing. After a specific time of mixing, sedimentation is controlled, and relative sedimentation rate (RST) is calculated. With the help of the software called HSPiP 5th edition programmed by Steven Abbott, the dispersibility sphere is created and the best solvent for the synthesis of silica nanoparticles is determined for the current system. Structural characterization of the synthesized silica nanoparticles is carried out by scanning electron microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and Dynamic Light Scattering (DLS).

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Keyword: SiO2 nanoparticle, Hansen dispersibility parameters, Sol-gel

# Investigation of Seeding Layer Effect on the Growth of MnO<sub>2</sub> Nanowires on Graphene Foam via Simple Hydrothermal Method

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The nanocomposite forms of graphene and manganese dioxide (MnO<sub>2</sub>) are one of the most studied materials in several applications, such as energy storage and biosensors. Accordingly, understanding the effect of hydrothermal process parameters on the synthesis of MnO<sub>2</sub> nanostructures plays a vital role in producing the nanocomposite in the desired morphology and polymorphic structure. This study intends to investigate the seeding layer effect on the growth of nanostructured MnO<sub>2</sub> on the chemical vapor deposition (CVD)-based graphene foam. For this purpose, for the comparison, MnO<sub>2</sub>-nanowires were synthesized via hydrothermal method on CVD-based graphene foam by two approaches: i) growth with a seeding layer, ii) direct growth without a seeding layer. Except for seeding layer, all parameters of the hydrothermal method were kept constant during both processes. Furthermore, samples were characterized via X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM-EDX), and Raman Spectroscopy. The experimental results demonstrate that the utilization of seeding layer directly influences the morphology of MnO<sub>2</sub> nanostructure by turning the structure into a wire-like shape. It is believed that this study will contribute to the studies for production of graphene/MnO<sub>2</sub> nanocomposites with high crystallinity and improved morphology for many applications.

Keyword: MnO2-nanowire, graphene foam, hydrothermal method

# Patterning and Chemically Tunable Electrostatic Interactions of BiSn@SnO Core-Shell Colloidal Particles

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Smart materials are able to sense, control and response to the changes in environment [1]. Anisotropic and multicomponent colloidal particles gain significant attention in recent years as they enable the directional movement and multifunctionality [2]. In addition to the size, chemistry and spatial distribution of phases in the particle, the surface characteristics are utmost importance to reveal the interactions between particles and the environment. In this study, we combine bismuth and tin metals in various forms and enclosed them in the tin oxide shell. This is an interesting structure as each of these components exhibit distinct properties which, if the particles are carefully prepared, can be combined in one particle. Bismuth-based materials are finding applications in photocatalysis, switchable plasmonic metamaterials and low toxicity control agents owing to their highly anisotropic Fermi surface, poor charge carrier density and very small band overlap energy [3,4]. Tin-based materials, on the other hand, are being used as an anode material in Li- or Na- ion batteries, as antimicrobial agents, and as electrocatalyst and photocatalyst particularly in water purification or CO<sub>2</sub> reduction reactions, etc. [5]. Moreover, metal (Bi-Sn) core and semiconductor (SnO) shell hybrid structures has a potential to alter the electronic and optical properties of Bi and Sn elements. In this presentation, we will first introduce the variety of BiSn core-SnO shell particle types that we have synthesized. Then, the electrical potential of particle surfaces in aqueous media will be reported. Our studies showed that the surface characteristics of BiSn@SnO core-shell particles can be altered by changing the spatial distribution of Bi and Sn in a particle, the composition and the surface oxide characteristics. The potential applications based on the tunable surface characteristics of BiSn@SnO core-shell structures will also be demonstrated.

#### Acknowledgement:

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Keyword: Core-shell particles, Multi-component Structures, Colloidal Particles

#### ID: 211 - Synthesis and Characterization of Nanomaterials

# Ordered Double Transition Metal MAX Phases and their Etching into MXenes

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Ordered Double Transition Metal MXenes (DTMs) and their MAX phases are a more recent addition to the rapidly growing MXene family of 2D materials. The few reports published on the electrochemical charge storage properties of DTMs suggests that they perform much better than their mono metal counterparts. This is true for both ordered and solid solution DTMs [1][2][3]. Despite the theoretical predictions on the stability of a number of double transition metal MAX phases, only a few have been synthesized and etched into their corresponding MXenes. In attempt to scale up the synthesis and processing of DTMs, we present the synthesis and structural studies of ordered Mo<sub>2</sub>Ti AlC<sub>2</sub>, Cr<sub>2</sub>TiAlC<sub>2</sub>, Cr<sub>2</sub>Ti<sub>2</sub>AlC<sub>3</sub> and solid solution Ti<sub>2</sub>NbAlC<sub>2</sub> MAX phases and their etching into corresponding MXenes. In-situ high temperature XRD data collected on the admix of activated metal powders was used to optimize and model the MAX phase synthesis in high temperature tube furnace. Electrochemical studies such as CV, EIS and CCD of the DTMs compared with Ti<sub>3</sub>C<sub>2</sub>Tx will be presented and discussed.

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Keyword: 2D Materials, MAX Phases and MXenes, Etching, Nanosheets

# Production of Nanoparticles Decorated Graphene-Based Materials

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Graphene based materials, such as few-layer graphene, multilayer graphene, graphene nano-platelets and reduced-graphene oxide (r-GO) are high surface area materials with outstanding mechanical, thermal and electrical properties. These properties can be further improved and/or additional properties can be added to these materials by coating them with other nanomaterials, such as noble metal nanoparticles. Those type of hybrid materials are promising for several different applications, e.g., surface enhanced Raman scattering, conductive inks, antibacterial applications and in energy related applications. Their performance can be improved if the nanoparticles are *in-situ* formed over graphene-based materials due to their uniform distribution. *In-situ* decoration of graphene-based materials with different metal nanoparticles and their potential applications will be discussed in this presentation.

# Graphene Oxide Particles Functionalized by Cold Atmospheric Plasma: Morphological, Physicochemical Features and Drug Release Performance

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Advances in biomaterial design principles and nanomaterial production and characterization methods have led to tremendous progress in the development of effective nano- and/or micro-sized particles with various functions in drug delivery systems. On the other hand, cold atmospheric plasma (CAP) use in clinical studies is mainly limited to the treatment of chronic wounds, but its application in a wide range of medical fields is now the goal of many analyses. It is therefore likely that its application spectrum will be expanded in the future. Graphene and its derivatives are the drug delivery system candidates that have attracted attention in nanomedicine applications in recent years [1-2]. Graphene-based nanomaterials such as graphene oxide (GO) are being evaluated in many medical applications, including drug release [3-4]. The use of plasma processes in nanomaterial synthesis and/or surface modification is limited due to a lack of understanding of the effects of plasma treatment on morphology and other properties [5]. In this work, the effects of cold atmospheric plasma treatment on the morphology and physicochemical properties of GO particles fabricated by the modified Hummers method were first investigated by Scanning electron microscopy/energy dispersive X-ray spectrometry (SEM/EDS), optical emission spectroscopy (OES), Fourier transform infrared spectroscopy (FTIR), and X-ray diffraction (XRD). Then, Quercetin (QU), which was chosen as the model drug, was loaded on the cold atmospheric plasma treated and untreated GO particles. The effect of cold atmospheric plasma modification of GO particles on QU loading efficiency, QU release profile and release kinetics was investigated. In vitro release of QU from the QU-loaded GO particles was examined in simulated physiological condition by ultraviolet-visible spectroscopy. The results showed that GO particles modified with cold atmospheric plasma increased the drug release efficiency by increasing the amount of oxygen on the surface.

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Keyword: Graphene Oxide, Drug Delivery System, Cold Atmospheric Plasma, Quercetin

#### ID: 248 - Synthesis and Characterization of Nanomaterials

# Nanomaterial Engineering as a Tool for Recent Developments in Radiation Shielding Materials

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Radiation science and technology has unique contributions to current science and technology applications ranging from medical, industrial applications to scientific research areas including recycle technologies. Nano metals having the advantage of high surface to volume ration has inherent advantage of gamma radiation attenuation. Nano level hexagonal boron nitrate, with a similar structure to graphite, was used for the neutron particle moderation. Composite materials highly filled with functional materials could end up with different material properties. A ceramic rubber composite with very high radiation stability has been developed. These materials could be used in many different applications including medical applications and space applications.

Keyword: radiation, nanomaterials, shielding

ID: 252 - Synthesis and Characterization of Nanomaterials

# Synthesis and Self-Assembly of Poly(2-isopropyl-2-oxazoline)-b-(2-phenyl-2-oxazoline)-b-(2-isopropyl-2-oxazoline)

# <u>Cağrı Turan</u><sup>\* 1</sup>, İrem Erel Göktepe<sup>1</sup>, İpek Terzioğlu<sup>2</sup>

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We report on synthesis and self-assembly of ABA-type amphiphilic triblock copolymer, namely as poly(2-isopropyl-2-oxazoline)-*b*-(2-phenyl-2-oxazoline)-*b*-(2-isopropyl-2-oxazoline) (PiPOX-*b*-PPhOX-*b*-PiPOX). PiPOX-*b*-PPhOX-*b*-PiPOX was synthesized through cationic ring opening polymerization technique by sequential monomer addition in a one-pot fashion and characterized through <sup>1</sup>H Nuclear Magnetic Resonance (<sup>1</sup>H NMR) Spectroscopy and Gel Permeation Chromatography (GPC). Self-assembly of PiPOX-*b*-PPhOX-*b*-PiPOX into polymersomes was achieved through solvent shifting method. The factors such as flow rate, vortexing, and concentration were examined to control the size and size distribution of polymersomes. PiPOX-*b*-PiPOX polymersomes were characterized through dynamic light scattering (DLS) technique, confocal laser scanning microscopy (CLSM) and transmission electron microscopy (TEM) imaging. Finally, the effect of increasing temperature on the morphology of the polymersomes was investigated and discussed within the context of LCST-type phase behaviour of PiPOX.

#### Acknowledgments

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Keyword: Poly(2-alkyl-2-oxazoline)s, polymersomes, temperature-responsive, self-assembly

#### ID: 269 - Synthesis and Characterization of Nanomaterials

# Light-Triggered Hydrogels for Folding Control with Pattern Design

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Controlling the shape change in responsive materials to external stimuli such as temperature, light, and pH attracts the attention of many fields including biomedical, tissue engineering, drug delivery, and soft robotics. *Poly(N-isopropylacrylamide)* P(NIPAm), a derivative of acrylamide, is one of the most widely used temperature responsive polymers. P(NIPAm) has hydrophobic and hydrophilic groups, so changes occur in its structure depending on the temperature. Aqueous solutions of P(NIPAm) swell by taking more water under the phase transition temperature ( $\sim$ 32 °C), which is called lower critical solution temperature (LCST), and shrink by releasing the absorbed water above that temperature.

By inspiring unique features of stimuli-responsive materials, we design a thermo-responsive trilayer hydrogel platform with different patterns and pattern colors. These hydrogel platforms are fabricated through crosslinking a non-responsive passive layer and two thermo-responsive active layers together in a 3D-printed mold. The difference in shrinkage between layers above the lower critical solution temperature (LCST) generates stress that results in the bending of the material. This bending is controlled by the external light stimulation of the responsive layer made in various patterns and colors. The colored upper layer absorbs the light in different degrees depending on the wavelength of light. This absorbance primarily provides the heating of the patterns and determines the folding direction. As proof of concept, the application of a design that gripes the target is also demonstrated. The results show that our approach might open up promising possibilities in the production of soft foldable materials.

Keyword: Stimuli responsive hydrogel, foldable material, soft gripper, smart material

# ID: 294 - Synthesis and Characterization of Nanomaterials

# **Graphene Quantum Dots Based Schottky Diode**

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The past decade has seen the rapid development of Graphene Quantum Dots (GQDs) in many areas. GQDs are excellent materials due to their large diameter, high surface area, high mechanical strength, high elasticity, thermal stability, and good electrical conductivity like graphene [1–4]. GQDs which have nanoscale small sections of graphene are a zero (0) dimensional nanomaterial. Compared to graphene, GQDs have a non-zero bandgap due to the quantum confinement effect in all dimensions [5]. This bandgap can be adjusted by varying the size and surface chemistry of the GQDs [6]. An objective of this study was to investigate GQDs on p-type Si-based hybrid structure diode parameters. These steps were followed to fabricate the GQDs Schottky diode. Firstly, nitrogen-doped GQDs were successfully prepared via a one-step hydrothermal method using citric acid (CA) and polyethyleneimine (PEI) as the carbon, nitrogen, and amino group precursors, respectively. Second, GQDs solutions was spin-coated on the p-type Si wafer. Finally, Aluminum (Al) (99.999% purity) was deposited to obtain ohmic and rectifying contacts. Current-voltage (I-V) characteristics of the diode were analyzed at room temperature. Diode parameters such as barrier height ( $\Phi_b$ ) and ideality factor (n) of the structure were extracted by Thermionic Emission (TE). The values of  $\Phi_b$  obtained from TE, were found to be 0.76 eV. Also, the values of n obtained from TE theory was found to be 3.71. The rectification ratio (RR) of the structure was found to be about 1000 at  $\pm$  5 V. The obtained results suggest that the NIR active GQDs hybrid structure can be used in various device applications such as solar cells and transistors.

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Keyword: Graphene Quantum Dots, N-doped GQDs, Schottky diode, I-V characteristic

ID: 298 - Synthesis and Characterization of Nanomaterials

# An Electrochemical Immunosensor Modified with Nanofibers for the Determination of a Carcinoembryonic Antigen

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Carcinoembryonic antigen (CEA) is considerably addressed for the clinical diagnosis of miscellaneous tumor types. In this study, an electrochemical immunosensor for the determination of the CEA biomarker was presented. Carcinoembryonic antigen (CEA) is of importance for the clinical diagnosis of various tumor types. In this study, an electrochemical immunosensor for CEA biomarker determination is presented. Nanofibers were prepared by electrospinning on the pencil graphite electrode (PEG) surface and loaded with CEA antibodies (Anti-CEA) as the CEA biomarker receptor. Finally, PGE/PAN+La0.25Fe0.75FeO3/Anti-CEA was used for CEA detection. The fabrication steps were characterized by cyclic voltammetry and electrochemical impedance spectroscopy in the presence of a  $[Fe(CN)_6]^{3-/4-}$  probe. The results showed that the nanofiber exhibited a very fine network for immuno detection. The use of this composite system is a novel immunosensor development approach for label-free detection of CEA. The results showed that even very small changes in CEA concentration could be detected with the presented system. In addition, immunosensor recovery was calculated in real serum samples containing dopamine and ascorbic acid. It has great potential in clinical screening of different cancer biomarkers.

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Keyword: Carcinoembriyonic antigen, Nanofiber, Immunosensor, cytosensor

# Nano-based Affinity Materials in Protein Separation Techniques for Diagnostic Applications

#### <u>Kerem Tok</u><sup>\*</sup>, Hichem Moulahoum, Faezeh Ghorbanizamani, Duygu Harmancı Karagülle, Simge Balaban Hanoğlu, Ceren Durmuş, Serap Evran, Candan Çiçek, Ruçhan Sertöz, Bilgin Arda, Tuncay Göksel, Kutsal Turhan, Suna Timur, Figen Zihnioğlu

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The identification and isolation of specific protein targets is a major field in bioscience and biotechnology. There is a variety of well-established chromatographic and electrophoretic techniques for this purpose. However, these conventional methods suffer from many disadvantages such as the lengthy processing time and experimented staff needed especially for emergency cases like pandemics. Hence, increased attention has been paid to the development and application of nano-based separation and detection techniques that have a great potential in overcoming many of the challenges mentioned. Nanomaterials have found widespread use in various fields such as electronic, material, and biomedical sciences. The fast advances in the development of tunable and controlled nanoparticles allowed the development of a variety of interesting nanoparticle-based systems for the separation, enrichment, and detection of target biomolecules. As opposed to complex and time-consuming conventional methods, affinity nano-based separation provides efficient separation and purification in terms of time, labor, and yield. The application of nano-based materials in the separation and purification of peptides and proteins can be of utmost importance in the case of antibodies and other biomarkers from pathogens for the development of sensing and diagnosis approaches.

We have developed a simple and quick magnetic nanoparticle (MNP)-based method for the isolation and separation of specific antigens and antibodies of SARS-CoV-2. These proteins were used for mass spectrometry profiling and diagnosis as well as the development of paper-based and electrochemical sensors. The development process of the nanomaterials was optimized to obtain a high yield of antibodies and antigens. The isolated antigens were then analyzed via mass spectrometry demonstrating that the use of MNP-based separation allowed a selective enrichment of SARS-CoV-2 antigens and eliminated unnecessary proteins. The combination of nano-based separation with mass spectrometry can be of great use for the detection and identification of original sequences with high potential for the identification of various variants indesciminatly. On the other hand, MNPs were also used in combination with the isolated antibodies for the development of a portable electrochemical immunosensor for SARS-CoV-2 diagnosis and its other variants. The sensor demonstrated indiscriminate detection of several COVID-19 variants with a high level of specificity and sensitivity that is comparable to the gold standard RT-PCR technique. These methodologies can pave a steppingstone for the creation of efficient tools for any eventual pandemic. This study was supported by TUBITAK (Project number: 120R021).

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Keyword: SARS-CoV-2, Antigen/antibody purification, Magnetic nanoparticle (MNP)-based separation, Mass spectrometry, Electrochemical sensors

# **Design of Polymeric Cathode Materials for Aqueous Zinc Ion Batteries**

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The use of sustainable energy sources as an alternative to fossil fuels places the study of energy storage systems as one of the important fields in science as well as industry. To store the electrical energy generated by sustainable sources such as solar or winds, batteries have been seen as the most promising storage systems. Although lithium ion batteries (LIBs) have already dominated the field of research and market, there are still demands for the new battery technologies serving cost effective. safe, and sustainable solutions, particularly for grid scale energy storage. In this regard, zinc ion batteries (ZIBs) have been seen as a promising rechargeable battery type due to their low cost, high capacity, and ability to work with aqueous electrolytes [1]. Although significant improvements can be achieved by using inorganic cathode materials, the low number of charge/discharge cycles and sustainability problems limit their practical usage. In this sense, the organic based electrode materials have been considered promising alternatives to their inorganic analogs. In recent years, several organic materials have been introduced as electrode materials in ZIBs. However, most of them usually suffered from low specific capacity, inadequate cycling stability, and most importantly solubility in aqueous electrolytes. On the other hand, porous polymeric frameworks have been considered promising electrode materials for rechargeable ZIBs due to their tailorable redox functionalities, high porosity, low cost, and environmental aspects [2]. In this aspect, we designed and synthesized a new covalent organic network (CON) to test its performance in Zn ion batteries as a cathode material. Due to its abundant and accessible carbonyl groups ready to interact with Zn ions, they show high reversible capacity up to 100 mAh g<sup>-1</sup> with high cyclic stability over 1000 discharge/charge cycles. We are currently exploring the zinc ion storage mechanism with the help of theoretical calculations and electrochemical analysis. These findings are highly important to gain a fundamental insight into the structure-property relationship, which paves the way for rationally designed next generation battery systems.

Acknowledgments: O.B. acknowledges financial support from the Scientific and Technological Research Council of Turkey (TUBITAK) under Project No.220Z024.

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Keyword: polymeric frameworks; porous organic polymers; energy storage; zinc-ion batteries



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#### ID: 323 - Synthesis and Characterization of Nanomaterials

# Synthesis and Characterization of Inherently Antibacterial Cationic Nanoparticles

## Shifa Alhamvi<sup>\* 1</sup>, Murat Topuzoğulları<sup>1</sup>, İlkgül Akmaya<sup>2</sup>, Tülin Özbek<sup>2</sup>

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Cationic polymers show considerable attention due to their inherent antibacterial activity, and biocompatibility, in addition to their relatively easy production and modification [1]. Polycations with quaternized ammonium groups such as 4-vinylpyridine are good examples of such polymers [2]. Polymeric nanoparticles synthesized from this type of polymer can be utilized in many biological applications such as drug delivery systems, surface coating, and wound dressing [3].

In this study, cationic polymer containing the monomers of 4-vinylpyridine (4VP) and oligo (ethylene glycol) methyl ether methacrylate 500 (OEGMA 500) (poly 4VP-co-OEGMA) was successfully synthesized. The produced polymer was modified with 1-bromohexane by quaternization reaction. In addition, Poly(lactic-co-glycolic acid) nanoparticles, coated with the quaternized polymer were synthesized. The synthesized nanoparticles were cross-linked with 1,6-dibromohexane by quaternization reaction. The produced materials were characterized with GPC, 1H-NMR, FTIR, DLS, ELS, and SEM methods. Finally, the antibacterial activity of the synthesized polymer and all the nanoparticles was examined using microdilution assay.

The results showed that the molecular weight of 4VP-co-OEGMA polymer was 29.9 kDa with 10% OEGMA and 90% 4VP content. The quaternization degree of the copolymer was 40%. Nanoparticles with hydrodynamic diameters ranging between 100 and 350 nm, polydispersity index below 0.2, and zeta potential values between 40 and 55 mV were obtained. In addition, the produced materials showed antibacterial activity in microdilution assays against both *E. coli* and *S. aureus*. The synthesized nanoparticles are expected to have the potential to be used in many biomedical applications.

#### Acknowledgement:

This project is supported by TÜBİTAK-2210C program-2021/2 - project Number: 1649B022113550.

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Keyword: 4-vinylpyridine, antibacterial, nanoparticles, polycations, quaternization.

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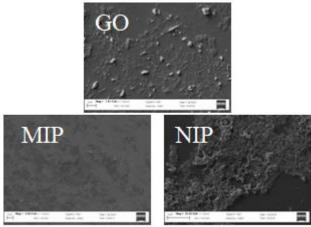
# Fabrication of imprinted polymer based reduced graphene oxide composite for the detection of 17-β -Estradiol

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Endocrine disrupting chemicals (EDCs) are now regarded as one of the main types of environmental pollutants that can affect how well the endocrine system works. Because EDCs are released into the environment without being treated, researchers in the field of environmental sciences have begun to pay more attention to them. Estradiol, commonly known as  $(17-\beta-estradiol)$ , is a naturally occurring steroid estrogen and one of these EDCs. By interfering with the regular physiological processes, it can have a wide range of negative consequences on the endocrine systems of both people and wild animals. Therefore, it is crucial to develop a sensitive method for analyzing and detecting this chemical in environmental samples [1,2].

In this study we develop the novel composite based on imprinted polymer on the surface of reduced graphene oxide for the selective detection of 17-β-estradiol. The two phase (organic and aquous phase) polymerization method was used to synthesize the imprinted molecule on to the surface of reduced graphene oxide. For this purpose, firstly the graphene oxide was synthesized by Hummer's method [3] and then it was reduced by 3-(trimethyoxysilyl) propyl methacrylate (3-MPS) [4]. The molecular imprinted polymerization was done on the surface of reduced graphene oxide to achieve the large surface area for the recognition of analyte 17-β-estradiol. The synthesized composite was thoroughly characterized to confirm the synthesis of imprinted polymer different characterization techniques were used to characterize the imprinted polymer on the surface of reduced graphene oxide such as Fourier transform infrared (FTIR), Surface enhanced microscopy (SEM), Raman spectroscopy and zeta sizer. Raman study shows that graphene oxide has successfully synthesize with remarkably D and G band position and after reduction it shows the single layer sheet. Moreover, the SEM shows that nanosized sheet of graphene was successfully synthesized and the MIP and NIP shows the narrow size distribution with spherical shape and size of around 126 nm.



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Keyword: Graphene oxide, Molecular imprinted polymer, 17- β-estradiol, Nanocomposite, Sensor

# Ruthenium Doped InP/ZnS QDs and Their LED Application

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Transition metal doping is a common approach to tune the optical properties, increase the thermal and chemical stability of QDs1. Due to its tunable photoluminescence (PL) emission, high photoluminescence quantum yield (PLQY), stability, and increased charge carrier density, transition metal ion-doped QDs are developing materials in this respect.2,3 Until now, transition metal (Ag, Cu, and Mn)-doped InP QDs have been reported. In our study, for the first time, we introduce ruthenium (Ru) element doping into the InP nanostructure.

InP core structure is synthesized by hot injection technique. Ru<sup>+3</sup> ion doping is performed at the temperature of 230°C by injection of Ru precurcor. We grew a zinc sulfide (ZnS) shell on ruthenium doped InP (Ru:InP) structure to reduce surface traps and increase PLQY. In accordance with the absorption spectra, PL peak of the undoped InP structure becomes red-shifted with Ru doping. According to InP core size and different Ru:In ratio, PL emission shift and PLQY change were optimized. Maximum PLQY of 26.7% was obtained with 0.003 Ru:In doping ratio in green InP core structure. The optimization studies of ZnS shell growth led to efficient Ru:InP/ZnS core/shell structures with PLQY of 77.6%. To gain insight into the non-linear absorption and ultrafast decay properties transient absorption spectroscopy (TAS) is employed for both undoped and doped InP QDs.

The transmission electron microscopy (TEM) results indicate that particle size of the InP core (3.15 nm) slightly increased after Ru doping (3.36 nm). After ZnS shell growth the QDs are enlarged to 6.01 nm. X-ray Photoelectron Spectroscopy (XPS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) results confirm the Ru presence in the crystal structure. Moreover, XRD results show that Ru is doped at interstitial sites of the InP crystal structure. Finally, we integrate the Ru:InP/ZnS QDs into light emitting diode (LED) die in liquid-state to reduce the host-material effect. The resulting liquid-LED device exhibited 7.92% of external quantum efficiency (EQE).

Acknowledgement: S.N. acknowledges support by the Technological Research Council of Turkey (TUBITAK) with Project No. 119F363.

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Keyword: Ruthenium doping, transition metal, indium phosphide

# Production, Characterization and In Vitro Applications of TiO2 Nanotubes

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In cell culture research, growing cells on a surface is one of the most essential experimental procedure and are widely used in bioresearch. With the rapid development of nanotechnology in recent years, the production and use of nanocomposite structures with more than one feature simultaneously have become widespread. In addition, various nanocomposite structures have been produced in Histology, cytology, and wound healing studies to evaluate the biocompatibility and in vitro toxicity of potential drug candidates. In this study, Titanium dioxide nanotubes were grown on titanium foil by anodization<sup>1</sup>. The structure of the final nanocomposite was investigated in detail by EDX, XRD, SEM, and AFM measurements. Human Cervical Epithelial Adenocarcinoma Cells (HeLa) and Mouse fibroblast cell line (L929) were used to prove the biocompatibility and low toxicity of decorated surfaces. UV spectrophotometry (MTT Assay (3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium Bromide))<sup>2</sup>, microscopy, and electrochemical sensing techniques<sup>3</sup> were applied to show the growth on the decorated and normal platforms. This nanocomposite is expected to be adapted into various bio-applications such as 'cell culture on a chip', biosensors and the design of tools for real-time viability assay. In addition, these applications will be supported by appropriate device software and artificial intelligence in future studies, and the results in the laboratory will be followed in real-time from mobile phones.

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# An Electric Field Induced Hot Electron Transport in GaAsBi Alloys

#### Mustafa Aydın, Selman Mutlu, <u>Omer Donmez</u>\*, Ayse Erol

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We report experimental and analytical results on hot electron transport in as-grown and thermally annealed n-type  $Al_{0.15}Ga_{0.85}As/GaAs_{0.96}Bi_{0.4}$  structures at room temperature. The drift mobility of as-grown and thermally annealed samples are determined from the slope drift velocity-electric field results at the low electric field. The drift velocity of both  $Al_{0.15}Ga_{0.85}As$  and  $GaAs_{0.96}Bi_{0.4}$  is theoretically calculated. Analyzing the experimental results with theoretical modeling shows that transport of the hot electrons is based on parallel conduction due to presence of electrons in both  $Al_{0.15}Ga_{0.85}As$  (barrier) and GaAsBi layers. The hot electron transfer from GaAsBi to barrier layer as real space transfer is suppressed at higher electric fields even being the lower energy barrier between the barrier and GaAsBi layers, whereas transferring of electrons from GaAsBi (Gamma-valley) to the nearest L-valley, inter-valley transfer, is dominated at high electric field. After thermal annealing, the drift velocity becomes lower due to the higher carrier density in the GaAsBi layer.

Keyword: Drift velocity, GaAsBi, hot electron, saturation velocity, electron temperature

#### ID: 84 - Properties of Nanoscale Materials

# Investigating the Factors Affecting the Specific Absorption Rate (SAR) of Magnetic Nanoparticles for Magnetic Hyperthermia

#### Beyza Abişoğlu<sup>\*</sup>, Cem Levent Altan

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Radiotherapy, surgery, and chemotherapy are mainly applied separately or in combination as conventional antitumor treatment methods, however exhibit several side effects that affect the efficiency of the treatment process. In recent years, magnetic hyperthermia has emerged as a potential and alternative treatment method in which, cancer cells are destroyed by increasing the temperature of a tumor area locally up to 40-45°C by using biocompatible magnetic nanoparticles that are either targeted or directly injected at a specified tumor site. Subsequently, an alternating magnetic field is applied at the region of interest and due to the magnetic hysteresis, particles generate heat which consequently increase the local temperature up to the desired limits and cause necrosis of cancer cells while healthy tissues are not adversely affected. The heating performance of magnetic nanoparticles is specified by the specific absorption rate (SAR), which is the power generated by magnetic nanoparticles per unit mass. The effective application of magnetic nanoparticles in hyperthermia depends on the frequency and the intensity of the externally applied magnetic field, exposure time, concentration, the magnetic properties even the size and morphology of the particles. In order to enhance the effectiveness of magnetic hyperthermia, magnetic nanoparticles that exhibit higher heating efficiencies which ensure adequate SAR values are needed and there are several conflicting studies illustrating the performance of magnetic nanoparticles that are prepared via several synthetic pathways. Therefore, in this study, biocompatible magnetic nanoparticles in the presence and absence of several surface-active agents and polymers was prepared via different synthesis methods in order to reveal the effect of surface coating, the morphology, particle size and magnetic properties over the heating performance of nanoparticles. In order to examine the efficiency of these nanoparticles in magnetic hyperthermia, specific absorption rates (SAR) were measured and additionally, the impact of field strength and frequency of the applied magnetic field as well as the particle concentration were analyzed for the optimization of SAR values that is directly affecting the performance of magnetic hyperthermia.

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Keyword: Magnetite, SAR, Hyperthermia, Magnetic Nanoparticles



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# The Effect of Hydrophobicity of Silica Nanoparticle Modified Surfaces on Bacterial Adhesion

#### Oznur Tiftik<sup>\*</sup>, Elif Sirin, Buse Camlıca, Zehra Beyza Erdekli, Merve Akmese, Merve Celik, Fatih Buyukserin TOBB ETU, Ankara, Turkey

Superhydrophobic surfaces, which is based on lotus effect, are an important research area and these surfaces gives the surface specific properties such as anti-icing, anti-fouling, anti-reflective and self-cleaning. [1] They also possess anti-adhesive properties so that they prevent any kind of attachement on the surface.[2] One of the most outstanding benefit of this property is that they can inhibit bacterial adhesion. Silica nanoparticles (Si NP) are frequently used in the production of superhydrophobic surfaces due to its low toxicity and easy fabrication.[3] In addition, among other techniques the use of spraycoating as an easy and facile production method allows mass production and by changing and modifiving the spray solution glass surfaces with different contact angles can be obtained. In this study, we researched the relation between the bacterial attachement/adhesion and the hydrophobicity of the surfaces by fabricating various spray-coated glass surfaces which were hydrophilic, hydrophobic and superhydrophobic. To obtain superhydrophobicity, two factors are necessary: surface roughness and low surface energy. (REF) In this study, superhydrophobic surfaces were prepared by using Si NPs to create surface roughness and octadecyltrichlorosilane (ODTS) and polydimethylsiloxane (PDMS) were used to reduce the surface energy. ODTS was used to decorate the Si NPs and PDMS was used as an adhesive which also enhances the durability of the coatings. Superhydrophobic surfaces were prepared by spray-coating the glass slides with Si NP/ODTS, Si NP/PDMS and and hydrophobic surfaces were prepared by spray-coating the glass slides with PDMS polymer solution. Contact angle of the surfaces were measured and roughness of the surfaces were characterized with atomic force microscopy. While the contact angle values are above 160° on superhydrophobic surfaces, it is above 100° on hydrophobic surfaces. Additionally, a variety of test were applied on surfaces such as duarbility of the coatings on different temperatures (+4, -20, 25 °C), autoclave test (121 °C, 1 atm) and tape test. Also the transparencies of the fabricated surfaces were determined by UV-Vis spectroscopy. To investigate bacterial adhesion, Escherichia coli (E. Coli) solution was drop-casted on the fabricated surfaces and the bacteria was incubated for 24 hours. After washing the surfaces, the remaining bacteria on the incubated surfaces were investigated via DAPI dye by fluorescence microscopy. Consequently, significantly less bacterial adhesion was observed on superhydrophobic and hydrophobic surfaces as expected.

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Keyword: Silica nanoparticle, Spray-coating, Hydrophobicity, Bacterial Adhesion, Durability

#### ID: 151 - Properties of Nanoscale Materials

# Effect of rapid thermal annealing on structural and morphological properties of n-type GaAsBi epilayer

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We investigate rapid thermal annealing effect on the structural, optical, and electrical properties of n-type GaAs<sub>0.98</sub>Bi<sub>0.02</sub> epilayer grown on semi-insulating GaAs substrate. Studies have shown that the annealing processes applied after growth has a significant effect on the optical, electronic and morphological properties of the GaAsBi alloy [1-3]. In this study, unlike the studies in the literature, the annealing effects of intentionally doped n-type doped triple GaAsBi alloy after growth were investigated. Rapid thermal annealing process were applied at 500 and 600°C for 60 sec, at 700°C for 60, 90, and 120 sec and at 800°C for 60 sec. Photoluminescence (PL) intensity and PL peak energies of the sample annealed below 600 °C are almost identical to the as-grown sample. Above 600°C annealing temperature, PL intensity increases, and PL peak energies blueshifts. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to investigate the effect of thermal annealing on the surface morphology of the sample. SEM and AFM images show that as-grown sample has droplets and clusters on the sample surface. The distribution and shape of the droplets and clusters are strongly affected by thermal annealing.

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Keyword: n-type GaAsBi, Thermal Annealing, Optical properties, Electronic properties, Electrooptic

#### ID: 163 - Properties of Nanoscale Materials

# **Gunn Effect in InGaAs Epilayer Structures**

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In this study, we have investigated emission characteristic and Gunn oscillations of InGaAs- based light emitter that depends on Gunn effect observed from domain transition along the device. The structures were grown by the Metal Organic Vapour Phase Epitaxy (MOVPE) with an alloy composition on %In = 0.53 and defined in a simple bar structure with different contact geometries using standard pholithograpy techniques. Threshold electric field was determined from the beginning of the NDR to observe Gunn oscillations. In the electroluminescence measurements at this threshold electric field value (3kV/cm) [1], it is observed that this structure emits at a wavelength of about 1600 nm. Above threshold electric value a drastic increase at the emission has been observed. Electrical measurements were conducted at a pulse width of applied voltage of 20ns, 40ns and 60ns. From the beginning of the NDR, Gunn oscillations have observed with a frequency of approximately between 0,5 GHz and 1GHz depending on the electric field.

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Keyword: Gunn effect, Gunn diode, Gunn oscillations, NDR, InGaAs-based Gunn diode

ID: 170 - Properties of Nanoscale Materials

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# Investigation of Gunn effect in GaAs and InGaAs epilayers

Not presented.

# Band renormalization of Ruddlesden-Popper Hybrid Lead Free Halogen Perovskites Under Strain

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Strain is an effective factor for designing the band structure of nano materials. The band gap and energy levels of semiconductor materials can be tuned by strain, and thus, semiconductor materials under strain show electrical properties that they do not have in equilibrium [1, 2]. The properties and stability of two dimensional perovskites regarding how strain affects are still largely unexplored, that's why it becomes great importance for fundamental research and designing high performance devices. Two-dimensional (2D) hybrid perovskites have better environmental stability compared to three-dimensional perovskites. In literature, Pb<sup>+2</sup> included hybrid perovskites are investigated in detail. However, lead is not suitable for use in devices due to its known toxic effect. So, in this work the 2D van der Waals Ruddlesden–Popper hybrid lead-free halide perovskites are investigated to eliminate the toxicity. The variation of electronic band structures of Ruddlesden-Popper hybrid halogen perovskites under strain calculated by generalized gradient approach using Perdew Burke-Ernzerhof parameterization as a first principle plane wave and exchange-correlation potential based on density functional theory. The results in this study show that band gap renormalization related to octahedra/ligand tilting motion. We found that by applying uniaxial strain the bandgap of the perovskites reduces monotonically, much similar to other inorganic semiconductors. However, increasing the applied strain displays surprisingly large blueshift/redshift with respect to the considered perovskite materials under external pressures.

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Keyword: Van der Waals Ruddlesden-Popper Hybrid Halogen Perovskites, Strain, Electrical Properties, Density Functional Theory

ID: 186 - Properties of Nanoscale Materials

# Investigation of Quantum Dot Dispersions in Various Vehicles with Hansen Dispersibility Parameters

#### <u>Secil Ünlütürk</u><sup>\* 1</sup>, Necati Güdümcüoğlu<sup>1</sup>, İlayda Melek Çelik<sup>1</sup>, Serdar Özçelik<sup>2</sup> <sup>1</sup> Kansai Altan Boya Sanayi Ticaret A.Ş., İzmir, Turkey <sup>2</sup> İzmir Institute of Technology, İzmir, Turkey

Since nanotechnology promises benefits to the various aspects of the industry, the automotive coating industry has also included nanomaterials to improve the performance of vehicles for both production and lab-scale research studies[1]. In automotive coatings, quantum dots could be used as solar paints [2, 3], antimicrobial surfaces[4], and even for revealing surface strains[5].

Nanoparticles with different organic capping agents have different dispersibility in a different vehicle(s). Regarding the application area, both aqueous phase and solvent phase compatible ligands are chosen as a capping agents of the nanoparticles. That is the reason why it is critical to choose the appropriate vehicle for the nanoparticle without executing any experiments to save the environment, cost, and time. Theoretical investigation of "good" and "bad" vehicles for the chosen system and nanoparticle type could be applied by using the known solubility approaches. In the Hildebrand approach - the older version of the solubility parameters - , the solubility is connected to the cohesive energy which is the energy of vaporization that provides global information on all interactions between molecules [6]. Later on, Hansen subdivided the whole cohesion energy into three contributions as polar  $\delta p$ , dispersive  $\delta d$ , and hydrogen bonding  $\delta h$ [7]. As a result, Hansen Solubility Parameters (HSP) have been established [8, 9]. Here, it would be better to note that although these approaches are the best fit for the solubility of molecules in the solvent systems, it is also found suitable for dispersion dispersants for the nanoparticles [10]. Consequently, in this study, we preferred to call it Hansen Dispersibility Parameters (HDP).

In this study, 6 different mostly used capping agents are chosen used for both aqueous and organic solvent-based systems. While thioglycolic acid (TGA), 3-mercaptopropionic acid (MPA), and N-acetyl-L-cysteine (NAC) are considered for the aqueous systems, trioctylphosphine (TOP), trioctylphosphine oxide (TOPO) and oleic acid (OA) are chosen for the organic solvent-borne systems. Regardless of the composition and the particle size of the nanoparticle, the capping agent effect on HSP is investigated for more than 20 different vehicles by HSPiP 5th edition programmed by Steven Abbott. The ligands and QDs are added to various vehicles. Observation of the dispersion visually and/or by centrifugation help to find the "happy" and "unhappy" vehicles by creating the HSP sphere. The results show that HSP is one of the promising methodologies to suit the best solvent system to disperse the nanoparticles for polymeric nanocomposites in coating technologies.

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Keyword: Quantum Dots, Hansen Dispersibility Parameters

# Carbon dioxide capture materials for deep decarbonization

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Enabling net emission reductions are by reducing the amount of greenhouse gases emitted from an activity and making use of decarbonization technology to capture CO<sub>2</sub> emissions. Until now, this has been achieved by minimizing energy waste or by introducing the use of renewable energy sources. However, to achieve net reductions, deep decarbonization technologies need to be applied to capture CO<sub>2</sub> emissions from hard-to-decarbonize sources such as iron and cement production, transportation, and so on. Therefore, decarbonization technologies including carbon capture from flue gas and direct air capture (DAC) are central technologies for ambitious climate change mitigation. Both of these techniques rely on carbon dioxide (CO2) sorbents or diffusion membranes, which can take many forms. I will describe the latest developments in carbon capture with liquid sorbents, solid sorbents in the form of nanoparticles, nanoscale metal-organic frameworks (MOFs), and nanoporous diffusion membranes. Their potential capture capacities and reaction kinetics, stability, and reusability are presented and compared. In addition, I will discuss potential alternatives to the conventional method of regenerating the sorbent capacity. Such a comprehensive summary of progress in this field can facilitate essential research, describe enabling technology innovations, and promote industrial implementations of carbon capture technologies for deep decarbonization.

ID: 314 - Properties of Nanoscale Materials

# Comparison of Electrochemical Properties of Raloxifene with Screen Printed and Boron Doped Diamond Electrodes

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Cancer is a disease that occurs when cells grow uncontrollably and abnormally as a result of damage to cell DNA, escape from the immune system, and invade and metastasize to neighboring tissues and subsequently to distant tissues and organs. Considering the types of cancer among women worldwide, breast cancer has a frequency of approximately 30%. The rate of breast cancer is constantly increasing worldwide, so it is important to develop therapeutic drugs that can be used in the treatment of breast cancer (Li, et al., 2019). Inresearch, the most important reports on the determination of raloxifene are based on ultra-performance liquid chromatography tandem mass spectrometry and isotopic dilution liquid chromatography tandem mass spectrometry (Bayle et al., 2020; Fouladgar et al., 2020). However, no study was found in which the results of electrochemical analysis of raloxifene were compared with both Boron Doped Diamond (BDD) and Screen Printed Electrodes (SPE). For this purpose, in order to increase the surface detection performance, the sensitive signals given by the SPEs prepared by using nanomaterials, which attract the attention of researchers today, and the continuously usable and cleanable BDD electrodes to the same drug under the same conditions were examined.

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Keyword: Raloxifene, Dropsense, Nanobiosensor

# **Optical and Electroluminescent Properties of Imidazole Based Small Molecules**

Elif Demirgezer<sup>\*</sup><sup>1</sup>, Eda Alemdar<sup>1</sup>, Özge Akkaya<sup>1</sup>, Ali Çırpan<sup>1</sup>, Gönül Hızalan Özsoy<sup>2</sup>, Şevki Can Cevher<sup>3</sup> <sup>1</sup> Middle East Technical University, Ankara, Turkey <sup>2</sup> GUNAM, Ankara, Turkey <sup>3</sup> Sivas University of Science and Technology, Sivas, Turkey

Organic Light-Emitting Diodes are the trend topic in the lighting and display industry because of their properties such as being flexible, highly bright, and thinner. In this project, the synthesis of imidazole small molecules with different substituents and their application to OLEDs were studied. Also, the effects of substituents in imidazole molecules on OLEDs were examined. In this study, imidazole-bearing small molecules with different substituents were synthesized. In order to investigate the electronic properties cyclic voltammetry studies were performed. Photoluminescence peaks were centered at 490, 492, 495, 488, 490, 489 nm for 2-(4-(tert-butyl)phenyl)-4,5-diphenyl-1H-imidazole (BIm-H-tBu), 2-(4-(tert-butyl)phenyl)-1-(4-chlorophenyl)-4,5-diphenyl-1H-imidazole (BIm-Ph-tBu), 2-(4-(tert-butyl)phenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,(4-methoxyphenyl)-2,(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-chlorophenyl)-2,(4-methoxyphenyl)-2,(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,(4-methoxyphenyl)-2,(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,(4-methoxyphenyl)-2,(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,(4-methoxyphenyl)-2,(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,4,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-1,4,5-triphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,4,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,5-diphenyl-1H-imidazole (BIm-Ph-*t*Bu), 2-(4-methoxyphenyl)-2,5-d

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Keyword: OLED, Small Molecule, Imidazole Derivative, Blue Light Emitting Materials

# Investigation of Vibrational Properties of Twisted Bilayer Graphene

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Demonstration of superconductivity in twisted bilayer graphene (TBG) in 2018 has brought great attention to twisted 2D materials. This discovery has opened a research area called *twistronics* where layers of two-dimensional materials twisted with respect to each other around their normal axis exhibit properties that are absent in their single, two or multilayered untwisted counterparts [1-2]. BCS theory -Nobel prize awarded conventional explanation for superconductivity relates the phenomenon to electron-phonon interaction [3]. Even though the nature of superconductivity observed in TBG is still open to debate, little theoretical work has been done in the investigation of vibrational characteristics of these materials. This is primarily because of the relatively large cell dimensions of emerging moiré superlattices. This work directly addresses these challenges by demonstrating an alternative computational approach to the problem. We theoretically investigate phonon dispersion in AB-stacked and TBG with various rotation angles. In order to provide a complete and clear understanding of the emerging patterns obtained from the theoretical calculations of the TBG, we employ machine learning (ML) methods.

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Keyword: Twisted bilayer graphene, moire patterns, molecular dynamics simulation, Machine Learning

# Langmuir Blodgett Deposition of Two Dimensional Oxide Nanosheets on Flexible ITO-PET Substrates

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Two-dimensional (2D) oxides are one of the members of the 2D family of materials. They have the monolayers of TiO<sub>2</sub>, MoO<sub>3</sub>, WO<sub>3</sub>, mica, and perovskites-like crystals [1]. They can be chemically exfoliated to produce 2D oxide nanosheets. The thickness of 2D oxide nanosheets can vary between 1 nanometer to a few nanometers according to the crystal structure and composition of the host layer. The lateral area dimensions were determined 1000 times greater than the thickness of the nanosheets [2]. They exhibit high dielectric properties and are suitable candidates for flexible and transparent capacitors that provide large specific space for energy/data storage. The studies on Dion-Jacobson type Ca<sub>2</sub>Na<sub>x-3</sub>Nb<sub>x</sub>O<sub>3x+1</sub> nanosheets exhibited an increase in x number would result in an increase in dielectric properties due to softening in polar phonon frequency [3]. This indicates that new forms of nanosheets with high dielectric characteristics can be produced when the perovskite Dion-Jacobson material is synthesised and exfoliated at the maximum x value. In this study, we have delaminated Dion-Jacobson-type perovskite layered material of KCa<sub>2</sub>NaNb<sub>4</sub>O<sub>13</sub> single Ca<sub>2</sub>NaNb<sub>4</sub>O<sub>13</sub> nanosheets. These 2D materials were then deposited on ITO-PET substrates grown on PET substrates, and nanofilms were obtained by repeating this process. Thus, 2D oxide nanosheets were used instead of thin films for deposition on ITO-PET substrates for the first time. These flexible ITO-PET substrates coated with 2D oxide nanosheets will provide a new perspective on flat-panel displays and wearable electronic device applications.

#### Acknowledgment

This work was supported by The Scientific and Technological Research Council of Turkey (TÜBİTAK; Grant number 218M517).

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#### ID: 45 - Graphene and 2D Materials

# Identification of Organic Solvent Nanofiltration Performances of MXenes via Non-equilibrium Molecular Dynamic Simulations

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Organic solvents have been widely used in a variety of industries, most notably the petrochemical, pharmaceutical, dye, and food industries, either as raw materials in chemical synthesis or as cleaning agents. Because of their high consumption, a huge amount of waste solvents has been generated, and significant portion of them were discharged into the environment without any processing. Considering both economic and environmental consequences of releasing solvents into the environment, it is definitely required to recover and reuse the solvents by the separation processes. Since financial issues head all activities in the industry, any separation process that can be used for solvent recovery should have a high separation yield and low cost. Therefore, organic solvent nanofiltration (OSN) processes have emerged as a promising method for solvent recovery and purification due to their advantages over traditional methods, such as low energy requirements, low carbon footprint, and high separation performance. Although polymeric membranes are highly used in the industrial applications, inorganic porous nanomaterials, especially 2D inorganic nanomaterials, are gained attraction as potential candidates that overcome the performance of traditional membranes. Specifically, MXenes, a new member of 2D nanomaterials, have begun to be used for OSN applications due to their unique properties such as high surface area, high stability, negatively charged surface, hydrophilic nature, and ease of functionalization.

In this study, non-equilibrium molecular dynamics simulations were used to determine the fluxes of nine different solvents (namely, water, ethanol, methanol, acetone, ethyl acetate, toluene, hexane, heptane, and dichloromethane) through the nanochannels of  $Ti_3C_2O_2$  MXene membrane. A system cell having approximately  $30 \times 30 \times 100$  Å<sup>3</sup> volume was designed as given in Figure 1 to calculate solvent flux and a specific external force was applied to mimic the experimental measurements. Water molecules modeled with SPC/E demonstrated a high flux (40.9 water molecules/ns under 0.3 kcal/mol×Å external force) due to the nano-confinement effect. Furthermore, fluxes of polar and nonpolar solvents were compared separately, and the relationships between some solvent properties (viscosity, polarity, diameter, etc.) and flux were clarified. The interactions between the membrane and the solvents that influence the solvent transport were revealed. This work will identify the mechanism responsible for the transport of each solvent through the nanochannels of  $Ti_3C_2O_2$  MXene membranes for specific solvent in OSN.

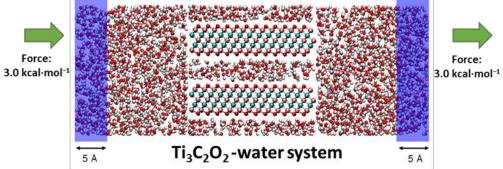


Figure 1. Representation of the initial configuration of the investigated Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub> MXene simulation systems. Oxygen, carbon, hydrogen, and titanium species are represented by red, cyan, white, and pink, respectively.

### Acknowledgements

The molecular simulations are performed at TUBITAK ULAKBIM High Performance and Grid Computing Center (TRUBA).

Keyword: Membrane-based separation, organic solvent separation, organic solvent nanofiltration, MXenes, NEMD simulations

ID: 55 - Graphene and 2D Materials

# Thermal Expansion Coefficient Determination of Graphene with machine learning type Gaussian Approximation Potentials

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Considering the ongoing technological pressure for developing ever smaller electronic devices, constituent two-dimensional (2D) materials and their thermal properties are becoming even more critical for the performance, reliability, longevity and safety of devices. As being the pioneer in 2D materials, graphene attracted much attention to be heavily used in next-generation device technologies. In this regard, thermal properties of graphene become very important and a comprehensive understanding of it is essential and required to control the thermal expansion and design superior devices. However, direct experimental measurement of thermal expansion coefficient without substrate effects is a challenging task for 2D materials and its accurate estimation with large-scale ab initio molecular dynamics is computationally very expensive. Hence, although graphene is studied heavily, there are contradictory reports on thermal expansion coefficients both theoretically and experimentally. Motivated by this ambiguity on the determination of thermal expansion coefficient of graphene, and the recent developments in the machine learning methodologies which enables large-scale calculations, here we present an investigation of thermal expansion properties of graphene by Gaussian Approximation Potentials type machine learning methods.

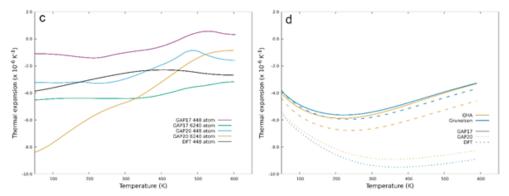


Figure 1: Calculated thermal expansion coefficients by MD, QHA and Grüneisen methods with GAP and DFT.

The one-to-one comparison of phonon frequencies hint that the GAP models catches the lattice dynamics of graphene very well, especially with GAP17 model. Thus, the TEC estimation from the Grüneisen framework is the closest to the DFT calculated value. On the other hand, there are larger differences in QHA due to the non-linear behavior of the vibrational frequencies at the limits in the selected strain range. The molecular dynamical simulations show that GAP17 model captures the origin of the thermal expansion similar to the DFT level calculations. The negative thermal expansion is associated with the rippling behavior caused by the out of plane vibrations (ZA mode) as the C-C bond lengths increase with the increasing temperature.

Keyword: graphene, Machine Learning, negative thermal expansion

#### ID: 85 - Graphene and 2D Materials

# Electromagnetic Absorber Based on Multilayer Graphene Reinforced Paint

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In this work, it is aimed to obtain electromagnetic absorber that can be applied on metal surfaces particularly for aircrafts. For this purpose, a special solvent-based paint is produced using graphene as the reinforcing element. Graphenes has many unique features, such as high electrical and thermal conductivity, high chemical and mechanical stability and corrosion resistance. Traditional radar absorber coatings are produced with carbonyl iron. On the other hand, compared with the carbonyl iron reinforcement, the anticorrosive performance can be increased with graphene filled polymeric paint. A solvent based epoxy resin is used as a binder. Solvents and the graphene nanoflakes were mixed and dispersed using high-speed dispersion machine in order to produce the absorber paint. The obtained paint was applied on a metal plate and its absorption properties were measured via free-space measurement setup. In the next stage, another paint sample was prepared by again using graphene with different ratio yielding absorption behavior at another frequency point. Combining both wet paint samples on a single metal plate yielded to electromagnetic absorption characteristics with high bandwidth.

Keyword: Graphene, Electromagnetic absorber, Layered absorber, RF, Paint

# The Synthesis and Characterization of Homogeneous High-Quality Graphene Encapsulated Metallic Powders via Plasma Enhanced Rotating CVD

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Graphene reinforced Cu composites are mostly produced by combining graphene flakes (synthesized by Hummer's method and derivatives) and Cu powders by using methods like ball milling. However, this approach has many issues like: • dispersion of graphene in matrix

• formation of interfacial bonding and interfacial products

• presence of structural defects in graphene

• the number of carbon layers in graphene

• presence of defects in the final product (e.g., porosity or interstitials)

• orientation of graphene relative to the loading direction

• % of graphene

Hence, it is difficult to directly examine the effect of graphene on mechanical properties using this method, and different, even contradictory, results have been found in the literature. The problems mentioned above are process-related, and within the scope of this study, a process design and development focused on the homogeneity and reproducibility of the graphene distribution has been made. To produce uniformly dispersed high quality graphene reinforced copper composites: 1 micrometer spherical Cu powder were coated via plasma enhanced CVD (PECVD), then pressed and sintered at 1000 °C. The results show that the yield strength and stress values of samples made from graphene powders are significantly higher than those of samples made without graphene: The yield strength of the graphene samples increased by about three times at room temperature, and the stress values obtained at 30 percent constant strain increased by about two times... achieving a breakthrough in the performance of copper-based materials. The improvement in mechanical performance was assessed in conjunction with the discussion of grain size reduction and strain hardening. This study is supported by TUBITAK grant number 118F491.

Keyword: Graphene, Copper, Plasma Enhanced Chemical Vapor Deposition, Mechanical Properties

# Development of Graphene/Silicon Composite Based Lithium ION Battery Anode

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Constantly increasing demand for energy storage devices requires the development of more efficient, high-capacity batteries. Due to their improved qualities compared to conventional batteries, lithium-ion battery cells have become the most common energy storage devices and are now widely utilized in our everyday lives. The most common application of lithium-ion batteries is in electric cars. It is expected that the Li-ion battery cells used in electric vehicles will have a rapid charging time. a long cycle life, a low weight per volume, and a large storage capacity. To obtain these desirable properties, the Li-ion battery anode structure must be improved. Graphite is the most commonly used active material in battery anode structures. Although graphite has greater electrical conductivity and a longer service life than its alternatives, its limited charge capacity and limited surface area require further development. Silicon is another popular Li-ion battery component. Silicon can store ten times as many Li ions as graphite, however anodes built of Si instead of graphite degrade faster and have a shorter service life due to structural fragmentation caused by the high volume changes during charge and discharge cycles. Graphene, a two-dimensional honeycomb structure of carbon atoms, offers a great deal of potential to address these issues due to its vast surface area, mechanical and electrical properties, and chemical resistance. Therefore, the objective of this study is to adopt a Gr/Si composite structure to enhance the energy storage capacity, mechanical properties, and chemical resistance of the battery anode. For the production of Gr for Gr/Si composites, top-down processes such as high vacuum furnaces, wet chemistry, and the flash method are used. Using OM, TEM, and SEM, the morphology of synthesized materials is examined. Their analysis was performed using Raman spectroscopy. BET analysis is utilized to determine the composite anode material's surface area. Using electrochemical characterization techniques, the charge capacity of Gr/Si composites will be studied and reported.

Keyword: Graphene, Silicon, Lithium Ion Batteries, Battery anode

# Investigation of EMI Shielding Effectiveness of Graphene Encapsulated Nickel/Epoxy Composites

#### <u>Begum Beril Incecik</u><sup>1,2,\*</sup>,Eren Atli<sup>3</sup>,Omer Refet Caylan<sup>1</sup>, Tarik Can Turkoglu<sup>1</sup>, Deniz Cakir<sup>1</sup>, Su Genelioglu<sup>3</sup>, Buse Yurdusever<sup>3</sup>, Bekhan Dogan<sup>3</sup>,Goknur Buke<sup>3</sup>

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In this study, the synthesis, characterization, and Electromagnetic Interference Shielding Effectiveness (EMI SE) measurements of Graphene Encapsulated Nickel (GNi)/Epoxy composites were conducted. Graphene encapsulation of Ni powders is achieved using custom made Rotating Plasma Enhanced Chemical Vapor Deposition Reactor (RPECVD). The process parameters such as gas amounts (Argon, Hydrogen, Acetylene), plasma power and plasma duration were studied. The spectroscopic analysis of graphene grown on the Nickel powders were characterized by Raman Spectroscopy. Morphological analysis of the synthesized materials was investigated via Optical Microscopy (OM) and Scanning Electron Microscopy (SEM). Neat Ni powders and synthesized Graphene Encapsulated Nickel powders were integrated into epoxy resin by hand mixing and to prepare EMI-SE test samples. Resin casting and curing processes were implemented respectively.

The EMI-SE of the Ni/epoxy and GNi/epoxy nanocomposites was measured in accordance with "ASTM D4935 Standard Test Method for Measuring the Electromagnetic Shielding Effectiveness of Planar Materials" using a vector network analyzer in the frequency range of 1.5–10 GHz. The EMI-SE measurements showed that pure epoxy samples fully transmitted the EM waves resulting in 0 dB EMI-SE value. Oscillations up to 2 dB throughout the frequency range are acceptable and within the tolerance range of the testing device and equipment. The composites with 50 wt. % Ni powders have the max. SE value of 7,4 dB and the composites with 50 wt. % Graphene Encapsulated Nickel powders have the max SE value of 18,3 dB. The results demonstrate that the graphene encapsulation process remarkably improves the EMI-SE of the composites and these materials have certain potential towards EMI Shielding applications of polymer matrix composites. This study is funded by TUBITAK grant no: 118F491.

Keyword: Electromagnetic Interference, Electromagnetic Shielding, Chemical Vapor Deposition, Graphene, Nickel, Encapsulation

# The Effects of Process Parameters on the Synthesis and Characterization of 2D Mo2C Crystals and Graphene Heterostructures Through CVD

# <u>Omer Caylan</u>\*, Furkan Turker, Derya Karadeniz, Elif Okay, Goknur Cambaz Buke

TOBB ETU, Ankara, Turkey

In this work, we have studied the effects of chemical vapor deposition processing parameters (effect of catalyst, catalyst type and thickness, reaction temperature and duration) on the growth of 2D Mo2C crystals. SEM and OM are used to investigate the morphology of the synthesized crystals and EDS and XPS are used to determine the chemical structure of Mo2C and finally Raman spectroscopy, TEM and XRD techniques are used to understand the structure of the hexagonal Mo2C crystals. The results showed that 2D Mo2C crystals which are orthorhombic, grow along the [100] direction together with graphene an amorphous carbon thin film on Cu and In, respectively [1, 2, 3]. Complementary experiments are performed in order to determine the activation energy for the growth of Mo2C on graphene and it was calculated to be 3.76 eV, and it was discovered that the rate-limiting step is the diffusion of Mo to the Cu surface through uncovered Cu or graphene vacancies/defects [2]. This growth mechanism is examined and discussed in detail, and a model is proposed. To confirm the model, AFM studies are used to measure the thickness of the transferred crystals and AFM studies agree well with the proposed model, showing that the vertical thickness of the Mo2C crystals decreases inversely with the thickness of catalyst (Cu or In) for a given reaction time [3] which confirms the previous works in the literature. This study is based on work supported by the Air Force Office of Scientific Research under Award Number FA9550-19-1-7048.1

# Engineering Energy Transfer from 0D to 2D

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Near-field interaction between the monolavers of two-dimensional materials has been recently investigated. Another branch of the matter to be probed is the interaction between 2D materials and lower-dimensional systems such as zero-dimensional nanostructures including quantum dots and metal nanoparticles. One more step to take is the ability to engineer the interaction between those systems. On that account, in this study, we probed the effect of mechanical strain on the non-radiative energy transfer (NRET) rate from a 0-dimensional material, CdSe/ZnS quantum dot (QD), to a 2-dimensional material, monolayer (1L) WS2. Our calculations show that the NRET rate is enhanced as the emission spectrum of CdSe/ZnS QD overlaps with the exciton resonances of 1L WS<sub>2</sub>. On that basis, the NRET rate is strongly dependent on the magnitude of strain, since applying strain shifts the exciton energies in 1L WS<sub>2</sub>. Based on the experimental results in the literature, we have computed the straindependent dielectric function of WS<sub>2</sub>. We calculate the NRET rate as a function of uniaxial strain and show that it can be greatly tuned by purely mechanical means. We choose WS<sub>2</sub> among the commonly used semiconducting group-6 transition metal dichalcogenides; WSe<sub>2</sub>, MoS<sub>2</sub>, MoS<sub>2</sub>, and MoTe<sub>2</sub> as it has the smallest A exciton linewidth at room temperature, which is relatively less sensitive to strain [1-4]. We also investigate the NRET rate from quantum dots to monolayer graphene. As graphene does not exhibit resonances in the emission range of the QD, the spectral dependence of the NRET is weak. Furthermore, the strain does not cause significant changes to the dielectric function of graphene, making it a reference material for strain-tuned NRET studies. Our results exemplify the use of mechanical strain to shed light on the interaction between lowdimensional material systems. We will follow up with experiments in which we will deposit quantum dots on 2D materials

#### and perform photoluminescence spectroscopy to demonstrate the strain-engineered NRET in QDs

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Keyword: non-radiative energy transfer, quantum dots, 2D materials, strain tuning

# Tailoring the Optical Properties of Suspended and Flat 2D Transition Metal Dichalcogenides

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UV-ozone (UV-O<sub>3</sub>) exposure and Focused ion beam (FIB) have shown great potential in material / surface modification, functionalization and defect engineering in 2D materials more recently, especially within the transition metal dichalcogenides (TMDCs) family, with the aim to tailor their optical and electronic properties. A better understanding and control of defects is important to move forward in the field of defect engineering in TMDCs. In this study, we investigated the effect of UV- $O_3$  exposure and focused ion (Ga+) beam irradiation (as a function of beam current and dose) on the optical and electrical properties of the suspended and flat 2D TMDCs.

Keyword: defect engineering, 2D materials, TMDCs, FIB, UV-Ozone

# **Quantum Monte Carlo Study of Semiconductor Artificial Graphene Nanostructures**

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Graphene is a two-dimensional material made of carbon atoms on a honeycomb lattice structure. Thanks to its linear energy dispersion near Fermi level, graphene has interesting electronic, optical and thermal properties leading it to be one of the most investigated materials in the last several decades[1,2]. However, the fabrication and reliability issues of nanostructured graphene, such as graphene quantum dots, draw lots of attention to similar two-dimensional materials in the recent years. Therefore, the artificial structures designed by imitating the 2D honeycomb pattern of graphene become more reliable and controllable sources for both fabrication and investigation of many physical phenomena[3]. These "artificial graphene nanostructures" can be formed using semiconductor materials or optical lattices.

In this study, we investigated the electronic and magnetic properties of semiconductor artificial graphene quantum dots using variational and diffusion quantum Monte Carlo (QMC) methods[4,5]. In QMC calculations, in which the many-body trial wave functions are obtained from localized gaussian orbitals, tight-binding and mean-field Hubbard calculations, we analyzed the effects of dot radius, dot depth, dot-to-dot distance, as well as the finite size effects. We show that metallic to antiferromagnetic phase transition can be probed depending on dot radius.

This work was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under the 1001 Grant Project Number 119F119. The numerical calculations reported in this study were partially performed at TUBITAK ULAKBIM, High Performance and Grid Computing Center (TRUBA resources).

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Keyword: quantum Monte Carlo, graphene, artificial graphene nanostructures, 2D materials

# ID: 197 - Graphene and 2D Materials

# Parameterization of Tersoff Inter-atomic Potential for Monolayer GaSe Crystal

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Monolayer materials are of great attention due to their remarkable physical properties and prospects to achieve the desired device performances for next-generation device applications in various fields [1]. GaSe, which is a new kind of layered metal monochalcogenide material and has been successfully synthesized by various kinds of methods in recent years. This layered material has a potential for photodetector, sensor, and field-effect transistor applications, owing to its intriguing properties such as direct band gap, small effective mass, high charge density and good thermoelectric properties [2]. In this study, we parameterize the empirical interatomic potential for monolayer GaSe crystal and evaluate the thermal properties of this crystal using classical molecular dynamics simulations. The interactions between atoms are defined by Tersoff-type empirical potential [3] that is developed to represent the structural, mechanical, and dynamic properties of this material. Parameters for the Tersoff potential are obtained with the particle swarm optimization method [4], which is a population-based stochastic optimization algorithm motivated by the social interaction behavior of some animal swarms such as birds or fish. The final Tersoff parameter set produces quite consistent results with first-principles calculations [5] in terms of lattice parameters, bond distances, equation of states, and vibrational properties. The calculated thermal properties by molecular dynamics simulations of large scale GaSe flakes are in good agreement with available first-principles and experimental data.

#### Acknowledgments

This work was supported by the Scientific and Technological Research Council of Turkey (TÜBİTAK), 2218-National Postdoctoral Research Fellowship Program, Project No: 118C455.

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Keyword: Monolayer GaSe, Tersoff Potential, Particle Swarm Optimization, Molecular Dynamics Simulations

ID: 233 - Graphene and 2D Materials

# Synthesis of Double Transition Metal (Ti<sub>2</sub>Nb)AlC<sub>2</sub> MAX Phase and Its Derivative (Ti<sub>2</sub>Nb)C2Tx MXene

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The MAX phases exhibit metallic properties because the partially filled d orbitals of the transition metals are close to the Fermi energy [1]. In addition, due to the metallic bonding between the transition metal atoms in the same layer, the MAX phases have electrical conductivity. Due to their high mechanical and thermal stability [2], some MAX phases can be used where materials must be resistant to thermal shock, fatigue, creep, oxidation or corrosive reactions [3]. Solid-state reaction (SSR) is the most used method to synthesize MAX phases. This method is based on high-temperature reactions between the basic component starting powders or other precursors such as carbides or hydrides. The synthesis temperature generally ranges from 1100 to 1700°C and is carried out in an Ar environment to prevent oxidation. Different synthesis methods include pressureless synthesis (PLS), self-propagating temperature synthesis (SHS), hot pressing (HP), hot isostatic pressing (HIP), spark plasma sintering (SPS), and microwave (MW). PLS is one of the most common synthesis methods because of its simplicity. Overall, PLS enables the production of MAX powders that are simple, cost-effective, flexible in terms of precursors, scalable to large quantities, and of relatively high purity. In this method, the pellets (green-body) are placed in a crucible and heated to a temperature of around 1400°C for several hours under a vacuum or Ar atmosphere. The formation of the MAX phases starts at about 1000°C, but the highest efficiency is achieved around 1300-1500°C. These temperature values may be higher for some MAX phases [4]. PLS allows obtaining high purity of pellets, about 95% by weight and relative densities up to 90-92%.

MXenes obtained from a layered transition metal carbide, nitride and/or carbonitride selectively etched from MAX phases stand out with their chemical and structural diversity beyond graphene to compete with 2D materials [5]. The MXene family has expanded since its discovery in 2011 and has grown further with the discovery of ordered double transition metal (DTM) MXenes. These DTM MXenes differ from mono-transition metal (mono-M) MXenes because the two transition metals can occupy the metal sites. Ordered DTM MXenes consist of in-plane or out-of-plane transition metals. In addition, some DTM MXenes are in a random solid solution structure defined by two transition metals randomly dispersed throughout the 2D structure. Their different structures and a range of transition metal pairs provide the ability to tune DTM MXenes for specific optical, magnetic, electrochemical, thermoelectric, catalytic or mechanical behavior. This degree of control over their composition and structure is unique in the field of 2D materials and will open new research possibilities for the application-based design of functional nanomaterials. In our study, the (Ti<sub>2</sub>Nb)AlC<sub>2</sub> MAX phase was synthesized using the pressureless synthesis method in a high-temperature inert gas environment. Then, the sequential phase (Ti<sub>2</sub>Nb)C<sub>2</sub>T<sub>x</sub> MXene structure was obtained by etching the Al atomic layers from this MAX phase using the selective etching method.

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ID: 245 - Graphene and 2D Materials

# Spray-coating of Self-adhesive Highly Conductive Graphene/ Silver Nanoparticles Ink for Flexible Printed Electronics

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Spray-coating of graphene inks using the layer-by-layer method is more preferred to produce the strain sensor with a higher gauge factor than drop-casting, spin-coating, and screen-printing methods [1]. In addition, the spray-coating method is quite successful in dispersed graphene coating like graphene nano pellets with high surface roughness. In the spray-coating process, many parameters such as substrate type, substrate ingredients, and ink content are effective on adhesion on polymer, and this process is required for a more effective analysis [2]. This study proposed an evaluation of what operation conditions are needed for the ink to adhere better to the polymer substrates.

### Acknowledgments

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 Ruhkopf, J., Role of Substrate Surface Morphology on the Performance of Graphene Inks for Flexible Electronics. ACS Applied Electronic Materials 2019, 1 (9), 1909-1916.

Keyword: Spray-coating, self-adhesive, flexible printed electronics, graphene ink

# 2D Heterostructures Formed by Graphene-like ZnO and MgO Monolayers

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Due to the enriched functionalities resulting from combining different properties of separate monolayers, van der Waals heterostructures (vdWHs) are considered a revolutionary class among the plethora of currently fabricated or predicted two-dimensional materials.

Alongside vdWHs, recent studies have reported 2D layered heterostructures with interlayer bonding [1]. Examples are borophene/graphene [2] and  $SnP_3/GeP_3$  heterostructures [3]. Besides, an ab initio study has demonstrated the feasibility of artificial controlling the physical properties of vdWHs by utilizing 2D donor-acceptor heterostructures to create strong bond-like interactions between layers [4]. Interlayer bonding in 2D heterostructures alters the properties of corresponding single layers, which is not so noticeable in vdWHs and thus creates a new playground for controlling the physical properties of 2D materials.

Single-layer graphene-like ZnO is already fabricated, and theoretical calculations based on density functional theory have shown a close lattice match between MgO and ZnO monolayers. Presently, ZnO and MgO layered structures have been utilized in various electronic devices. ZnO/MgO dielectrics for metal-insulator-metal capacitor, felid-effect transistor and Au/MgO/ZnO metal-insulator-semiconductor ultraviolet light emitters are currently fabricated. Besides, enhanced stability of self-powered lead-halide perovskite is achieved by using a microspherical MgO/ZnO bilayer. Furthermore, a previous theoretical study has shown that monolayer MgO is an excellent dielectric gate oxide for encapsulating ZnO-based optoelectronic devices [5].

Motivated by the flourishing properties of lateral heterostructures, we systematically investigated four different heterostructures assembled by binary hexagonal monolayers of ZnO and MgO. Structural relaxation has revealed two vdWHs and two structures with interlayer bonding. All of the four possible stacking across the heterostructure are mechanically stable. In addition, stability analysis using phonon dispersion reveals that the AB stacking formed by placing the Mg atom on top of the O atom of the ZnO layer is also dynamically stable at zero temperature. Our band structure calculation based on DFT shows that the orbital of the Zn atom dominates the first conduction band of these structure. We employed GW approximation for a better description of the electronic properties. Besides, the optical properties are determined by solving the Bethe-Salpeter equation. Our results show that strong excitonic effects reduce the optical band gap to the visible light spectrum range.

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Keyword: Excitons, Electronic structure, Optoelectronics

#### ID: 364 - Graphene and 2D Materials

# Precursor Dependent Bandgap Engineering of Graphitic Carbon Nitrides

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The properties of graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) can be tuned by the various reaction parameters such as precursor type [1] and thermal treatment temperature [2]. Engineering the bandgap. is critically essential in energy and environment-related applications. [3] Herein, five different g-C<sub>3</sub>N<sub>4</sub>s were prepared using urea (U), dicyandiamide (DCDA), thiosemicarbazide (TSC), semicarbazide hydrochloride (SC-HCl), and thiosemicarbazide hydrochloride (TSC-HCl) precursors by heating at 600 °C for 4 hours. X-Ray Diffraction (XRD) suggested that SC-derived g-C<sub>3</sub>N<sub>4</sub>s had low crystallinity and small crystallite size (3.59 nm). The bandgap and valence band energy of the prepared g-C<sub>3</sub>N<sub>4</sub>s were studied using DR-UV-vis spectra and X-ray Photoelectron Spectroscopy (XPS). The bandgaps of U-, DCDA-, TSC-, SC-HCl-, and TSC-HCl-derived g-C<sub>3</sub>N<sub>4</sub>s were found as 2.97 eV, 2.84 eV, 2.74 eV, 1.98 eV, and 2.61 eV, respectively. Relatively narrow-band gap and high valence band (2.07 eV) oxygen-rich g-C<sub>3</sub>N<sub>4</sub>s were obtained when SC-based precursors were used.

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Keyword: graphitic carbon nitride, bandgap energy, absorption spectroscopy, X-ray photoelectron spectroscopy

ID: 100 - Nanotubes and Nanowires

# The Synthesis and Characterization of Carbon Nanotubes on SiC via Vacuum Decomposition

Not presented.

# Atmospheric Cold Plasma assisted Anticancer Drug Release from Hyaluronic acid-based Micromotors

#### <u>Gozde Karaca</u>\*, Yunus Emre Bülbül, Aysegul Uygun Oksuz Sulevman Demirel University, Isparta, Turkey

The field of nano-/micromotors possess remarkable physical, mechanical, chemical, and biological properties, which can offer exceptional opportunities for bio-applications [1-3]. They are promising platforms that offer rapid drug delivery, high tissue penetration and motion control [4-5]. The most important feature that distinguishes micro/nanomotor structures from other superior structures is that they have movement mechanisms. This mechanism of action makes micro/nanomotors prominent in applications such as chemical sensors, controlled drug release, nanorobotic studies, and nanoscale transport.

In this research, Gold-Hyaluronic acid (Au-HA) based micromotors will be synthesized by electrochemically and important cancer drug doxorubicin (DOX) release profile depending on pH will be investigated for biomedical applications. In addition, atmospheric cold plasma (CAP) will be applied to drug-loaded micromotors and its effect on drug release will be examined. DOX will be prepared at 4 different concentrations (50, 100, 200, 300 uM) in pH=8 phosphate buffer solution (PBS) and will be incubated on Au-HA micromotors for 24 hours. At the end of 24 hours, the micromotors will be placed in pH=5 PBS and UV-Vis spectroscopy analysis will be performed. UV-Vis spectroscopy measurements will be measured by applying atmospheric cold plasma on drug loaded micromotors for investigate the effect of CAP on the release of DOX. Scanning electron microscope (SEM) and elemental analyzes of the synthesized microtube as micromotors will be performed, and the presence of polymer and drug will be verified with Fourier transform infrared (FTIR) analyzes at each stage, X-ray diffraction (XRD) analysis will analyze the crystallographic properties of the micromaterials. In this research aimed to minimize the side effects of DOX with HA-based micromotors and to increase drug loading and release efficiency due to the functional groups HA.

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Keyword: microtube, hyaluranic acid, Doxorubicin, atmospheric cold plasma

# **MEMS Shear Force Sensor Integrated in a Microchannel**

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Shear stress in fluids, including liquids and gases, due to the viscosity of the fluid, arises from the tangential force of the moving fluid along a solid boundary. Shear stress is of importance for aerodynamics and hydrodynamics in aerospace and naval industries. From a biological perspective, fluid shear stress acts on the cells has a great impact on cell differentiation, proliferation, adhesion, motility, and fate. For example, endothelial cells experience shear stress resulting from the blood flowing along the vessels. Measurement of the shear stress is great of importance in understanding the behavior and type of the flow field to better design and build up the system according to the structure of the flow field. Amongst the different measurement methods which are employed in the literature, namely direct and indirect measurements, the floating element from the direct methods category is preferred in this study. In this method, a flat plate, here proof mass hold with springs, is subjected to the fluid shear stress, and the displacement of the plate is measured employing different read-out schemes, such as piezoresistive, piezoelectric, capacitive, optical, etc. In this study, a piezoresistive transduction scheme with silicon nanowires as sensing elements, which one of its key advantages in comparison with the conventional schemes, is the potential for extreme miniaturization, is simulated inside a microfluidic channel, where applied fluid shear stress causes a change in the electrical resistivity of the doped silicon nanowires. Electromechanical sensors miniaturization gives rise to outstanding advantages such as higher resonance frequencies resulting in increased sensitivity, lower power requirements, and cost reduction due to wafer-level production. According to the results of the simulation of the individual sensor, an array of sensors can be integrated to have multiple measurements at multiple locations simultaneously.

Keyword: Microelectromechanical Systems, Microfluidics, Shear Force Sensor, Piezoresistive, Floating-Element, Simulation

#### ID: 386 - Nanotubes and Nanowires

#### Electrochemical Approach for Nitrite Sensing via MWCNTS/Pt Modified Electrode from Water Samples

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A modified platinum electrode with multi-walled carbon nanotubes (MWCNTs) was fabricated to detect nitrite in an aqueous solution. First, the electrocatalytic activity of MWCNTs/Pt was investigated with cyclic voltammetry (CV), chronoamperometry, and electrochemical impedance spectroscopy (EIS). Then the quantitative analysis of nitrite was studied using square wave voltammetry (SWV) in 0.1M phosphate buffer solution (PBS) at pH 7.0. This modified electrode exhibited high electrocatalytic activity and a large specific surface area for the NO<sub>2</sub>- oxidation. Subsequently, the prepared electrochemical sensor MWCNTs/Pt exhibits a high sensitivity for the NO<sub>2</sub>- determination and a low detection limit (0.1  $\mu$ M) in a wide linear concentration domain (1.0  $\mu$ M - 1000  $\mu$ M). The sensor has also a profitable anti-interference ability as well as good stability, reproducibility, and applicability. The results demonstrate that the designed sensor has potential application in water analysis.

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Keyword: Modified electrode, Nitrite ion, Electrchemical detection, Multi-walled carbon nanotubes

**ID: 9 - Nanoelectronics and Spintronics** 

# Preparation of Ultrathin Molybdenum oxide film using Atomic Layer Deposition System for UV Photonic and Optoelectronic Applications

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Molybdenum oxides (MoO<sub>3</sub>) have gained a lot of attention as one of the transition metal oxides because of their enormous electron affinity, broad bandgap, various valence states, and layered structure, which could be used in sensors, optics, catalysis, electronics, energy units, and bio-systems. In this study, we prepared ultra-thin Molybdenum oxide (MoO<sub>3</sub>) using an atomic layer deposition (ALD) system using Bis(tbutylimido)bis(dimethylamino)molybdenum(VI) as a Molybdenum (Mo) source. To understand the effect of depositing temperatures, we prepared the films at 100, 150, and 250° C. The ultra-thin films were then annealed in the air for a brief time at 600°C. Different film thickens have arranged from 0.1nm to 10nm. The morphological and elemental properties were assessed using scanning transmission electron microscopy and energy-dispersion X-ray spectroscopy. The thickness of the films is increasing with increasing deposition temperature. Using atomic force microscopy we discovered highly homogeneous thin films with minuscule particle sizes. The thickness films show n-type semiconductor behavior with electron mobility of 9.80E+2 cm^2/V. These findings were examined and interpreted in light of temperature-dependent atomic interdiffusion, surface evaporation, and/or melting of MoO<sub>3</sub>, shedding fresh insight into ALD MoO<sub>3</sub>'s electrical applications.

Keyword: Nanostructured thin films, Atomic layer deposition, Optoelectronics, Photodetector, MoO3 ultrathin film

# Fabrication and Characterization of Titanium Oxide Memristors with Graphene Top Electrodes

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The memristor, memory resistor, is a resistive switching device which has nonlinear properties and time dependent resistance. Due to their novel properties, including similarity to biological synapses and nonvolatile memory, memristors are particularly suitable for beyond CMOS and von Neumann neuromorphic applications [1].

Typically, memristive devices are made of two electrodes (usually metal) with an active layer in between. The active layer is commonly made of transition metal oxides. This research aims to utilize the inherent input dependent resistive switching properties of memristive devices along with the attractive properties of graphene, as such, we fabricated devices with an active layer of stoichiometric and doped Titanium Oxide. The bottom electrode is platinum, the top electrode is made of graphene. Graphene and its derivatives are being used in memristive devices as electrodes and interface materials [2]. Fabricating memristors with graphene top electrodes enables utilizing the intrinsically sensitive structure of memristors due to their time-dependent resistance which causes hysteresis, along with graphene which has properties such as high surface-to-volume ratio, biocompatibility, strong adsorption. A reasonable hypothesis would be that the combination of these characteristics will render selective and sensitive biosensors.

This work presents a novel fabrication methodology by which graphene, synthesized via CVD and transferred onto the wafer, was patterned with photolithography using lift-off. Graphene was characterized using Raman spectroscopy after being patterned. Electrical characterization of Pt/TiO<sub>2</sub>/TiO<sub>x</sub>/Graphene memristors as well as preliminary sensing measurements will be discussed.

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Keyword: memristor, graphene, device fabrication, bioinspired devices

# First Demonstration of Enhancement-Mode Recessed Gate β-Ga2O3 MOSHFETs

#### **Gokhan Atmaca**\*, Ho-Young Cha

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Recently, among other WBG semiconductors,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> draw more attention due to its ultrawide bandgap (4.5-4.9 eV), high expected breakdown electric field of about 6–8 MV/cm. However, the lack of p-type is a serious issue to make enhancement-mode transistors for  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> power devices. To realize enhancement-mode  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSFET, a recessed-gate approach has been widely used. A gate recess process partially removes the epitaxial channel under the gate and it depletes electrons in the channel at V<sub>GS</sub>=0 V. The same gate recess process can deplete the electrons in the integrated heterojunction channel below the MOS-channel. The 2-dimensional confined electrons in the heterojunction channel can enhance the maximum drain current and reduce ON-resistance maintaining a high threshold voltage. The MOSHFET device structure contains a  $\beta$ -Al<sub>x</sub>Ga<sub>(1-x)2</sub>O<sub>3</sub> barrier layer and an undoped Ga<sub>2</sub>O<sub>3</sub> channel layer below the MOS-channel. The  $\beta$ -Al<sub>x</sub>Ga<sub>(1-x)2</sub>O<sub>3</sub> barrier layer consists of a 10 nm undoped  $\beta$ -Al<sub>x</sub>Ga<sub>(1-x)2</sub>O<sub>3</sub>, a 4 nm Si-doped  $\beta$ -Al<sub>x</sub>Ga<sub>(1-x)2</sub>O<sub>3</sub>, and a 1 nm  $\beta$ -Al<sub>x</sub>Ga<sub>(1-x)2</sub>O<sub>3</sub> spacer layer. In this study, firstly, 2D simulations of enhancement-mode recessed-gate  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSFETs were performed in a Silvaco ATLAS TCAD environment to calibrate the transfer characteristics with measured data of the investigated device reported in reference [1]. Secondly, using calibrated physical models and parameters, transfer and transconductance characteristics, output, and off-state characteristics of enhancement-mode recessed-gate  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSHFETs have been comprehensively investigated. It was found that the calculated maximum drain current at V<sub>GS</sub>=8 V and V<sub>DS</sub>=10 V was increased from 21.8 mA/mm to 38.5 mA/mm with the MOSHFET for the same threshold voltage.

This work was supported by Material Component Development Program of MOTIE/ KEIT (10080736), the Basic Science Research Programs (2015R1A6A1A03031833) and Brain Pool Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (2020H1D3A1A0410562511).

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Keyword: β-Ga2O3 MOSFETs, TCAD, Power electronics, e-mode operation

# Geniş yelpazedeki analiz ihtiyaçlarınız için GÜÇLÜ ÇÖZÜM ORTAĞINIZ

ODTU MERLAB www.merlab.metu.edu.tr

MERLAB; üniversitelere, sanayiye, Ar-Ge şirketlerine ve kamu kuruluşlarına, kar amacı gütmeksizin, koşulsuz hizmet vermektedir.

> Kolay Erişilir Güvenilir Kaliteli Öncü

MERLAB; çeşitli branşlardan kırkın üzerinde konusunda deneyimli uzmanı ve yüze yakın cihazı ile verdiği kaliteli hizmetle araştırmacıların ve sanayinin güvenini kazanmıştır.

MERLAB; düzenli katıldığı karşılaştırma ve yeterlilik testleri ile hizmet verdiği alanlarda kalitesinin devamlılığını ve kontrolünü sağlamaktadır.

Ar-Ge Eğitim ve Ölçme Merkezi

MERLAB; Türkiye'nin ilk üniversite merkez laboratuvarı olarak hizmet vermeye başladığı 2004 yılından bu yana ulusal ve uluslararası araştırmalara doğru, tarafsız, hızlı ve güvenilir veriler sağlayarak alanında öncü olmuştur.

# Moleküler Biyoloji ve Biyoteknoloji Ar-Ge Merkezi



# **ODTÜ Merkez Laboratuvarı**

# High-Throughput Computational Screening Evaluating the MXene Adsorbents: Ideal CO2/H2 Separation Performance and The Impact of Interlayer Distance

#### Sirin Massoumılari\*, Sadiye Velioğlu

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The dramatic increase in greenhouse gases emitted to the atmosphere induces the depletion of energy resources as well as global warming. Considering that hydrogen is produced from a wide range of resources and show high energetic efficiency [1, 2], it appears as an environmentally friendly and sustainable energy source for the future of the world. However, hydrogen is mostly in the combination with the other gases such as  $CO_2$ , CO,  $CH_4$ , and  $H_2S$  depending on the resource and process. In this sense, the separation of  $CO_2$  which has a high concentration in hydrogen stream ( $CO_2/H_2$  separation) during hydrogen production can be considered as an unavoidable strategy. Among several separation methods, adsorption-based separation is taken attention due its reversibility and low energy consumption as well as high adsorption efficiency for  $CO_2$ .

MXene family are growing rapidly since its first discovery in 2011. There are more than 150 different MAX phases providing us a large number of precursors for MXenes [3] to produce and mostly design theoretically. Although they have superb properties such as large surface area, adjustable interlayer spacing and surface terminations for gas separation [4], adsorptionbased separation performance of MXenes is examined by the limited number of studies. Identification of adsorption performance of each MXene structure is required a much effort, time, and resource especially during synthesis, characterization, and testing. Therefore, we investigated adsorption performances of the whole MXene family for  $CO_2/H_2$ separation via molecular simulation methods in this study. This high-throughput computational screening approach allows to scan over hundreds of MXene members concurrently.

Novel MXene database including 730 MXene structures was employed for the first time. Each structure was collected from different experimental and quantum-based theoretical studies. Single CO<sub>2</sub> and H<sub>2</sub> adsorption performances of MXene family were evaluated with grand canonical Monte Carlo (GCMC) simulation for pressure swing adsorption (PSA) and vacuum swing adsorption (VSA) processes. To identify the effect of interlayer spacing of MXene nanolayers on gas adsorption performance, simulations were repeated for the MXenes having enhanced interlayer distance. Depending on specific adsorbent metrics, best ten MXene structures were reported for each process. Ti<sub>0.4</sub>Nb<sub>1.6</sub>C, V<sub>2</sub>Ti<sub>2</sub>C<sub>3</sub>, Ti<sub>2</sub>VC<sub>2</sub>, and Ti<sub>1.2</sub>Nb<sub>0.8</sub>C were identified as common MXenes on the basis of several adsorbent metrics and at each process. Their common features are comprising of two types of metal, being un-functionalized, and including Ti element accompanying to the second metal type. However, MXenes including double transition metals and bulky functional groups of –(NCS<sub>2</sub>) were ranked as prominent after the enhancement in interlayer distance of MXenes for both PSA and VSA. Thanks to the enhancement of interlayer distance that regenerability percentages reached to 98% and 95% of all MXenes for PSA and VSA, respectively which were higher than the other adsorbent material reported in the literature. The novel MXene database established by this study has paved the way for not only a road map to the experimentalists and theoreticians to design efficient MXene-based adsorbent, but also a change to transform this database into a big library among the other 2D nanomaterials.

#### Acknowledgements

The molecular simulations are performed at TUBITAK ULAKBIM High Performance and Grid Computing Center (TRUBA). Financial support by the Scientific and Technological Research Council of Turkey (TUBITAK, Grant No. 120M180) is acknowledged.

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# Thousands of Hypothetical MXene Adsorbents for CO<sub>2</sub>/CH<sub>4</sub> Mixture Separation: Highthroughput Computational Screening Study

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Greenhouse gas emissions have been increased day by day and resulted in severe climate changes that lead to natural disasters in all over the world. According to the Paris Agreement, it is expected to reach carbon neutrality by 2050 [1]. Therefore, predominantly the source of greenhouse gases, especially fossil fuels should be cleansed from the acidic gases like CO<sub>2</sub>, H<sub>2</sub>S, etc. As a result, considering the impact of CO<sub>2</sub> on global warming, natural gas separation is gained importance for the environmental safety as well as green energy. Adsorption-based separation is emerged due to its low energy requirement, simplicity and high efficiency compared to the other methods such as absorption, cryogenic distillation, and chemical looping combustion. Among the best performing adsorbents, MXene, which is a very young nanomaterial family, have taken attention related to their high surface area, adjustable interlayer spacing, abundant active sites, and high-regenerability features. As a consequence of different modification approaches, several types of MXene structures have been designed such as MXenes having in-plane and out-of-plane ordering of the metal atoms, in-plane vacancies of metal atoms, solid solution of metal or carbon/nitrogen atoms, and various surface terminations. Since the fabrication of all types of MXenes is time-intensive and costly period, many of them are designed theoretically. However, the number of MXene structures in the literature are less than 1,000. In this study, initially, we created a database of hypothetical 19,800 MXene structures by creating all possible MXene structure combinations. Then, grand canonical Monte Carlo simulations were carried out to compute the performance of MXenes for pressure (PSA) and vacuum (VSA) swing adsorption processes in a high-throughput computational screening manner. Therefore, we have investigated the adsorption performance of 4,000 different MXene structures for CO<sub>2</sub>/CH<sub>4</sub> mixture separation so far. This extensive hypothetical MXene database would be beneficial to suggest a proper MXene design for CO<sub>2</sub>/CH<sub>4</sub> separation. It will be publicly available for other researchers to conduct further analysis and to calculate other desirable properties for the interested separation applications.

#### Acknowledgements:

The molecular simulations are performed at TUBITAK ULAKBIM High Performance and Grid Computing Center (TRUBA). Financial support by the Scientific and Technological Research Council of Turkey (TUBITAK, Grant No. 120M180) is acknowledged. We thank for their support in structure construction to Selin Adıgüzel.

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[1] Oshiro, K., Masui, T., & Kainuma, M. (2018). Transformation of Japan's energy system to attain net-zero emission by 2050. Carbon Management, 9(5), 493-501.

Keyword: MXene nanomaterials, CO<sub>2</sub>/CH<sub>4</sub> Separation, GCMC Simulations, Adsorption-based Separation

# Electrical Conductivity Enhancement Mechanism of Acid Treated PEDOT:PSS by Molecular Modeling Methods

#### Erhan Özdemir<sup>\*</sup>, Erol Yıldırım

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Poly(3,4-ethylenedioxythiophene):polystyrenesulfonate (PEDOT:PSS) is a conductive polymer which attract widespread interest both in the organic electronic literature and industry due to its high stability, processability and high rate of conductivity. It has good film-forming, transparency and thermal stability. Its electrical conductivity can be increased by solvent treatment such as with organic solvents, ionic liquids, acids etc. It was demonstrated that 500 folds of increase from 0.2 Scm<sup>-1</sup> to 100 Scm<sup>-1</sup> in the electrical conductivity of PEDOT:PSS can be achieved by solvent treatment. PEDOT:PSS treated with aqueous solutions of various salts showed that soft cations like  $Cu^{2+}$ ,  $Ag^+$  and  $In^{3+}$  increased the conductivity by 2 orders of magnitude while the effect of hard cations like Li<sup>+</sup>, Na<sup>+</sup>, Mg<sup>+</sup> was negligible. Experimental groups reached electrical conductivity over 4000 Scm<sup>-1</sup> by treating PEDOT:PSS film with H<sub>2</sub>SO<sub>4</sub>.<sup>5</sup> Proposed mechanism for this enhancement is that, H<sub>3</sub>SO<sub>4</sub><sup>+</sup> and HSO<sub>4</sub><sup>-</sup> ions from the autoprotolysis of H<sub>2</sub>SO<sub>4</sub> hold PEDOT and PSS nanofibrils together and disordered PEDOT:PSS becomes highly ordered. Another proposed mechanism is that, PSS is removed from the surface of PEDOT:PSS film during solvent treatment, resulting in the enhancement of conductivity since PEDOT is the conducting part of the film. It was also claimed that after organic solvent treatment and removal of PSS, PEDOT with coiled structure turns into extended coil or linear structure. In another study, conductivity enhancement is proposed to be due to the change in resonant structure of PEDOT from benzoid to quinoid structure.9 We previously showed that conductivity enhancement of PEDOT:PSS with DMSO treatment was examined with density functional theory (DFT) calculations, molecular dynamics (MD) studies and hydrophobicity studies and removal of the PSSH with DMSO is suggested to be the enhancement mechanism. In this study, enhancement mechanism of the electrical conductivity by the H<sub>2</sub>SO<sub>4</sub> treatment will be investigated by first principle methods and classical simulation studies.

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Keyword: PEDOT:PSS, Molecular Modeling, Conductivity, Acid Treatment, Molecular Dynamics

# Enhancement of Physical and Mechanical Properties of Epoxy Resins by Graphene/Graphene Oxide Additives

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Epoxy is a commonly used thermosetting resin with superior mechanical properties, high chemical and thermal resistance and adhesion properties. It has a wide range of application areas including aerospace, coatings, automotive, adhesives, electronic materials and biomedical devices. Although high crosslinking density provides high stiffness and mechanical strength, it also makes epoxy resins rigid and brittle, resulting in poor resistance to crack initiation and growth. To improve mechanical properties of epoxy resins, fillers such as graphene can be embedded into an epoxy matrix.

Graphene is a promising reinforcing material for polymer composites with its large specific surface area, highest Young's modulus ever known as high as 1 TPa, excellent electrical and thermal conductivity.<sup>[1]</sup> In order to achieve the desired mechanical, thermal and electrical properties of the structure; effective dispersion and strong adhesion of graphene sheets into the epoxy matrix are required. Graphene sheets are insoluble in most solvents, which is making them difficult to process. They tend to agglomerate in the polymer matrix due to strong vdW forces between them. Functionalization of graphene sheets with oxygen containing groups is an effective method to reduce this interaction and increase their compatibility with epoxy system.<sup>[2]</sup>

In this project, type and number of functional groups on graphene oxide (GO), mass percentage of GO in the epoxy matrix, epoxy structure and crosslinking density will be optimized by molecular dynamics simulations and physical and mechanical properties will be investigated. Improvement of the interaction energy between GO sheets and a well-known epoxy system DGEBA (Bisphenol A diglycidyl ether)/DETA (Diethylenetriamine) will be calculated by changing the number, type and position of functional groups on the GO via all-atom molecular dynamics simulations. This theoretical study will provide an insight into the design of the structure of GO nanofillers and enable them to perform better in the epoxy matrix.

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#### ID: 80 - Computational Nanoscience

# Theoretical Modeling of Single-Atom Catalysts on Titania Anatase Surface

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Catalysts are atoms, molecules, or crystal structures that do not directly participate in a reaction but accelerate its rate by lowering the amount of energy necessary for the reaction to occur. Heterogeneous catalysts are typically made up of surfaces to which gaseous components are connected and on which the reaction occurs. Reducing the size of the metal component in catalysts containing valuable metals is tremendously advantageous both chemically and commercially. It is critical to boost efficiency while also lowering costs. The single-atom catalyst (SAC), which is made by putting single metal atoms on surfaces in a regulated and homogeneous manner, is the upper limit.

Due to the enormous number of options available for both the metal component and the underlying substrate, identifying the best catalyst for a given reaction only by experimental means is a challenging process. By using Density Functional Theory (DFT)-based approaches we provide a theoretical study to calculate binding geometries, adsorption energies, activation barriers, vibration frequencies and contribution of metal atoms' reaction and diffusion barriers for Titania Anatase (TiO2) support surface. Ir and Rh chosen as additive metals. We have picked CO oxidation as the reaction that will be used to test the activity of these SACs. This reaction involves the conversion of hazardous CO gas to CO2 by interacting with O2.

Our research aims to fill a gap in the literature by evaluating the potential of these two metals. The metal oxides were chosen as the support material due to differences in their electronic structure, specifically their degree of charge interchange with the metal component. Successful completion will provide the experimental community with a reference for the best surface-metal pair selection.

## Acknowledgements:

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ID: 116 - Computational Nanoscience

Molecular Mechanism of the Aromatic Macrocycle Self-assembly: A Theoretical Study

Not presented.

# Potential of MXene Membranes for H<sub>2</sub>/CO<sub>2</sub> Separation

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According to the Paris Agreement on climate change, the European Union and its member states among the 190 parties have agreed to reduce greenhouse gas emission. Because it is predicted that the amount of  $CO_2$  in the atmosphere will reach 570 ppm in 2100 and the temperature will increase by  $3-4^{\circ}C$  [1]. This situation not only threatens our health, but also endanger the production of agricultural products necessary for our survival. For this purpose, the source of  $CO_2$  emissions like syngas, natural gas, flue gas, etc. should be separated via the most appropriate gas separation processes. Since low cost, high efficiency, and purity are required in gas separation, membrane technology is a promising technology due to its simplicity of operation and low energy consumption, cost-effectiveness, and environmentally friendly features. Polymeric membranes dominate the commercial application, whereas recently, mixed matrix membranes (MMMs) have been emerged as prominent alternatives to polymeric membranes. MMMs are fabricated by combining a continuous polymeric phase and an inorganic dispersed phase. Since the mass transfer resistance is hindered by the use of thin membranes, 2D materials as inorganic filler in MMMs attracted great attention. Among them, Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> from MXene family, revealed superior H<sub>2</sub>/CO<sub>2</sub> separation performance. Therefore, we aimed to reveal the membrane based H<sub>2</sub>/CO<sub>2</sub> separation potential of whole MXene family at a molecular level.

Initially, 730 MXene structures from experimental and theoretical studies in the literature were collected to establish the online freely accessible MXene database. Then, boundaries for H<sub>2</sub> permeability and H<sub>2</sub>/CO<sub>2</sub> selectivity of MXene membranes were determined as  $19.3-4.4 \times 10^6$  Barrer and  $1.1 \times 10^{-2}$ -635.2, respectively. We specified a criterion for H<sub>2</sub> permeability and H<sub>2</sub>/CO<sub>2</sub> selectivity to define the best performing members. Accordingly, 20 best performing MXene membranes were identified, displaying H<sub>2</sub>/CO<sub>2</sub> selectivity between 10.6 and 20.2, and CO<sub>2</sub> permeability of  $7.8 \times 10^4$ -8.2×10<sup>5</sup> Barrer. Surprisingly, all the best performing MXene structures either had surface functional groups of  $-O_2$  and  $-F_2$  or were unfunctionalized. Compared to the highly preferred inorganic materials as MOFs, and COFs, 95.9% of MXene structures from its family exceed the Robeson upper bound [2] whereas this number was 92.7% and 23.3% for COF [3] and MOF [4] structures, respectively. Finally, the performance of top four structures, namely VCrNF<sub>2</sub>, MoWCF<sub>2</sub>, Y<sub>2</sub>NO<sub>2</sub>, and Sc<sub>2</sub>NO<sub>2</sub>, were also evaluated by non-equilibrium molecular dynamics approaches and combined with the performance of common polymers to propose possible MMMs for H<sub>2</sub>/CO<sub>2</sub> separation. Results of this study will guide the experimentalists who can further explore the actual separation performances of the proposed MXene membranes by this study.

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Keyword: Membrane-based gas separation, MXene family, H<sub>2</sub>/CO<sub>2</sub> separation, GCMC+EMD, and NEMD simulations.

**ID: 147 - Computational Nanoscience** 

# Binary CO<sub>2</sub>/H<sub>2</sub> Separation Performance of MXenes Under Different Adsorption Processes: High-throughput Computational Screening

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Separation of CO<sub>2</sub> from H<sub>2</sub> is a very crucial process for petroleum refining and in the production of hydrogen, methanol, or ammonia due to the requirements in their end-use areas. In addition, CO2 is a greenhouse gas, and its rapid increase in the atmosphere leads to global warming. Therefore, it is essential to remove  $CO_2$  from industrial gas streams such as syngas, natural gas, and biomass. Commonly used methods such as amine purification and cryogenic distillation processes for CO2 capture have given rise to the alternatives due to their high cost. One of the most promising alternative separation technologies is the adsorption which can be diversified based on operational conditions such as pressure swing adsorption (PSA), vacuum swing adsorption (VSA), temperature swing adsorption (TSA), pressure-temperature swing adsorption (PTSA), and vacuumtemperature swing adsorption (VTSA). MXenes, a new family of two-dimensional (2D) materials, appeared to be promising materials for the adsorption-based CO<sub>2</sub> capture with their high thermal conductivity, adjustable pore structure and ability to be functionalized. In this study, the binary CO2/H2:25/75 adsorption performance of almost 730 MXenes was determined by classical molecular simulation approaches. Depending on several adsorption performance metrics, best performing 10 MXene structures were determined for each adsorption process. For instance, Cr, Mo, and W including MXene structures were dominating in the top list of PSA and VSA. However, top lists of TSA, PTSA, and VTSA processes were completely different due to the alteration in the performance of adsorbents at desorption conditions. Therefore, MXenes functionalized with bulky -NCS<sub>2</sub> group and in-plane ordered vacancy MXenes such as Nb<sub>1.33</sub>C and W<sub>1.33</sub>C appeared as best candidates. This type of high throughput computational screening studies enables to test many adsorbents for the specialized applications to guide the experimental research.

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Keyword: MXene nanomaterials, adsorption processes, binary gas separation, GCMC simulations

ID: 202 - Computational Nanoscience

# Designing and Comparing the Catalytic Activity of Molten Metal Catalysts for Methane Pyrolysis

#### <u>Arda Erbasan</u><sup>\* 1</sup>, Hande Toffoli<sup>1</sup>, Uğur Sökmen<sup>2</sup>, Gökhan Çelik<sup>2</sup>, Esra Eroğlu<sup>3</sup>, Rasiha Nefise Mutlu<sup>3</sup>, İskender Gökalp<sup>3</sup>, Gülfeza Kardaş<sup>4</sup>

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Hydrogen is a vital source of energy and indispensable for the chemical industry. Today, hydrogen is globally supplied by steam reforming of natural gas: a process emitting greenhouse gases, including enormous amounts of CO2. Therefore, the need for environmentally friendly hydrogen production technologies is clear. Catalytic pyrolysis of methane is one of the efficient and environmentally friendly methods to produce  $CO_2$  -free hydrogen. The reaction also produces carbon, which causes product build-up in the reactor when pyrolysis is performed in the gas phase. To avoid carbon poisoning in the reactor, bubble column reactors using molten metal alloys as catalysts are used where carbon leaves the reactor bed due to the density difference under reaction conditions. Herein, we provide a theoretical study on the catalytic activity of molten ternary alloys towards methane dehydrogenation. The rates of the methane dehydrogenation reaction are obtained with ab-initio Molecular Dynamics simulations for different ternary alloying ratios for Ni, Cu, Al, Bi Ga, In, and Sn. Further, the ternary alloy systems are assessed in terms of reactivity descriptors such as d-band center and Bader partial charges using Density Functional Theory.

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Keyword: Methane Pyrolysis, Density Functional Theory, Molecular Dynamics, Hydrogen Production, Bubble Column Reactors

ID: 239 - Computational Nanoscience

# Investigations on the Hydrolysis Mechanism of Aluminum for Hydrogen Generation: A First-Principles Study

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Due to its high energy efficiency and environmentally friendly characteristics, hydrogen is known as one of the most ideal energy carriers and fuels [1]. In recent years, the reaction of aluminum materials with water to produce hydrogen has received significant attention owing to efficient and cheaper hydrogen generation from aluminum compared to other metals [2-3]. This work is a density functional theory (DFT) investigation of the detailed reaction mechanisms of the hydrolysis of water on the oxidized Al (111). We first explore the adsorption properties of all species involved as both reactants and products. We

then proceed to carefully construct and calculate the energy barriers of a multiple-step reaction mechanism. Water splitting potential energy profiles for each hydrolysis process and hydrogen generation on both O pre-adsorbed Al

(111) and clean Al (111) surfaces are mapped out via the nudged elastic band (NEB) method calculations. All calculations were conducted using the Vienna Ab Initio Simulation Package (VASP). The activation barriers of an eight-step surface reaction mechanism (0.16 eV-0.65 eV) are compared with the experimentally estimated barrier and yield a very good agreement. These results validate the proposed reaction mechanism involving the mixture of dissociated water molecules and direct surface adsorption of free OH<sup>-</sup> radicals from the solution.

#### Acknowledgement

This work is financially supported by the Scientific and Technological Research Council of Turkey (TÜBITAK), Grants No:118C291 and 118C287.

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Keyword: Hydrogen Energy, Hydrolysis, Aluminum, DFT

# An Investigation of ion Transport Through the SARS-CoV-2 E Protein ion Channels

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The E protein is one of the major structural proteins of RNA viruses. It is involved in replication, budding, and assembly, E proteins are known to form ion channels which slightly favor cation transport over anion. In the light of the ongoing pandemic, we compared SARS-CoV-1 and SARS-CoV-2 E protein ion channels in terms of their selectivity. The impact of the bath concentration and concentration gradients across the channel on the binding ratios of sodium and chloride ions have been also studied. Ion transport is described through the fourth-order Poisson-Nernst-Planck-Bikerman (4PNPBik) model which generalizes the traditional model by including ionic interactions between ions and their surrounding medium and non-ionic interactions between particles due to their finite size. The immersed boundary-lattice Boltzmann method (IB-LBM) is used for the solution of the system. The mathematical model has been validated by comparing analytical and experimental ion activity. Ion transport through SARS-CoV-2 E protein ion channel shows that cation selectivity is not as prominent as in E proteins of other RNA viruses. Furthermore, the chloride binding ratio increases as the concentration gradient increases. A potential gradient has a minimal effect on the binding ratio. A potential gradient has a minimal effect on the binding ratio. A potential gradient has a minimal effect on the binding ratio. Ion transport through SARS-CoV-2 E protein ion channel shows that cation selectivity is not as prominent as in E proteins of other RNA viruses. Furthermore, the chloride binding ratio increases as the concentration gradient increases. A potential gradient has a minimal effect on the binding ratio.A potential gradient has a minimal effect on the binding ratio. A potential gradient has a minimal effect on the binding ratio. Ion transport through SARS-CoV-2 E protein ion channel shows that cation selectivity is not as prominent as in E proteins of other RNA viruses. Furthermore, the chloride binding ratio increases as the concentration gradient increases. A potential gradient has a minimal effect on the binding ratio. A potential gradient has a minimal effect on the binding ratio. A potential gradient has a minimal effect on the binding ratio.

ID: 179 - Nanomembranes, Catalytical Nanostructures, and Electrochemical Nanomaterials

# Silver (Ag) Based Electrocatalysts for Oxygen Reduction Reaction

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The environmental problems such as 'global warming' caused by the heavy consumption of fossil fuels have accelerated the research toward clean energy technologies such as fuel cells and metal-air batteries. The high over-potential required for the oxygen reduction reaction (ORR) at the cathode is one of the most critical challenges that these technologies face. To overcome the sluggish ORR kinetics, it is critical to developing suitable electrode materials other than the expensive and scarce platinum (Pt), known as the most effective electrocatalyst. In this study, we present how to manipulate the activity of bimetallic AgCu alloy nanoparticles by dealloying Cu in an acidic medium. Analyzes reveal that dealloying in HCl on AgCu alloy NPs results in the formation of relatively large nanostructures composed of Ag/AgCl that present a superb ORR activity with a high onset potential (E0) of  $\approx$ 0.97 V vs. RHE, comparable to commercial Pt/C catalysts. We propose that Ag+ stabilized in the presence of sub-stoichiometric Cl- plays a critical role in the superior activity of the catalyst.

#### ID: 208 - Nanomembranes, Catalytical Nanostructures, and Electrochemical Nanomaterials

# The Lab-made and Bio-made Precursors of Carbonaceous Catalysts for Fuel Cells

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There is a growing need for the advances in designing the new efficient electric power sources to substitute traditionally used combustion systems. For instance, the modern electricity-driven cars rely on onboard Li-ion batteries. Unfortunately, this technology has its limitations too. The electrochemical fuel cells (FCs) as sustainable energy conversion and storage devices are considered as a promising alternative. FC and battery powered hybrid systems for mobility and off-grid applications are in the focus of ongoing scientific and technical research [1].

FC comprises two porous electrodes immersed into a conducting electrolyte and separated by a membrane. Its operation is driven by redox reactions when a fuel gas (typically hydrogen) passes through the anode while oxygen goes through the cathode. The oxygen reduction reaction (ORR) is sluggish, and a catalyst is required to boost the reaction kinetics. The most efficient are Pt-based catalysts, although the scarcity and high cost of its noble metal hinders broad application of FCs. Extensive efforts are ongoing on optimization of the catalyst's structure to achieve the low-cost and high-activity Pt-based material [2].

An alternative approach to combine some transition metals (Cd, Fe) and nonmetals (N, P) in a composite material able to reach the overall catalytic efficiency comparable to the Pt-based benchmark has been rapidly developing. These nanostructured carbons doped with heteroatoms are obtained by a variety of techniques. Metal-organic frameworks comprising the 3D ordered metal sites separated by organic ligand spacers have become popular precursors to obtain active carbons via pyrolysis. Earlier we adopted this approach to produce a series of electrochemically active Fe,Co,Zn-N/C catalysts for ORR from bimetallic ZIF structures [3].

In this contribution another emerging trend of preparing the biomass-derived carbon catalysts will be considered as well by discussing the concept, the synthesis approaches, characterization techniques and applications. Biomass is a renewable source, and its purposeful utilization as a precursor for novel materials of industrial relevance contributes to a sustainable economy [4].

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Keyword: carbon-based catalysts, oxygen reduction reaction, fuel cells, electrochemistry, biomass-derived carbon materials

ID: 243 - Nanomembranes, Catalytical Nanostructures, and Electrochemical Nanomaterials

# Synthesis and Characterization of Titanium Dioxide Nanotube Based Membrane Systems for Blood Filtration Applications

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Due to high biocompatible properties, titanium dioxide nanotube surface arrays have widely been used in orthopedic and dental implants, biosensor and drug releasing systems. In the presented thesis study, titania nanotube-based membrane structures, which preserving its bulk stability, had been fabricated by three-step electrochemical anodic oxidation and sudden change in application potential at different temperatures. Availability of fabricated titania nanotube-based membrane structures at blood filtration applications were investigated for wearable/portable and implantable artificial kidneys; their chemical and morphological properties had been determined by scanning electron microscopy (SEM), energy dispersive x-ray analysis (EDX), x-ray diffraction analysis (XRD), water contact angle (WCA) and atomic force microscopy (AFM). In this aim, uremic toxin filtration performances of these nanostructures had been tested in the flow cells which had been manufactured with 3D printing by modernized fused deposition modelling technology of poly(ethlyene tereftalat – gyclycol) (PETG). Two different membrane structures, which having nanotubes with 50 nm radius and 30  $\mu$ m length on 36% of their surfaces, had been investigated for crossflow pure water flux (PWF), rates of creatinine clearance and 20% in BSA rejection. The nanoceramic ultrafiltration membranes shows 95% in creatinine clearance applicable as the results of digital and experimental failure analysis.

Keyword: nanoceramic, nanoporous membrane, titanium dioxide nanotube, anodic oxidation, artificial kidney

ID: 336 - Nanomembranes, Catalytical Nanostructures, and Electrochemical Nanomaterials

## P(VDF-TrFE) and Sulfonated Silica-Based Electrospun Membrane-Electrode-Assemblies (MEAs) for PEM Fuel Cells

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In the present study, sulfonated silica (S-SiO<sub>2</sub>) nanoparticles (NPs) which are cheap and stable at low humidity are synthesized and employed in both membrane and electrode structure of PEM fuel cells [1,2]. Here, electrospinning is utilized to prepare hybrid nanofiber based PEM fuel cell membranes containing S-SiO<sub>2</sub> particles, poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) binder (carrier polymer); and electrodes containing commercial Pt/C catalyst, S-SiO<sub>2</sub>, and P(VDF-TrFE) carrier polymer. Additionally, in order to investigate the effect of reinforcing polymer, poly(vinylidene fluoride) (PVDF) carrier polymer included membranes and electrodes were fabricated. Firstly, the morphology of both electrospun membranes and electrodes have been investigated by scanning electron microscopy (SEM) to determine optimum electrospinning conditions to achieve a uniform nanoparticle distribution along the carrier polymer. In order to prepare hybrid membranes, fiber mats were transformed into dense membranes by hot-pressing and Nafion® impregnation steps. After obtaining compact membrane, ionic conductivity, water uptake and mechanical strength of the hybrid membranes have also examined [3]. Electrospun electrodes also are characterized by transmission electron microscopy (TEM) to investigate catalyst (Pt/C) distribution along the Nanofibers. Additionally, porosity of electrospun electrodes have been investigated by mercury porosimetry. After obtaining nanofiber-based hybrid membrane and electrodes, membrane electrode assemblies (MEA) are fabricated, and fuel cell tests are performed with using H<sub>2</sub>/air at different humidity levels. Moreover, the durability of electrospun electrodes were investigated with accelerated stress tests (AST) in fuel cell. These novel electrospun hybrid membranes and electrodes possess a superior PEM fuel cell performance especially at low humidity conditions compared to Nafion® based membranes and electrodes. The hybrid electrodes showed remarkable durability after Pt-dissolution and carbon corrosion AST.

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Keyword: Electrospinning, Catalyst layer, polymer electrolyte membrane, PEM fuel cells, Sulfonated silica

ID: 325 - Organic and Inorganic Nanocomposites

## Nanoscale Patterning of Liquid Crystal-Aqueous Interfaces

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Liquid crystals (LC) are defined by their long-range ordering of the constituent molecules (mesogens) while possessing liquidlike mobility. Cholesteric LCs (CLCs) are the phases where helical twist is present orthogonal to the director of the individual mesogens. Under confinement, LCs may not maintain a uniform helical twist and the ordering of the mesogens deform significantly, forming localized topological defects. Depending on the characteristics of the confining medium such as size. interfacial orientation of the mesogens and the helix pitch length, defined structures, the so-called liquid crystal configurations are formed. One of the most common configurations observed is where all the defects transform into a single line defect just below the LC-water interface, wrapping the droplet from one end to another<sup>1</sup>. LC defects cause significant elastic energy penalty; and thus, are used in directed assembly of molecular or particular species<sup>2-4</sup>. We hypothesize that the CLC configurations maintained in droplet geometries can be used to assemble nanoparticles at LC interfaces with high precision. For this purpose, we first characterized the configurations of the CLC droplets as a function of their sizes, helical pitch length, and interfacial LC orientation, and showed that polymerization using a reactive mesogen did not cause a significant change in their configurations. Experiments with nanoparticles at interfaces revealed the nanoparticle assemblies to follow the underlying defects, erasing of which by heating to isotropic phase resulted in the loss of such assemblies. We showed that the patterns formed can be tuned by altering the properties of the LCs, the nanoparticles and the composition and the ionic strength of the medium. Parameters effecting the symmetry and characteristics of the nanoparticle patterns are investigated in motivation to provide insight into the mechanism of the patterning. The study suggests a novel method for directed particle assembly which can be utilized for applications in the fields of microelectronics, sensors, patterned surfaces and energy harvesting.

#### Acknowledgments:

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Keyword: Nanoparticle, Colloid, Self Assembly, Liquid Crystal

## Coating of Thin Molecularly Imprinted Films onto Magnetic Nanoparticles for Removal of Antibiotics from Real Water Samples

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Antibiotics may be the most useful family of drugs improved for human health. In addition to this basic application, they are widely used to treat animal and plant infections. Tetracyclines are the second most commonly used family of antibiotics used in animal husbandry to treat bacterial infections. More than 75% of tetracyclines are excreted in their original form and derivatives and released into the environment via human and animal urine and feces, which cause a serious threat to the ecosystem and human health. The removal of antibiotics from environmental water supplies is of vital importance due to the ongoing release of these pharmaceuticals [1]. There are several conventional techniques to remove tetracyclines from environment such as adsorption and degradation. However, the main disadvantage of these methods is the lack of the selectivity. At that point the molecular imprinting, a method to prepare tailor made materials with high specific selectivity and binding capacity is a useful alternative. In this work, tetracycline imprinted thin films were prepared onto the magnetic iron (III) oxide nanoparticles (MNP) by admicellar polymerization of styrene and divinylbenzene. The detailed structural and physical characterization of modified magnetic nanoparticles was carried out by FTIR, XPS, XRD, TEM and BET. The size of the magnetic nanoparticles before and after modification was determined as approximately 35 nm and 115 nm, respectively. Binding properties were evaluated by employing adsorption isotherms. The specific selectivity of the tetracycline imprinted polymers was evaluated for structurally similar tetracyclines. The imprinting factor was determined as 3.41, 1.55, 1.52 and 1.23 for tetracycline, oxytetracycline hydrochloride, doxycycline hyclate and chlorotetracycline, respectively. The binding capacity of the molecularly imprinted polymer modified MNP was investigated for tap water and natural waters samples. The adsorption percentage of tetracycline was determined as 83.2, 66.3, 54.7 and 51.5 for ultra-pure water, tap water and natural water samples as Pazar Creek and Halys River, respectively [2].

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Keyword: Molecular Imprinting, Tetracycline

ID: 126 - Polymer Nanotechnology

## Surface Functionalization via Layer-by-Layer Films of Chitosan/Tannic Acid and Chitosan/Poly(acrylic acid) for Biological Applications

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In the present study, the effect of polyacid type on chitosan (CHI) based layer-by-layer (LbL) films was investigated in terms of chemical structure, surface morphology, wettability, drug release and biological properties of the multilayers. Tannic acid (TA), a polyphenol and poly(acrylic acid) (PAA), a polycarboxylic acid were chosen to fabricate multilayers of CHI. It was demonstrated that chemical structure of the polyacid affected LbL film growth, surface morphology, wettability, and multilayer stability at pH 7.4/37°C. The antiadhesive behaviour of the films against protein adsorption was assessed using bovine serum albumin (BSA) and lysozyme (LYS). The antibacterial activity of ciprofloxacin (CIP) embedded multilayers were examined against Escherichia coli (E. coli), Staphylococcus aureus (S. aureus), and Listeria monocytogenes (L. monocytogenes). TA/CHI films were found to be antiadhesive against protein adsorption when topmost layer and the protein were similarly charged. PAA/CHI multilayers did not resist protein adsorption. The amount of CIP release was higher from PAA/CHI films. Therefore, they showed enhanced antibacterial activity compared to TA/CHI films. Results showed that biomaterial surfaces can be modified through PAA/CHI multilayers for enhanced antibacterial activity, while material surface gains antiadhesive property via TA/CHI multilayer coating.

Keyword: chitosan, layer-by-layer technique, drug release, protein adsorption, antibacterial activity

## Production of Graphene Oxide and Polysulfone Based Porous Films via Breath Figure Method

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Porous polymers/porous polymer films have found applications in many research areas as membranes, templates, supports for sensors and catalysts. Most of these areas have the need for porous structures having distinct structural, interfacial, compositional, and morphological properties to increase the surface area, to provide low density etc. Therefore, structural characteristics of porous polymers such as pore geometry (spherical, tubular, network-type), pore size, surface functionality of the pores as well as composition, topology and functionality of the framework structure play an important role on the decision making for the desired application. Recently in order to produce porous polymers, novel self-assembly/templating methods are developed [1]. Breath figure (BF) method is an example of self-assembly process. A breath figure (BF) is the fog that is formed upon breathing onto a cold surface, and it gets its name from this process. Such a technique has important advantages over conventional approaches, including the use of largely available and nontoxic template and a reduced amount of solvent as well as the requirement of only one fabrication step [2]. Therefore, it is a convenient, adjustable and inexpensive technique which uses the ordered arrays of water droplets as the template. They are formed when a cold surface is brought in contact with moist air. If the surface is not wetted by the vapor, moisture condenses on the cold surface forming water droplets that grow during the evaporation giving rise to distinct water droplet arrangements on the surface.

Graphene is a two dimentional and one-atom thick material in which carbon atoms are arranged in a honeycomb lattice [3]. Following the isolation of graphene and identification of its properties by Andre Geim and Konstantin Novoselov, graphene and related materials have become the focus of research in different fields owing to their superior properties such as high surface area, high modulus, and high thermal and electrical conductivity. Among them, graphene oxide (GO) has been commonly used since it contains carboxyl, hydroxyl and epoxide groups anebling further functionalizations.

In this study, it was aimed to produce porous films of polysulfone with regular pores using a GO based surfactant, GO – dimethyldioctadecylammonium (GO-DODA) via breath figure method. Graphene oxide, which was synthesized using Tour Method [4], was used to obtain GO-DODA complex. GO and GO-DODA were characterized (using ATR-FTIR, UVVis, TGA, SEM etc.). The effects of parameters such as relative humidity, polymer and GO-DODA concentrations on pore formation and regularity were investigated using optical microscopy and SEM.

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Keyword: Breath Figure, Porous Film, Graphene, Graphene Oxide

## Synthesis and Characterization of Autonomous, Self-Healing Waterborne Polyurethane Dispersions

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One of the most severe problems in today's world is the massive amount of waste produced by the consumption of polymeric materials. Herein, self-healing polymers' role can be critical as ameliorate the durability and extend the service time of polymeric materials, thereby reduce the related volume and cost waste materials [1]. Particularly, autonomous self-healing materials are highly desirable as they prevent the use of external energy or stimuli [2]. In this sense, polyurethanes have emerged as a promising class of self-healing polymers due to their versatile chemistry, segmental structure, and tunable bond structure [3-4-5]. In this study, environmentally friendly waterborne polyurethane (WPU) dispersions bearing anionic groups on the backbone were synthesized via acetone method from an aliphatic diisocyanate and a polyester polyol to investigate the synergistic effect of the ionic interactions and H-bonding on the room-temperature, autonomous self-healing behavior of resulting films and coatings. The WPU latex nanoparticles were characterized by Dynamic Light Scattering (DLS), and the resulting films were characterized by structural, thermal, and mechanical analyses using Fourier Transform Infra-Red Spectroscopy (FT-IR), Thermo-Gravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) and tensile tests. It was demonstrated by optical microscope images and tensile tests that the final coatings with an optimum content of hard segment and ionic groups show an unexpectedly high degree of self-healing behavior at room temperature compared to their non-ionic analogues, and thus, offer an enormous application potential for next-generation smart protective coatings, adhesives, and films.

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Keyword: waterborne polyurethane, self-healing, non-covalent interactions, coatings, films

## Investigation of the Use of Antiimflammatory Riboflavin Induced Periodically Nanopillar Decorated Collagen/Polycaprolactone Membranes for Wound Healing

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Skin is the largest organ that acts as a physical barrier towards the environment. The deviations and damages in the skin is called as wounds and the healing of these wounds without any complications is crucial.[1] Activation of the immune system triggers the inflammation cascade and delays healing. Therefore, the use of a suitable wound dressing is essential for not only healthy and fast recovery of the wound area, but also to protect the area. However, using a dressing could increase the risk of infection.

The wound dressings that will be used for such applications are expected to be biocompatible, biodegradable,non-toxic,antiinflammatory,physically and chemically enhance wound healing, cost-effective and a barrier for external factors. Thus, the inflammation caused by the external factors can be avoided and even if there is an inflammation, it will be suppressed.

In order to fulfill these needs, in this study the use of riboflavin induced collagen/polycaprolactone membranes as wound dressing are investigated. Polycaprolactone(PCL) is a resorbable and FDA-approved biomaterial and using PCL with collagen(Col) the biocompatibility and efficiency of the membrane will be enhanced.[2] In order to control the degradation, riboflavin(Rb) will be used as photocrosslinker.[3] On the other hand, it is reported earlier in literature that riboflavin has anti-inflammatory effect but there is no study in literature about anti-imflammatory effect of a riboflavin containing biomaterial.

The proposed membranes will be fabricated via drop-casting from periodically decorated anodic aluminum oxide membranes(AAMs) that can be obtained via two-step anodization. As AAMs posses periodic hexagonal nanopores, the obtained polymeric membranes will have periodic nanopillars. Therefore, highly controlled nanofeatures with a specific chemical composition can be achieved with a non-lithographic method. Especially the size and morphological similarity between these structures and natural symmetric arrays of extracellular matrix makes AAMs valuable biomaterial and mold in tissue engineering.[4]

In order to investigate morphological effects, flat counterparts were fabricated via drop-casting on silicon wafer and to show the effect of riboflavin the specimens for the following tests were flat PCL/Col, flat PCL/Col/Rb, nanopillared PCL/Col and nanopillared PCL/Col/Rb. The morphologic characterizations of the membranes were performed via atomic force microscopy(AFM) and scanning electron microscopy(SEM) and both the flat and nanopillared morphology were investigated. Then the mechanical analysis was conducted. In vitro degradation and swelling characteristics were determined for 120 days and more than 80% weight of the membranes preserved itself. Also, riboflavin release was determined and the effect of the nanofeature on the release was determined.

By using a fibroblast cell line(L-929), in vitro cytotoxicity and cell adhesion tests were performed and all of the membranes showed biocompatibility.(viability more than 90%) Lastly, in order to report the anti-inflammatory effect of the fabricated membranes, macrophages(RAW 264.7) were seeded on the membranes and the inflammation was chemically induced by lipopolysaccaride. Then the expression of selected anti-inflammatory and pro-inflammatory genes were analyzed and results will be represented in the presentation. As a result, the potential of the use of riboflavin induced periodically nanopillar decorated collagen/polycaprolactone membranes for wound healing in skin tissue engineering will be reported.

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Keyword: riboflavin, collagen, nanobiomaterial, wound dressing, wound healing, tissue engineering

## Nanostructures on Titanium Significantly Affects the Conformation of Surface Adsorbed Protein

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Due to their good biological compatibility and mechanical properties, titanium (Ti) and its alloys are widely used in hard tissue repair as implant material. One of the crucial factors affecting the bonding between the Ti implant and the bone is the surface roughness at the nanometer scale [1]. Hence, the current trend in Ti biomaterials development is focused on generating surfaces with nanoscale topographic features in an attempt to influence or control in vivo tissue response at the molecular and cellular level. The cellular response to nanoscale surface topography is known to be governed by the initial protein layer that is adsorbed to the surface of a biomaterial immediately after implantation. Furthermore, the adsorption of proteins is also affected by the surface nanotopography. For this reason, while designing biomaterials, the amount and conformation of proteins merits further investigation. However, the overall effect of nanoscale properties of surfaces on protein adsorption is not fully understood yet. There are a limited number of reports on the effect of surface topography on protein adsorption albeit with contradictory results [3-5]. In order to contribute filling in this gap in the literature we investigated the effect of nanotopography on protein adsorption using Ti as the model surface and bovine serum albumin (BSA) as the model protein. Nano-structures, in the form of TiO<sub>2</sub> nanotubes were generated by anodic oxidation. Surface characterization was performed using scanning electron microscopy, atomic force microscopy, water contact angle measurements and X-ray photoelectron spectroscopy. The behavior of BSA upon surface adsorption was investigated in terms of the amount and the conformation of the protein of the protein adsorbed on the surfaces. The secondary structure of surface adsorbed proteins was investigated using the second derivative and curve fitting methods applied to the Fourier transform infrared spectra of the surfaces with surface adsorbed BSA. The results obtained for Ti specimens with nanotubes were compared with the amount of protein adsorption on bare and sanded Ti surfaces. Our results showed that the amount of protein adsorbed on the surfaces increased with increasing surface roughness as expected. We observed a dramatic change in the secondary structure of BSA upon adsorption onto surfaces having nanoscale structures. Furthermore, the conformation of the surface adsorbed protein was unique to each surface. BSA has undergone significant conformational changes on all surfaces upon adsorption irrespective of surface hydrophilicity and roughness and the extent of the changes in the secondary structure of BSA was not directly correlated with the surface hydrophilicity and the surface roughness. For anodized samples a correlation between the pore diameter and the secondary structure of surface adsorbed protein adsorbed was observed.

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Keyword: Titanium implants, Nanotubes, Anodic oxidation, Protein adsorption, Protein conformation

#### ID: 20 - Nanobiotechnology: Biomaterials and Biosensors

#### **RNA Capture with High Magnetic Field Gradients**

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Magnetophoretic devices are utilized to control, manipulate, and capture bio-entities. In this work, the novel and innovative magnetophoretic-based method to fabricate a well-patterned patch [1] has been adapted for nucleic acid isolation. The developed patch is simple to use as a test kit for specialists and patients, easy to manufacture, quick to respond, and cost-effective. A magnetophoretic patch was synthesized by utilizing well-patterned Nd-Fe-B flakes embedded in two different polymer matrices: polydimethylsiloxane (PDMS) and epoxy. (Figure 1) Epoxy-based patch has better capturing performance than PDMS-based patch, which can be attributed to the former's larger magnetic field gradient of up to 6.7x104T/m.(1,2) According to RT-PCR experiments, the magnetic gradient patch effectively captures RNA under a variety of situations. The viral RNA sample got interacted with different types of magnetophoretic patches during this study. RT-PCR testing was performed on the interacting RNA samples. Positive control RFU peaks were compared to RFU peaks of magnetic field-manipulated RNA. When compared to the positive control sample, the RFU peak maximum values of interacted RNA were reduced by 40% and 75% for PDMS, and epoxy, respectively. (2) Ergo, the analyses and tests performed, confirmed that the magnetic patch is capable of capturing RNA. In the further steps of the research, the magnetic patches produced were combined with microfluidic polymer channels to study vascular network by mimicking. The magnetic capturing ability of the channel was tested with iron nanoparticle flow.

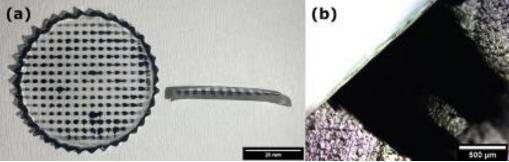


Figure 1. Magnetic Gradient Patch (left) and Cross-section image of the Magnetic Gradient Patch under the light microscope. (2)

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Keyword: RNA capture, magnetic gradient field, isolation, magnetophoresis, Nd-Fe-B

## ID: 34 - Nanobiotechnology: Biomaterials and Biosensors

## Electrospun Nanofibers containing carbohydrates for the application in environmental biotechnology: The removal of textile dyes

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The types of pollutants of today's water resources and the increase in the amount of these pollutants threaten the lives of living things more and more every day.

Current research shows that 1.3 billion people have limited access to safe and hygienic drinking water, and millions of people die each vear from unhygienic water-borne diseases (Sustainable Development Goals - UNDP). Recently, nanotechnology combined with nanomaterials has offered great potential to improve water treatment technologies. Electrospinning to produce nanofiber membranes has emerged as an efficient technology for producing durable and potential membranes for water treatment and advanced desalination (Ray et al., 2019). Membrane fibers, which act as semi-permeable barriers, allow only certain molecules to pass. Membrane structures formed from Nanofibers obtained by electrospinning are materials developed for the removal of pollutants from the environment.

Among the hydrophilic polysaccharide polymers, sodium alginate (SA) is considered as a possible dehydration membrane material due to its unique properties such as water solubility, good hydrophilicity, and favorable film-forming properties (Nigiz et al., 2012; Aminabhavi et al., 2002). On the other hand, Polycaprolactone (PCL) is a semi-crystalline polyester with outstanding properties such as biodegradability, wide compatibility with various types of polymers, and good mechanical properties (Hung et al., 2014).

PCL-SA Nanofibers were formed within the scope of this study by using the interoperable structure of polymers and the hydrophilic properties of SA. Using the hydrophilic properties of PCL-SA nanofiber and its suitability for enzyme immobilization, laccase (Lac) was conjugated to PCL-SA for usage of the removal of textile waste dves. The textile azo dyestuffs were treated with PCL-SA/Lac Nanofibers. Absorbance monitoring was performed at 580 nm before and after treatment of dye.

#### Acknowledgement:

Authors thank to The Scientific and Technological Research Council of Turkey (2210/D Master Project).

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Keyword: Water treatment, Nanofibers, nanobiotechnology, nanomaterial, nanotechnology

#### ID: 77 - Nanobiotechnology: Biomaterials and Biosensors

## **Applications of AFM in Bioscience and Biotechnology**

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Since its discovery in the late 1980s, the atomic force microscope (AFM) has revolutionized scientifically many fields, both in surface science and in biological physics. Although in the early years of its invention it was applied almost exclusively to characterize nonbiological material surfaces, it is now frequently used in the examination of biological samples. To better understand the behavior of complex biological systems, it is important to study biological samples in their physiological environments or natural conditions modifications and improvements in AFM in recent years have made it possible to conduct many studies under physiological conditions that are not possible with other methods. For example, high resolution observation of biological molecules has enabled studies such as specific molecule detection and localization, bonds at the single molecule level, detection of intramolecular and intermolecular interaction dynamics (Sevim et.al., 2017; Sevim et.al., 2016a; Sevim et.al., 2016b), and understanding of the mechanics of cells.

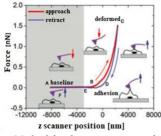


Figure 1: Force Spectroscopy Method for the investigation of mechanobiology of living cells

The observation of several dynamic biological processes such as antibody-antigen binding (Hu et.al., 2021), bending of DNA, infecting living cells by microorganisms, and the mechanobiology of cells has also inspired exploration of the potential of AFM (Viljoen et.al., 2021). There are also studies on mapping the properties of cells such as flexibility and stickiness. AFM-based mechanobiological measurements are now widely applied, especially for living normal and sick (eg cancerous) cells. We contributed to the literature with our studies on this subject. In one of our studies, we designed a modular AFM for biomolecular experiments. The AFM can be operated in different modes such as molecular pull or force clamp by operating the console with available actuators. Binding-dissolving experiments were performed on the biotin-streptavidin couple using piezoelectric and electromagnetic cantilever actuation. It has been determined that the most probable breaking force as a function of loading speed is obtained using both electromagnetic actuator and conventional piezo actuator (Sevim et al., 2016a). We also developed a new AFM technique with dual actuation properties that uses both piezo and magnetic bead activation for advanced single-molecule force spectroscopy experiments. This has led to a deeper understanding of biomolecular interactions (Sevim et al., 2016b). In another study, we demonstrated the nanomechanical mechanism of the interaction between heparin and fibroblast growth factor 2 (FGF-2), a paracrine growth factor, with a modular AFM design. Binding-dissolving events between FGF-2-heparin complexes have been found to be specific and short-lived. The binding between FGF-2 and heparin had strong shear bond properties, as indicated by the tensile force on the complex and the reduced lifetime. The non-binding forces between FGF-2 and heparin have been described in more detail with respect to (patho-)physiological conditions at different pH. An acidic pH environment (5.5) modulated FGF-2-heparin binding, as demonstrated by the enhanced tear forces required to release FGF-2 from the heparin-FGF-2 complex compared to physiological conditions. Thus, a mechanistic and hypothetical model of how molecular forces can affect FGF-2 release and storage during tissue remodeling and repair is provided (Sevim et al., 2017).

This study covers the fundamental principles of AFM and current developments in bioscience and biotechnology applications, including the fields of microbiology, cell biology and biomedical studies. We think that both our own study results on the subject and the information shared as a result of the literature review will be useful for researchers who are just starting to use AFM in the field of biotechnology.

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Keyword: atomic force spectroscopy, mechanobiology, single cell, force spectroscopy

#### ID: 83 - Nanobiotechnology: Biomaterials and Biosensors

## Development of Molecularly Imprinted Polymer-based FET Biosensor via Oxidative Chemical Vapor Deposition

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Biosensors have been attracting an increasing interest in various fields including medical diagnosis and health monitoring due to its rapid, selective and sensitive detection of target analyte in real-time. As biological receptors require special environmental conditions, they limit the durability and long-term storage of the biosensors. However, molecularly imprinted polymers (MIPs) are artificially synthesized to mimic the recognition of biological macromolecules at a significantly lower cost and no need for any special storage. Here, we reported the usability of the polypyrrole (PPy) MIP as a synthetic biorecognition element on a FET based biosensor to detect CA-125 ovarian cancer biomarker. We used oxidative chemical vapor deposition (oCVD) technique which allows the conformal and controlled thin film conductive polymers, to produce MIP onto a sacrificial layer. Synthesized MIP then integrated onto the interdigitated electrode arrays to make a conductive bridge between source and drain terminals for the development of the FET biosensing platform. The oCVD technique has a great potential to be used in the development of MIP-based biosensors for the detection of target proteins without wasting as in the traditional bulk polymerization method.

## Acknowledgments

This work was supported by the Scientific and Technological Research Council of Turkey (TUBITAK), Grant No: 119Z342.

Keyword: oxidative chemical vapor deposition, molecularly imprinted polymer, FET biosensor

## Electrospun Nanofiber Based Electrochemical Immunosensor for Serum Amyloid A Detection

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Modern biomedical researches require accurate, sensitive and rapid measurements to facilitate biomarker discovery diagnosis, disease monitoring, personalized medicine and new drug development. An important application includes measurement of protein levels in blood serum of biomarkers for disease diagnosis (Baumann et al., 2016).

Serum amyloid A is an acute phase protein which as an inflammation marker (Soler et al., 2012). Detection of serum amyloid A (SAA) can provide medical diagnostic and potential for developing point of care devices (Xia et al., 2015). In this study, electrochemical immunosensor was developed for detection of SAA. Screen-printed electrode (SPCE) was modified with polymer Nanofibers as a support platform for antibody immobilization. The nanofiber possess highly surface area and hydrophilic surfaces provide covalent conjugation of biomolecules (Thenmozhi et al., 2017). With these properties, it has become one of the popular materials in applications in the field of sensors (Gordegir et al., 2019). The polymer Nanofibers were characterized with Scanning Electron Microscopy (SEM), X-Ray photoelectron spectroscopy and Fourier-transform infrared spectroscopy (FTIR) and contact angle measurements. Electrochemical measurement was carried out by cyclic voltammetry (CV), differential pulse voltammetry (DPV) and impedance spectroscopy (EIS). The calibration plot was linear in the 0.1 to 10 ng/ mL of SAA concentration range, and the detection limit was determined as low as 0,061 ng/mL. In the presence of potential interferences, they did not affect the immunosensor response to SAA. In addition, the level of SAA was determined in artificial serum and saliva. Finally, it is a promising study to be able to analyze in the clinical field in the future.

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Keyword: nanobiotechnology, nanomaterial, nanotechnology, nanofiber, immunosensing of serum amyloid A

# Fabrication of Bilayer Small Diameter PCL-Heparin/TPU-Chitosan Vascular Graft (artificial blood vessel) via Electrospinning Method

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According to World Health Organization (WHO), over 17 million people died hence of cardiovascular diseases (CVD) in 2019 [1,2] One of the most common CVD is arteriosclerosis [1,2], defined as the narrowing of arteries by cholesterol plaques, and it causes congestion of arteries [3]. Therefore, many treatment methods are used in this scenario including cardiovascular grafting. The saphenous vein, taken from the patient itself or other donors, is commonly used as an implant vessel in advanced arteriosclerosis cases [3,4]. However, this necessitates a secondary operation. To overcome this, synthetic blood vessels (SBV) are developed for decades. This SBV might be both biodegradable and non-biodegradable. One of the problems encountered in biodegradable SBV is the loss of mechanical strength during endothelization (defined as the rate of forming endothelial cells by the implant degrading) [5]. In our study, we are focusing on this phenomenon. Our study brings a new perspective to SBV, including both biodegradable and non-biodegradable materials. The vessel consists of two layers having various amounts of PCL, Heparin, TPU, and Chitosan. Both layers are the same thickness, and the vessel's inner diameter is 4 mm. In the first layer, PCL is a matrix material due to its biodegradable properties, and Heparin is used to prevent the formation of thrombosis [5]. In the second layer, TPU is used as a matrix and Chitosan is used as an additive material. TPU is used as a matrix because of its flexibility and biocompatible properties, and Chitosan for its increased mechanical properties [5]. Besides, TPU is nonbiodegradable; hence, while all other materials are degrading within the body, the TPU skeleton will stay and provide extra support for the new vessel. To produce a vessel, the electrospun method is used. To characterize the properties of the SBV, SEM, FT-IR, XPS tensile test, and blood flow test methods are used.

## Acknowledgments

This study was supported by Ondokuz Mayıs University Project No. PYO.MUH.1908.22.007.

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Keyword: Nanofibers, artificial blood vessel, vascular graft, cardiovascular diseases, electrospinning

## SERS Mapping on Surface of Nanofibril and Lateral Flow Assay for Detection of Bacteria

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In this work, we provide a disposable, low-cost cellulose nanofibril substrate embedded with gold nanoparticles for use in surface-enhanced Raman scattering (SERS) mapping for the quick enumeration of Escherichia coli (E. coli). Cellulose Nano Fibril CNF and gold chloride solution were mixed in a water bath at 120 °C to create a disposable SERS substrate. Enrichment and SERS detection of E. coli were used to implement the obtained substrate. As a result, E. coli was employed to scavenge gold nanoparticles from a cellulose nanofibril substrate. Using orientated antibodies, the target bacteria, E. coli, were first isolated from the matrix. Next, 5,5-dithiobis-(2-nitrobenzoic acid) (DTNB)-coated Au nanorod particles were used as SERS mapping probes in a sandwich experiment. With SERS mapping, we were able to clearly display the DTNB distribution density, and the experiment took only one hour to complete. Within the concentration range of 15 cfu mL1 to 1.5 105 cfu mL1, a linear relationship was discovered between the SERS mapping signals and the E. coli concentrations. Using a SERS mapping assay, we were able to demonstrate that a concentration of 2 cfu mL1 was the lowest level at which detection was possible. *Micrococcus luteus* (M. luteus), *Bacillus subtilis* (*B. subtilis*), and *Enterobacter aerogenes* (*E. aerogenes*) were used to test the selectivity of the devised approach, however none of these bacteria showed a significant response.

The SERS mapping is effective for the identification of biological analytes. Fe<sub>3</sub>O<sub>4</sub>/Au-PEI nanoparticles were synthesized in aqueous solution and characterized. In order to be able to use the lateral flow immunoassay method and sandwich complex with higher performance in *E. coli* analysis, it is aimed to three steps; a) Firstly, Nanomagnetic extraction of the sample by using *E. coli* antibody modified magnetic nanoparticles, b) then Enzymatic cleavage of the connection of the magnetic particles with bacteria after extraction, c) finally SERS analyze in paper based lateral flow immunoassay strips. All of steps was optimized on lateral flow immunoassay such as casein amount.

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Keyword: SERS mapping, Lateral flow immunoassay, Nanoparticles, Bacteria

ID: 189 - Nanobiotechnology: Biomaterials and Biosensors

## RuO<sub>2</sub> Supercapacitor and PEDOT:PSS Pseudocapacitor Based Optoelectronic Neural Stimulation

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Applications of optoelectronic neural interfaces present alternatives for understanding neural circuits and treatments for neurodegenerative diseases such as Parkinson's disease, epilepsy, hearing loss, and sight loss. In such devices, light is converted to ionic currents at the interface to stimulate nerve cells to create action potentials. Using optoelectronic devices offers wireless stimulation, minimal invasiveness, and higher spatiotemporal resolution. Such devices consist of an electron transfer layer(ETL), photoactive layer, hole transport layer(HTL), back electrode, and interlayers for conversion of the light. Those layers are generally made of materials such as silicon, nanoparticles, semiconductor thin films, polymers, and organic dyes. Depending on the fabrication technique and materials used, thin-film device layers are mostly between 10-300 nm thickness.[1]

For optoelectronic interfaces, stimulation mechanism and generation of ionic currents are important for safe operation without tissue damage. Light-activated modulation needs to be controlled for irreversible faradaic reactions that can change the cellular environment. [1] To avoid such harm, operations using double-layer capacitance or reversible faradaic reactions carry critical importance. Pseudocapacitive materials[2] or supercapacitors[3] are lately reported as functioning for such purposes: reversible reduction-oxidation reactions at the interface with large capacitance, and high-level control of charge injection density.

In this work, we present a photovoltaic device fabricated onto glass-indium tin oxide(ITO) subtrates, with zinc oxide (ZnO)/ poly(3-hexylthiophene-2,5-diyl)(P3HT) photovoltaic heterostructure, PEDOT:PSS organic polymer pseudocapacitor as electrode-electrolyte interfacial layer and RuO<sub>2</sub> supercapacitor as back electrode. In order to achieve a stable interface between non-polar P3HT surface and hidrophyllic PEDOT:PSS, surfactant Triton X-100 is used with conductivity enhancer ethylene glycol(EG). With this modification, spin coating of thin PEDOT:PSS films of different thicknesses (30-300 nm) directly onto P3HT was possible. Photocurrent generated by the device is optimized with different PEDOT:PSS solution content and RuO<sub>2</sub> return electrode layer thickness (10-60nm). As result, ITO/ZnO/P3HT/PEDOT:PSS device with RuO<sub>2</sub> return electrode achieved increased capacitive photocurrent and charge injection than ITO/ZnO/P3HT control device. The biointerface showed improved performance and efficient neural stimulation, without causing any damage to the cell environment.

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Keyword: Neurostimulation, Bioelectronics, Photovoltaics, Supercapacitor, Pseudocapacitor

## SAW Based biosensor Determining Cell number in Cell Culture

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Cell culture analysis are essential studies in biomedical research such as stem-cell, cancer researches, tissue engineering and more(1). In these studies, one of the most fundamental processes is counting number of living cells(2). Conventional method used for cell culture analysis are done by counting cells under a microscope, but here, the result highly depends on the experience of analyst and requires more time(3). Furthermore, it is an endpoint assay which activity in cell culture cannot traced during all course of experiment in real-time. There are other approaches for quantification to meet the need in this field in last decades. These systems are based on the change in real-time electrical impedance(4), high-resolution image processing(2) or the SAW based approach(5-7). Surface Acoustic Wave (SAW) Based sensors are now widely used in many fields such as mechanics, chemical, electronics, biomedical.(8-9) Their sensing capabilities SAW devices are also used as actuators in biomedical area(10). In this study a surface acoustic waves (SAW) based biosensor is developed for Quantification of Cell number in the culture. Our work consists of the simulation and fabrication of a SAW based biosensor chip and also the experimental studies to demonstrate its efficiency. IDT Sensor chip is simulated using COMSOL Multiphysics software to optimize the design parameters. An SH-SAW device with 17 MHz center frequency was designed. Sensor structure consist of two IDT-electrodes placed oppositely on a piezoelectric plate (ST-Quartz wafer)(Figure-1). An IDT structure consists of two interlocking comb-shaped arrays of metallic electrodes. One of the IDT works as transmitter and the other is receiver. The transmitter is excited by using a HF-sine signal to create SH-Waves on the piezoelectric surface. Receiver IDT converts these acoustic waves into electrical signals back. The received signal carries the information to measure small load changes on the surface that is between the transmitter and receiver IDTs. A well placed between the sensor's input and output terminals(Figure 1). The cell culture containing the living cells and nutrient medium are put inside the well. The total volume inside the well is 50µl and 50000cells were placed inside to observe the operation. A control group cell cultivations are also placed with same ratio of fluid. We encounter evaporation during the experiment therefore the fluid containing nutrient added at intervals to avoid this problem. Cells harvested are incubated in incubator at 37°C for 4 hours and at two hours intervals development of S12 parameter and phase have been measured using network analyzer at 17.12 Mhz. We also used the sensor to count the cells in the well while the well has no cells. These results are presented in Figure-2, which shows phase measurements without a cell line inside the well (red,-.-) and phase measurements with cell culture (red,--). The blue side in the same figure shows the control group measurements (conventional method).

The results show that the sensor responds to the cell number inside the well, and the phase measurements agrees well with the cell numbers measured by using conventional method. The study demonstrates the capability of in situ cell number measurement using SH-SAW biosensor

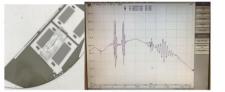
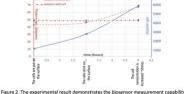


Figure 1. The fabricated biosensor (left), the transmission parameter (s12) of the sensor(right)



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Keyword: SAW. Biosensor. In situ cell counting

## A Dual-Action Ag Nanowire Filter Foil: Pathogen Isolation and SERS Substrate

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In recent years, surface enhanced raman spectroscopy (SERS) has demonstrated its potential as a powerful label-free approach for pathogen detection. To expand the applicability of this approach in fluid environments, suitable SERS active substrates are required as current approaches are not effective on large objects such as viruses, bacteria and unicellular parasites. The most challenging part of pathogen detection is the isolation and amplification step, which can take up to three days, which is too long for most clinical needs [1]. Here we propose a single solution with dual-action of "isolation" and "signal amplification" in pathogen detection. In this work, we demonstrate fabrication of a low-cost, label-free, flexible and free-standing silver nanowire (AgNW) filter foil SERS substrate as a candidate for ultrasensitive and specific detection of bacteria and viruses. Thus, the AgNW filter foils combine two functions in a single unit: (1) a porous 3D substrate can capture and isolate pathogens by performing an efficient mechanical filter due to ideal geometrical shapes of nanowires, (2) a high density of hot-spots provide enhanced Raman signals. The free-standing model eliminates the background signal that may be caused by the filter membrane. Additionally, the SERS activity can be highly enhanced by removing the capping agents of the AgNWs by applying chemical treatments, as the presence of surface termination agents such as polyvinylpirolidone (PVP) reduces plasmonic coupling between the AgNW junctions, resulting in weak localized surface plasmon resonance [2]. Since the uncapped AgNWs do not show themselves a Raman signature, the spectra would not need correction for the capping agent Raman spectra [3]. We will also present SERS results obtained with brilliant cresyl blue and crystal violet probe molecules and several pathogens. We kindly thank support of TÜBİTAK under grant nr 119N413.

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Keyword: Surface enhanced Raman scattering, silver, nanowire, filter, pathogen detection

## ZnO Thin-Films Grown by Atomic Layer Deposition as a Biosensor Platform for the Detection of Human Transferrin

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#### Introduction

Transferrin is an important transporter of iron ions synthesized in the liver. An increase in the amount of transferrin in the blood may be correlated with some diseases such as rheumatism, cirrhosis, leukemia, and tumor. On the other hand, acute hepatitis, anemia, and pregnancy are related to the increased levels of transferrin in the blood. Though transferrin in the blood can be detected via conventional techniques such as ELISA, these methods require expensive instruments and a laborious process [1]. Therefore, the development of fast, compact, practical, and sensitive devices to be used in point-of-care diagnostics has gained great importance. In this respect, biosensors can be a good candidate to be used in point-of-care diagnostics due to their ease of use, compact, and portable features.

One of the most important parts that determine the performance of a biosensor is the transducer element. Among various transducers, quartz crystal microbalance (QCM) is a mass-sensitive device that offers an affinity-based and label-free biosensor platform. In addition, it provides a selective and highly sensitive platform to antigen by binding the antibody (receptor) to the sensor surface. Consequently, QCM-based immunoassays gained great importance in the application of biosensors [1-2].

Another important parameter that affects the immunoassay performance is antibody immobilization and its stabilization [3]. The biocompatible nanomaterials showed promising results to develop new generation biosensors. Among various nanomaterials, ZnO nanostructures have attracted great interest in biosensing applications due to their low cost, biocompatibility, high isoelectric point, and relative chemical stability [4]. Atomic layer deposition (ALD) is a chemical vapor deposition (CVD) technique that offers uniform film growth with angstrom precision. Thus, ALD grown ZnO thin films can be used for biosensor applications [5].

In this study, ZnO thin film coated QCM biosensors were fabricated to detect transferrin molecules. ZnO thin films were grown on QCM oscillators by the ALD technique. Structural and morphological characterizations of ZnO thin films were performed by scanning electron microscopy (SEM), electron dispersive spectroscopy (EDS), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and Ultraviolet-visible spectroscopy (UV-Vis). The sensor surface was modified with the antibodies (specific MAM TRC2) of the transferrin to obtain selectivity against the target analyte. The fabricated sensors were tested against different concentrations of human transferrin (hTF).

#### Experimental

ZnO thin films were grown on Au-coated 5 MHz AT-cut QCM oscillators via an ALD system. Structural and morphological characterizations of the thin films were performed by XPS, AFM, and SEM. The surface of the ZnO/QCM sensor was functionalized with hTF-specific monoclonal antibody "MAM TRC2", which was obtained from TUBİTAK MAM Genetic Engineering and Biotechnology Institute, to make the sensors selective towards hTF. TRC2 immobilized ZnO/QCM sensors were tested against hTF.

#### **Results and Discussion**

ZnO thin films grown by the ALD method homogenously covered the entire substrate surface. According to the XPS results, it was observed that the surface defects increase significantly with the decrease of the film thickness. With the increase of the film thickness, the binding energy of the lattice oxide peak shifted to lower energies.

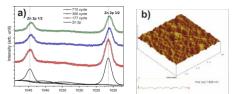


Figure 1:a) number of ALD cycle dependent Zn 2p spectra of ZnO thin films, and b) AFM image of a ZnO thin-film grown by ALD.

The antibody (TRC2) immobilizations on the ZnO surfaces were successfully performed. The fabricated sensor exhibited 91, 196, 303, and 375 Hz sensor responses (frequency shift) against 100 ng, 150 ng, 250 ng, and 500 ng hTF, respectively. According to the results, TRC2/ZnO biosensor platform gives consistent results in the range of 100-1000 ng hTF.

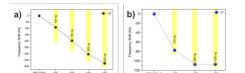


Figure 2: Frequency shifts of ZnO/QCM biosensor platforms against different concentrations of hTF.

#### Acknowledgements

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Keyword: Biosensor, Zinc Oxide, Atomic layer deposition, Human transferrin, Quartz cyrstal microbalance

## Biosensor Applications of Metal Nanoparticles and Their Interaction with Nucleic Acids

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Biosensors are analytical devices that convert a biological response into a measurable signal. In biosensors, there is a molecular recognition element called a bio-receptor for the sensing process and a physicochemical transducer that converts the biological or chemical signals into a physical signal. In electrochemical biosensors, the physicochemical transducer could be an electronic conductor, semiconductor or ionic conductive material [1, 2]. Electrochemical biosensors provide low cost analysis in a short time [3]. In order to achieve improved sensitivity and lower detection limits, nanomaterials are generally incorporated into electrochemical biosensors due to providing high surface to volume ratio, good electrical conductivity, stability, and chemical robustness. Nanomaterials allow the detection of nucleic acids, miRNAs, pathogens, cancer, and biomarkers at very low concentrations [3, 4]. In this talk, we will talk about the electrochemical results of the interaction between novel nickel-based metal nanoparticles and nucleic acids. In addition, we will discuss the advantages of metal nanoparticles incorporated with polymers to create molecularly imprinted polymer (MIP) structures with molecular recognition abilities. Moreover, different applications of metal nanoparticles within the biosensor systems will be emphasized.

In our experiments, metal nanoparticles characterization studies were performed, then electrochemical properties of these novel metal nanoparticles were obtained. The changes in the oxidation signals of metal nanoparticles and guanine bases of ssDNA and dsDNA were evaluated with using differential pulse voltammetry (DPV) and cyclic voltammetry (CV). We also examined the changes in charge-transfer resistance (R<sub>et</sub>) as a result of the interaction with the electrochemical impedance spectroscopy (EIS). We determined that the oxidation signals of the metal nanoparticles were significantly reduced as a result of interaction with DNA and RNA. We confirmed our DPV results with EIS. In particular, we observed that the interaction of the metal nanoparticle with ssDNA and dsDNA occurred at different rates. Therefore, we think that the metal nanoparticle could also be used as a hybridization indicator. We also found that the metal nanoparticle was electrically conductive and increased the surface area of the electrodes. In another application, we combined these metal nanoparticles for creating MIP to achieve sensitive detection of target analyte by mimicing recognition units of biological molecules.

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Keyword: electrochemical biosensors, metal nanoparticles, nanomaterials, DNA, RNA

## Nanomaterial Modified Electrochemical Sensor for Ultrasensitive Phenylalanine Detection in Human Blood

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Phenylketonuria (PKU) is a genetic disorder related to the metabolic malfunctioning of phenylalanine hydroxylase enzyme which breaks down phenylalanine amino acid. When phenylalanine builds up in the bodily fluids of the patients, such as blood and urine, it starts affecting the central nervous system by disturbing the myelinization process and thus causes mental retardation (1). Today, the most common methods, used for PKU diagnosis, are the Guthrie test, liquid chromatography, tandem mass spectroscopy, etc. which require well-developed infrastructure and expensive instruments (2). On the other hand, electrochemical detection methods show promise technology in clinical diagnosis with the advantages of accuracy, fast response and simple use. Electrodes, used in these methods, should provide high sensitivity and optimal analytical performance.

Here, we report the performance of different nanomaterial-modified electrodes and compare their response to the enzymatic oxidation reaction of phenylalanine and detection performances in a complex human blood matrix (3,4). Four of the compared six screen-printed electrodes (SPE) have carbon (DRP 110) and two have gold (DRP 220AT) working electrodes. Two of the carbon electrodes were used as received, modified with graphene with gold nanoparticles (C-GPH-GNP) and carbon nanotube with gold nanoparticles (C-CNT-GNP). Electrochemical reduction of graphene oxide (ERGO) was used to modify both carbon and gold bare electrodes, named C-ERGO and Au-ERGO respectively. The graphene oxide solution used in the ERGO reaction was prepared by mixing 700 µL of 2 mg/mL graphene oxide solution with 300 µL of 0.1 M, pH 6 phosphate buffer. 40 µL of the mixture was loaded onto the electrode and GO was reduced by applying 75 cycles at 100 mV/s between 0.1 and -1.5 V.

For the electrochemical detection of phenylalanine (Phe), blood samples received from laboratory volunteers were used by spiking Phe to 2, 4, 10 and 20 mg/dL. The blood sample was diluted 1:3 (blood:buffer) with glycine buffer to maintain 10.5 pH, the optimum working pH of the phenylalanine dehydrogenase enzyme. Samples were centrifuged at 5500 rpm for 3 minutes to remove red blood cells and obtain blood plasma. After 46  $\mu$ L of plasma was added to the electrode, amperometric measurement was initiated at potentials determined by cyclic voltammetry for each electrode. After the current stabilized, the reaction was started by adding 4  $\mu$ L of enzyme mixture to final concentrations of 1.6 U/mL PheDH and 2.5 mM NAD<sup>+</sup>. Current increases were analyzed by plotting against concentration.

The results are presented within the study in terms of limit of detection (LOD), limit of quantification (LOQ), sensitivity and repeatability. Among all electrodes ERGO gold electrode showed lowest LOD (0.0524 mg/dL), LOQ (0.1587) and highest sensitivity (0.3338  $\mu$ A/(mg/dL)) and it is reusable up to 3 times. On the other hand, the bare gold electrode showed 75% of its activity after 5 measurements. This study reveals that ERGO-modified gold electrode can pave the way for further diagnosis purposes with its ability to enhance electrocatalytic activity.

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Keyword: electrochemical analysis, enzymatic biosensors, phenylketonuria, carbon-based nanomaterial, gold nanoparticle

## Laser-Scribed Graphene Electrochemical Sensors for Health Applications

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Electrochemical sensing platforms including nanostructured materials have attracted increasing attention for diagnostic applications in recent decades. People in resource-limited places, particularly in low- and middle-income countries, continue to face problems finding high-quality medical treatment and technologies. The use of LSG sensors for diagnostic purposes has been gaining attention [1]. Point-of-care (PoC) diagnostic technologies are in high demand for early diagnosis due to their ability to analyze a biological event directly from a real sample by displaying the result without any further sample processing or expertise [2]. Compared to established methods for graphene synthesis, laser scribing provides many advantages, such as cost-effectiveness, fast electron mobility, mask-free production, green synthesis, good electrical conductivity, porosity, mechanical stability, and large surface area. The electrodeposition technique was chosen to enhance the electrocatalytic activity with high surface coverage, higher sensitivity, and ease of surface modification. We also focused on possible surface activation techniques on LSG electrodes to achieve an enhancement in surface area through electrochemical strategies [3]. LSG-AuNS electrodes are realized by electrodeposition of gold chloride (HAuCl4) solution, which gave~2-fold enhancement in sensitivity and electrocatalytic activity compared to bare LSG electrode. Moreover, we focus on surface functionalization methods for the development of self-diagnostic devices. LSG based electrochemical sensors have been applied to screening of acute myocardial infarction and human epidermal growth factor receptor 2 (Her-2) biomarker detection for breast cancer screening. As a readout system, we developed a portable potentiostat with smartphone application, called KAUSTat. Together with a customized smartphone app and Bluetooth connection, this point of care diagnostic platform has the potential to replace costly health care instrumentation with simple and practical miniaturized smart systems [4].

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Keyword: Biosensors, point-of-care diagnostics, Laser-scribed graphene, electrochemical sensors, affinity sensors

## 'All In One' SARS-CoV-2 Recognition Platforms: Laser Scribed Graphene Based Point of Care **Diagnostics**

Duygu Beduk<sup>\*</sup><sup>1</sup>, Duygu Harmanci<sup>1</sup>, Suna Timur<sup>1</sup>, Tutku Beduk<sup>2</sup>, José Ilton de Oliveira Filho<sup>3</sup>, Khaled Nabil Salama<sup>3</sup>, Figen Zihnioglu<sup>4</sup>, Candan Cicek<sup>5</sup>, Ruchan Sertoz<sup>5</sup>, Bilgin Arda<sup>6</sup>, Tuncay Goksel<sup>7</sup>, Kutsal Turhan<sup>8</sup>

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The worldwide pandemic caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) virus has revealed the urgent need for accurate, rapid, and affordable diagnostic tests for virus detection and monitoring. Although modern diagnostic techniques, such as real-time polymerase chain reaction (RT- PCR), can detect SARS-CoV-2 with high sensitivity, they require sample preparation, highly qualified personnel and long processing times.[1] Laser-scribed graphene (LSG)-based biosensing platforms have received great attention as miniaturized electrochemical systems with excellent potential as pointof-care (POC) diagnostic tools.[2] In the first section of our study, we described LSG-based electrochemical sensing combined with three-dimensional gold nanostructures for COVID-19 diagnosis. Following the required surface modifications, electrodes were modified with the SARS-CoV-2 spike protein antibody. Due to its simplicity of use, accessibility, and organized data administration, the system was also integrated into a portable POC detection device that was controlled by a customized smartphone application. With a detection limit of 2.9 ng/mL, the standard solution of S-protein was used to test the analytical capabilities of the electrochemical immunoassay. A clinical research investigation on 23 patient blood serum samples has showed highly compatible results of COVID-19 diagnosis with commercial RT-PCR, antibody blood testing, and enzymelinked immunosorbent assay (ELISA) IgG and IgA tests.[3] In the second part of the study, main focus was to provide high accuracy and be adaptable for the new variants of SARS-CoV-2. Laser-scribed graphene (LSG) sensors are coupled with gold nanoparticles (AuNPs) to create sensitive and accurate biosensing platforms for detection of SARS-CoV-2 variants. Angiotensin Converting Enzyme 2 (ACE2), an enzymatic receptor, is chosen to be the biorecognition unit due to its high binding affinity towards spike proteins as a key-lock model. The sensor was integrated to a handmade and portable potentistat device, wirelessly connected to a smartphone having a customized application for easy operation. LODs of 5.14 and 2.09 ng/mL was achieved for S1 and S2 protein in the linear range of 1.0-200 ng/mL, respectively. Nasopharyngeal swabs from 63 patients with alpha (B.1.17), beta (B.1.351), and delta (B.1.617.2) variations, patients without variants, and negative patients were used for a clinical research. With 99.37% accuracy rate, a machine learning model was created to quickly identify the SARS-CoV-2 variants.[4] By delivering accurate and rapid variant detection without the need for expertise or prior sample preparation, the PoC platform demonstrated its potential for real-time monitoring.

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Keyword: COVID-19, Laser-scribed graphene, SARS-CoV-2 Sensor, Machine learning, Point-of-care

ID: 257 - Nanobiotechnology: Biomaterials and Biosensors

## Development of Non-enzymatic Flexible Glucose Sensors Using Closed Bipolar Electrode Coupling

## Elif Muslu<sup>\*</sup>, Beyza Beşkardeş, Esin Eren, Aysegul Uygun Oksuz

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Recently, much scientific research focused on the study of development of non-enzymatic glucose sensors due to their facile of manufacturing, long operational life, or durability [1,2]. Graphene and its derivatives have gained a considerable significant material due to their advantageous properties including high surface area, easy functionalization, excellent electron transfer, and good biocompatibility. Designing of non-enzymatic glucose sensor using graphene and its derivatives could supply high reliability and durability during glucose sensing [3].

Herein, graphene oxide (GO) was prepared from pure graphite powder by using a modified Hummer's method. Scanning electron microscopy energy-dispersive X-ray (SEM-EDX), X-ray diffraction (XRD) analysis, Fourier-transform infrared spectroscopy (FTIR) were used for GO characterizetion. GO-based flexible thin film was produced using spin-coating technique. Bipolar electrodes (BPEs) were prepared using graphene oxide thin film, electrochromic gel electrolyte which was coupled electrochemical detection to optical sensing in two cells. The color change was monitored in the presence of different glucose concentrations.

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Keyword: non-enzymatic, glucose sensors, graphene oxide

## Construction of Boron-Silicon Networked Wool Keratin/Jellyfish Collagen Artificial Skin Grafts

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The process encountered in wound healing is overly complex and difficult. Skin infections, especially chronic wounds such as burns, diabetes ulcers, and skin injuries, are laborious and long-term treatment processes that require a high cost to health systems worldwide.[1][2] In this context, it is crucial to develop wound dressings that support tissue regeneration, accelerate the healing process, and provide optimal conditions around the wound.[3] Considering all this, working on developing innovative skin substitutes following the fields of regenerative medicine and skin tissue engineering has become an important topic for translational medicine. In addition to this, synthesis of organic-inorganic hybrid structures in tissue engineering has enormous potential for skin tissue defects.[4][5][6] In this study, innovative wound dressings were developed using keratin obtained from waste sheep wool and collagen isolated from jellyfish. Wool keratin and jellyfish collagen were networked with boron (B) and silica (Si) nanoparticles thanks to sol-gel reactions to obtain novel wound dressing substitutes. The obtained films were then analyzed by Fourier transform-infrared (FT-IR) spectroscopy, thermogravimetric analysis (TGA), X-Ray Diffraction (XRD), Raman spectroscopy, Brunauer-Emmet-Teller (BET) test. The tensile strength and suture retention test of the prepared wound dressing were investigated by a micromechanical test device. We conclude that prepared artificial skin grafts may have the potential to boost the wound healing process. We would like to acknowledge Canakkale Onsekiz Mart University Scientific Research Projects Coordination Unit for financial support (Project ID: FYL-2022-3983).

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Keyword: Boron, wool keratin, jellyfish collagen, silica nanoparticles, skin tissue engineering

## Natural Polymeric Bone Fillers from Keratin Paste and Silk Fibroin for Bone Tissue Engineering

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Bone tissue has the ability to regenerate without scarring, but its regenerative capacity is insufficient due to major defects, tissue loss, and aging. Currently, tissue engineering approaches are of great interest due to the limitations of autografting, which is the clinical gold standard in cases where bone tissue regeneration is inadequate. Keratin is one of the attracting attention polymers in regenerative medicine due to its superior properties such as excellent biocompatibility, mechanical strength, enzymatic stability, cell attachment, and providing a suitable microenvironment for cellular proliferation. On the other hand, Bombyx mori silk is a material that has been used as a suture material for centuries and is regarded for its strength and luster. Within this scope, we aimed at developing an innovative and environmentally friendly bone filling material using wool keratin and silk fibroin. Isolated proteins and keratin/silk fibroin filler construct were characterized in-depth via sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) analysis, Fourier transform-infrared (FT-IR) spectroscopy, thermogravimetric analysis (TGA), and Brunauer-Emmett-Teller (BET) methods. In addition, the keratin/silk fibroin filler was crosslinked with methanol to improve mechanical integrity. Overall, we believe that obtained construct has the potential to use as a filler in treating significant bone defects. The financial support of Canakkale Onsekiz Mart University Scientific Research Projects Coordination Unit is acknowledged (Project ID: FYL-2022-3981).

Keyword: Keratin paste, silk fibroin, bone filler, bone tissue engineering

## **Electrochemical Nanoaptasensor for Diagnostics and Monitoring of Multiple Sclerosis**

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Neurodegenerative diseases are associated with progressive and irreversible loss of neurons in specific areas of the central nervous system (CNS). Multiple sclerosis (MS) is a recurrent and progressive inflammatory, demyelinating disease of the CNS. Nowadays, the number of MS patients is increasing, but the diagnostic process is still quite difficult and costly and requires combination of various methods and analysis. Myelin is a structure made up of a few proteins located between two lipid layers tightly wrapping the axons of neuro cells, which is necessary for rapid providing of electrical signal between CNS and body. Myelin basic protein (MBP) makes up to 30% of myelin and it is known to be released into the cerebrospinal fluid (CSF) as a bioindicator of MS (1). In addition, in case of another demyelinating disease or trauma of CNS, MBP is present as a biomarker in human blood serum (2).

Within the scope of the present study, MBP specific aptamer earlier developed for possible therapeutic purposes (3) in mouse model was applied as a bioreceptor for human MBP recognition. A biosensor for MBP detection and monitoring was developed by using graphene oxide nanomaterial integrated onto the pencil graphite electrodes with aptamer immobilized to create a bioactive layer on the sensor surface for MBP binding. The measurements were carried out using electrochemical impedance spectrometry technique. Using carbon-based nanomaterial with large surface area aggregated with aptamer allowed us to achieve high specificity and affinity to the target molecule and enabled selective and sensitive MBP determination.

The biosensing system designed in this study can be implemented for development of prototype product for further clinical use in the MBP determination and monitoring in both CSF and blood serum.

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Keyword: Multiple Sclerosis, Graphene Oxide, Myelin Basic Protein, Aptasensor

## Development of Natural Bioactive Compound Containing Poly(ε-Caprolactone) Nanofibers as a Potential Scaffold for Skin Tissue Engineering

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Many synthetic and natural materials are used in tissue engineering applications. In recent years, the use of nanofibrous materials in biotechnological and medical applications has attracted a lot of attention. One of the reasons for preference; features such as very large surface area-to-volume ratio, flexibility in surface functionality, superior mechanical performance and small pore diameters between fibers can be listed (Li et al., 2002; Pham et al., 2006). Among the nanofiber production techniques, electrospinning is the most versatile and most preferred technique (Xue et al., 2019). Electrospun Nanofibers have been used successfully in various fields such as health, biotechnology, engineering, environment, sensor systems, defense and security (Barnes et al., 2007; Ding et al., 2005, 2004; Ramakrishna et al., 2006; Wu et al., 2015). In these areas, the production of filtration membranes, fiber-based sensors and tissue engineering scaffolds draw attention (Li et al., 2005; Pham et al., 2006; Yoo et al., 2009).

In this study, Nanofibers were prepared with poly(ε-caprolactone) (PCL), carbohydrate polymer (Car) and seed oil (SO) for the purpose of developing the skin tissue engineering matrices. Nanofibers were produced via electrospinning technique by using various PCL-Car/SO solution ratios. Cell proliferation experiments of PCL-Car/SO Nanofibers were performed on HaCaT (human immortalized skin keratinocyte cell line) cell lines. For the choosing of appropriate composition for PCL-Car/SO Nanofibers; cell imaging experiments were carried out by fluorescence microscopy after DAPI staining. The wound healing activity of PCL-Car/SO Nanofibers was investigated with culture inserts by taking pictures of the gap at different time points.

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Keyword: Nanobiotechnology, Nanotechnology, Nanomaterial, Nanofiber, Tissue Engineering

## Polymeric nanostructures for diagnosis applications of small molecules and viruses

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The development of diagnostic tools and biosensors has seen tremendous developments throughout the last decades especially with the introduction of portable and on-site formats that lessen the economical and human resources burden. The evolution of biosensor opened new paths of research regarding sensing materials, strategies, and device structures. Polymeric structures and composite materials can be sculpted into various nanostructures and networks such as nanovesicles and nanogels with high biocompatibility and tunability. They are a promising tool in current and future lab-on-chip devices due to their accessibility and ease to manufacturing. In addition, the application of portable biosensing devices is of great importance for large-scale screenings (i.e., pandemics like COVID-19) or road control (i.e., substance of abuse). These approaches were made more accessible using smartphone-assisted imaging allowing for the decentralization of diagnosis. In here, we share our latest findings in the development of polymeric-based materials and biosensors aimed for the detection of viruses (COVID-19) and small molecules of drug abuse (cocaine, methamphetamine, cannabinoids) through simples approaches like colorimetric paper-based assays and electrochemical sensors. The use of nano-scaled materials became an integrated component in sensing applications due to their various structural advantages in producing highly sensitive tools that rival bench-top instruments. The developments in material design open a new door for decentralized medicine and public protection that allows effective onsite and point-of-care diagnostics.

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Keyword: Diagnostics, Biosensors, COVID-19, Drugs of abuse, Nano-polymers, on-site testing

## **Development of 3D Printed Electrodes for Biosensing Applications**

## Pınar Kara\*, F. Selen Günden, Sezin Yüksel

3D printing provides a wide range of technology for electrochemical sensing, as it offers advantages such as different design possibilities, minimizing waste, rapid prototyping, and low cost (1-2). Although there are different 3D printing techniques, the most affordable 3D printing technique used in terms of dimensional accuracy, durability and production of more stable parts is the Fused Deposition Modeling (FDM) technique. It is more often preferred for electrochemical sensing. In the manufacturing process, 3D printing takes place by layering the polymeric material (filament) on a platform with a temperaturecontrolled head. The filaments used are different. The filaments frequently used in 3D printers are polylactic acid (PLA) and acrylonitrile-butadiene-styrene (ABS) and are often used in electrochemical devices (3-5). Polylactic acid (PLA); It belongs to a family of polyesters called "biodegradable plastics". The building blocks can be lactic acid or lactide monomers. They then polymerize in PLA. PLA's versatility is closely related to its biodegradability, which is one of its main advantages. It is widely used to fabricate materials using the FDM technique. PLA and ABS are the most commonly used raw materials for the construction of electrochemical cells and their composites, along with conductive materials for sensors. To improve the electrical properties of 3D printed devices conductive carbonaceous materials are used mostly nanomaterials such as carbon nanotubes, carbon black, and graphene. Their selection is due to their high surface area, good thermal and mechanical resistance, high chemical inertia and high electrical conductivity (3). Graphene/PLA and carbon black/PLA filaments are the most commonly used materials for electrode construction with the FDM technique. These materials have made possible the electrochemical detection of various species by developing 3D-printed electrochemical sensors (5).

In this study carbon black&PLA based filament is used for sensor surface production. Physical, chemical and electrochemical pretreatment methods are applied for optimum electrode performance. A fish sperm dsDNA and a ssDNA oligonucleotide representing E. Coli bacteria are biomodified onto cbPLAe's (carbon black&PLA electrodes for label free voltammetric detection. Diffreansial pulse voltammetry technique is used as label free bioelectronic detection of hybridization.

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Keyword: biosensor, electrochemistry, 3D printing

ID: 282 - Nanobiotechnology: Biomaterials and Biosensors

## Biofunctional Surface Based on Conductive Polymer-Clay Nanocomposite for Cell Adhesion

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Advances in nanotechnology and nanomaterials provide many innovations in fields such as biomedicine and tissue engineering. The unique properties of nanomaterials and nanocomposites are greatly utilized in systems developed for use in these areas. Cellular interactions with polymer-clay nanocomposites have been the subject of recent research focusing on their potential use in biomedical applications such as tissue engineering, gene therapy, food preservation, biosensing, bioimaging and drug delivery (Kerativitayanan et al., 2017). Clay minerals are layered minerals that are typically highly charged and characterized by large surface areas (Abduljauwad., 2019). Because of these properties, clay minerals can be considered as suitable candidates for cell adhesion.

In this study, a conductive polymer-clay nanocomposite was synthesized applied to monitor cell adhesion. The nanocomposite surface was modified with aptamer, which has a high affinity for the U87-MG cells. The created surfaces were characterized using SEM-EDS, XRD, ATR-FTIR, TEM techniques. Application of the bio-nanocomposite for U87-MG glioblastoma cell adhesion were carried out. Measurements to follow success of the study was made using electrochemical techniques.

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Keyword: Nanobiotechnology, Nanotechnology, Nanomaterials, Nanocomposites, Cell Adhesion

## ID: 285 - Nanobiotechnology: Biomaterials and Biosensors

## Effects of Controlled Surface Micro Modification on the Biocompatibility of Biomedical Alloys

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Effects of surface properties such as roughness and surface energy are critical for determining the biocompatibility of all types of biomaterials, as in the case of biomedical alloys. Recently, in addition to common surface topography related parameters, microstructure induced surface energy changes have also started attracting attention in surface property related biocompatibility analysis of metals [1-3].

The current study mainly aims to focus on the effects of surface micro modification on the biocompatibility of metallic biomaterials, in order to get an understanding of the underlying mechanisms that affect surface properties and biocompatibility. For this purpose, a thorough biocompatibility analysis was conducted on a conventional biomedical alloy; 316L stainless steel, whose surface was modified by forming micro-deformation areas of different patterns. The controlled micro-deformation areas of the different patterns, which consist of various indent depths and spacings, were formed via using a micro-hardness testing device

Following the characterization of the topographical features of the micro-deformed surfaces in terms of their surface roughness, wettability and their overall examination via SEM; their biocompatibility properties were tested at the *ex situ* and *in vitro* levels.

Initially with the *ex situ* experiments, interaction of the created surfaces with synthetic body fluid were analyzed. These tests were followed by *in vitro* experiments where osteosarcoma cells were seeded on the surfaces of the samples and the adhesion, proliferation and osteogenic differentiation behavior of these cells on the micro-deformed areas as well as non-processed surfaces were investigated.

The findings revealed that in addition to surface roughness, micro-deformation pattern characteristics such as the depth of and spacing between the indentations and the microstructural mechanisms triggered close to the surface by the formation of these structures are also very critical parameters in terms of determining the biocompatibility response of biomedical alloys. Moreover, apparent improvements were achieved in the biocompatibility response of the tested material as compared to the control sample with the application of the surface micro-deformation process.

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Keyword: biomedical alloys, surface micro-deformation, biocompatibility, 316L stainless steel

ID: 289 - Nanobiotechnology: Biomaterials and Biosensors

## Carbon Nanofiber and Conjugated Polymer Architecture for Futuristic Flexible Biosensor Applications

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A flexible carbon nanofiber (CNF) and a conjugated polymer including three moieties of benzotriazole, benzodithiophene, and benzenediamine (P-BDT-BTz:BDA) modified electrodes were designed and used for glucose analysis. First of all, the sensing platform was assembled with the combination of CNF on a defined area of a flexible polyethylene terephthalate (PET) substrate. Then, a random conjugated polymer; P-BDT-BTz:BDA was synthesized, characterized, and used for modifier of a CNF modified transducer surface. Finally, glucose oxidase was immobilized onto the modified surfaces for glucose detection. The chronoamperometric technique was used to monitor glucose at room temperature under mild stirring conditions by applying a -700 mV constant potential (vs. Ag/AgCl) in phosphate buffer (50 mM, pH 7.0). The effects of each parameter on biosensor response were evaluated. Under the optimized conditions, the newly designed biosensor offers a wide linear range, and a low detection limit with a high sensitivity. Moreover, it was observed that the designed biosensor has a good sensing ability for glucose in a beverage sample with a high specificity.

Keyword: Glucose detection, Carbon nanofiber, Conjugated random polymer, Enzyme immobilization, Glucose oxidase

ID: 296 - Nanobiotechnology: Biomaterials and Biosensors

## Combination of ECM Inspired Hydrogel and Swimming Incubation Platform for Improving Tissue Fidelity of 3D Cell Culture

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The development of 3D cell culture models mimicking native environment of tissue has been the focus of numerous studies seeking the closest approximation to real tissue. The cellular responses significantly differentiate under different physiological conditions and therefore chemical and physical features of the ECM must be considered carefully while designing a tissue-like cell culture model.

ECM is mainly composed of water, protein and polysaccharide and existence of each component is essential for providing proper conditions for cellular survival. Pectin is one of the most easily attainable biopolymers which is preferably used for cell culturing due to its similar properties to extracellular polysaccharides. In previous studies, pectin biopolymer was cross-linked with chemical agents or calcium mineral for the gel formation. Even these methods seem convenient, these techniques are not adequate to present extracellular matrix like microenvironment. Recently, self-assembling peptides emerged as promising, adoptable, and facile protein mimics. Besides their biological protein-like functions, peptide Nanofibers also can be employed for crosslinking of the other biopolymers for rich-content hydrogel formation. So far, pectin and peptides are cross-linked via covalent conjugation, non-covalent crosslinking via entanglement of peptide Nanofibers with pectin biopolymers is not yet considered for 3D cell culturing. Moreover, peptide sequences can be tailored with short signals to generate target tissue-like environment.

Besides the components of the matrix, for cell preservation also the incubation methods are also critical for determining cellular behavior. Static techniques usually suffer from multidimensional media penetration since one side of the gel is resided on the cell culture plate. Reactors enables closest tissue environment for 3D cell culturing whereas these techniques are elaborate and requires complex equipment. Herein, we designed a swimming module which enables interaction-penetration in all dimensions and non-static environment. ECM-like peptide pectin gels were in these modules which swims in cell culture media and the combination of a new gel formation with cell culturing technique will provide a new method to create closest tissue mimics to replace *in vivo* test models.

#### Acknowledgements

The authors gratefully acknowledge the TUBITAK Project (No: 121M973) for the financial support throughout the research.

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Keyword: 3D cell culture, pectin, peptide, hydrogel, ECM mimicking

ID: 308 - Nanobiotechnology: Biomaterials and Biosensors

## Nanobioconjugates for Diagnosis: Design and Applications in Point-of-Care Devices Based on Surface Modification

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Successful combination of nanomaterials with biorecognition molecules such as antibodies, aptamers, DNA and enzymes, provides excellent molecular recognition surface in well-oriented and nanoscale form. Nanomaterials with different sizes, surface functionalities, optical, electrical and mechanical properties, enable the development of different bioanalytical systems in desired surface decorations and intended use with various detection methodologies. Advances in nanotechnology and bioconjugation strategies have made significant contribution to the evolution of typical biosensor systems to Point-of-Care (POC) diagnostics tools. For instance, visible test signals could be obtained due to colorimetric properties of nanoparticles. On the other hand, color generation/change could be measured by smartphones or hand-held devices. Hence, the nanobioconjugation strategies are critical for the obtainment of detectable test signals as well as accuracy, sensitivity, and stability of a POC diagnostic system. Additionally, functional nanoparticles enable multiplexing capability, ease of use and cost-effectiveness [1,2]. The diversity of both nanomaterials and molecular recognition elements can adapted to surface modification of different test devices including lateral flow assays [3], micro-well assays [4], lab-in-a-tube based assays [5] and dot-blot assays [6] etc. We succeeded the fabrication of different biosensing tools including paper/tube-based tests via using nanobioconjugation-enabled specific surfaces. Within these studies, design strategies for the integration of nanostructured molecular architectures to *in vitro* diagnostics will be presented.

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Keyword: Nanobioconjugates, Biosensors, Lateral flow assays, Point-of-Care diagnostics

## Development of selective SPR sensor chip for the detection of aflatoxin M1 in milk

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Mycotoxins are secondary metabolites produced naturally by moulds, and which may contaminate food and feed. In the food chain, the original mycotoxin may be transformed in other toxic compounds, reaching the consumer. A good example is the occurrence of aflatoxin M1 (AFM1) in dairy products, which is due to the presence of aflatoxin B1 (AFB1) in the animal feed. Aflatoxins have carcinogenic, hepatotoxic, teratogenic, and mutagenic effects in humans and animals, even at very small concentrations, and exposure may occur through ingestion, inhalation or absorption through the skin. For this reason, the establishment of allowed maximum limits in dairy products and the development of methodologies for its detection and quantification are of extreme importance [1-3]. In recent years, sensors have emerged as a quick, low–cost, and reliable platform for the detection of aflatoxins. Molecularly imprinted polymers (MIPs) have been broadly applied in recent years as biomimetic receptors in the development of sensors. The molecularly imprinting technique involves a polymerization process of one or more functional monomer and crosslinking monomers in the presence of the template molecule, in a suitable solvent [4,5].

A sensitive molecularly imprinted polymer film-based plasmonic sensor was developed for the detection of AFM1 in milk sample. For this purpose, we designed gold–nanoparticle–(AuNP)–integrated polymer nanofilm on a SPR gold sensor chip. The MIP nanofilm was prepared using the light–initiated polymerization of N–methacryloyl–l–phenylalanine (MAPA) and ethylene glycol dimethacrylate in the presence of AFM1 as a template molecule. The removal of the template leads to the formation of cavities that are able to recognize and bind AFM1 with high affinity. The performance of the developed sensor for the detection of AFM1 was investigated by the change of resonance angle of the SPR sensor device adjusted with a mirror system using a pH 7.4 PBS containing 0.05% Tween-20 solution. The developed method enabled the detection of AFM1 with a detection limit of 0.4 pg/mL and demonstrated good linearity (0.0003 ng/mL–20.0 ng/mL). Compared to the non-imprinted sensor, the molecularly imprinted SPR sensor chip exhibits high affinity for the binding of AFM1. Moreover, selectivity studies, performed towards binding of the other mycotoxins such as aflatoxin B1, ochratoxin A, and citrinin with similar chemical structure, proved high sensor selectivity. Designed SPR sensor allows the estimation the real contamination level of spiked raw milk samples.

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Keyword: Aflatoxin M1, Mycotoxins, Sensors, Gold Nanoparticles, Surface Plasmon Resonance, Molecularly imprinted polymers

## Designing of Piezo-Composite Scaffolds Using Boron Nitride Based Nanomaterials for Bone Tissue Engineering

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Tissue engineering, a promising and an interdisciplinary field of regenerative medicine, aims to develop solutions by mimicking tissue/organ using natural, synthetic or semi-synthetic materials within the required functionality for the recovery/regeneration of lost or damaged tissue or organs. The currently used scaffolds in tissue engineering have inadequacies to be applicable due to need of more physical, chemical and biological enhancements to provide better cell adhesion, penetration, growth and regeneration. At this point nanotechnology idea comes into stage by using nanomaterials that have significant contributions to tissue engineering applications as reinforcement material so far. Nanomaterials can be preferred to manufacture high-performance biomaterials with tailored physical, chemical and biological features due to their superior mechanical, physical and chemical as well as greater biocompatibility properties [1, 2]. In this study, boron nitride based nanomaterials were used by embedding into poly(&-caprolactone) (PCL) polymer due to their high piezoelectric properties to introduce piezoelectric feature to the composite scaffolds. Electric-responsive Human Osteoblast cells (HOb) cells on scaffolds were stimulated by applying low-frequency ultrasound (US) stimulation during cell growth. Biocompatibility, cell adhesion, alkaline phosphatase activities and mineralization of HOb cells on piezo-composite scaffolds were investigated. Utilization of these piezo-composite scaffolds will be helpful for wireless tissue stimulation studies using piezoelectric phenomena in electrically sensitive cells or tissues to decrease the conventional invasiveness of in vivo electric stimulation.

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Keyword: Bone tissue, scaffold, piezoelectricity, nanomaterial

ID: 379 - Nanobiotechnology: Biomaterials and Biosensors

## Fabrication of Carbon Nanotubes-Gold Nanoparticles Based Screen-Printed Electrodes for Enzymatic Biosensor Platforms

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High electron transfer between enzyme and electrode surface without loosing any catalytic activity is crucial in the construction of enzymatic biosensors. Nanomaterials like carbon nanotubes, graphene, gold and iron nanoparticles shows great advantages for enzyme immobilization with their superior properties like high surface area ratio, electrocatalytic activity and biocompatibility [1,2]. Combining multi-walled carbon nanotubes (MWCNTs) and gold nanoparticles (AuNPs) with carbon screen-printed layers can further improve the electrochemical properties of these nanomaterials and thus the sensitivity of the biosensor. The aim of this work is to show how the combination of screen printing layers of carbon screen printing ink, MWCNTs and AuNPs could represent potential advances in the development of superior biosensor surfaces. In this context, MWCNTs-AuNPs based carbon screen-printed electrodes (MWCNTs-AuNPs-SPCE) were produced for biosensor platforms. Silver/silver chloride screen printing ink for reference electrode and carbon screen printing ink for counter electrode were used in the production of these electrodes. In the content of the working electrode, MWCNTs and AuNPs were added in carbon viscous screen printing ink and the preparation was performed as layers or mixtures. Screen printing inks were used by printing on polyvinyl chloride (PVC) substrate. The electrodes were produced on a semi-automatic screen printing machine, and then the modifications were completed on a manual screen printing table with constant pressure. Electrochemical characterizations of the produced electrodes were evaluated by cyclic voltammetry (CV), differential pulse voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) methods. Surface homogenization and topography were evaluated by scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDX). The produced electrodes were used for glucose biosensing.

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Keyword: Screen-printed electrode, carbon nanotubes, gold nanoparticles, enzyme electrode

# Graphene and Tungsten Disulfide Containing Polypyrrole Based Enzymatic Electrodes for Glucose and Urea Detection

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One of the important tasks in healthcare system is to design and develop diagnosis systems that can detect various problems or disorders accurately and sensitively. At this stage, (bio)sensor platforms have been attracted great attention. Diabetes is a serious health problem and sugar level should be kept in certain intervals. Therefore, development of sensing platforms to detect glucose which is the indicator of sugar level is crucial. Besides this, detection of urea which is a waste product of the body is prominent since it is related to kidney function and protein intake. Electrochemical methods have been widely used for the detection of glucose and urea since they offer high sensitivity, selectivity and good stability [1,2]. This work describes the preparation of polypyrrole-based enzymatic electrodes for glucose and urea detection. For glucose detection, graphene and tungsten disulfide (WS<sub>2</sub>) containing polypyrrole was prepared by cyclic voltammetry (CV). The prepared electrode was immobilized with glucose oxidase enzyme and used for amperometric glucose detection. For urea detection, polypyrrole-based electrode was immobilized with urease and used for amperometric urea detection. The electrodes were characterized by using electrochemical methods, scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS). Two-dimensional (2D) materials have brought new insights into sensor technology [3,4]. Thus, it can be concluded that 2D materials supported polymer electrodes showed enhanced electrochemical responses for the analytes used in this study.

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Keyword: Electrochemical sensor, Enzyme electrode, Glucose, Urea

#### ID: 394 - Nanobiotechnology: Biomaterials and Biosensors

#### A novel microfluidic electrochemical sensor using angiotensin-I converting enzyme and its application in highsensitive SARS-CoV-2 antigen sensing

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The COVID-19, coronavirus disease is an infectious disease caused by a novel virus called Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) [1,2]. This ongoing pandemic urgently requires an accurate testing device that can be used in the field in a fast manner [3,4]. Serological assays to detect antibodies have been proven to be a great complement to the standard method of reverse transcription-polymerase chain reaction (RT-PCR), particularly after the second week of infection [5]. Therefore, it is crucial to construct diagnostic features that can rapidly identify infected individuals to limit the spread of the virus and assign treatment choices. Herein, we constructed a novel and selective method using a microfluidic system and electrochemical method to rapidly detect spike protein Covid-19 through a label-free electrochemical immunoassay. The development of innovative approaches for direct viral detection employing simplified and ideally reagent-free assays is a pressing and difficult topic. The absence of speedy and effective ways to diagnose viral diseases, especially SARS-CoV-2 on demand has worsened the issue of combating the COVID-19 pandemic. The developed method illustrated a wide dynamic range of 100.0 fg mL<sup>-1</sup> to 10.0 ng mL<sup>-1</sup> with low limit detection. Therefore, the advanced strategy SARS-CoV-2 S-protein sensor suggests an appropriate perspective in the point-of-care system, within 5.0 min, in nasal samples with satisfactory recovery.

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Keyword: COVID-19, Microfluidic system, Label-free, Nasal sample

#### ID: 7 Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Characterization of Triple Medicaments Loaded Electrospun Polymeric Nanofibers as Endodontics Drug Delivery Systems

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The newest regenerative endodontics method applies either the triple antibiotic paste related to minocycline or the double antibiotic paste form. The best form has an antimicrobial effect, and due to the proven clinical efficacy related to antibiotic mixtures containing MINO (TAP), this study investigated the characterization of biodegradable polymer-based electrospun antibiotic-containing nano/microfibrous with triple-antibiotic-loaded systems. These systems can potentially be applied as drug delivery systems for root canal disinfection before the regeneration procedure of endodontics.

Besides cell-friendly and antimicrobial features, an ideal electrospun system to be translated into clinics for regenerative endodontics must show sufficient clinical handleability. Based on the results we achieved from SEM and EDX analyses, we selected 9 wt% DA-NFs as the main experimental groups and PVP-NFs as a control group for the rest studies. We worked on coating GP cons which are commonly used in dental clinics, with the produced electrospun mats. After that, we analyzed these coated GP cones' chemical and physical impacts on the dentine surface. FTIR and Nano-SEM tests confirmed no modification on the dentine surface, which suggests their ability to endure placement in clinical conditions.

The SEM micrographs showed triple antibiotic-containing Nanofibers (MET-CIP-MINO-PVP) as being generally smaller in fiber diameter than the antibiotic-free PVP control group. This holds a potential benefit because the smaller diameter creates more surface area and, theoretically more drug release over an extended period. The concentrations of the medicaments used in all experiment groups instigated no demineralization of radicular dentin which was calculated by the ratio phosphate/amide. ATR-FTIR presented the efficacy of intracanal medicaments on the root canal dentins, and the change they cause in the chemical structure of the dentine surface. There was no substantial difference in the ratio of phosphate/amide at 1 week and 4 weeks in samples treated with TA-NFs. Thus, this treatment group has no demineralization effect on the dental tissues with time. All specimens treated with medicaments displayed the existence of crusts/agglomerates partially covering the dentin surface. These agglomerates showed a slightly heterogeneous component. It can be shown that even low concentrated nanofibers' groups resulted in a slight creation of these crusts, denoting that the contact of the medicaments with the substrate, regardless of the concentration or vehicle used, is important to produce these mineralized agglomerates. Conversely, the specimens that did not receive medicament treatment exhibited neither tubule obliteration (control) nor only slight obliteration (scaffold).

My study further demonstrated the antibacterial efficacy of the antibiotics released from the fibrous mats against *E.coli*, *P. aeruginosa*, and *E. faecalis*. These bacteria were chosen as the test species due to endodontic bacterial infections. MIC values confirmed the incorporation and release of medicaments from the polymer fibers. Overall, all samples provided bacterial inhibition significantly greater than that of the control group, with varying degrees of success. Analysis of cell viability data groups (PVP-NFs as a negative control group) presented no significant decrease in cell viability in the first 24<sup>th</sup> hours (p> 0.05). 3T3 cell viability decreased significantly at the 72nd hour at 1.7 mg/mL the concentration of both TAP and TA-NFs groups compared to the control group (containing 0.1% DMSO) (\*\*\* p <0.001). Although the present study did not consider the kinetics of drug release, it demonstrated long-term antimicrobial activity and good cell viability over time.

In sum, this study showed that antimicrobial (MET-CIP-PVP) double antibiotic Nanofibers and (MET-CIP-MINO PVP) triple antibiotic Nanofibers could be successfully manufactured at much lower concentrations via electrospinning. The data gathered herein demonstrates the clinical protentional of these electrospun systems based on significant antimicrobial, low cytotoxicity, and handleability. Therefore, the clinical connection of these drug delivery systems should be further estimated by preclinical animal models of preapical disease that could supply the means to analyze their impact on humans.

Keyword: Regenerative Endodontic, Nanofibers, Drug Delivery Systems, Triple Medicaments

#### ID: 66 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## **Development of New generation Diamagnetic Microswimmers**

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Restrictions on medical treatment due to the impossibility of accessing some sensitive, delicate, and inaccessible parts of the body could be eliminated using micro-robots. There is a need for careful and complex design by considering materials. movement, and control so that micro-robots can perform their tasks accurately. By utilizing 3D printers and additive manufacturing technologies, micro-robotic swimmers could be developed and controlled by magnetic-, photo-, and acoustic actuation. Since magnetic actuation shows better performance to control mechanisms in biological systems to provide force or torque on magneto responding objects, it's preferred to the others. This method with an electromagnetic coil system can be used for different purposes such as cargo and drug delivery, sensing, and in-vivo studies [1]. Bismuth is one of the applicable diamagnetic materials in the therapeutic and diagnostic field. In the last decades, Bismuth was heavily used to treat gastrointestinal disease, hypertension, and syphilis but now researchers are interested to use Bismuth for hard-to-treat diseases such as heart disease and cancer [2]. Bismuth is one of the choices of scientists because of its significant properties which include low toxicity, biodegradability, cost-effectiveness, and high stability. In this work, Bismuth diamagnetic microswimmers were successfully synthesized by utilizing a 3D printer. This research will investigate the movement kinetics and speeds of microswimmers in a magnetic field gradient system depending on their shapes and sizes. Figure 1 shows the XRD, SEM, and particle size distribution histogram of the mortared and pulverized sample that was separated with a sieve shaker to the size of 300µm. XRD peaks were indexed to Hermann Mauguin R3m [166] phase [3] (figure 1a). The SEM image shows the irregular morphology of the particles. (figure 1 b), The standard deviation of the powder from the histogram plot is 45.77 nm (figure 1 c).

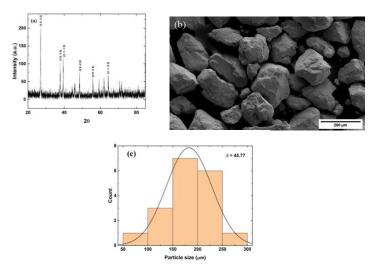


Figure (1). (a) XRD, (b) SEM, and (c) Histogram results from 300 µ Bismuth powders.

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Keyword: Microswimmers, Diamagnetic Materials, Bismuth, Drug Delivery, 3D printer, gradient system

ID: 87 Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Cytotoxic Effect of Palbociclib Conjugated Pamam Dendrimer Coated Magnetic Nanoparticles on Different Types of Breast Cancer Cell Lines

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Drug targeting and controlled drug release systems in cancer treatment have many advantages over conventional chemotherapy in terms of limiting the systemic toxicity and side effects and also overcoming drug resistance. PAMAM dendrimer coated magnetic nanoparticles (DcMNPs) maintain suitable drug delivery system due to their surface functional groups, internal cavities and targeting ability under magnetic field. Palbociclib is a chemotherapeutic agent which is used to treat ER-positive and HER-negative metastatic breast cancer. The aim of this study was to show the anti cancer activity of Palbociclib conjugated DcMNPs on different types of breast cancer cells. Palbociclib was conjugated to G5.5 PAMAM dendrimers which were characterized previously by our group. In this study, the cytotoxicity of free Palbociclib and PalDcMNPs on MCF7, MDAMB231 and SKBR3 cells were tested by LDH and cell viability assays. Quantification of expression levels of Bax, Bcl2, CDH1, MDR1 and mTOR genes due to the treatment of free Palbociclib and PalDcMNP were performed by qRTPCR analysis. The results show that cytotoxicity of Palbociclib and PalDcMNPs were dose dependent. At the higher concentrations (50µM), free Palbociclib have more cytotoxic effect on breast cancer cell lines. However, with PalDcMNP treatment, it has been observed that drug doses that inhibit 50% of the cell viability can be achieved with even lower drug concentrations (15µM) with respect to free Palbociclib for all of the breast cancer cell lines. The observed effects were more evident for MCF7 cells than for MDAMB231 and SKBR3 cells. In addition, the association between cell viability data and LDH release was also observed at a lower dosage (2.5 and 5 µM) of PalDcMNPs. The values of LDH are relatively high, considering that viability decreased to 30% at 2.5µM treatment of PalDcMNPs at MCF7 cells. According to qRTPCR results, Bax/Bcl2 ratio and CDH1 gene expression increased followed by PalDcMNP in all three cell lines. MDR1 and mTOR gene expression levels significantly downregulated only in SKBR3 and MDAMB231 cell lines, respectively after treatment with PalDcMNP. The results of this study show that PalDcMNPs have more cytotoxic effect on different types of breast cancer cells at lower doses comparing to free drug and can be further investigated as a potential Palbociclib delivery system in the in vivo studies.

#### Acknowledgments:

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Keyword: Palbocicilib, Magnetic nanoparticles, PAMAM dendrimer, Breast cancer

ID: 105 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Graphene Oxide-Silica Composite Aerogels as Pharmaceutical Nanocarriers

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After the isolation of graphene at the beginning of the 21st century, studies on the production of different materials gained momentum and the synthesis of new generation materials including graphene-based structure became possible. In addition to having unique physicochemical properties, graphene can be produced and modified in a wide variety of ways according to the requirements of different applications. Graphene has great potential to be used in drug delivery systems due to its large surface area and high biocompatibility [1]. Aerogels, on the other hand, are the most porous materials known, and they stand out with their much larger surface areas compared to other nanomaterials. Large surface areas and ultra-porous structures of aerogels are great advantages for drug carrying capacity, so aerogels constitute an important potential for targeted drug delivery applications [2]. Within the scope of this work, graphene oxide-silica composite aerogel nanostructures were produced based on the incorporation of the unique properties of graphene into the ultra-porous structure of aerogels using Sol-gel and ambient pressure drying method, which is advantageous in terms of time and cost. An important step in material production is the physicochemical characterization of these materials. Common and advanced techniques such as electron microscopy and X-Ray diffraction analysis were used for the characterization of materials. Biocompatibility and drug loading performance of the clear and in-situ functionalized aerogels were revealed. The biocompatibility of the nanocarriers were tested using cell viability assay and drug loading tests were done by using curcumin. Functionalization done with sodium dodecyl sulphate, polyvinylpyrrolidone and ethylenediaminetetraacetic acid affected the cytotoxicity and entrapment efficiency of the composite aerogels significantly. Sodium dodecyl sulfate functionalized aerogel showed the highest rate of cellular proliferation while all the samples presented high cellular proliferation rates in a dose dependent manner. Entrapment efficiency of ethylenediaminetetraacetic acid functionalized aerogel (59%) was higher than the other three samples (between 20%-50%) which is a crucial parameter to evaluate the nanocarriers. According to these promising results, we consider this study as the first step in the development of targeted new aerogel based carrier platforms for cancer therapy.

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Keyword: graphene, aerogel, nanocarrier, curcumin, cancer therapy

#### ID: 136 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Implantable Nanofiber Patch for Long-Term Treatment of Breast Cancer

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While breast cancer can be effectively treated in early stages thanks to the drugs developed, the treatment is more difficult in late stages due to rapid metastasis, and also it has a high risk of recurrence after the treatment. The lack of effective drug delivery systems for the chemotherapies used in the clinical practices today results in reduced success rate of the treatment on the tumor. Nowadays, in the vast majority of breast cancer treatment, radiotherapy and systemic chemotherapy are applied to prevent cancer recurrence and metastasis after the tumor is removed by surgical operation. However, in women diagnosed with breast cancer, recurrence of the disease has been observed within 5-20 years following the treatment [1, 2]. Therefore, there is a need for reliable long term preventive methods against the high probability of recurrence of the cancer. In this study, implantable nanofiber patches will be developed to prevent recurrence and metastasis risk of breast cancer. The patches will be applied to the patients just after the tumor removal surgery and will provide effective long term treatment. The nanofiber patches will be produced by solution blow spinning (SBS) method using a biocompatible and biodegradable polymer and will contain antigen epitopes that will trigger the immune system and generate long-term immunity against breast cancer. The surface of the patches will be coated with pH sensitive polymer thin films using the initiated chemical vapor deposition (iCVD) technique to control the release of antigen epitopes from the patches. The degradation rate of the patches will be calculated after various incubation times in phosphate buffered saline (PBS) solution and lysosome-mimicking solution (LMS). The changes in the fiber structure of the patches due to their degradation will be investigated by scanning electron microscopy (SEM), and the change in their chemical composition will be examined by Fourier-transform infrared spectroscopy (FTIR). Release of the antigen epitopes will be controlled by compositional changes of the patches and will also be quantitatively determined by enzyme-linked immunosorbent assay (ELISA). The success of the patches in the stimulation of the immune system will be investigated in vitro on T helper cells and B cells with dendritic cell morphology (BDCM). This therapy will be a promising candidate for long-term treatment of breast cancer.

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Keyword: Cancer, Controlled release, Immune response, Blow spinning

## ID: 149 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Ultra-Small Lipid Nanoparticles for Controlled Release of Coenzyme Q10: Hemocompatibility, Antioxidant Activity and Stability

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Oxidative stress is a measure of the mismatch between the ability of cells to defend themselves against free radicals and the amount of free radicals present in the environment. It is one of the major problems in different pathophysiological conditions and is characterized by elevated level of various free radicals. Coenzyme Q10 (CoQ10) is a potent antioxidant, anticancer and anti-inflammatory agent [1]. However therapeutic applications of CoQ10 are greatly limited by its lack of solubility in aqueous media. In this study, CoQ10-loaded ultra-small lipid nanoparticles (LPs) were prepared by melt-emulsification method. In order to examine the effect of the usage of liquid lipid in the LPs, besides solid lipid nanoparticles (SLNs), nanostructured lipid carriers (NLCs) were also prepared by the use of olive oil in 2 of 5 LPs. The effects of different formulations on the physicochemical properties of the carriers including size, zeta-potential, crystallinity, thermal-stability and storage-stability. These LPs were subjected to in vitro release studies, antioxidant activity analysis and hemocompatibility tests. The kinetic model of the release rate as well as the release profile of CoQ10 showed that the release profile can be controlled with the composition of the LPs in terms of lipid and emulsifier type. Antioxidant activity results showed that, nanoencapsulation of CoQ10 improved the hydroxyl scavenging activity of CoQ10 and decreases its EC50 value, and the best one was NLC2 with 30% olive oil content respect to total lipid. In addition, it is found that CoQ10-LPs can protect the human erythrocytes from free radical attack by HOCl, more than free CoQ10. Furthermore, compared to CoQ10 solution, SLN1 and SLN3 exhibited excellent sustained release profiles. In conclusion, it's proved that the ultra-small LPs can improve the stability, bioavailability and antioxidant ability of CoQ10 whereas offered personalized and customizable biocompatible drug delivery systems with adjustable release kinetics.

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Keyword: Coenzyme Q10, solid lipid nanoparticles, nanostructured lipid carriers, antioxidant, hemocompatibility

#### ID: 155 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## A Novel Nanoparticle Design for Combined Photothermal and Photodynamic Therapy

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Phototherapy has gained attention as it provides many advantages over the conventional treatment methods, such as increased efficacy and minimally invasive tumor treatment [1]. Photodynamic and photothermal therapies are two kinds of phototherapy that provide treatment by the use of photosensitizer and photothermal agents to induce cell destruction via Reactive Oxygen Species (ROS) production and hyperthermia, respectively [2]. Herein, a novel nanoparticle design to be used in the combined photodynamic and photothermal therapy is introduced. The nanoparticle system is comprised of three functional subunits one of which enables site-specific delivery as it includes specific protein, and the others provide treatment by photothermal and photodynamic therapies. These functional nanoparticles will be excited by two different Near Infrared (NIR) lasers which are of 808 nm and 1060 nm to trigger the treatment at the intended site. While the success of the NIR radiation in the generation of ROS will be analyzed by chemical indicator, the success in cell targeting will be investigated by the visualization of cellular uptake with microscopic technique. Fourier transform infrared spectroscopy (FTIR) will be used to investigate the chemical composition of the nanoparticles. The morphologies and the zeta potentials of the fabricated nanoparticles will be characterized by Scanning Electron Microscopy (SEM) and Dynamic Light Scattering (DLS), respectively. This novel nanoparticle design will offer a promising site-specific treatment through combined photothermal and photodynamic therapy.

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Keyword: Photodynamic therapy, Photothermal therapy, Targeted delivery, Nanoparticles

#### ID: 162 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Magnetic Nanoparticles as Smart Carriers for Cancer Immunotherapy

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Magnetic nanoparticles (MNPs), which can be collected with a magnet, provide rapid delivery of biomolecules to the target (Mitchell et al. 2021). MNPs have different magnetic properties according to their content. In this study, zinc doped iron oxide MNPs were produced and coated with silica shells (MSNP) to ensure their biocompatibility and stability. The NPs were characterized by TEM, XRD, and XPS. TEM images indicated a typical morphology of the core/ shell MSNPs. As a result of the Wide-scan spectrum of XPS, it was determined that Zn was in the 2+ oxidation state and Fe was in the 3+ state in the MNPs. Interferon-stimulating DNA (ISD) was transferred to cancer cells by using the obtained MSNP. The targeting of the DNA in cancer cells was achieved with folic acid. A cationic polymer of polyethyleneimine was used to link folic acid, ISD, and MSNPs. Folic acid was covalently bound to the polyethyleneimine which was confirmed by FTIR. The stability of the DNA-loaded nanoparticle system was tested by DLS measurement, and it was demonstrated by ELISA test that it increased the amount of interferon in cancer cells. As a result, when the ISD is wrapped with folic acid-modified polyethylene imine and attached to the magnetic platform, it is rapidly taken into the cell by helping a magnet. When ISD is released in the cell, it induces interferon-beta production by activating its target pathway (Barber et al., 2015) in cancer cells.

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Keyword: cancer, interferon, immunotherapy, Magnetic nanoparticles

#### ID: 165 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Magnetic Hyperthermia and Gene Therapy for Breast Cancer Treatment

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Dual therapies are suggested as a more effective strategy for cancer which is an important health problem in the world. In this study, two different anti-cancer strategies were proposed for breast cancer treatment by combining magnetic hyperthermia and gene therapy. In magnetic hyperthermia, it is aimed to kill cancer cells based on thermal energy by relaxation of MNPs under AC magnetic field (Liu et al., 2013). The azurin protein was preferred for gene therapy to induce apoptosis and inhibit growth in human cancer cells (Huang et al., 2020).

Firstly, amine modified magnetic silica nanoparticles (MSNP-NH<sub>2</sub>) were synthesized. It was determined that the sizes of MSNP-NH<sub>2</sub> were smaller than 50 nm based on TEM images. It was observed that MSNP-NH<sub>2</sub> increased the temperatures under AC magnetic field and their magnetic saturation was 30 emu/g. On the other hand, green fluorescent protein (GFP) expression under the control of heat shock promoter (HSP) which will be used for dual therapy was investigated in MCF-7 cells before dual therapy. Cells were incubated for 90 minutes in an incubator set at 38 °C or in a magnetic hyperthermia device. GFP expression was observed in cells in flow cytometry analysis. Therapeutic DNA (pHSP-Azu) was obtained to be used for dual therapy after promoter control. pHSP-Azu was transferred to MCF-7 and MCF-10A cells and exposed to magnetic field in magnetic hyperthermia device for 90 minutes. Apoptosis tests were performed after treatments in MCF-7 and MCF-10A cells and it was revealed that the recommended treatment led the cells to the non-apoptosis path. As a result, it was observed that the proposed dual therapy affected MCF-7 cells more than MCF-10A cells.

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Keyword: magnetic hyperthermia, gene therapy, dual therapy, magnetic nanoparticle, azurin

ID: 277 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Polyplexed Nanovesicles for in Vitro Intelligent Stimuli-oriented Drug Delivery Systems Against Breast Cancer: Case of Cell Penetrating Peptides

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Chemotherapy has seen great progress in the development of multifunctional tools for theranostic applications. The cancer environment has many complicated mechanisms induced at the tumor level following contact with therapeutic agents which results in tolerance and drug resistance in some patients [1-4]. Therefore, developing novel approaches for treatment remains an important subject of research. The use of polymeric structures coupled with intelligent targeting properties is an important part of the current employed strategies. These approaches can enhance tumor targeting and lower the disadvantages seen with classical chemotherapy such as toxicities and treatment load on patients [2-4]. Drug delivery systems provides many therapeutic advantages, such as the ability to encapsulate multiple molecules including hydrophobic ones. Additionally, they can be readily modified on their surface for specific targeting using various molecules such as antibodies, receptors, proteins, and peptides [2]. From the many drug delivery systems available, nanovesicles (such as niosomes, polymersomes, etc.) are of great interest as they are structures inspired from cellular membranes and made from biocompatible materials [2]. In addition to their advantages mentioned earlier, they can also be made to respond to specific stimuli which enhances the drug delivery process during therapy [2-4]. The term of polyplex nano-delivery system is gaining more attraction as the structures are given multiple functions that can target, treat, and monitor the disease at the same time. In here, we share some of our progress in the development of polyplexed nanocarriers made from polymersomes and niosomes with pH-responsive features and the use of cell-penetrating peptides (CPP) to facilitate penetration and drug delivery [5]. We used doxorubicin (DOX) as a therapeutic molecule which possess fluorescent features allowing for real-time tracking of the treatment progress. The advantage of this combination is further appreciated at high DOX concentrations where the proposed formulation can overcome therapy tolerance in MCF-7 cell lines. The combination of natural peptides that possess special functions such as pH-responsiveness and cell penetration with novel polymeric-based nanocarriers offers an important tool for chemotherapy and biomedicine applications

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Keyword: Theranostics, Drug delivery systems, Bioconjugation, Stimuli-responsive systems, Cell-penetrating peptides

#### ID: 195 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## **Development and Evaluation of Risperidone Loaded Orally Dissolving Films**

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Orally dissolving films (ODFs) are drug delivery systems that allow rapid disintegration when applied on the tongue or release the active ingredient it contains and provides its swallowing with saliva after disintegration (1). Risperidone is a second-generation antipsychotic drug used in the treatment of schizophrenia. In patients with schizophrenia, there is a resistance to taking drugs (2,3). Thus, Risperidone loaded ODFs have a good potential for use in the treatment of schizophrenia. The aims of the present study were to manufacture risperidone ODFs and to characterize the prepared ODFs.

ODF formulations containing hydroxypropyl cellulose (Brand name: Klucel) and polyvinylpyrrolidone (Brand name: Kollidon 90F) were prepared by the solution/solvent casting method. The formulations containing Klucel and Kollidon 90F were prepared using distilled water and methanol as the film forming solvents, respectively. The polymer solutions were mixed under continuous stirring, cast onto petri dish and kept at room temperature for 48 h until drying. Then the films were cut into 15 x 20 mm pieces. The prepared formulations were coded from F1 to F5. F1 and F2 were prepared using 100 mg and 200 mg of Kollidon 90F, respectively. F3, F4, and F5 were prepared with 100, 200, and 300 mg Klucel, respectively. 30 mg of mannitol was also added as a sweetener to formulations. The formulations F2 and F5 were found to be suitable for the preparation of risperidone loaded films. Other film formulations could not be removed from the Petri dishes. The drug loaded formulations of F2 and F5 were manufactured by adding 100 mg risperidone into the polymer solutions. The morphological properties of the films were evaluated using an optical microscope. The thickness of the films were measured via a digital micrometer. The disintegration time of the films were measured in pH 6.8 buffer solution. In vitro drug release studies of the film formulations were performed by using USP type II dissolution apparatus at 37± 0.5°C and rotating speed of 50 rpm in 500 mL pH 6.8 buffer. In order to investigate the solid-state properties of the ODFs, an XRD analysis was also performed. Optical microscope images of the films showed that the formulation F2 was more homogenous than F5. This is because risperidone dissolved in formulation F2 and dispersed in formulation F5. The thickness of the obtained film formulations was found to be 57.5±1.9 µm and 69.3±3.4 um for the formulations F2 and F5, respectively. Formulation F2 disintegrated in 30 s and F5 disintegrated in 48 s. Both formulations were in accordance with the European Pharmacopoeia, where the dosage forms are defined as 'orodispersible' if disintegration time is less than 3 min. Comparative in vitro drug release profiles of the formulations F2 and F5 showed that the drug release was completed within 30 min for both of them. The immediate drug release of 70% in the first 10 minutes of both formulations showed that the films were completely wetted and disintegrated during this period. XRD analysis results showed that risperidone was in crystal form in F5 and amorphous form in F2.

Consequently, risperidone loaded ODFs were manufactured and characterized successfully. The results obtained from the characterization of the film formulations prepared in the study also showed their suitability for the intended use to increase patient compliance.

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Keyword: orally dissolving film, risperidone, hydroxypropyl cellulose, polyvinylpyrrolidone

ID: 209 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Preparation of Chitosan-based Biocomposite Hydrogel Sponges for Wound Dressing Application

Not presented.

#### ID: 212 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Stimuli-Responsive Nanogels: Small Agents with Big Goals

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Stimuli-responsive nanogels have emerged as a promising platform for targeted drug delivery. These nanoparticles can be loaded with therapeutic agents either physically or through chemical linkages, as well as they can be functionalized with different targeting groups and imaging agents.[1,2] Due to their swollen and soft nature, nanogels can easily adapt to their environment by changing their physical or chemical structures, thus making them attractive candidates. Interest in the design of delivery agents that are responsive to changes in endogenous stimuli such as changes in pH and redox environment is on the rise due to their promising attributes.[3] The presentation will outline the fabrication of a nanogel system driven by thermally promoted self-assembly of a thermoresponsive polymer. After the formation of the transient nanosized aggregate, crosslinking is induced through chemical transformations to yield stable nanogels. The polymeric building blocks are designed to impart these nanogels with redox-responsiveness. Thus fabricated stimuli-responsive nanogels can be loaded with chemotherapeutic agents, and their surfaces are equipped with a targeting group that promotes internalization into cancer cells. Apart from their enhanced internalization into breast cancer cells, these nanogels release their cargo efficiently under the reducing environment encountered inside the cells. One can envision that the modular nanosized drug delivery system developed here can be tailored to carry a variety of therapeutically active agents in a targeted fashion to combat a complex disease such as cancer where systemic toxicity of chemotherapy continues to pose a major hurdle.

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Keyword: Nanogel, Nanoparticle, Drug Delivery, Stimuli-Responsive

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## Phenylboronic Acid-Based Catalytic Motors for Drug Delivery

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In recent years, laboratory-made motors have captured significant attention with their excellent properties including sensing, cell isolation, cargo transport and drug delivery abilities. They have achieved important tasks with their adjustable surface functions and distinctive motion mechanisms [1,2]. Drug delivery and controlled release are important topics of scientific investigations in the field of nanobiotechnology. It is known that the conventional drug delivery systems have been inadequate to reduce systemic cytotoxic effects on healthy tissues. However, active drug delivery systems can maintain side effect reduction of the drugs and better therapeutic efficacy. Studies point out the facile use of nano/micromotor systems as drug carriers to inaccessible areas with adequate delivery time and increasing penetration depth rate [3]. Polymeric motors have had efficient performance for drug loading and delivery [4]. In this study, paclitaxel loaded nanomotors were prepared and used for targeted drug delivery. The tubular catalytic nanomotors were synthesized electrochemically and the segments were composed of poly(3-aminophenylboronic acid) (PAPBA) outer layer, platinum (Pt)-nickel (Ni) segment and Pt catalytic inner layer. The propulsion of the motors was achieved under hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) and Triton-X 100 with a velocity of 127  $\pm$  6 mm/s. Drug delivery function was designed to release paclitaxel via external stimulations such as Near-Infrared irradiation (NIR) and acidic pH condition towards human breast cancer cell line (MCF-7). The drug loading process was carried out by the interaction of the antitumor agent with the outer polymeric layer of the robots. Motors exhibited promising viability results by using 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide tetrazolium reduction (MTT) assays.

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Keyword: Nano/micromotors, drug delivery, anticancer drug, MCF-7 human breast cancer cell line

#### ID: 376 - Synthetic Materials Biology

## Parity-time symmetry breaking in biological active matter

## <u>Aşkın Kocabaş</u>\*

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Symmetry is a fundamental property of physical systems. However, it is generally broken in nature. Our heart is always on the left and our left and right hands are mirror images of one another. How and why nature breaks these fundamental symmetries remains a long-standing scientific mystery. We recently observed that active biological systems consisting of multiple interacting components can break left-right symmetry. Interestingly, this symmetry-breaking process originates from the non-Hermitian nature of the systems resulting from nonreciprocal physical interactions between active and passive components. In this talk, I will present our recent experimental and theoretical results revealing the secrets of this complex symmetry-breaking phenomenon.

Keyword: Active matter

ID: 3 - Nanooptics, Nanophotonics, and Nanoplasmonics - Oral

## LIPSS for SERS: Metal Coated Direct Laser Written Periodic Nanostructures for Surface Enhanced Raman Spectroscopy

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In this work, a novel method of fabricating large-area, low-cost surface-enhanced Raman spectroscopy (SERS) [1] substrates is explained which yields densely nanostructured surfaces utilizing laser-induced periodic surface structuring (LIPSS) [2] of crystalline silicon (Si). Two different interaction regimes are utilized to yield low-spatial frequency (LSFL) and high-spatial-frequency (HSFL) LIPSS patterns. Nanostructuring of Si surface is followed by deposition of a thin noble metal layer to complete the fabrication procedure. A 50-70 nm thick Ag layer is shown to maximize the SERS performance. The SERS effect is attributed to the electromagnetic field enhancement originating from the nanoscale surface roughness of Si that can be controlled by LSFL and HSFL nature of the structure. The SERS substrates are found to be capable of detecting a Raman analyte down to  $10^{-11}$  M. SERS performance of the Ag deposited substrates are compared at 532, 660 and 785 nm excitation wavelengths. Both LSFL and HSFL Si surfaces with 70 nm thick Ag are found to exhibit strongest SERS under 660 nm excitation exhibiting Raman enhancement factors (EFs) as high as  $10^{9}$ . The Raman EFs are calculated both by SERS spectra experimentally, and using finite elements method simulation of the electric field enhancement where a good agreement is found [3].

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Keyword: Raman spectroscopy, Laser induced periodic surface structuring, nanostructuring, enhancement factor

ID: 54 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Highly Efficient White Light-emitting Diodes by the Integration of Near Unity Emitting **Quantum Dots in Liquid State**

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LEDs are predicted to monopolize illumination applications in the close future, with the ability to save 62 quads (quadrillion British thermal units) of energy by 2035 [1]. As a result, the energy effect of LED technology will expand in the future. It is critical to create solid-state lighting devices apart from phosphors for next-generation LED technologies. These alternatives can improve their functioning and suit the demands of various applications. Because of their high efficiency and unique spectrum tuning capabilities via the quantum confinement effect [2,3], quantum dots (QDs) offer considerable promise for this purpose.

Liquid-state usage of QDs enables precise control of optical device properties by easy QD injection, suppresses the hostmaterial effect [4], and maintains a high photoluminescence quantum yield (PLQY) of QDs in device structures. However, the record efficiency of white LEDs (WLEDs) has been maintained at around 100 lm/W when utilizing this technology.

We demonstrate WLEDs with a brightness of more than 150 lm/W employing QDs in liquid in this work. We achieved this by carefully optimizing nucleation-growth conditions and obtaining highly efficient green- and red-emitting ZnCdSe/ZnSe QDs with near-unity PLQY of 94.1 and 94.2%, respectively, by post-synthetic removal of surface traps. We also tested the cadmium content of ZnCdSe/ZnSe core/shell QDs, which revealed that the cadmium concentration is less than 100 ppm, meeting current EU RoHS rules. We combined simulated quantities of green- and red-emitting QDs in a liquid state onto blue LED chips based on optical simulations, resulting in red-green-blue (RGB)- and green-blue (GB)-based WLEDs with maximum luminous efficiency of 129.6 and 170.4 lm/W, respectively. Our simulations also revealed that by employing ultraefficient blue LED pumps, we can achieve an efficiency level of more than 230 lm/W. As a result, liquid-state integration of efficient nanomaterials has the potential for high-performance WLEDs.

#### Acknowledgments

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Keyword: quantum dot, white light-emitting diodes, quantum efficiency, luminous efficiency, external quantum efficiency

#### ID: 59 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Single-Pixel, Picometer Scale Spectral Characterization of Light Through Scattering Media

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Nanoscale (sub-wavelength) imaging has various applications in nanostructures such as cells and biomolecules. Controlling the wavefront of light traveling through a scattering medium having sub-wavelength spatial modes may result in sub-wavelength focusing, which may be used in nanoscale imaging [1]. Single-pixel imaging is another preferred technique in nanophotonics applications seeking low-cost production and compactness [2]. In this study, we propose a single-pixel multimode fiber spectrometer with picometer scale resolution by controlling the light via wavefront modulation. We use a spatial light modulator (SLM) to focus individual wavelengths at the distal end of the fiber. The calibration of the spectrometer is done by exploiting the sensitive response of multimode fiber to variations in the wavelength. The calibrated data is later used to successfully reconstruct unknown arbitrary input spectra. The technique developed in this study can be used in nanoscale spectral characterization, investigation of scattering nanostructures, and sub-wavelength imaging.

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Keyword: single-pixel, spectrometer, fiber optics, wavefront shaping, imaging

## Facile Fabrication of Plasmonic Nanostructures for Surface Enhanced Vibrational Spectroscopy

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Detection and analysis of even a minute concentration of molecules is important in various fields such as environmental monitoring, food quality control, and clinical analysis. One of the convenient and non-destructive techniques that can be used for such purposes is vibrational spectroscopy, due to unique vibrational fingerprint of molecules. However, the detection capability of conventional spectroscopic techniques such as Fourier transform infrared (FTIR) and Raman spectroscopy is limited to due to weak signal. Fortunately, signals of analyte molecules placed close to plasmonic nanostructures can be enhanced millions of times, due to the strong confinement of light. These results in enhanced absorption of IR light and strong Raman scattering, as used in surface enhanced IR absorption (SEIRA) and SERS techniques.<sup>1</sup> Coinage metals (Au, Ag, Cu) can support surface plasmons, which can be confined to surfaces to achieve strong localized surface plasmon resonances (LSPR) by engineering nanostructures made of those metals. Plasmonic nanoparticles can be conveniently synthesized via colloidal chemistry, though structural (size, shape, etc.) control is difficult, especially so for high aspect ratio particles that needed for SEIRA. On the other hand, precise nanostructures can be prepared using conventional lithographic techniques such as e-beam lithography, laser lithography, etc. However, these techniques involve complex processes, and require specialized facilities and expensive equipment, hindering development of novel plasmonic nanostructures for surface enhanced vibrational spectroscopy applications.

In this study, we explore two convenient approaches that can be used to fabricate plasmonic nanostructures, focusing on their applications in SEIRA. In the first approach, we employ electrohydrodynamic jet printing (e-Jet) to print arrays of narrow (~200 nm) polymer brushes that is a few  $\mu$ m long, followed by immobilizing commercial gold nanoparticles (NPs) or growing them in situ.<sup>2</sup> This results in plasmonic nanoantenna arrays whose LSPR can be tuned to be in the mid IR region (3-20  $\mu$ m) so that traditional FTIR instruments can be used to measure SEIRA spectroscopy of various molecules. It turns out this is an effective and low-cost approach to fabricate substrates for SEIRA, especially for prototyping purposes. Furthermore, enhancement and quality factor of the plasmonic nanoantenna is compared against nanoantenna's fabricated using traditional lithographic techniques, as well as against finite difference time domain simulations (FDTD) performed using open-source python package MEEP.<sup>3</sup>

In a second approach, we utilize dewetting to fabricate micron-scale islands of polymers, followed by immobilizing Au NPs. The results indicate that both structural and plasmonic effect led to patterns in the visible range, as well as multiple LSPR bands in the mid IR region. Furthermore, it is observed that the coupling between molecular vibration of the underlying polymer and the LSPR results in Fano type line shape in the SERIA spectra.<sup>4</sup> These plasmonic substrates can used for SEIRA as well as for SERS applications.

## Acknowledgement:

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Keyword: Plasmonics, Nanophotonics, Polymer brushes, SEIRA, SERS

#### ID: 134 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Passive Reconstruction of Sound through a Multi-Mode Fiber

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When an object is stimulated with sound waves, it vibrates. Using a camera, these vibrations can be observed and reconstructed to sound (1), providing a photo-acoustical signal. In our work, we managed to bring a new perspective to this approach using a multi-mode fiber (MMF). We analysed the speckle pattern coming out from the MMF. We use an InGaAs camera to image the speckle pattern of a multi-mode fiber operating at the telecom range. The resolution of our camera is 350x256; however, we chose a region of 128x8 pixels which provides us with faster data acquisition at an increased frame rate. We analyse different regions of interest and compare the reconstructed sound quality. With this approach, we find the point where the correlations with the original sound are maximum. This method helps us reduce the background noise and eliminate the non-existing frequencies in the original sound. As a result, we managed to successfully reconstruct sound signals that are emerging from a source positioned next to the optical fiber.

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Keyword: photo-acoustics, visual microphone

#### ID: 143 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Sensing the Fiber Bent via Deep Learning

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Multimode fibers (MMFs) are extremely sensitive against external perturbations, such as bending. The increased number of modes as well as the modal coupling are the main reasons for this increased sensitivity. Under perturbative effects, the optical paths of the fiber modes change, and the perturbation causes energy redistribution between modes [1]. At the distal end of an MMF, interference between propagation modes can be observed in the form of random interference patterns called speckles. As a type of external perturbation, the bending of the MMF is a considerable problem, therefore bending is considered a limiting factor for such systems [2]. But some studies make use of this fiber sensitivity and utilize bending sensors [3]. In this study, we used a Deep Learning (DL) algorithm to classify the radius of curvature of a bent MMF as well as to predict the bending location through the fiber. Intensity only speckle images that are corresponding to the bending curvature and bending location are used as input for the training of a Convolutional Neural Network (CNN). Our experiments showed that the CNN model can find each bending location with a Root Mean Square Error (RMSE) of  $\approx$ 1.4 cm and predicts the curvature radii with an RMSE of  $\approx$ 0.2 mm. This is a clear indication that the applied CNN model can learn to resolve the perturbation effects caused by bending and can classify not just the bending radii but also the bending location at the same time.

With the help of digital spatial modulators, MMFs can be used to transfer images. Being able to know how the bending affects the ability to transmit multiple spatial modes of light, MMFs can be a good candidate to replace bundles of single mode fibers used in endoscopy, which are usually few millimeters thick. The replacement will reduce the thickness up to a 50 microns, which is close to the limits of nanotechnology and revolutionizing medical endoscopy[4].

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Keyword: Fiber specklegram sensing, multimode fiber, bending, deep learning, convolutional neural networks

## ALD Based Al<sub>2</sub>O<sub>3</sub> Ring Resonator Devices for Application in Avionics

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The use of light and optics dates to a long time ago. This has led to the invention of devices with working principles based on the transmission and reflection of light. One of the most important usage areas of this system is aviation applications. Because high sensitivity and low noise rates, which are important in aviation, are well provided by optoelectronic detection devices. In our studies we focus on CVD and ALD based 2D materials (such as graphene, MoS<sub>2</sub>, MXene and similar) and devices for specific applications in avionics.

In this study, design and analysis studies focusing on integrated ring resonator-based sensors as an accelerometer and temperature sensor. A Micro-Opto-Electro-Mechanical System (MOEMS) refers to an optical accelerometer with a similar working principle to traditional Micro-Electro-Mechanical Systems (MEMS), but which gives better outputs in important parameters such as sensitivity, noise, shock value. In the designed devices is formed with an Atomic Layer Deposition (ALD) grown  $Al_2O_3$  based ring resonator and a single-mode ridge waveguide structure. The waveguide of the ring resonator is designed with a width between 2-2.5 micrometer, a height between 0.6-0.8 micrometer, a radius between 150-1000 micrometer, and a gap between 0.75-1 micrometer. The quality factor is  $5x10^5$ , temperature sensitivity  $10 \pm 0.1$  pm/K, and thermo-optic coefficient is  $1.86 \times 10^{-5}$  RIU/K are the target design.<sup>[1]</sup>

Al<sub>2</sub>O<sub>3</sub>, an innovative optical material, was used when designing the device. [2] This material provides the integrated circuit with superior properties such as high refractive index, doping with rare earth ions, high light trapping, minimum loss, stability, transparency, and adaptability to optical fibers.[3] In addition, the Atomic Layer Deposition (ALD) method used in the production of the material provides high controllability and doping ratio and low cost. [4]

The usage of Al2O3 based ring resonator structure, enables MOEMS accelerometer to be obtained. The system works on the principle that the bending of the cantilever structure as a result of acceleration, changes the refractive index of the ring resonator and the measurement of the shift in the wavelength. (figure1.a) Temperature changes are detected, and a temperature sensor is obtained.(figure1.d) Optical and mechanical analyzes of the designed accelerometer and temperature sensor were made using Ansys program. Numerical methods such as Finite Different Time Domain (FDTD) and Finite Element Method (FEM) were applied in these optimization studies. (figure1.b,c) Improvements were made in the device through the parameters obtained as a result of the analysis. As a result of the study, it has been observed that an accelerometer and temperature sensor that are more sensitive, have a low noise ratio, have a high impact resistance and a low cost compared to the ones in the market has been obtained.

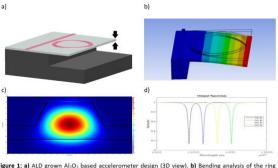


Figure 1: a) ALD grown Al<sub>2</sub>O<sub>3</sub> based accelerometer design (3D view). b) Bending analysis of the ring resonator using ANSYS. c) Electric field profile of the fundamental mode of the Al<sub>2</sub>O<sub>3</sub> waveguide at a wavelength of 1550 nm. d) Temperature caused resonance wavelength shift.

#### Acknowledgments:

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**Keyword:** Al2O3, ALD, MOEMS, accelerometer, temperature sensor, waveguide, micro-ring resonator, single mode, quality factor, thermo-optic coefficient, aviation technology

#### ID: 238 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Enhanced Raman Spectroscopy with Laser Processed Tips

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A combination of Raman spectroscopy and scanning probe microscopy (Fig. 1.a), either atomic force microscopy (AFM) or scanning tunneling microscopy, seemed particularly promising as a nanoscale resolved detection tool called tip-enhanced Raman spectroscopy [1]. Morphology and size of the tips, surrounding medium, wavelength, and polarization of the field are crucial parameters for the spectral response of the AFM tips [2]. Plasmon nanofocusing provides high-efficiency coupling of the far-field radiation to the near-field zone via propagation of surface plasmon polariton (SPP) through the end of the tip following exciting the SPP on the metal tip shaft. The formation of the grating for the propagation of SPP and conversion of it into a localized SPP at the tip apex is achieved by focused ion beam milling [3]. We aim to modify the AFM tips by non-linear laser lithography (Fig. 1.b) exploiting feedback mechanisms to regulate the formation of regularly spaced nanolines in long-range uniformity induced by femtosecond (fs) pulses [4]. This method is applicable for surfaces having curvatures owing to the insensitivity to the laser intensity variations. In order to find the optimum parameters, ripple formation on flat substrates and tips was studied with different power of fs pulsed laser and different velocities and hatch distances of galvoscanner head.

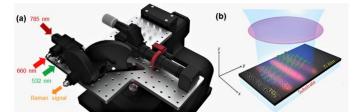


Figure 1: (a) 3D drawing of the integrated AFM and Raman spectroscopy system and (b) schematic of the nanostructure formation process.

#### Acknowledgement

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Keyword: Plasmonics, Tip-enhanced Raman Spectroscopy, Femtosecond laser structuring

# Bu gördüğünüz sadece bir potansiyostat değil.



µStat-i Multi16

# Yeni Metrohm DropSens µStat-i MultiX ile tanışın!

Yeni µStat-i MultiX ile, elektrokimyasal araştırmalarınız için verimli, çok yönlü ve güvenilir kullanıcı deneyimine dayalı gelişmiş olanaklar artık elinizin altında. Bu çok-kanallı bipotansiyostat, galvanostat ve empedans analizörü (çift-kanallı Elektrokimyasal Empedans Spektroskopisi gerçekleştirmek için MultiplES®teknobojisine sahip), çoklu kullanıcı ve çoklu disiplin çalışmalarınız için özellikle uygundur.

İhtiyaç duyduğunuz kanal sayısını seçin (opsiyonel floting nordu da nervcut), aynı anda bir den fazla kullanıcının aynı enstrüman ile çalışabilmesinin avantajlarından yararlanın, isterseniz uzaktan çalışın ve kullanımı kolay yazılım arayüzü ile araştırmanızı destekleyin.

Elektrokimya gerçek hayattaki analitik problemleri çözebilme potansiyelini kanıtlamıştır. uStat-i MultiX bu yolda analitik araştırmalarınızı basitleştirmekte ve günlük iş akışlarınızı dönüştürmektedir.

Daha

µStat-i MultiX'i daha yakından keşfetmek için internet sitemizi ziyaret edin: https://www.metrohm.com/tr\_tr/products/electrochemistry/portable-line/ustat-i-multix.html

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#### ID: 90 Nanomechanics, Nanotribology, and Nanomanipulation

## **Comparison of Control Approaches in High-Speed Dynamic Atomic Force Microscopy**

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High-Speed Atomic Force Microscope (AFM) is a versatile instrument used for imaging biological processes in millisecond time frame. In this study, the state-of-art high-speed dynamic-AFM is modeled in MATLAB/Simulink in both air and liquid environments. To increase the scan rate further we use Q-controlled fundamental eigenmode in place of a conventional piezo actuator while the higher-order eigenmode amplitude is used in feedback. Conventional PI controller and a robust controller are compared in terms of scan speed and accuracy of obtaining the sample for a small high frequency cantilever. In addition, the performances of these controllers are assessed under noise, disturbance and uncertainty for the same topography.

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Keyword: High-Speed Dynamic-AFM, Multi-Frequency AFM, Q-Controlled Eigenmode, Robust Control

## Mechanical Properties of Nanostructured Copper-Tantalum Metallic Glass Thin Films

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Metallic glasses (MG) are alloys with an amorphous structure, as opposed to crystalline alloys. The amorphous structure can be obtained by utilizing different combinations of a wide range of metals, providing a vast design space for the development of new engineering materials [1]. MGs demonstrate desirable properties such as high hardness, wear resistance, corrosion resistance, and biocompatibility based on their composition and alloying elements [2-4]. MGs can also be obtained in thin-film form, making them promising for coating applications of wear resistance, corrosion resistance, and biocompatibility [5]. In this work, we probe the mechanical properties of copper-tantalum metallic glasses, to understand the structure-property relationships in FCC-refractory alloy binary MGs. In addition, we design nanostructures formed by these alloys to further improve the mechanical properties.

The experimental work started by depositing 1  $\mu$ m-thick Cu-Ta alloy coatings on an oxidized single crystal silicon substrate using magnetron sputtering. We employed combinatorial sputtering to obtain a continuously varying alloy composition over a single substrate. After the deposition process, we analyzed 12 different compositions of Cu-Ta by X-ray diffraction, electron microscopy, and nanoindentation. The findings identified the glass-forming compositions and the respective mechanical properties.

Based on the findings of the first stage of experiments, two types of nanolayered films were deposited on dog bone-shaped polyimide sheets for tensile testing. The first type contained alternating layers of two different fully amorphous Cu-Ta compositions. The second type was made of alternating layers of amorphous Cu-Ta and semi-crystalline Cu-Ta. Both sets of samples had a total film thickness of 1  $\mu$ m and a layer thickness of 20 nm. In addition to the standardized microstructural and micromechanical characterization, we performed tensile tests on the polyimide-supported thin films, which provided a more accurate picture of ductility and fracture resistance trends.

The result demonstrated that the Cu-Ta system can form a fully amorphous structure in the compositional range of 37 at.% to 75 at.% Cu. The amorphous alloys exhibited a wide range of hardness values between 6 and 12 GPa, where higher Ta content led to higher hardness. Implementation of nanostructures improved the ductility and toughness of the glassy films. The enhanced properties of the MG films combined with their grain boundary-free structure provide a promising route for the development of more effective wear-resistant, corrosion-resistant, and biocompatible coatings.

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Keyword: Mechanical Properties, Metallic glasses, Ductility, Toughness

## Intercalation Leads to Inverse Layer Dependence of Friction on Chemically Doped MoS<sub>2</sub>

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We present results of atomic-force-microscopy-based friction measurements [1, 2] on Re-doped molybdenum disulfide ( $MoS_2$ ). In stark contrast to the widespread observation of decreasing friction with increasing number of layers on twodimensional (2D) materials [3, 4], friction on Re-doped  $MoS_2$  exhibits an anomalous, i.e., *inverse* dependence on the number of layers. Raman spectroscopy measurements combined with *ab initio* calculations reveal signatures of Re intercalation. Calculations suggest an increase in out-of-plane stiffness that inversely correlates with the number of layers as the physical mechanism behind this remarkable observation, revealing a distinctive regime of puckering for 2D materials. This study opens the way for selective tuning of friction in micro- and nano-scale mechanical systems, by the combined use of undoped 2D materials and those with intercalated dopants (which are most probably not limited to the Re-doped  $MoS_2$  system investigated here).

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Keyword: atomic force microscopy, chemical doping, density functional theory, friction, molybdenum disulfide

## Lubricant Degradation Monitoring Using Triboelectric Sensor

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Lubricating oil is vital for the operation of internal combustion engines, since they reduce friction, wear, heat, and corrosion. Their usage helps to prolong the machine life and reduce the carbon footprint. Especially, energy consumption of the machine is reduced with using high quality of lubricants. Lubrication is degraded because of some factors such as pressure, heat, moisture, dust, water, metal cations and its service life. These effects results in oxidation of lubricant and change its mechanical and rheological properties<sup>1</sup>

In our approach, we correlated chemical changes of lubricant due to oxidation and depletion of additive materials with triboelectric signals. Triboelectric signals were generated by contacting a polymer film to a lubricant-wet paper. Metal electrodes that were placed behind these materials (polymer and paper) were connected to the probes of an oscilloscope which was used to monitor triboelectric signals in Volts.

We investigated the contacted polymer surface by AFM and surface topographical analyses showed that the triboelectric signal is associated with deformations on the surfaces. We observed that at the polymer surfaces that are in contact with oxidized oil exhibited less deformations. It can be surmised that the less efficient contact between polymer and paper in the presence of oxidized oil caused less deformation on the polymer surface (less mechanical bond-breaking). It was revealed that tribocharging of the contacting surfaces were reduced for the oxidized lubricant due to changes in the lubricant's composition, changes in its electrical properties, and surface deformations on the contacting materials<sup>2</sup>.

Finally, we built an example of a portable online triboelectric liquid lubricant condition monitoring sensor<sup>2</sup>. We believe that this oil oxidation monitoring method can help to prevent economic losses and protect the environment.

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Keyword: Triboelectric, Lubricant, Engine oil, contact charging, polymer

#### ID: 256 - Nanomechanics, Nanotribology, and Nanomanipulation

## Vibration of Axially Graded Timoshenko-Ehrenfest Nanobeam with Follower Force

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Transverse vibration of axially functionally graded cantilever carbon nanotubes with follower force effect has been studied in the present work. Timoshenko-Ehrenfest beam model [1-3], Eringen's Nonlocal Elasticity Theory [4-6] and variational principle have been used in modeling of the nanobeam. Material properties variation of nanotube is considered in exponential form. Solution of the governing differential equation of motion with variable coefficients [7] have been obtained with approximate Ritz method. Effect of material grading index, nonlocal parameter and non-dimensional follower force on the dynamics of axially graded nanobeam have been investigated. Present work can contribute to design of nano scale sensors or energy harvesting applications.

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Keyword: nanobeam, axially graded, nonlocal elasticity, follower force, Ritz method

#### ID: 266 - Nanomechanics, Nanotribology, and Nanomanipulation

## Metallic Glass-High Entropy Alloy Nanolayered Composites with Ultra-High Strength

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This study investigates the mechanical behavior of nanolayers comprised of metallic glasses (MG) and high-entropy alloys (HEA). The MG/HEA nanolayered structure provides an effective model system to study the length scale-dependent mechanical behavior of advanced alloys in confined geometries [1]. In addition, the new design space enabled by MG/HEA composites offers an effective route to the design of new generation structural materials [2].

 $Cu_{50}Zr_{50}/Nb_{25}Mo_{25}Ta_{25}W_{25}$  nanolayers were prepared by magnetron sputtering on oxidized single crystal silicon substrates. The total film thickness was 1  $\mu$ m and different specimens were prepared with layer thicknesses in the range of 5 – 200 nm. X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM) characterized the microstructure of the films. The mechanical properties were investigated through hardness measurements using nanoindentation.

Microstructural analysis showed that the composite consists of fully amorphous CuZr layers and nanocrystalline NbMoTaW exhibiting a single-phase BCC structure. As the layer thickness decreases, the hardness of the composite dramatically increases from about 9 GPa to 14 GPa.

The increasing hardness with decreasing layer thickness is analogous to the Hall-Petch behavior observed in polycrystalline structures. In our case, the decreasing layer thickness increases the density of the interfaces, which act as obstacles to dislocation motion [3].

Further analysis of the nanoindentation response provided means for estimating the fracture toughness. The nanolayered morphology exhibits improved toughness compared to the monolithic versions of both the HEA and the MG film.

In summary, we demonstrated a novel nanocomposite that combines the features of HEAs and MGs, providing high hardness and toughness values that exceed those of the constituents in monolithic form. The findings will guide future studies for the development of next-generation high-performance coatings and structural materials.

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Keyword: mechanical properties, nanoindentation, high entropy alloys, metallic glasses, nanostructured alloys

ID: 309 - Nanomechanics, Nanotribology, and Nanomanipulation

## Simulation of Ferrofluid Magnetic Actuation with Dynamic Magnetic Fields Using Permanent Magnets in Small Channels

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Magnetic actuation of ferrofluids is one of the most interesting research topics because of the extensive range of possible applications, including aerospace, microfluidics, and medical areas [1]. A ferrofluid can be described as the colloidal suspension of ion oxide nanoparticles (Fe<sub>3</sub>O<sub>4</sub>) in oil-based or water-based carrier fluid which becomes magnetized when exposed to a magnetic field. Ferrofluid has been used in nanoscience and nanotechnology since the beginning because of the small particle sizes of nanoparticles it contains. Based on the Web of Science data, the increment in the number of published articles on Ferrofluid is over three times in the last 20 years which is mostly attributable to cutting-edge audio devices, energy harvesters, lubrication systems, sensors, pumps, valves, and healthcare fields [2].

The ferrohydrodynamic behavior of the ferrofluids in microchannels is yet to be fully understood due to the complexity arising from different properties of the nanoparticles as concentration, coating, size, stability, and so on [3]. However, from the microfluidics point of view, ferrofluid is mostly considered in micropump and microvalve applications. In this study, the modeling of ferrofluid actuation in a circular microchannel with a number of neodymium permanent magnets which are integrated into a circular rotating system that creates a dynamic magnetic field is studied using the COMSOL Multiphysics software to better understand the ferrofluid actuation phenomenon. Ferrofluid flow in microchannels was investigated using superparamagnetic iron oxide nanoparticle-based ferrofluids at various angles of rotating permanent magnets. Our novel ferrofluid actuator design model might assist in the design and development of microfluidic pumps as well as be used to investigate ferrofluid flows with dynamic magnetic fields.

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Keyword: ferrofluid actuation, microfluidics, dynamic magnetic field

# A Novel Antibacterial and Low-cost Ceramic Membrane Coated with Ni-doped ZnO Nanoparticles for Water Purification

#### Arvin Alvandi<sup>\* 1</sup>, Mohammad-Hossein Sarrafzadeh<sup>1</sup>, Seyed-Behnam Ghaffari<sup>1</sup>, Ali Mohammad Hadian<sup>2</sup>

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The lack of access of about one billion people around the world to safe water and the prevalence of waterborne diseases rise the demand to the development of simple and cost-effective approaches to disinfect water. Since membrane filtration technologies provide several advantages for pathogen-free water production compared to the conventional processes, they are recently attracted attentions as an advanced alternative one. In this study, a low-cost ceramic membrane coated with Ni/ZnO nanoparticles was synthesized for bacterial removal from contaminated water. The ceramic membrane was fabricated via a slip casting method containing starch, alumina and kaolin with the ratio of 30, 35 and 35 wt.%, respectively (1). Ni/ZnO nanoparticles (Ni/ZnO NPs) were synthesized by the sol-gel method (2) and the coating process was done via the dip coating method and the membranes were soaked into the nanoparticles suspensions with different concentrations for 10 minutes (3). The physicochemical properties and the morphologies of Ni/ZnO NPs and the membranes were characterized by FTIR, XRD, FESEM and EDS. The bactericidal efficiency of the samples against E. coli was investigated by the plate counting method (4). Based on the results, the optimum concentration of Ni/ZnO NPs was 5 wt.% in the suspension. For this sample, the concentration of bacteria reduced from 1.5\*10^8 CFU/ml to 3\*10^4 CFU/ml after 12-h treatment (99.98% removal efficiency). The results qualify the efficiency of the modified membranes for bacteria removal and their potentials for the development of portable point-of-use (POU) technology for purify water.

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Keyword: Ceramic membrane, Ni-doped ZnO, Antibacterial, Water and wastewater treatment

ID: 117 - Nanomaterials in Food, Agriculture and Water Purification

# Extending the Shelf Life of Bananas with Cinnamaldehyde Essential Oil Impregnated Halloysite Nanotubes/polypropylene Nanocomposite Films

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Active food packaging materials that can prevent the spoilage of fresh fruits and vegetables provide an important solution to food loss-based economic problems[1][2]. Ethylene gas produced by most fruits and vegetables as a ripening hormone is an important parameter that needs to be investigated in terms of its inhibition or elimination to prolong the shelf-life of fresh fruits and vegetables[3]. With an attempt to obtain a sustained-release system that can decrease the ethylene production of bananas, cinnamaldehyde (CA) essential oil was encapsulated in halloysite nanotubes (HNT). The slow release of CA from the HNT-CA nanohybrids has been demonstrated to last for over 180 days and cause inhibition of ethylene production in fruits. In order to obtain food packaging films, which have the ability to inhibit ethylene production based on the release of CA, HNT-CA nanohybrids were incorporated into polypropylene (PP) by 0.25 and 1 wt % via melt extrusion followed by film blowing extrusion. The resulting PP/HNT-CA nanocomposite films were demonstrated to present the thermal and mechanical properties required for use as food packaging materials. Bananas packaged with PP/HNT-CA nanocomposite films containing 1 wt % HNT-CA nanohybrids were shown to present significantly higher firmness values and higher color scores indicating freshness, compared to bananas packaged with control neat PP films. Nanocomposite food packaging films presented in this study were shown to increase the shelf life of bananas by inhibiting the ethylene gas production via the slow release of CA and they have strong potential as active food packaging materials that can prevent food loss.

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Keyword: Active food packaging, Nanocomposite film, Sustained-release, Cinnamaldehyde essential oil, Halloysite nanotubes

ID: 166 - Nanomaterials in Food, Agriculture and Water Purification

# CNT@Ag@ZnO Multifunctional Nanomaterial for Solid Phase Extraction and Photocatalytic Degradation-based Removal of Sildenafil Sitrate

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Recently, wrong and excessive drug use is among the major problems encountered. Drugs that are taken into the body and released into the nature after the use of other supportive drug derivatives during drug use are among the major polluting sources in nature. There are many methods used in the literature for minimizing/destroying the pollution activity in nature, separating the polluting sources from the matrix environment and at the same time analyzing the pollutant active drug species in the environment. One of the most used methods in the literature is Solid Phase Extraction (KFE). By using this method, the separation, purification and enrichment steps of the drug active species or derivatives to be analyzed in the environment are made possible in systems such as UPLC or HPLC<sup>1-3</sup>. The properties of the adsorbent to be used for the separation and purification steps allow the synthesis of multifunctional nanomaterials with desired properties with the designed and controlled synthesis methods.

In this study, CNT@Ag@ZnO multifunctional nanomaterial was synthesized as adsorbent for SPE. The characterization of the synthesized nanomaterial was performed using X-ray diffraction (XRD), Raman spectrometry, Fourier Transform Infrared Spectroscopy (FT-IR), scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDX) techniques, and its structure was elucidated. CNT@Ag@ZnO multifunctional nanomaterial was used both as an adsorbent in KFE and as a photocatalyst in photocatalytic experiments.

In addition to its high commercial share, sildenafil citrate (SS), which is one of the most widely used drug active species, is used for separation, purification and enrichment by solid phase extraction and ultra-high performance liquid chromatography (UPLC-DAD) after photocatalytic decomposition of SS. analyzes were carried out. pH effect, eluent type and volume, adsorbent amount, sample volume and real sample analyzes were succesfully applied as optimization parameters. Analytical performance parameters (limit of quantification (LOQ), limit of dedection (LOD), correlation coefficient (r2), calibration line, enrichment factor, preconcentration factor, etc.) were determined for the optimized and developed method. The developed solid phase extraction method was successfully applied to real samples.

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Keyword: SPE, Photocatalysis, UPLC-DAD, Multifunctional nanomaterial

# The Effect of Film Thickness on Photocatalytic Activity of the ALD ZnO Films Deposited on Glass Fibers

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Fresh water is vital for the whole ecosystem, and industrial wastes are threatening the resources due to increased production. More efficient and eco-friendly wastewater treatment mechanisms and systems are desired to reduce the impact of such wastes on the environment. Photocatalytic elimination of organic pollutants is a promising approach since the mechanism reduces the toxicity of the pollutants while using sunlight in an ideal scenario [1]. Like any other catalytic mechanism, the surface area of the photocatalyst plays an important role in the performance of the material. A convenient way to increase the surface area is to reduce the particle size to the nanoscale which results in several problems including the removal of particles out of clean water. Our approach aims to eliminate such problems by immobilizing the photocatalyst materials onto high surface area substrates such as textiles [2]. Atomic layer deposition is an ideal technique to deposit conformal films on high surface area substrates. We investigate the effect of the thin film thickness of ALD deposited ZnO films on fibrous substrates by measuring methylene blue and methyl orange degradation under a solar simulator. Results suggest an optimum film thickness in the range we studied for better photocatalytic performance. We investigate the changes in the surface properties of the textile substrate by forming various thicknesses of ZnO films to understand the results better. We also characterize the film materials to explain the phenomena observed.

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Keyword: photocatalysis, atomic layer deposition, textiles, ZnO, thin film

# Green Synthesis of Silver Nanoparticles Using Instant Coffee and Their Usage in Extension of Food Shelf Life

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Nanoparticles show different activity on materials due to their large surface area and quantum field effects. For example, although the antibacterial effect of silver is known [1], the antibacterial properties of silver nanoparticles (Ag NPs) used in this study are considerably higher than that of bulk silver metal [2].

In this study, Ag NPs were synthesized using a green chemistry approach where silver nitrate (AgNO<sub>3</sub>) was reduced using instant coffee extract as both a reducing agent and a stabilizer under very mild conditions. Investigation of synthesis conditions was performed by the variation of temperature, reaction time, and use of different coffee extracts [2,3]. Produced Ag NPs were characterized using Ultraviolet-visible region (UV-VIS), Fourier-transform infrared (FTIR), Dynamic light scattering (DSL), X-Ray Photoelectron Spectroscopy (XPS) and X-Ray diffraction (XRD) spectroscopies as well as Scanning electron microscopy (SEM) and Tm.ransmission electron microscopy (TEM) [3]. Furthermore, their usage in the extension of food shelf life was studied by the incorporation of them into packing films for some vegetables/fruits. The samples taken from the food samples through the cell spreader were inoculated into lysogeny broth (LB) agar medium. The potential for bacterial colonization in LB agar media was investigated for antibacterial activity analyses [4]. Our efforts will continue on the development of composite systems for packaging in food security.

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Keyword: Silver Nanoparticles, Antimicrobial, Green Synthesis, Coffee, Food Shelf Life

# Functionalized Carbon Nanotube Embedded Thin Film Nanocomposite Membranes for Desalination

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Increasing population, industrialization and climate change increases the demand for potable and irrigation water. Even though 70 percent of the Earth is covered with water, most of it is saline. Hence, there exists a large interest in desalination technologies to ensure water sustainability and production of potable water from brackish or seawater via reverse osmosis (RO) stands out as the leading technology (Jones et. al., 2019). Polyamide (PA) based thin film composite (TFC) membranes are extensively used in seawater reverse osmosis (SWRO) applications due to their superior separation performance and stability. Thin film nanocomposites (TFN) are promising to overcome the important limitations in SWRO applications, such as permeability-selectivity trade-off and rejection of small and neutral species such as boron.

Incorporation of carbon nanotubes (CNTs), with their exact pore diameter and smooth inner surface, into the PA layer of TFC membranes show interesting water and ion permeability features. While addition of CNT into TFC structure during interfacial polymerization process enhances water permeability by a factor of 4 and maintains its salt rejection around 98% (Chan et. al. 2013), it is also crucial to remove neutral solutes like boron. CNTs can prefer water over boron via smooth inner surfaces and could increase selectivity by increasing water passage. Furthermore, functionalization of CNTs could be a solution to narrow the pore tips and functional groups with an affinity to boron could act as gate-keeper for boric species (Thomas and Corry, 2016, Werber et. al. 2016).

In this work, we explore the possibility of tailoring the desalination performance to add new functionality of high boron rejection to RO membranes by incorporating functionalized single walled CNTs (SWCNT) into the polyamide layer. We used commercial SWCNTs with diameter around 1 nm. First, we functionalize SWCNTs using different functional groups, namely biotin (BIO), 8-amino caprylic acid (ACA), and zwitterion (ZW), which are bulky, long chain, and have zwitterionic properties, respectively. Then, we incorporated SWCNTs by using vacuum filtration to allow CNTs partially aligning in the pore structure of the support membrane. Finally, thin film nanocomposite membranes are prepared by interfacial polymerization using mphenylenediamine and trimesoyl chloride as monomers. SWCNTs are characterized by TGA, XPS and Raman Spectroscopy while membranes are characterized by structural and surface analysis via SEM and AFM. All prepared membranes are tested using feed solutions with 2000 ppm NaCl and 5 ppm boron at ambient temperature and 15.5 bar feed pressure. TFN membrane with zwitterionic SWCNT yielded the highest boron rejection with higher pure water flux than TFC membranes without compromising salt rejection performance at neutral pH.

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Keyword: carbon nanotube, desalination, reverse osmosis, membrane

# Ni Loaded on Dealuminated Mordenites for Aqueous-phase and Gas-phase Hydrodechlorination of Trichloroethylene

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Trichloroethylene (TCE) is one of the frequently observed halogenated organic contaminant in groundwater and it brings serious concerns about human health and environment. Among different water treatment methods, catalytic hydrodechlorination is an effective approach to removing chlorinated hydrocarbons from water<sup>1</sup>. Hydrodechlorination (HDC) is an elimination based remediation method where the reaction takes place by the interaction of chlorinated hydrocarbons with adsorbed hydrogen on a metal catalyst surface, resulting in formation of HCl and chloride free hydrocarbons. HCl as a product is deleterious since it is irreversibly adsorbed on active sites and causing to deactivation, in other words, chloride poisoning, In some of the studies conducted so far, nickel-based catalysts have been concluded to have promising catalytic activity towards hydrodechlorination<sup>2,3</sup>. In this study, Ni loaded mordenite (MOR) type zeolites dealuminated with different HNO<sub>3</sub> concentrations are synthesized via ion exchange and impregnation, tested for catalytic activity using an aqueous phase batch reactor at atmospheric conditions and a gas phase fixed bed reactor, and characterized via several techniques such as N2 physisorption (BET), X ray diffractometer (XRD), isothermal desorption of CO (TPD), temperature programmed reduction (TPR) of H<sub>2</sub>, transmission electron microscopy (TEM) and Fourier Transform Infrared Spectroscopy of adsorbed pyridine (FTIR). ICP results demonstrate that dealumination of mordenite resulted in support materials with three different Si/Al ratios (10, 58, and 101) having slight differences in crystal structure and major differences in acidity and textural properties. Although no catalytic activity was obtained in aqueous phase up to 60 °C, samples were found to be highly active in gas phase at elevated temperatures, above 100 °C, and ambient pressure. Characterization results, when combined with catalytic activity performance, allowed us to obtain structure activity relations that shed a light on the effect of acidity and mesoporosity on chloride poisoning in HDC of TCE.

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Keyword: Hydrodechlorination, zeolite, nickel, mordenite, trichloroethylene

# A novel and rapid pesticide test: aptamer-based lateral flow assay for detecting and monitoring imidacloprid in water

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One of the most important requirements for sustainable agriculture is pesticides. Although they are used to protect agricultural products, they also have toxic properties that cannot be ignored. The uncontrolled use of pesticides quickly pollutes resources such as soil and water. For this reason, sensitive and rapid detection of pesticides in soil and water is of great interest. In recent years, lateral flow assays have become increasingly popular in agricultural and environmental applications. In particular, they are often preferred for monitoring the use of pesticides such as imidacloprid (Imi). Here, for the first time, we have developed an aptamer-based lateral flow assay (LFA) for the detection and monitoring of Imi levels in the water. This innovative, costeffective LFA system allows specific determination of Imi when the Imi aptamer has been conjugated to cysteamine-coated gold nanoparticles and has bound the biotinylated complement. Thus, when no Imi is present in the water sample, the biotin in the complementary interacts with the streptavidin line to form a pinkish-red line. The line disappears as the Imi content in the wastewater increases because recognition of the Imi causes a conformational change in the aptamer that replaces the biotinylated complementary sequences. The intensity of the assay gradually decreases in response to the target concentrations. A calibration plot was prepared for the different concentrations (0.5; 1.0; 5.0; 10; 25; 50 and 75 ug/mL) of Imi. This test is characterized by a high sensitivity (LOD: 0.414 ug/mL) and the absence of cross-reactions with other pesticides commonly found in soils and waters. The developed test was successfully used for the detection of Imi in water. The validity of the method and the applicability of the test were successfully evaluated by the detection of Imi in spiked water and the wastewater sample from the Konya closed basin. Confirmatory studies were also carried out by chromatographic means. The duration of the test was about three minutes. In conclusion, this innovative system is easy to use and does not require lengthy preparations. It has the potential to be used and adapted in the future for the detection and monitoring of Imi and other pesticides in wastewater

Keyword: Lateral Flow Assay, Paper-based Sensor, Imidacloprid, Agrosensor

#### ID: 267 - Molecular and Supramolecular Materials, Organic and Hybrid Electronics: OLED, OTFT, PLED

# Preparation of New High Refractive Index Hybrid Polymers for the Production of Optical Waveguides

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Recently, the most widely used optical devices for data transmission are fiber optic cables and optical waveguides. The development of these devices is a very important topic for both academic and industrial environments. Advances in the material technology of optical devices play a vital role. Controlled refractive index, good adhesion to a wide variety of surfaces, and thermal stability of optical materials are key issues for the development of modern technology [1, 2]. The fact that polymer materials have properties such as easy processability, tunable refractive index, and optimum thermal stability have made them very important in this area. In particular, the development of high refractive index polymers has led to innovations in optical devices [3]. In today's rapidly renewing telecommunications technology, there is a serious demand for novel polymer materials for the application of new optical devices in a variety of fields. Aromatic polysiloxanes which are very interesting structures for academic and industrial environments have unique properties such as optical transmittance, and chemical and thermal stability due to their hybrid structure consisting of inorganic-organic units. It is remarkable that siloxane-based hybrid polymers have been attractive materials for optical and thermal properties of their films were investigated. Carbazole, a well-known molecule in materials science due to its electroluminescent and photoconductive properties, also exhibits high polarization by exhibiting a high refractive index over a wide atomic field [5].

#### Acknowledgments:

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Keyword: Organic and Hybrid Electronics, Optical Devices, Polymers, Organic and Inorganic Polysiloxanes

# Development of an Easily Applicable Heterogeneous Catalyst by Anchoring Palladium and Gold Nanoparticles onto Chemically-modified Wool Fabrics

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In this work, one of the most sustainable textile polymers, wool fabric, was converted into a practical material for developing a heterogeneous catalyst through successive modification steps. For this purpose, the wool keratin was permanently modified by chemical reduction to make its surface attractive for crosslinking with thiol moiety. Then, reduced wool's surface was enriched by immobilizing the 2-amino thiophenol (2-ATP) molecule, followed by graft copolymerization of 2-ATP through in-situ oxidative polymerization using ammonium persulfate as an oxidant. The homogenous deposition of palladium nanoparticles (PdNPs) and gold nanoparticles (AuNPs) was then ensured onto this modified fabric surface. A composite sample without 2-ATP immobilization was also prepared to compare the PdNPs deposition efficiency of the copolymer fabric. The changes in wool's structural, morphological, and surface properties were evidenced by ATR-FTIR, XPS, SEM, and contact angle measurements. Finally, the applicability of the developed composite in the catalytic reduction of nitroaromatics to aminoaromatics was examined using model nitro compounds in the presence of excess NaBH4. It was observed that the catalytic performances of the samples against selected nitro compounds were differentiated depending on their preparation route and the deposited metal nanoparticles.

Keyword: wool fabric, palladium nanoparticles, gold nanoparticles, catalytic reduction of nitroaromatics, poly(2-aminothiophenol)

# Vanadium Dioxide Cathode Electrodes for Aqueous Zn Ion Batteries

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Vanadium dioxide (VO<sub>2</sub>) is commonly utilized in thermochromic devices due to its metal-insulator-transition (MIT) feature between monoclinic (M) and rutile (R) phases at 68 °C; however, its demonstration in energy storage devices is very limited. It has unique physical and chemical properties such as high theoretical capacity, good chemical stability, and cyclability. It is emerged as a promising active material for aqueous batteries. In this work, we report on the fabrication and characterization of aqueous Zn-ion batteries (ZIBs) with VO<sub>2</sub> (M) cathodes to investigate the heat-activated capacitive properties. VO<sub>2</sub> (M) was fabricated by hydrothermal method and then annealed at 700 °C under Argon gas. Fabricated VO<sub>2</sub> (M) cathodes in this work provided MIT transition and high electrochemical capacity. Electrochemical properties such as specific capacity and cycling ability of aqueous ZIBs were then investigated through cyclic voltammetry, chronopotentiometry, and electrochemical impedance spectroscopy. A specific capacity of 200 mAh/g was obtained for the fabricated VO<sub>2</sub> (M) cathodes. We will present a detailed analysis of the electrochemical properties of the fabricated ZIBs to underline their capacitive behavior. Our results reveal the potential of the use of VO<sub>2</sub> (M) in ZIBs that can be simply adapted to an industrial scale for sustainable energy storage systems.

#### Acknowledgments:

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Keyword: vanadium dioxide, cathode, battery, energy storage

### Electrochemical Determination of Sunset Yellow in river water and some food samples

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Food dyes play an important role in the food industry, as food quality and food flavor are nearly related to the color of the food. The industrialization of food systems and the increase in food processing have rised the use of food additives like food dyes, preservatives and sweeteners (1). The synthetic food color is called Sunset Yellow (SY) (Figure 1). It is also known as 1-p-sulphophenylazo-2-naphthol-6-sulfonic acid disodium salt. It is often used as an additive in soft drinks, desserts and jellies. (2).

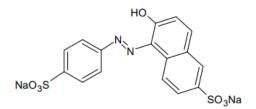


Figure 1. Chemical structure of Sunset Yellow

Metrohm-Autolab potentiostat/galvanostat system (PGSTAT128N, Netherlands) was utilized in the electrochemical analyses. All of the experiments were measured in a three-electrode system using a platinum wire, an Ag/AgCl (saturated KCl) as a reference electrode, and a glassy carbon working electrode (GCE). For the experiment, the electrode surfaces were polished with 0.3 mm alumina slurries. The alumina residues were then washed in a mixture of ethanol and water (1:1, v/v) solution and were dried. Then, 1 mg of functionalized multi carbon nanotubes (F-MWCNTs) was dispersed in 1.0 ml water and waiting for 30 min in ultrasonic bath. It was then modified by dropping F-MWCNTs onto the glassy carbon electrode and drying the modified electrode.

The electrochemical analysis was for river water and cola samples. River water and cola liquid samples were filtred 0,45 µm CA syringa filter. The Cola sample was diluted with buffer solution. Prepared samples were determined sensitively.

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Keyword: Sunset yellow, determination, electrochemical method, F-MWCNTs

# **Bio-Waste Based High Performance Supercapacitor System Design**

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As the world's population grows, so does the energy demand, necessitating the development of efficient energy storage technologies. Supercapacitors are substantial energy storage devices with the capability of supplying large amounts of power unlike, batteries. In today's world, many research and development efforts have been dedicated for developing low-cost and efficient electrode components. Herein, we present the performance of supercapacitor device which are obtained from biowaste based sources. The development of supercapacitor electrode material from biowaste materials aims to convert wastes into useful products and contribute to recycling. The morphological structure of the used biowaste and the effects of synthesis processes on supercapacitor performance were systematically investigated. The physical properties, morphology and specific surface area of the synthesized structures were defined by X-ray powder diffraction (XRD) and scanning electron microscopy (SEM). In this study, we demonstrate that biowaste can be appropriately activated as an electrochemical energy storage materials is attributed to the well electrochemical performance of the device performance. Furthermore, this research could guide the development of nontoxicity, high-performance, and low-cost electrodes which will be useful in energy storage devices.

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Keyword: Bio-waste, Supercapacitor, Energy storage

ID: 74 - Nanotechnology for Energy

# Silver Nanoparticle Immobilized Anion Exchange Membranes for Reverse Electrodialysis to Generate Salinity Gradient Power

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Recently, energy conversion and storage technologies have gained a significant interest. Reverse electrodialysis (RED) is very widely investigated, non-polluting and sustainable electromembrane process [1,2]. It extracts electrical energy from the mixing of two salt solutions with different salinity, such as river water and seawater. Cation- and anion-exchange membranes (AEMs) are used for selective ionic transport in this process. Among those, AEMs are more complex to fabricate, usually requiring multiple steps including toxic chemicals such as chloromethyl groups. Furthermore, biological fouling of ion exchange membranes is another limiting phenomenon that is usually valid for this type of membrane in the case of the use of natural feed waters [3]. Thus, to overcome these major issues and to increase the power generating performance in RED, polyepichlorohydrin based AEMs with inherent chloromethyl groups were simply fabricated using a single-step chemical reaction by solvent evaporation [2]. Subsequently, dipcoating method was used to integrate 100 nm-silver nanoparticles onto AEMs to enhance antifouling property. Finally, RED performance was measured using artificial salt solutions as feed. The results show that AEMs with high hydrophilicity and low electrical resistance (i.e. high conductivity) were obtained. The optimum composition of the membranes provided the highest ion exchange capacity (3.470 mmol/g dry membrane), highest fixed charge density (5.250 mmol/ g H<sub>2</sub>O), and lowest swelling degree (66 %). Silver nanoparticle integrated AEMs also exhibited high resistance towards biological activity. In addition, these AEMs when coupled with commercial Neosepta cation exchange membranes provided satisfyingly high power density (0.4 W/m<sup>2</sup>).

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Keyword: salinity gradient power, reverse electrodialysis, silver nanoparticle, anion exchange membrane, antifouling

### Synthesis of co-doped PANI Based Electrode Materials for Electrochemical Energy Storage

### Beray Alvakut<sup>\* 1</sup>, Hasan Altınışık<sup>1</sup>, Bengü Getiren<sup>2</sup>, Furkan Soysal<sup>3</sup>, Zafer Çıplak<sup>4</sup>, Aslıhan Öztürk<sup>1</sup>, Nuray Yıldız<sup>1</sup>

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In this work, it is aimed to prepare co-doped polyaniline (PANI) including graphene family materials such as graphene oxide, reduced graphene oxide (macherla et al. 2021), via one-step in-situ polymerization in H<sub>2</sub>SO<sub>4</sub> and DBSA aqueous media having high specific capacitance, high energy, and power density for supercapacitor applications (Ajay et al. 2021). Herein, the effects of doping agent concentrations and aniline monomer amount on the capacitive behavior were investigated. The chemical structure and morphology of synthesized binary nanocomposites were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, X-ray photoelectron spectroscopy (XPS), and Fourier transform infrared (FTIR) spectroscopy. Moreover, the electrochemical properties were characterized by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The results showed that co-doping of PANI promoted electrochemical properties of PANI based electrode materials. The maximum specific capacitance was obtained with NrGO/PANI as 566.25 F/g at a scan rate of 10 mV/s and 341.07 F/g at a current density of 1 A/g in a two-electrode configuration. The unique morphologic structure of the nanocomposite, and synergistic effect of graphene family materials and PANI ensure the binary nanocomposite to be a promising electrode material for supercapacitor applications (Ji et al. 2021).

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Keyword: Polyaniline, reduced graphene oxide, nitrogen doped reduced graphene oxide, nanocomposite, supercapacitor

# Synthesis of Au-MnO<sub>2</sub>/PANI Nanocomposites for Electrochemical Energy Storage

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In this work, it is aimed to synthesize Au-MnO<sub>2</sub>/PANI nanocomposites via in-situ polymerization using H<sub>2</sub>SO<sub>4</sub> and DBSA dopants having (Cıplak and Yıldız, 2019) high specific capacitance, high energy, and power density for supercapacitor applications. For the synthesis of Au-MnO<sub>2</sub>/PANI, gold(III) chloride (HAuCl<sub>4</sub>) is used as a precursor for Au nanoparticles, potassium permanganate (KMnO<sub>4</sub>) is used as an oxidizing agent for aniline polymerization (Zeplin and Neiva, 2021) and manganese(II) chloride (MnCl<sub>2</sub>) as the precursor for MnO<sub>2</sub> nanoparticles. In this report, the effect of gold nanoparticles on the capacitive behavior was investigated (Jadhav vd., 2021). The chemical structure and morphology of synthesized Au-MnO<sub>2</sub>/PANI nanocomposites were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and Fourier transform infrared (FTIR) spectroscopy. Moreover, the electrochemical properties were characterized by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) using a potentiostat/galvanostat. The results showed that the maximum specific capacitance of Au-MnO<sub>2</sub>/PANI reached up to 520.6 F/g at a scan rate of 10 mV/s and 307.4 F/g at a current density of 1 A/g in a two-electrode configuration. The unique morphologic structure of the nanocomposite, and synergistic effect of Au-MnO<sub>2</sub>/PANI ensure the nanocomposite to be a promising electrode material for supercapacitor applications.

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Keyword: Polyaniline, metal nanoparticles, metal oxide nanoparticles, supercapacitor

# Development and Application of New Non-toxic and High Performance Supercapacitor cell:La<sub>2</sub>O<sub>3</sub> @CuO

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Developments of contemporary and quilted multifunctional materials play a pivotal role in today's technology-oriented life. Recently, the necessity for modern, economical, high efficiency yet ecological and non-toxic energy storage systems also come to the forefront. Among energy storage devices Supercapacitors (SC) compel attention due to having almost limitless lifespan, and outstanding charge-discharge capability with high power density [1-2]. However, the low energy density of SCs, in contrast to batteries, is the most drawback restricting their utilization. Although, pseudocapacitors can boost the specific capacity via battery–like redox reactions they also contend water decomposition that limits the voltage window of aqueous electrolytes. Ultimately, enhancing the working potential window of aqueous SCs is one of the main problems that need to be addressed [3-4].

The goal of this study was to develop a novel supercapacitor cathode electrode material owing to a high potential window in an aqueous electrolyte with a nontoxic structure. The study exhibits the rationale form and synthesis of a hybrid material (La<sub>2</sub>O<sub>3</sub>@CuO) with binary functionality: at high voltage supercapacitor electrode and excellent antibacterial agent. The La<sub>2</sub>O<sub>3</sub>@CuO hybrid structure was obtained by conjoining Copper Oxide molecules towards La<sub>2</sub>O<sub>3</sub> by ultrasonication route at 60°C, after the calcination at 300°C for 1 hour at a rate of 1°C min<sup>-1</sup>, in flowing air. When the specific capacitance of pure CuO was 243 F g<sup>-1</sup> at a current density of 1 A g<sup>-1</sup> with a potential range of 0-0.42 Volt, La<sub>2</sub>O<sub>3</sub>@CuO hybrid material achieved 354 F g<sup>-1</sup> at the same current density with -1.2-0.42 voltage range (1.2 volts more than pure CuO) with good rate capability even at 20 A g<sup>-1</sup>. Moreover, the cyclic stability of the hybrid material was also better than pristine Copper oxide, the degradation was just 8% after 10000 cycles while the retention of the specific capacitance of CuO was 83% after 10000 continuous cycles. Additionally, the antimicrobial kinetic test results of E. coli; it was obtained that the composite (La<sub>2</sub>O<sub>3</sub>@CuO) owned improved bactericidal activity. With these outstanding results, the formed non-toxic hybrid material is ponderable a promising cathode material for aqueous SCs.

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Keyword: supercapacitor, antimicrobial, hybrid material

ID: 253 - Nanotubes and Nanowires

Tactile Sensors Based on Nanocomposites of Multi-walled Carbon Nanotube and Alginate

Not presented.

#### Effect of Different Solvents in the Synthesis of Boron Doped Ordered Mesoporous Carbons

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Fuel cell technology has the potential to replace the conventional, fossil fuel based technology in transportation applications. However, there is a need for development of cost-effective nanomaterials for the electrocatalysis of oxygen reduction reaction occuring at the fuel cell cathode. Boron doped ordered mesoporous carbons (B-OMC) are promising materials as metal-free electrocatalysts for the cathode reaction [1-4]. The catalytic activity of these materials depend on their chemical and structural properties such as the surface groups, boron doping amount, surface area and pore size. Synthesis of B-OMC is typically carried out in ethanol/water solution, primarily due to the availability of its constituents [5,6]. In this study, B-OMC synthesis was carried out in different solvent media, including isopropanol, n-propanol, acetone and acetic acid. Materials were synthesized using a one-pot self assebly technique, where boric acid was used as boron dopant, resorcinol and formaldehyde as carbon sources and pluronic F127 triblock copolymer was used as the structure directing agent. Polymers were carbonized at 750 °C under a controlled inert atmosphere. Resultant B-OMC samples were characterized by X-ray diffraction analysis (XRD), fourier-transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), nitrogen adsorption, Xray photoelectron spectroscopy (XPS) and cyclic voltammetry (CV). It was observed that all samples except for that prepared in isopropanol possessed ordered and mesoporous structures with surface areas varying between 381 and 607  $m^2/g$ . The samples prepared by ethanol and n-propanol had more ordered structures and higher BET surface areas compared to other samples. Pore sizes varied between 5-10 nm. The boron contents of samples varied between 0.48 and 1.38%. Cyclic voltammetry measurements showed higher activity in samples prepared in ethanol/water and n-propanol/water, due to advantageous structural properties such as high surface area and boron doping content.

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Keyword: Ordered mesoporous carbon, Boron doping, Fuel cell, Cathode

# Electrodeposition of Nanosized PbOx-doped poly(pyrrole-co-carbazole) in Acetonitrile on Stainless-steel Electrode for Supercapacitor Application

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As energy storage devices become popular, research into electrochemical supercapacitors has sped up because of their similarities to capacitors and batteries [1]. They have higher specific energy and power than regular capacitors, making them suitable for faster charging in advanced technology applications. In recent years, metal oxide/conducting polymer composites as supercapacitor electrode active materials have attracted considerable attention due to their large specific surfaces, good ion accessibility, high conductivity, and mechanical durability. The most studied electrode material is polypyrrole (PPy), which exhibits high conductivity, low cost, reversible redox property, large power density, and ease of penetration. Metal oxides are preferred because of their excellent conductivity, relative stability, and affordability [2].

*In this study, the electrochemical synthesis of poly(pyrrole-co-carbazole) (p(Py-co-Cz))/PbO<sub>x</sub> composite on stainless steel mesh electrode in acetonitrile/LiClO<sub>4</sub> solution with pyrrole, carbazole, PbClO<sub>4</sub>, HClO<sub>4</sub>, H<sub>2</sub>O, and sodium carboxymethyl cellulose (CMC) using galvanostatic pulse deposition method. Since the current is applied for short periods in the presence of both monomers, p(Py-co-Cz) copolymer chains occur in short lengths, suitable for supercapacitor electrodes. The tricyclic carbazole units located between the pyrrole rings were obtained in copolymer chains. The composite coating was characterized using SEM, EDX, XRD, and XPS. XRD analysis exhibited the presence of PbO.H<sub>2</sub>O, Pb<sub>3</sub>O<sub>4</sub>, a-PbO<sub>2</sub>, and b-PbO<sub>2</sub>. In the XPS analysis of the composite, Pb(IV)4f<sub>7/2</sub>, 4f<sub>5/2</sub> and Pb(II)4f<sub>7/2</sub>, 4f<sub>5/2</sub> were observed. While SEM images of the composite film displayed small grains on a cauliflower structure of the polymer, EDX mapping results indicated the grains of PbO<sub>x</sub> (3% atomic percentage of Pb) encapsulated into the composite. The effect of additives on the capacitive behavior of p(Py-co-Cz)/PbO<sub>x</sub> composite (10 mg cm<sup>-2</sup> loading) was studied in 0.1 M Na<sub>2</sub>SO<sub>4</sub> solution using cyclic voltammetry and electrochemical impedance spectroscopy. Despite the small quantity of nano-size PbO<sub>x</sub> in the composite, it contributed significantly to specific capacitance due to the homogeneous distribution. The specific capacitance of the composite was 325 F g<sup>-1</sup> at 100 mV s<sup>-1</sup>. The copolymer has higher C<sub>m</sub> and lower R<sub>et</sub> values as well as higher porosity that improves ion transport, thus greater stability than the homopolymers. An asymmetric cell was constructed and tested in PVA/Na<sub>2</sub>SO<sub>4</sub> gel electrolyte.* 

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Keyword: Supercapacitor, Electrosynthesis, Composite, poly(pyrrole-co-carbazole), Lead oxide, PVC

# Controlled Calcination of TiO<sub>2</sub> Bronze Nanotubes and its Enhanced Electrochemical Performance as an Anode for Li-ion Battery Application

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In the current study, titania's bronze phase, TiO<sub>2</sub>(B), were synthesized, characterized, and tested as a high-capacity and durable anode for Li-ion battery from the naturally abundant and low-cost anatase precursor, TiO<sub>2</sub>(A). As a result of hydrothermal process in an alkaline media, TiO<sub>2</sub>(A) powders can be converted to the titanate's nanotubes (TNT) [1]. Thanks to the TNTs' elongated and scrolled morphology, the Li-ions can easily intercalate and be reduced within these channels, and this leads to the pseudocapacitive behavior and an enhanced capacity during cycling [2]. The calcination process can extract the extra water existing in TNT and brings about a phase with a wider van der Waals gap, TiO<sub>2</sub>(B) [3]. So far, studies concerning the TiO<sub>2</sub>(B) synthesis have utilized  $O_2$  -containg atmosphere for calcination of the TNT, and this results in a structure comprising a combination of TiO<sub>2</sub>(B) & amp; TiO<sub>2</sub>(A). In the current study, for the first time, the effect of various calcination temperatures and durations under an Ar-controlled atmosphere were thoroughly investigated to minimize the presence of contributing TiO<sub>2</sub>(A) due to its limited Li-ion diffusivity. Firstly, X-ray diffraction (XRD) patterns showed that calcination at 500 brings about the highest TiO<sub>2</sub>(B) contributing phase. Results of scanning electron microscope (SEM) and transition electron microscope (TEM) proved that 10 hrs of calcination at 500 (HT-10) could preserve the nanotube morphologies, and elongated calcination resulted in a spherical morphology. The peak current existing in cyclic voltammograms (CV) showed that the higher contribution of TiO<sub>2</sub>(B) could be attributed to HT-10. Galvanostatic charge/discharge tests after 100 cycles illustrated that HT-10 obtained the comparatively highest capacity, around 250 mAh/g at 99.5 mA/g. Electrochemical impedance spectroscopy spectra illustrated that the fastest charge transfer kinetics belongs to HT-10. After 500 cycles, HT-10 could preserve the capacity around 225 mAh/g at 99.5 mA/g. The obtained electrodes showed a potential of this material as a safe and promising alternative for the commercial graphite.

# Sintering CuSbSe<sub>2</sub> Alloy and Characterization of CuSbSe<sub>2</sub> Thin Films for Photovoltaic Applications

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The solar market is expeditiously growing to satisfy the increasing energy demand in a sustainable way [1]. Therefore, the diversity of materials which are used for photovoltaic applications is increasing. Although CuInSe<sub>2</sub> is a promising material in this area with an ideal band gap, high absorption coefficient and high conversion efficiency, it is not a low price material due to the cost of indium (In) [2,3]. In this study, our motivation is introducing a cost efficient alternative material to CuInSe<sub>2</sub>. For this reason, indium (In) is replaced with Sb and CuSbSe<sub>2</sub> structure is obtained. Besides its relatively low cost, it is known that CuSbSe<sub>2</sub> has orthorhombic structure with 2-D behavior and this is highly desirable to prevent dangling bonds [4,5]. In this study, the elements were filled in a crucible after their weights are measured carefully. Then, the crucible was sintered in a furnace whose temperature was increasing fractionally for obtaining a homogeneous CuSbSe<sub>2</sub> alloy. As a next step, CuSbSe<sub>2</sub> thin films were deposited on glass substrates by e-beam physical vapor deposition by using the CuSbSe<sub>2</sub> powder which was obtained by grinding the sintered alloy. Furthermore, a group of samples were annealed in nitrogen (N) environment to analyze the effect of heat treatment. The stoichiometries of as grown and annealed samples were investigated by Energy Dispersive X-Ray Spectroscopy (EDAX) and the stuctural parameters have been calculated by using the outcome of X-Ray Diffraction (XRD) measurement. Also, absorption coefficients were measured by using UV-Vis Spectroscopy and optical band gap values have been obtained. The conductivity values and the effect of annealing on the structural, electrical and optical properties have been investigated.

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Keyword: Sintering, Thin Film Deposition, Thin Film Characterization

# Experimental Investigation of Hydrogen Production as a Result of the Reaction of Aluminum with Water.

#### <u>Rasiha Nefise Mutlu</u><sup>\*</sup>, Esra Eroğlu, Hande Toffoli, Mehmet Karaca, Jayaraman Kandasamy, İskender Gökalp Middle East Technical University, Ankara, Turkey

Hydrogen generation via water splitting is an important part of the clean energy production effort. Thanks to its abundance, high reactivity and low toxicity, aluminum (Al) has broad application in this field. The hydrolysis reaction of aluminum is utilized for producing hydrogen [1,2]. Aluminum is found in nature with an oxide layer on its surface. Even if the oxide is removed, aluminum tends to reoxidize upon contact with air. It is known that the oxide dissolves upon contact with NaOH. The hydrogen production occurs on a bare aluminum surface under the oxide layer. During the hydrolysis experiments, the removal of the oxide layer is monitored by employing impedance measurements. The change of real resistances versus time are recorded to detemine aluminum oxide disappearance times for different (0.5-4 M) NaOH concentration and for different temperature (25-70°C) in 0.5 M NaOH. The pure wire form (99.86 %) aluminum is used for these measurements. The activation energy for the two different forms of aluminum, powder and wire, was determined experimentally through the Arrhenius equation.

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Keyword: Hydrogen Energy, Hydrolysis, Aluminum, Green Energy

# Sunlight-Triggered Controlled Release System Based on Polydopamine Coated Halloysite Nanotubes

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An environmentally friendly sunlight-triggered controlled release system, which allows control of when and at what dose an active substance will be released, is presented. The smart controlled release system consists of a photothermal nanocarrier, that can be remotely heated by sunlight and a heat-activatable stopper that can be removed via sunlight-triggered heating of the nanocarriers. Photothermal nanocarriers that heat up when exposed to sunlight were obtained by the functionalization of halloysite nanotubes (HNTs) with a polydopamine (PDA) layer. Obtained HNT-PDA nanocarriers were impregnated with carvacrol, an essential oil, that served as a model active substance. Lauric acid (LA), an active component of coconut oil, is utilized to further the functionalization of HNT-PDA nanocarriers as a stopper by plugging their pores and tube ends. The LA stopper was demonstrated to slow down and hinder the carvacrol release in dark. When the HNT-PDA nanocarriers were irradiated with sunlight. When the HNT-PDA nanocarriers were irradiated with sunlight irradiation for 6 h, and the carvacrol release stopped when the sunlight irradiation was turned off demonstrating that the release of carvacrol molecules that were entrapped in the HNT-PDA nanocarriers can be controlled with sunlight. The potential application of the presented controlled release system for sunlight-activated pesticide release will be discussed.

Keyword: halloysite nanotube, photothermal nanomaterials, phase change materials, lauric acid, sunlight-triggered controlled release

# Facile Fabrication of Electrospun Fiber-Based Green Slippery Lubricant Infused Surfaces for Antimicrobial Activity

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Bacteria found in all kinds of synthetic and natural environments tend to adhere on the surface and form biofilm layers that can be defined as multicellular communities. The adhesion and biofilm formation on surfaces by bacteria causes loss of capital, labor and energy in terms of materials. Due to their resistance to large-scale antibiotics, treatment of biofilms is difficult and overcostly. Lately, researchers have been aimed to fabricate antimicrobial surfaces to prevent bacterial adhesion and biofilm formation by changing the topography of surfaces with the help of bio-inspiration. *Nepenthes*-inspired a novel material named slippery liquid-infused porous surfaces have been developed as a new strategy. SLIPS contain an operationalized hydrophobic substrate and a lubricant layer for slippery effect. Under favour of porous structure on its surfaces, operationalized hydrophobic surface traps the lubricant liquid in its pores. However, most of the reported SLIPS were produced by infusing silicon oil, fluorine containing oils and petroleum-based hydrocarbons and synthetic oils as lubricant. In this regard, the use of these expensive, ungreen and chemical-based lubricants conflicts with this non-toxic approach.

Within this scope in this research, fiber-based SLIPS were produced by using a medicinal, antimicrobial St. John's Wort oil as a lubricant. Firstly, porous cellulose acetate (CA) Nanofibers were coated on substrate. The porous morphology was showed in SEM micrographs and fiber diameter and pore size diameter was measured as  $1356.37 \pm 496.287$  and  $413.91 \pm 173.52$  nm by using ImageJ software.

Subsequently, porous CA fibers were coated to glass substrate by placed to collector via electrospinning technique at voltage 15 kV, flow rate of 1 mL.h<sup>-1</sup>, 10 cm needle-collector distance, room temperature and 20% relative humidity. Super hydrophobicity of produced surface was showed in static water contact angle (WCA) measurements, and it was determined as  $160.94 \pm 16.02^{\circ}$ . For produce SLIPS, St. John's Wort Oil was infused into produced superhydrophobic surface. Integration between bio-lubricant and fiber was proven and the pores in the fiber structures was filled with bio-lubricant was demonstrated with obtained SEM micrographs properly. WCA value of produced SLIPS was measured as  $74.65 \pm 2.30^{\circ}$ . Moreover, the antimicrobial effects of fabricated SLIP surface using bio-lubricant were demonstrated against *Staphylococcus aureus*. CAcoated glass surfaces were demonstrated poor antibacterial activity which 520 colonies of *S. aureus* was counted on the agarplate. Through infusion of bio-lubricant into surfaces, antibacterial activity was increased and produced SLIP surfaces exhibited 100% antibacterial activity.

Keyword: antimicrobial activity, electrospinning, green lubricant, slippery liquid infused surfaces

# Self-assembly of redox-active nano/microstructures at the air/water interface

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Self-assembly can be achieved with the help of molecular level interactions such as hydrophobic/hydrophobic interactions, van der Waals interactions,  $\pi$ - $\pi$  stacking and hydrogen bonding [1-2]. Amphiphilic molecules such as peptides, proteins and especially lipids can self-assembly form nanostructures in solution, as well as form nanostructures with nanotube, helix or planar morphology at air/water interfaces [3]. These nanostructures obtained by the proper alignment of the molecules at the interfaces can find a place in various areas such as microfabrication for medical applications, microelectronics and biosensing according to their functions [4]. Among those applications, synthesis of hybrid materials or nanocomposites with desired properties such as having biocompatibility and still pertaining catalytic activity or conductance could be crucial [5]. An anionic and amphiphilic (Anthraquinone) molecule, AQua (AQ-NH-(CH2)10COOH), which has two stimuli responsive functionalgroups, can form self-assembled interfacial aggregates at the air/water interface and, their morphologies can be controlled by changing the subphase conditions such as the pH of the subphase. These interfacial morphologies may be altered from planar structures to wormlike aggregates which is a very rare observation in the literature. Moreover, the unique functional groups of AQua give possibility to reduce metal cations and allow the formation of organic/inorganic nanocomposite structures at the interface. The main feature that makes the AQua molecule different from other lipids is the presence of AQ group in its molecular structure. The AQ group can be reduced chemically and electrochemically with a potential of the combination of self-assembling properties with redox activity and charge transport properties. By this way, these structures may find usage as redox-switches in molecular electronics or charge transporting organic semiconductors in photovoltaics, field-effect transistors and light-emitting diodes. This study demonstrates that interfacial configuration of the AQua molecule at the interface as well as its orientation has a vital role in the morphology of either organic or inorganic self-assemblies formed. The morphology may be adjusted and designed interfacial structures may be obtained. Based on these results obtained within the scope of the study, these unique structures will create the potential to be used in different fields from medicine, biotechnology, and engineering to sensor applications with various modifications.

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Keyword: AQua, Air/water interface, Self-assembly, Worm-like aggregates

#### ID: 32 - Novel Applications of Nanostructured Materials

# Mechanical Properties of TiO2 Nanoparticle-coated Glass Fibers

# <u>Mustafa Ordu</u>\* Bilkent University UNAM, Ankara, Turkey

Glass fibers are widely explored as reinforcement materials for composites due to their low cost, lightweight, high strength and reliable mechanical properties. In our study, different concentrations of nanoparticle coatings were applied to the surface of E-glass fibers to reduce the defects density, thereby enhancing the mechanical property of glass fiber. Tensile strength of glass fibers increased up to 12% with TiO<sub>2</sub> nanoparticle coating. In addition, fractographic examinations of the broken fibers have revealed a linear relationship between the tensile strength and the morphology of fibers' cross-sectional areas. The nanoparticle-coated fibers are expected to have a positive impact on the mechanical properties of the fiber-made composite.

Keyword: Nanoparticle coating, glass fibers, Titanium dioxide

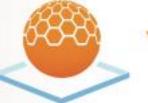
# A Novel and Highly Efficient Electrochemical Nanosensor for the Determination of an Anticancer Drug Nelarabine

#### <u>Md Zahirul Kabir</u><sup>\*</sup>, Cem Erkmen, Sevinc Kurbanoglu, Gözde Aydoğdu Tığ, Bengi Uslu Ankara University, Ankara, Turkey

Nelarabine is an FDA-approved potent anticancer drug used for the treatment of T cell acute lymphoblastic leukemia and T cell lymphoblastic lymphoma. In this study, the sensitive detection of nelarabine was carried out at the bare and the modified glassy carbon electrodes (GCEs) using differential pulse and cyclic voltammetry techniques. The decoration of bismuth oxide (Bi<sub>2</sub>O<sub>3</sub>NPs) and silver nitrate nanoparticles (AgNPs) as well as electrochemically reduced graphene oxide (ERGO) onto the surface of GCE developed a novel and highly efficient electrochemical nanosensor. The nanosensor based on Bi2O3NPs-AgNPs-ErGO/GCE was characterized using field emission scanning electron microscopy, electrochemical impedance spectroscopy, and cyclic voltammetry investigations. Effects of the loading of different nanoparticles on the modified GCE, electrolyte pH, accumulation potential and time, and scan rate were optimized for the drug response. The current responses toward the oxidation of nelarabine was more than 14 times higher with the suggested nanosensor compared to the bare GCE. The nanosensor exhibited a linear range between 0.025 and 1 µM with a limit of the detection value of 1.59 nM. The designed nanosensor showed excellent reproducibility, repeatability, and storage stability, which clearly indicated the effective accuracy of the developed nanosensor. The involvement of diffusion-controlled and adsorption-controlled mechanism processes was found at the bare GCE and the nanosensor, respectively, for the electrochemical manner of nelarabine. The DPV results revealed the linearity in the calibration curves at both the bare and the nanosensor, upon increasing concentrations of nelarabine. Satisfactory recovery results were obtained from 98 to 103% at the suggested nanosensor in nelarabine detection from its pharmaceutical dosage form and human serum sample. Moreover, the designed nanosensor was found selective toward nelarabine in the presence of various interfering agents.

Keyword: Nelarabine, Ag nanoparticles, Bi2O3 nanoparticles, Reduced graphene oxide, Electrochemistry





# Yüzey ve Malzeme Karakterizasyonu

- Biyomalzeme Geliştirme Sistemleri
- Fizîksel Test Cîhazlan
- Ince Flim Oluşturma ve Karakterizasyon Sistemleri
- Kalorimetreler
- Katalizör Karakterizasyon Sistemleri
- Partikül ve Gözenekli Malzerne
- Karakterizasyon Sistemleri

- Piroliz Üniteleri
- Plazma Karakterizasyon Sistemleri
- RGA Kütle Spektromentre Sistemleri
- Taramalı Uç Mikroskopları (SPM)
- Temas Açısı ve Yüzey Gerilimi Ölçüm Cihazları
- Yúzey Kaplama Sistemleri
- Yůzey ve Gôzeneklilik Karakterizasyon Sistemleri



ID: 73 - Novel Applications of Nanostructured Materials

# From the Nature of Chaotic Instabilities to High-level Security Applications: Physically Unclonable Systems via Electrospraying

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In today's world, where global commerce and information technologies are rapidly developing, the economic losses caused by counterfeit goods, currency, or identity, as well as the health and safety risks associated with counterfeiting cannot be underestimated. Conventionally used cryptographic primitives are clonable due to their deterministic fabrication processes as well as predictable encoding and decoding mechanisms. A promising solution that has gained recent attention involves the exploitation of physically unclonable functions (PUFs)[1,2]. In this approach, the response of the encoded surface against a challenge is determined through a physical and stochastic process[3]. This stochasticity and inherently random responses against challenges prevent the replication of encoded surfaces by third parties or even by the manufacturer itself. However, simultaneously meeting the requirements of an ideal PUF including low-cost fabrication, versatility, practical coding-decoding-and-authentication, and high-level security with multi-layered security measures is still challenging.

Herein we present a novel strategy for integrating all the benefits of low-cost fabrication, easy authentication, and multi-layered high-level security into a PUF system via electrospraying technique. The approach called "E-spray PUFs" has many peculiarities. The key advantage of this strategy is that electrohydrodynamic instabilities resulting from the chaotic interaction of different intertwined forces that occur during the process offer a very useful way to generate random complex features. It has been shown that nanoscopic, microscopic, and/or nanostructured features are obtained effectively and in a controlled manner by simply adjusting the electrospraying parameters. Besides the randomness in the spatial positions and sizes of the features, another enabling characteristic of the presented approach is the ability to generate complex 3D shapes, which are very challenging to fabricate with the most advanced fabrication techniques. E-spray PUFs obtained by using a wide range of polymers have very high encoding capacity and near-ideal figure of merits (randomness, uniformity, reliability, etc) values.

Thanks to the solution-based and additive operation nature of the process, it enables polymeric structures functionalized with multiple materials to be sequentially electrosprayed on the same substrate. In this way, fluorescence molecules with distinct photophysical properties, quantum dots emitting at specific wavelengths or metallic nanoparticles with plasmonic properties can be directly cooperated into the features or site-specificly immobilized on the surface of the features[4]. The resulting multiplexed PUFs can be authenticated at different levels, which can be performed independently. Extra coding layers are established with coherent aspects such as spatial random positions and complex morphologies on the surface of sequentially deposited structures, photophysical behavior of functional materials in the structure, structural colors, specific wavelengths, surface-enhanced plasmon properties, etc. In addition to the direct application of PUFs on the label of goods, practical and precise authentication approaches of these PUFs are also presented The authentication steps of optical responses are effectively performed using ORB algorithm without the need for markers and precisely defined rotation angles, greatly relaxing constraints associated with the imaging. Finally, authentication via compact microscopes demonstrates the practical utility of the presented strategy.

#### Acknowledgements:

This work was supported by TUBITAK under Grant No: 119F384.

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Keyword: physically unclonable functions, quantum dots, functionalized polymers, encoding, electrospraying

# Evaluation of Effect of Nano Molybdenum Disulfide on Performances Characteristics of Lithium Soap and Calcium Sulfonate Complex Greases

#### <u>Sevda Şahan</u>\*, Ece Korkut

Petrol Ofisi Technology Center, Kocaeli, Turkey

Molybdenum disulfide mostly used for developing especially extreme pressure properties of different type of lubricating products. In this study, we have been investigated and reported the performance effects of particle size of molybdenum disulfide on final product as a grease additive on lithium soap and calcium sulfonate complex greases. Both fine powder molybdenum disulfide and nano molybdenum disulfide have been applied with % 1, % 3 and % 5 ratios on lithium soap and calcium sulfonate complex greases. Tribological performance tests have been applied and reported. We have been evaluated the usage of nano molybdenum disulfide as a performance additive on different type of greases. And we have been reported the performance advantages and disadvantages of nano molybdenum disulfide as a grease extreme pressure additive according to fine powder molybdenum disulfide.

Keyword: Nano molybdenum disulfide, Fine powder molybdenum disulfide, grease, extreme pressure, tribology

# Photovoltaic Synaptic Biointerfaces based on InP-ZnS Quantum Dots

#### <u>Ridvan Balamur</u><sup>\*</sup>, Güncem Özgün Eren, Hümeyra Nur Kaleli, Onuralp Karatum, Sedat Nizamoğlu Koç University, Istanbul, Turkey

Humans are capable of perceiving and reacting to external stimuli such as light, sound, and chemicals. One can easily lose the ability of vision with the degeneration of those photoreceptors in the retina. Therefore, there is a need for an artificial synaptic device to replace the degenerated retina. Instead of biological cells, light activated synapses should combine sensing, synaptic functions, and bioelectronic stimulation in one device. Biologically inspired silicon-based devices have been developed and successfully emulated common synaptic functions such as, short-term plasticity (STP) and long-term plasticity (LTP). While those studies perform the detection and signal processing functions, they are limited in transferring these signals to the biological environment.

Here, we combine a photovoltaic artificial synaptic device based on InP/ZnS quantum dots with hippocampal neurons to establish a biohybrid synapse with ROS-mediated synaptic plasticity. Unlike other studies, our synaptic devices not only mimic basic synaptic behaviors by applying stimuluses depending on intensity, duration, and frequency, but are also capable of stimulating hippocampal neurons dependent on modulated input. The use of organic-biocompatible QDs can create significant impact on future retinal implants and neuromorphic computing systems.

Keyword: Neuromorphic, Synapse, Plasticity, Quantum dot, Biointerface

ID: 193 - Novel Applications of Nanostructured Materials

# Fabrication, Characterization and Sensing Performance of ZnO Based Surface Acoustic Wave Gas Sensors

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#### Introduction

Volatile organic compounds (VOCs) such as acetone, ethanol, benzene, toluene, and xylene are widely used in the industry and daily life. Monitoring of VOCs is essential due to their harmful effects to human health [1]. Therefore, there is a big demand for the fabrication of highly sensitive, selective, and stable gas sensors in recent years. To meet these requirements various types of sensors such as chemiresistive, surface acoustic wave (SAW), optical, electrochemical, etc. have been developed. Among them, SAW sensors have attracted much attention due to their advantages such as low cost and high sensitivity [2].

Sensing layer plays a key role in the SAW sensors [3]. It is known that semiconductor ZnO-based materials have been widely used in gas sensor applications for many years due to their superior properties such as low cost, easy nanostructural production, good adsorption ability against various gases, and adaptability to microelectronic fabrication [4, 5].

In this study, the SAW sensor platform has been coated with nanostructural ZnO sensing layer to investigate gas sensing properties towards VOCs such as acetone, ethanol, xylene, and toluene.

#### Experimental

The SAW sensor platforms were fabricated by photolithography. ZnO nanorods were coated by hydrothermal technique on SAW sensor platforms. A scanning electron microscope (SEM) equipped with electron dispersive spectroscopy (EDS), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) were used to characterize the fabricated samples. The fabricated SAW sensors were tested against acetone, ethanol, toluene, xylene, and relative humidity.

#### **Results and Discussion**

Figure 1 shows SEM images of ZnO nanorods. As seen in Figure 1, nanorods have homogenously covered the SAW sensor platform. ZnO nanorods are vertically aligned and average 44 nm in diameter.

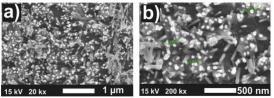


Figure 1. SEM images of ZnO nanorods sensing element.

Gas sensing measurements of SAW sensors were performed against VOCs with various concentration. Moreover, the sensing performance of SAW sensors in relative humidity ambient was investigated. As seen in Figure 2, gas sensor tests showed that ZnO-based SAW sensors could be used for monitoring the VOCs.

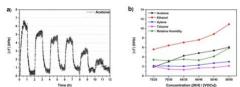


Figure 2. Gas sensing performance of ZnO based SAW sensor: a) Dynamic sensor response peaks against various concentration of acetone and b) Sensor response curves against various VOCs and relative humidity.

#### Acknowledgements

This work is financially supported by Scientific and Technological Council of Turkey (TUBİTAK) project number 119E396. **References:** 

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Keyword: Surface Acoustic Waves (SAW), Gas Sensor, ZnO, VOCs

#### ID: 216 - Novel Applications of Nanostructured Materials

# Controlled Growth of Mo<sub>2</sub>C MXene Films and Flakes by Copper and Indium Metal Catalysts

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Transition metal carbides provide a widely attended two-dimensional compound as MXenes concept used in biomedicine to energy conversion fields. Molybdenum carbide ( $Mo_2C$ ) is a MXene family member with a promising photoelectric behavior that has been mainly formed by the chemical vapor deposition technique. The fabrication specifications are refined to produce a wide and thin structure1,2. In case, better physical characteristics and flake transfer capability are affected by catalyst metal intrinsic properties, precursor gases flow rate and process temperature2,3.

As the gas flows and temperature are the most controllable parameters, this approach delineates the precisely engineered copper and indium metals used as catalysts in order to achieve and control the growth of MXene flakes. In this process, PVD and CVD methods are applied respectively to coordinate metal catalyst thickness and homogenous overlap in nano and micrometres scales, providing uniform MXene formation. The operational temperature is adjusted between 1000 -1150 °C. As result, the optical microscope analysis elucidates that MXene flakes incline to change their shape from dendritic to the planner by extended growth formation in average 2-30 µm diameter as the thickness of the copper thin film is increased. Also, Micro-Raman spectroscopy measurements exhibit shows that graphene layers also form under specific conditions. In summary, metallic catalysts provide us to control MXene formations with different thicknesses and substrate coverages.

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# Nanofiber Surface Coating Applications for Natural Leather

<u>Fatma Akpolat</u><sup>\* 1</sup>, Hüseyin Ata Karavana<sup>2</sup>, Mehmet Özgür Seydibeyoğlu<sup>3</sup> <sup>1</sup> Uşak University, Uşak, Turkey <sup>2</sup> Ege University, İzmir, Turkey

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In this study, it was aimed to create a new leather production system with using Nanofibers obtained from electrospinning mechanism instead of the classical leather production finishing process. It has been thought that the effect of studying in nanoscale can be expanded the working area, improved the adhesion properties, provided using less chemicals and increased the functionality of healty and comfortable natural leather materials then classical.

After beamhouse process, drum dyed leathers without finishing were placed to electrospinnig system for nanofiber coating and it has been tried to determine the functionality of the application with trials. Thermo plastic polyurethane (TPU), using in classical leather finishing process was created for nanofiber production (8% TPU-dimethylformamide) Prepared solution was applied to leather surface at different flow rate (1,2,3,4,5 ml/h), different voltage (20,25,30kV) and distance. Solution dispersion and adhesion to leather surface was characterized by SEM (scanning electron microscope), WVP (water vapor permeability) and flexometer tests. According to results, micro pores on leather surface were clearly visible and WVP was good but there were some adhension and fiber structure problems. Nanofiber optimazition parameters were controlled and solution was modified. Viscosity of solution was increased up to certain consentration (10,12,14,16,18%) and new solvents (ethyl acetate) and crosslinkers (aldehydes) were added to solution for adhesion and homogeneity of fibers. New solutions were applied to samples and results were determined again, samples were showed improvement. Co-axial electrospinning aparatus were used for the coating and some mechanical affects using for classical leather were applicated to leather samples. Then they were characterized by SEM, TGA (termogravimetric analyses), FT\_IR (frourier transform infrared spectroscopy) and AFM (atomic force microscopy) analyses and dry rubbing test.

It was concluded from all data, nanofiber coating mechanism can be suitable for leather production and can be developed by controling the system parameters. And some studies was planned with using co-axial fiber technology, these studies can be open new roads for leather features like enthalpy, water and dirt repellent, windproof etc

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Keyword: leather, nanofiber, electrospinning, TPU

# Simulation Based Design and Fabrication of a PPy Coated PDMS Based Pressure Sensor

Ece Naz Erülker<sup>\* 1</sup>, Tuğhan Ece<sup>1</sup>, Ayşe Ekicioğlu<sup>1</sup>, Faruk Can<sup>1</sup>, Güllü Kızıltaş Şendur<sup>1</sup>, Gözde İnce<sup>2</sup>

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Flexible sensors have attracted widespread attention because of their highly desired multifunctionality such as flexibility, high sensitivity, and large workable range in electronic skin or wearable health monitoring applications. Among these, piezoresistive pressure sensors are expected to deliver these functions in a stable fashion whilst being produced in a low cost and scalable manner. It is known that sensor performance directly depends on the 3D geometrical and material composition. In this study a flexible pressure sensor with a unique interconnected and porous geometry is designed and fabricated using a simulation based design approach and a two-step manufacturing technique. The substrate of the sensor is cast using Polydimethylsiloxane (PDMS) which is known for its mold-release properties and ability to replicate fine features with low shrinkage and excellent elastic properties. The 3D PDMS structures were prepared by mixing base solution and curing agent at a weight ratio of 10:1 following poured onto 3D printed molds and cured at 80 °C for over 2 h. The sensing capability of the composite material was achieved by the facile solution based dip coating method of polypyrrole (PPy) thin film onto the PDMS structure. The mechanical and electrical response of the proposed PPy coated PDMS sensor was characterized using compression tests via a multimeter setup integrated to Universal Testing Machine and a four-point probe measurement system. Micro-computed tomography characterizations were used to analyze the cast sensor's geometrical features. Simulations were carried out using Finite Element Analysis software COMSOL Multiphysics. Both simulations and measurements demonstrate that the proposed sensor delivers a stable piezoresistive behavior with high sensitivity. The proposed production technique's flexibility to produce sensors with complex 3D geometries combined with the tuning potential of the sensor's sensitivity should prove useful for a wide range of applications with different desired pressure ranges. Keyword: Pressure sensor, Piezoresistivity, PDMS, PPy, Finite element analysis, 3D printing

#### ID: 334 - Novel Applications of Nanostructured Materials

## Encoded Surfaces based on deterministic and stochastic patterning of nanomaterials

### M. Serdar Onses<sup>\* 1</sup>, N. Burak Kiremitler<sup>1</sup>, Abidin Esidir<sup>1</sup>, Nail Gunaltay<sup>1</sup>, Mustafa Kalay<sup>2</sup>

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There is an urgent need for novel encoded surfaces in anti-counterfeiting and authentication applications. Particularly, counterfeit products and infringement of intellectual property constitute a significant threat to national security, world economy and human health. Almost 10% of the commercial goods in the world are either counterfeit or pirated. In addition to their significance for anti-counterfeiting, encoded surfaces are becoming critical in hardware and data security, driven by the rapid digitization of the world.

Encoded surfaces have been conventionally prepared by deterministic pathways. In this approach, discrete geometries are patterned on the surface of objects for encoding.<sup>1</sup> One-dimensional and two-dimensional barcodes are widely utilized examples to this approach. Despite their effectiveness in addressable encoding and rapid read out, these patterns can be duplicated due to their deterministic nature of fabrication using reproducible processes. A solution to this challenge is the use of stochastic processes in surface encoding. Physically unclonable functions (PUFs) consist of random structures with a specific response and are impossible to replicate by both the manufacturer and third parties.<sup>2-5</sup> PUFs can be fabricated by using stochastic physical and chemical processes. Novel hybridization of deterministic and stochastic pathways is needed to benefit from the advantages of both approaches.

Herein we present strategies for integrating deterministic and stochastic encoding approaches in the same platform. The random domains of nanoscale materials are formed by electrospraying. PUFs can be constructed in a rapid, low-cost and versatile manner based on random placement of polymer materials, thanks to the electrohydrodynamic instability.<sup>6</sup> To fabricate PUFs within one-dimensional and two-dimensional barcodes, electrospraying is adapted with conventional microfabrication methods. In one approach, electrospraying is performed through stencil masks fabricated by laser engraving. The use of same masks with screen printing, allows for practical patterning of materials within barcoded regions for effective read-out of the first security layer, whereas the random patterns directly formed on these barcodes constitute the second layer. In a complementary approach, the use lithographically prepared templates will be discussed. Nanoscale materials can be effectively incorporated for generating complex and difficult to replicate responses. The additive characteristic of electrospraying allows for multiplex deposition of these nanomaterials, thereby improving the encoding capacity. The addressable PUFs will facilitate rapid and accurate authentication of the encoded surfaces.

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Keyword: encoded surfaces, nanomaterials, patterning

## Amphiphilic Polymer Based Nano-Reactor Systems: Organometallic Catalysts in Confined Spaces

#### Bengi Özgün Öztürk\*, Mina Aşkun, Zeynep Tunalı, Solmaz Karabulut Şehitoğlu

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Amphiphilic polymers are of great importance owing to their unique ability to form nano-sized micelle structures in water, thus providing hydrophobic reaction centers for catalytic reactions to take place[1]. In these catalytic systems amphiphilic polymer act as both surfactant and ligand precursor. The organometallic complexes that are air and moisture-sensitive can be stabilized in these pre-defined hydrophobic spaces generated by micelles in water [2]. Following the tremendous interest in the synthetic reactions catalyzed by organometallic complexes, the researchers have focused on more environmentally friendly approaches. The substitution of toxic and harmful organic solvents with water and the integration of these catalytic systems to aqueous media is a ongoing challenge. In this study, we have focused on the integration of well-known ruthenium and gold catalysts to be used in water media in various catalytic reactions such as olefin metathesis, transfer hydrogenation and alkyne hydration. Amphiphilic ring-opening metathesis polymers, as well as commercially available non-ionic and ionic surfactants are used to generate micellar catalytic systems in water media. In this contribution, we are going to summarize our recent results based on novel nano-reactors systems that were developed in our research group. The ruthenium and gold-based nano-reactor systems work smoothly in pure water and show high recyclability in metathesis, transfer hydrogenation and alkyne hydrogenation reactions.

#### Acknowledgments:

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Keyword: Nano-reactors, amphiphilic polymers, Gold, Ruthenium, Transfer hydrogenation, alkyne hydration, olefin metathesis

#### ID: 250 - Social, Economic and Environmental Effects About Nanotechnology, and Ethical Issues

## Nano-Circular: Nanotechnology for Circular Built Environment

#### <u>Hatidza Isanovic</u>\*

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Being driven by the linear 'take-make-waste' economic model, built environment has become the largest consumer of material and energy resources, and the greatest producer of emissions and waste. This can be countered by implementing the principles of the new circular economy model which is "...restorative and regenerative by design and aims to keep products, components, and materials at their highest utility and value at all times." [1] To achieve a sustainable future where buildings will no longer be detrimental for the environment, but an active part of its restoration, building solutions should utilize the novel approaches and technologies that aim for minimized consumption of raw materials, sustainable management of waste and reduced environmental impacts of material choices throughout the life cycle.

The recent advances in nanotechnological building materials demonstrate the prospect for significant improvements to performance of buildings and reduction of material consumption [2]. However, much of this is unknown among practitioners in the built environment, hence the lack of development and widespread application in building solutions. A synergy between nanoscience and built environment will be critical for the development of nanomaterials that will ensure resource efficient and circular material lifecycles and address the unmet needs for sustainable built environment.

This study explores potentials and limitations for the applicability of nanomaterials in building scale by identifying and analyzing a comprehensive array of criteria that maximize performance within a circular economy framework. These include the development of solutions for:

- *Material reduction* using less material without compromising the structural integrity, utility or aesthetics;
- Less polluting substitutes and alternatives to materials that generate harmful emissions during the manufacturing process;
- *Reusable materials* of better quality and durability thus reducing the need for production of new materials;
- *Extending the materials lifespan* instead of demolishing and rebuilding existing structures, renovating buildings in an energy-efficient way to prolong the building's longevity.

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Keyword: Nanotechnology, Circular economy, Built environment, Building materials, Resource efficiency

#### ID: 82 - Machine Learning Approaches for Nanotechnology Applications

## Machine Learning for Predicting Lead-Free Hybrid Double Perovskites

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Inorganic–organic halide perovskites represent a major break-through in the development of highly efficient photovoltaic materials. Within only several years, polycrystalline thin-film perovskite photovoltaic (PV) devices have achieved a certified power conversion efficiency (PCE) of 25.5% with lead based formamidinium lead tri-iodide (FAPbI3)[1].

Double perovskites (DPs) have attracted interest due to their ability to form highly efficient lead-free absorber materials. For finding new DPs, high throughput calculations is an efficient and widely used approach to be able to screen a large number of DP candidates. Although many inorganic lead-free perovskite cells have been studied and synthesized, there are vast prospects in researching organic-inorganic DPs, replacing lead with a mix of tin and germanium. For example, recently a stable DP, Cs2SnGeI6, has been successfully used as the absorber layer delivering a PCE of 7.11 % [2]. This success urged us to discover other possible combinations of DPs with a general formula of ABSnyGe1-yX6 with A and B are organic or inorganic cations and X= Cl, Br and I. This selection will produce thousands of possible DPs which need to be computationally screened with the density functional theory (DFT) based calculations.

Currently there are fewer structural and electronic properties of DPs in the well-known open source material databases, compared to their single counterparts, which shows us that we are still far away from considering all possible DPs. Therefore, our attempt to produce a specific computational repository on DPs will serve as a highly reliable data set, which can also be considered in machine learning (ML) studies.

To screen such perovskites, we propose a workflow employing a combination of preprocessing data with sampling methods and training the data with ML methods, and consequently conducting hybrid DFT computations for verifying the results.

We train a ML model on experimental data of perovskites, which is quite imbalanced in terms of stability of perovskites, meaning while there's an abundance of data of stable perovskites, data regarding unstable perovskites is quite few, as failed experiments go unreported. Whilst training data, this unevenness in class distribution can cause bias and prejudice in the model. To handle this problem in this study, statistical methods which help adjust the class distribution by removing unwanted noise, or producing synthetic data, e.g. undersampling and oversampling and methods, are employed in preprocessing the dataset, before training an ML model.

Having obtained an ML model with various algorithms, it can be used to predict the target criteria, such as band gap, formation energy, and formability, of new candidate structures, which are generated to create unique compositions of different stoichiometry, different cations in the A site, and halides in the X site, which amount to approximately 10000 possible DPs.

The predictions are then verified by highly precise and accurate band gap calculations carried out using hybrid DFT functional (HSE06).

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Keyword: machine learning, double perovskites, density functional theory, band gap prediction, computational screening

#### ID: 206 - Machine Learning Approaches for Nanotechnology Applications

## Hyper-Spectral Imaging Through a Multi-Mode Fiber via Machine Learning

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The use of optical fibers is of utmost importance, which provides super resolution and a small footprint [1]. Compared to a single-mode fiber, a multi-mode fiber (MMF) provides much more information due to a larger core diameter resulting in an increased number of modes. However, the increased number of modes result in scrambling of the images due to inter-modal mixing through the MMF since each of these individual modes propagates at a slightly different velocity. Therefore, the image at the fiber output appears as a random speckle pattern. This effect completely scrambles and destroys the input image. We present hyperspectral imaging through an MMF with a spatial light modulator (SLM). We developed neural network [2] to reconstruct hyper-spectral images and classify corresponding speckle patterns at telecommunication wavelength.

# Accelerating Materials Discovery with Machine Learning: A case study with Graphene and DFT

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Studying various properties of chemicals, drugs, biomaterials and alloys requires intense work over many years. Also, the properties of the materials that have been investigated may turn out to be unsuitable for the specific application at hand. For example, a doped graphene quantum dot (GQD) with a specific dopant percentage may not have the desired absorption spectrum for solar cell applications, or a specific derivative of a known drug may not have the right docking properties for the relevant protein. A grid search in the chemical or structural parameter space is one way to find the material with the desired properties. However, this is extremely time consuming and costly for both lab synthesis and in silico simulations. Materials discovery paradigm tries to reverse this process: Instead of studying the properties of a chosen material or its limited number of structural derivatives, one first determines the target property such as "graphene quantum dot with maximum absorption in the 300-400 nm range of the spectrum", and then a smart search algorithm augmented with artificial intelligence swiftly searches the chemical or structural parameter space to find the physical structure or chemical configuration of the material that has the exact desired property. We present a case study showcasing a Bayesian optimization algorithm working with Gaussian and artificial neural net kernels and finding the particular GQD that has the desired absorption maxima at the given range of the UV-Vis spectrum as defined by the objective function. Here we have the parameter space of GQDs as dopant element type (B, N, O, S and P), dopant percentage (pristine, 1.5%, 3%, 5% and 7%) and graphene size (1, 1.5 and 2 nm), where the absorption spectrum of each GQD was calculated with time-dependent density functional theory (TDDFT) in advance in this proof-of-concept study. Our results show that the machine learning algorithm with artificial neural nets can find the GQD with the desired absorption characteristics, set by the objective function, among many possible GQDs in a few steps, much more quickly than a grid search algorithm does. This algorithm provides a time- and resource-efficient way of discovering new materials since it tests only limited number of variations of the material from the parameter space, and for each tested material variation, there is usually an expensive and time-consuming procedure such as lab synthesis of the material or calculation of the material's properties via computer simulations. So, it's important to find the desired material without testing all possible configurations in the parameter space. This procedure can be used not only with in silico simulations but also with actual synthesis of materials in the lab environment.

Keyword: machine learning, artificial intelligence, artificial neural networks, Bayesian optimization, graphene

## **Poster Presentations**

ID: 11 - Synthesis and Characterization of Nanomaterials

## Investigation of Pair Distribution Function Method on Structural Analysis of Nanocrystalline Powders

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This self-consistent computational work presents the minimum errors of structural parameters (e.g. lattice parameters, crystalline size, atomic displacement parameters) expected from Pair Distribution Function (PDF) analysis of nanocrystalline gold powders. Recently, PDF analysis has gained momentum in nanocrystalline powder characterization by X-rays, however, current literature does not contain expected error bounds of the resulting structural parameters. For an accurate interpretation of X-ray diffraction data, the error bounds must be analyzed. We aim to address this problem in three steps: 1. Simulation of ideal powder diffraction experiments with the use of the Debye scattering equation, 2. PDF analysis of the diffraction data, and 3. Determination of the errors from PDF analysis by comparing them with real-space analysis of spherical gold nanocrystals with sizes of 30 nm and smaller. Our results demonstrate that even for the ideal nanocrystals in ideal diffraction conditions, the extracted structural parameters from PDF analysis diverge from their true values. These deviations are dependent on the average size of the nanocrystals and the wavelengths of the illuminating X-rays. In diffraction analyses of nanocrystalline powders, lower X-ray energies and smaller crystal sizes are prone to greater uncertainties in extracted structural parameters.

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Keyword: Pair Distribution Function, X-ray Diffraction, Nanocrystalline, Powder Crystallography

#### ID: 14 - Synthesis and Characterization of Nanomaterials

## Problems of Rietveld refinement in nanocrystalline materials

#### Hamidreza Hekmatjou<sup>\*</sup>, Hande Ozturk

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Powder X-ray diffraction (PXRD) is a widely used method to investigate the structural and microstructural properties of crystalline materials. For the past few decades, this technique has been used to investigate the properties of nanocrystalline powders. However, some incompatibilities are present between the atomic configurations in nanocrystals and the theoretical constructs used to build x-ray analysis algorithms. Therefore, the structural properties of nanocrystals obtained by x-ray based quantitative analyses include some uncertainties. In the present study, the performance of Rietveld refinement in terms of evaluating structural parameters of gold nanoparticles and the related challenges within their Rietveld refinements are investigated using computer simulations of diffraction from nanocrystalline powder models. Furthermore, a workflow has been proposed for Rietveld refinement of nanocrystalline diffraction data showing the essential steps required for a successful refinement. It is demonstrated that the accuracy of thermal atomic displacements, including isotropic displacement parameters and microstrains, depends strongly on the average sizes of the investigated nanocrystals.

Keyword: Powder X-ray diffraction, Rietveld refinement, Thermal atomic displacement, Nanocrystal

ID: 17 - Synthesis and Characterization of Nanomaterials

## Using of Pistachio for Synthesis of CQDs with a Hydrothermal Method, Investigating Optical Properties, and Application for Co<sup>2+</sup> Sensing

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In this research, carbon quantum dots (CQDs) were synthesized by using pistachio as precursor for the first time with a hydrothermal method in aqueous media. Synthesized QDs were characterized by different analyses such as X-ray diffraction (XRD), transmission electron microscopy (TEM), Zeta potential, Raman, photoluminescence (PL) and UV-visible (UV-vis) spectroscopies. The XRD pattern of CQDs indicates from a main peak at  $2\theta = 20^{\circ}$  and d = 4.5415 A which is related to (002) plane of JCPDS card no. 26-1076 [1]. Raman spectrum of CQDs indicates of two sharp peaks at 1311.87 cm<sup>-1</sup> and 1585.82  $cm^{-1}$  which are related to D-band and G-band, respectively. The D-band peak (sp<sup>3</sup> hybridization) shows the amount of defect. functionalization and edge effect corresponds to the A<sub>1g</sub> symmetry photons near K-zone boundary and G-band peak (sp<sup>2</sup> hybridization) corresponds to the amount of graphitization associated with CQDs. The ratio of G/D, which means the intensity of G-band peak divided on the intensity of D-band of Raman spectrum, obtained about 3.54 that is much higher than other G/D reported ratios [2-4]. Zeta potential measurement of CQDs showed that CQDs had negative charge in their surface and it confirmed a great stability for CQDs. TEM images showed that synthesized CQDs are spherical with a size of about 7 nm. CODs had blue photo emission with a broad PL peak between 300 to 600 nm with quantum yield of 12%. For investigating effect of solvent on PL intensity of CQDs, 5 mg of synthesized CQDs were dispersed in 5 ml of different solvents and showed that the highest PL intensity of CQDs was in acetone and lowest of intensity was in dimethylformamide (DMF). These results shows that the PL of synthesized CQDs is dependent to solution due to surface trap or interaction of oxygen, nitrogen and sulfur bonds with environment around of QDS. Heavy metal sensitivity of CQDs were investigated by different heavy metal ions and results showed that PL intensity of CQDs in presence of  $Co^{2+}$  ions decreased and showed CQDs had sensitivity versus  $Co^{2+}$  ions. There is a good relationship with linear equation of y=0.0027 x + 0.193 and R<sup>2</sup>=0.9944 between degree of decreasing in PL intensity and Co<sup>2+</sup> concentration.

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Keyword: CQDs, synthesis, Co<sup>2+</sup> sensitivity

## Development of Gold Nanoparticle Decorated, Micro/Nano-channeled PCL/PLGA Film Scaffolds for Neural Tissue Engineering Applications

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In the field of neural tissue engineering, intensive work is being done to develop alternative nerve guidance channels with the new techniques offered by nanotechnology and biomaterials science [1]. Polycaprolactone (PCL) and poly-lactic-glycolic acid (PLGA) are highly biocompatible, biodegradable and FDA-approved biopolymers, and they have been frequently preferred in the field of tissue engineering due to their superior mechanical properties [2, 3]. Due to the innovative approaches offered by electron beam lithography technique, highly stable and reliable micro/nano patterns can be applied on biomaterial surfaces [4]. Gold nanoparticles (AuNPs) have wide range applications in the biomedical field due to their unique physical, chemical and biological advantages [5]. The aim of this study was the design of conductive and micro/nano-channeled PCL/PLGA (10:1 v/v) film scaffolds for neural tissue engineering applications. PCL/PLGA films with three different channel widths (500 nm, 1µm and 5µm) were produced by e-beam lithography technique and their surfaces were decorated using medium sized-AuNP<sub>50</sub>. Also, polypyrrole (PPy, 1% v/v) coating was applied on the films as an alternative surface conductivity design. In addition, poly-L-lysine (PLL, 10% v/v) and pentapeptide-IKVAV (0.2 mg/mL) surface modification were performed for subsequent neural cellular studies. PCL/PLGA (10:1 ratio) hybrid polymer composition has been shown to increase mechanical strength. Although there was a slight decrease in the mass of polymers within the scope of degradation test, film scaffolds preserved their physical stability. PLL/IKVAV surface modification significantly increased the hydrophilicity of the scaffolds. Fourier transform infrared spectroscopy (FTIR) was used to identify functional groups found on the scaffolds with various surface chemistry. It was concluded that it can help to guide the progression of cellular neurites and axons along linear lines within the scope of future potential neural tissue engineering studies of the developed biomaterial. It has also been evaluated that the designed material can promote regeneration after implantation at a nerve injury site.

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Keyword: Neural tissue engineering, Polycaprolactone/poly-lactic-glycolic acid, Gold nanoparticles, Electron beam lithography, Micro/nano-channels

## Synthesis, Characterization and Electrochemical Behavior of rGO Supported MoS<sub>2</sub>/Nafion Nanocomposite for Wearable Energy Storage Applications

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Recently, energy storage devices have gained tremendous attraction as the solution to overcome the drawback of energy deficiency worldwide [1]. The development of innovative nanomaterials has improved the electrochemical performance of energy storage systems [2]. Herein, we report the synthesis of MoS<sub>2</sub>/rGO /Nafion hybrid nanocomposite as the electrode material for supercapacitor applications. One-pot hydrothermal synthesis has been applied for the preparation of the positive electrode which has a carbon fiber current collector. The structure, morphology, and surface area of prepared samples are characterized by XRD, XPS, DRIFT, FESEM, and TEM. The electrochemical performance of both electrode and supercapacitor device has been investigated using cyclic voltammetry (CV), and galvanostatic charge-discharge (GCD) techniques in the 1 M Na<sub>2</sub>SO<sub>4</sub> supporting electrolyte. The maximum energy and power densities of the asymmetric supercapacitor device have been found as 232 Whkg-1 (at 25 mVs-1) and 94 kWkg-1 (at 1 Vs-1), respectively. Furthermore, the device has shown excellent cycling performance (~99%) after 10000 dynamic CV cycles.

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Keyword: wearable energy, MoS<sub>2</sub>, supercapacitor, high-performance

#### ID: 72 - Synthesis and Characterization of Nanomaterials

## **Colloidal Synthesis and Characterization of Carbon Quantum Dots**

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Carbon nano particles, also called C-dots [1], have drawn considerable scientific interest owing to their water solubility, unique optical properties as luminescent semiconductor nanostructures [2, 3, 4]. C-Dots are useful in bioimaging [3] and drug deliveries [3] due to biocompatibility and low toxicity. In this work, the fluorescent CDs were synthesized from fresh orange juice by microwave heating method which is simple, safe and environmentally friendly. Fresh orange juice contains citric acid which is carbon source and thiourea was used for doping the CDs with S and N. The amount of thiourea, synthesis time and power of microwave were vital for the CDs properties. The results show that the amount of thiourea and emission are directly related. CDs exhibit maximum PL emission at the blue-light region. The emission peak of the sample with 0.84 gr thiourea is 124.52 Au on 445 nm with 380 nm extraction, but the emission peak of the sample with 0.94 gr thiourea is 162.58 Au on 446.95 nm with the same extraction rate. Furthermore, the absorbance peak of the sample with 0.105 gr thiourea that was heated at 800 W and it was stirred in 3h is 0.2349 Au on 278nm. In contrast, the peak of the same sample that was stirred in 2:30h is 0.1463Au on 280nm.

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Keyword: C-dots, Carbon Dots, Synthesis CDs, Characterization CDs, Carbon Dots with Orange juice, CDs by microwave heating

## Preparation and Characterization of Hybrid Materials (NiMoO<sub>4</sub>+GO) for Simultaneous Determination of Acetaminophen and Tryptophan

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Metal molybdates compounds can be prepared by several methods and are considered as prospective electrode materials in many fields because the metal ions possess the ability to exist in several oxidation states. Recently, researchers have proven that metal molybdate compounds  $MMoO_4$  (M = Co, Zn, Mn, Fe, Ni, etc.) are remarkable materials in various fields such as catalysts, humidity, gas sensors, energy storage devices and so on. [1-3] Due to the synergistic effect between different metal molybdate components, nanocomposites with many metal molybdate compounds have been successfully synthesized.[4-7]. In addition, together with these synthesized hybrid materials, graphene-based materials have become remarkable for electrochemical sensor applications [8-12]. Because of unique crystal structure of graphene oxide it makes it extremely attractive as a support material for metal and metal oxide catalyst nanoparticles[13].

Tryptophan (Trp; 2-amino-3-(1H-indol-3-yl)-propionic acid), is an essential amino acid, which is mainly used as the precursor in the synthesis of melatonin, serotonin etc.,[14] that are involved in mood swing and synthesized by Trp hydroxylase [15–17]. The intake of Trp is vital in food products or through pharmaceutical preparations because it is not synthesized in human body and is necessary for maintaining and establishing a positive nitrogen balance in human system. Paracetamol (N-acetyl-p-aminophenol or acetaminophen, denoted as ACP) is one of the most common analgesic and antipyretic drugs. It is an effective and safe analgesic agent used for the relief of mild to moderate pain associated with headache, backache, arthritis and postoperative pain. In therapeutic doses, it is a suitable alternative when the patient is sensitive to aspirin

Overdose consumption of ACP can alter TRP metabolism by inhibiting tryptophan 2, 3-dioxygenase activity thus increasing the availability of tryptophan for the production of serotonin in brain [18]. Thus, the simultaneous determination of acetaminophen and tryptophan compounds could be of considerable value.

A nanocomposite electrode containing NiMoO<sub>4</sub> and GO was fabricated for simultaneous determination of acetaminophen and tryptophan using differential pulse voltammetry. Under optimized conditions, with a pH 5.00 AcH/Ac buffer solution; the ratio components of the composite 5% NiMoO<sub>4</sub> and 95% GO, the method have been the best results. The NiMoO<sub>4</sub>/ GO nanocomposite electrode exhibits low limits of detection ( $4.89 \times 10^{-8}$  M and  $4.01 \times 10^{-8}$  M), wide linear ranges ( $0.1 \mu$ M to 10  $\mu$ M and 0.6  $\mu$ M to 60  $\mu$ M), and well-separated oxidation peaks (at 0.497 V and 0.744 V vs Ag/AgCl) towards acetaminophen and tryptophan, respectively. The nanocomposite electrode was characterized by scanning electron microscopy (SEM), energy dispersion X-ray (EDX), X ray photoelectron spectroscopy (XPS) and electrochemical impedance spectroscopy. The fabricated electrode and developed method has been successfully applied to the determination of acetaminophen and tryptophan in synthetic urine samples.

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## Characterization and Determination of Selenium Nanoparticles in Dietary Supplements by Single Particle Inductively Coupled Plasma Mass Spectrometry

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Selenium nanoparticles (SeNPs) attract attention with their anticancer, antioxidant, antibacterial properties and wider therapeutic range compared to inorganic selenium forms (1). Although there is no approved pharmaceutical formulation containing SeNP, several dietary supplements containing inorganic selenium in syrup form are commercially available. The presence of ascorbic acid in these preparations provide a favorable chemical environment for SeNP formation. Therefore, the detection of selenium forms in these products is important. On the other hand, one of the main challenges during NP characterization is the low concentration in the real samples. Methods such as transmission electron microscopy (TEM), scanning electron microscopy (SEM) and Dynamic light scattering are the techniques commonly used for the characterization of NPs. However, they are time consuming, and their sensitivity is insufficient for the characterization and/or detection of NPs at low concentrations. Therefore, analytical techniques are needed for NP characterization and determination at low concentration levels.

Single Particle Inductively Coupled Plasma-Mass Spectrometry (SP-ICP-MS) is a new technique that provides simultaneous information on NP size, size distribution, mass and particle number concentrations down to ng  $L^{-1}$ . The principle is based on the fact that each particle, upon reaching the plasma, is ionized and reaches the mass detector as an ion cluster which creates a transient signal. When the signal integration time is short enough, each transient signal represents a single particle event. The number of events is proportional to the particle number concentration, while the intensity of the event is proportional to the particle diameter of the tracked element within the particle (2).

In this study, the effects of experimental parameters such as torch distance, aspiration rate, organic solvent addition, plasma conditions and dissolved selenium concentration on the signal intensity of SeNPs were studied and optimum conditions were determined. SeNPs synthesized in our laboratory were characterized by UV-VIS and SEM and the results were compared with SP-ICP-MS. The mean diameter of SeNPs, which was found to be  $136\pm26$  nm by SP-ICP-MS, was found to be  $144\pm10$  and 130 nm by SEM and UV-Vis techniques, respectively. The size detection limit by SP-ICP-MS was calculated as 35 nm. Nanoparticles were detected in four of the five food supplements analyzed with the developed method, and it was found that 33-55% of the total selenium was in the form of nanoparticles and their sizes were in the range of 55-130 nm. SP-ICP-MS is a highly sensitive and rapid technique with minimum sample preparation steps for metal nanoparticle characterization in complex matrices.

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Keyword: selenium nanoparticle, nanoparticle characterization, single particle inductively coupled plasma mass spectrometry

## Synthesis and characterization of Nickel loaded ZIF-8/Silica Aerogel hybrid material

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Metal organic frameworks (MOFs) are important porous materials for the applications such as gas separation and catalysis. As a subclass of MOFs, ZIF-8 has come to the forefront because of its high thermal and chemical stability, high surface area and crystallinity [1]. As a catalyst support, ZIF-8 provides dispersion of metallic active phase uniformly. However, ZIF-8 has microporosity which can cause agglomeration of macromolecules and coke formation during the reaction. So, transforming the structure as hierarchical can be utilized to overcome the mentioned problem [2]. In this study, it was aimed to synthesized Nickel doped ZIF-8/Silica aerogel catalyst for further using catalyst in cyclic carbonate production reaction. ZIF-8 was joined to synthesized silica aerogel structure by using in-situ method. Precursor of silica aerogel was selected as Tetra ethyl ortho silicate (TEOS). Silica aerogel was synthesized by using two step acid base sol gel method and drying at atmospheric pressure. Metal loading was done to the aerogel with wet impregnation. Metal loading ratio in final aerogel was planned as 5% by mass. Mass ratio of Nickel loaded Silica aerogel/ZIF-8 was chosen as 15. Synthesized catalyst was characterized by taking advantage of Scanning Electron Microscopy (SEM) with Energy Dispersive X-Ray Analysis (EDX), Fourier-transform infrared spectroscopy (FTIR), Diffuse reflectance infrared fourier transform spectroscopy (DRIFTS) and X-ray diffraction analysis (XRD).

#### Acknowledgement:

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 Razavian, M., Fatemi, S., & Nouralishahi, A. (2021). Nickel supported ZIF-8. PEG modified catalyst: A designed active catalyst with high H2 productivity in steam reforming of ethanol at moderate temperature. Journal of Environmental Chemical Engineering,

Keyword: Silica aerogel, Metal Organic framework (MOF), Zeolitic Imidazolate Framework (ZIF), ZIF-8, nanocatalyst synthesis and characterization

## Growth and Characterization of Magnetite Fe<sub>3</sub>O<sub>4</sub> Thin Films for Application of Ferromagneticinsulating Josephson Junction in Quantum Computing

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Josephson junctions containing ferromagnetic tunneling barrier so-called  $\pi$ -junctions exhibit both magnetic and superconducting characteristics. The rich physics concept in the tunneling characteristics of the  $\pi$ -junctions open a new path in developing new cryogenic devices for applications of superconducting spintronic memory circuits and superconducting qubits. In a number of ferromagnetic materials, magnetite Fe<sub>3</sub>O<sub>4</sub> as a tunneling barrier have recently great deal of interests in the development of  $\pi$ -junctions due to their unique electrical and magnetic properties. In our study, we investigate ideal conditions in our magnetron DC sputtering chamber to grow high-quality magnetite thin films for the  $\pi$ -junction applications. Structural, stoichiometric, and topological characterizations of a series of magnetite films grown by the sputtering system have been investigated by X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscope spectroscopy (SEM-EDS). Moreover, we have studied annealing effects in the crystalline structure of the as-grown thin films. We discuss their sputtering and annealing conditions to improve the crystalline quality of the magnetite films upon their electrical and magnetic characteristics.

## Optimization and Characterization of MoO3 Thin Films Deposited by RF Magnetron Sputtering

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Molybdenum oxide thin films exhibit a variety of stable phases. They possess interesting structural, optical, chemical, and electrical characteristics that are appealing for a number of applications in energy storage, sensors, solar cells, infrared detectors, and smart windows. Additionally, molybdenum oxide thin films are mostly preferred in chemiresistive gas sensors, for sensitive detection of nitrogen dioxide (NO<sub>2</sub>), carbon dioxide (CO<sub>2</sub>), hydrogen (H<sub>2</sub>), and ammonia (NH<sub>3</sub>). In this study, optimized conditions of MoO<sub>3</sub> have been investigated for gas sensor applications. Molybdenum oxide thin films have been deposited by Radio Frequency (RF) magnetron sputtering on silicon wafers using a metallic molybdenum target in the presence of oxygen (O<sub>2</sub>) and argon. In situ heat treatment was applied to form a crystalline structure of molybdenum oxide thin films followed by X-Ray Diffractometer (XRD), Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM) were used for the structural, stoichiometric, and morphological characterization. The optical characteristics were analyzed by ellipsometry to gain insight into the semiconducting character of the samples and sheet resistance was measured by the 4-Point Probe method. In the light of the information gathered from the experiments, we discuss the growth conditions in the sputtering system to improve their structural qualities affecting their optical and electrical characteristics.

Keyword: molybdenum oxide, thin film, RF magnetron sputtering

## ID: 188 - Synthesis and Characterization of Nanomaterials

## Vanadium Dioxide Based Thermochromic Films on Silver Nanowire Electrodes

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Today, among various oxide materials, monoclinic/rutile phase vanadium dioxide (VO<sub>2</sub>) is used as the most promising candidate for smart windows due to its unique reversible metal–insulator transition. Also, the selection of electrode material is one of the important parameters for the energy-saving performance of VO<sub>2</sub>-based smart windows. In this study, vanadium dioxide based thermochromic films are fabricated on silver nanowire (Ag NW) electrodes for the application in smart windows. Firstly, VO<sub>2</sub>(B) phase was synthesized from vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) precursor by hydrothermal method to obtain high purity thermochromic VO<sub>2</sub>(M) nanoparticles, and then VO<sub>2</sub>(B) powder was annealed in argon atmosphere. The structural properties of these nanoparticles and their surface morphologies were examined by the XRD and SEM, respectively. Then, VO<sub>2</sub> (M) nanoparticles were deposited onto silver nanowire (Ag NW) electrodes on glass substrates. Optoelectronic and morphological properties of the Ag NW/ VO<sub>2</sub> (M) films were investigated in detail. Schematic representation of the fabrication route is provided in Fig. 1. Lastly, thermochromic transition of VO<sub>2</sub> was triggered using Ag NW electrodes as heaters.

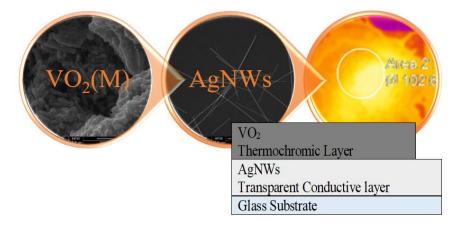


Figure 1. Schematic representation of the fabrication route

#### Acknowledgments:

This work was supported by the Scientific and Technological Research Council of Turkey (TUBITAK) with Grant no. 121N708.

Keyword: Vanadium dioxide, silver nanowires (Ag NWs), electro-thermochromic film

ID: 196 - Synthesis and Characterization of Nanomaterials

## Synthesis and Characterization of Ag Nanoparticles Using Syzygium Aromaticum by a Mild Green Synthesis Approach

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Researchers are interested in silver nanoparticles (AgNPs) due to their unique features and uses in sectors such as medicine, catalysis, textile engineering, and pollution control. The green synthesis of AgNPs offers several benefits, including a shorter time requirement, extremely stable AgNPs, improved control over crystal development and shape, scalability, and economic feasibility.

Herein, we report the synthesis and characterization of Ag NPs produced via green synthesis method using *Syzygium aromaticum* (SA) extract both as a reducing agent and a stabilizer under mild circumstances. Synthesized Ag/SA NPs were characterized by Ultraviolet-Visible Region (UV-VIS), Fourier-Transform Infrared (FTIR), Dynamic Light Scattering (DSL), X-Ray Photoelectron Spectroscopy (XPS), X-Ray Diffraction (XRD) spectroscopies; Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) in order to determine their morphology and composition. Preliminary studies were also performed to investigate the antibacterial properties of the produced Ag/SA NPs.

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Keyword: Green synthesis, Syzygium aromaticum, antibacterial, characterization

#### ID: 203 - Synthesis and Characterization of Nanomaterials

#### Covalent Modification of Magnetic-Single Walled Carbon Nanotubes with Bovine Serum Albumin

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Magnetic nanomaterials have attracted attention in biomedical engineering due to their physical and chemical properties. The main advantage of magnetic nanomaterials is their capacity to be magnetically targeted in a specific zone in the human body by an external magnetic field. Carbon nanotubes (CNTs) have been used as nanocarriers for anticancer drugs because of their high surface area, high drug loading capacity, and easy modification. Non-functional CNTs were intrinsically hydrophobic and toxic. To overcome this problem, modification of a CNT surface has mediated by adsorption, electrostatic interaction or covalent bonding of different molecules. These modifications have improved the water solubility/dispersion of the CNTs and facilitates the incorporation of different drugs via surface adsorption, entrapping, or encapsulation. Proteins are an essential group of organic structures used to improve the water solubility/dispersion and biocompatibility properties of nanocarriers. Among the proteins, bovine serum albumin (BSA) has attracted interest because it is soluble in water and has different drug binding sites in the albumin molecule. CNTs are able to adsorb proteins via the  $\pi$ -stacking interaction, electrostatic interaction or hydrogen bonding. However, the physical adsorption process is non-steady and uncontrollable compared to covalent functionalization. Thus, the protein adsorption capacity of CNT is restricted in this method. In this study, carboxylated magnetic CNTs were functionalized with BSA via carbodiimide mediated reaction. Successful coating of magnetic CNTs (mCNTs) with BSA was confirmed by Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy, thermogravimetric analysis (TGA), X-ray photoelectron spectroscopy (XPS), and zeta potential measurement. According to the results of Raman spectroscopy and TGA, the intensity ratio of D to G band of the BSA coated mCNT was found as 0.82 and functionalizing of mCNT with BSA leads to an increase in weight loss between 200 and 400 °C. The zeta potential values of pristine and coated mCNT were measured as -16.3 and -20.5 mV, respectively. The FTIR spectra of coated mCNT exhibited new peak at 1020 cm-1 (C-N), corresponding to the amide bond between mCNT and BSA, and this result is also compatible with XPS.

Keyword: carbon nanotubes, bovine serum albumin, covalent modification, magnetic nanomaterials

## ID: 234 - Synthesis and Characterization of Nanomaterials

## Preparation and Characterization of Polymeric Nanobiomaterials by Electrospinning

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Nowadays, nanotechnology has been of great importance in science, industry and many fields. The synthesis of nano-sized materials is also quite common. Electrospinning technique is very important for the synthesis of these nano-sized materials and it shows great performance and efficiency especially in nanofiber production [1]. Electrospun Nanofibers are a suitable platform to fabricate such novel antimicrobial materials due to their desirable properties, including small size, high specific surface area, multi-porosity, and high surface functionalization potential. Giving antimicrobial properties to Nanofibers; medical devices, drinking water, food and textiles have the potential to prevent a major public health threat. Therefore, the development of new and potent antimicrobial materials is vital for the protection of human health by increasing bacterial resistance [2]. In this study, hydrophobic and hydrophilic polymers were used together to obtain electrospun Nanofibers with antimicrobial agent to investigate its antimicrobial properties. In the first stage, Nanofibers with hydrophilic character was obtained by electrospinning technique with homogeneous distribution without beads. In the second step, Nanofibers with appropriate morphology and character were modified with antimicrobial agent. The morphology of obtained Nanofibers was followed by scanning electron microscopy (SEM). The contact angle measurements were carried out to identify surface hydrophilicity.

#### Acknowledgments:

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Keyword: Nanobiotechnology, Nanotechnology, Nanomaterials, Electrospun Nanofibers, Antimicrobial coatings

## Porous Cryo-Dried MXene Supported Pd (0) Nanoparticles for The Methylamine-Borane Hidrolysis as An Effective and Stable Catalyst

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In this study, palladium doped porous MXene (Pd@MXene) and cryo-dried MXene (Pd@cryo-MXene) were synthesized by a wet impregnation method for the methylamine-borane hidrolysis. In order to obtain MXene phases, the prepared  $Ti_3AlC_2$ compounds denoted as  $M_{n+1}AX_n$  were etched with 39 wt% of HF solution to remove the Al phase. Then, MXene particles prepared by the same process were cryogenically treated at -80 °C for 25 min using liquid nitrogen to get the cryo-dried MXene. The morphological and structural characterization of the prepared Pd@MXene and cryo-Pd@cryo-MXene materials was performed using a field emission scanning electron microscope, transmission electron microscope, and X-ray diffraction equipped with Cu K $\alpha$  radiation. The surface and bonding types of the materials were determined by fourier transform infrared and <u>Brunauer-Emmett-Teller Method (BET) analyses</u>. Surface and morphological characterizations confirmed that the surface area of MXene particles increased after cryogenic treatment. Finally, catalytic performance of prepared catalysts was investigated in the hydrolysis of methylamine-borane. Consequently, palladium-doped MXene based catalysts exhibited excellent catalytic performance in the methylamine-borane hydrolysis compared after cryogenic treatment compared to the nontreated particles.

Keyword: Catalyst, Cryo-MXene, Hydrogen, Hydrolysis, Methylamine-borane, Nanoparticle

## Investigation of Electrochemical Performance of RF-plasma Modified Prussian Blue Composites

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Prussian blue (PB) is one of the broadly investigated compounds due to the promising features such as electrochemical behavior, chemical durability, biocompatibility [1-3]. PB containing silver (Ag) is a promising nanoformulation compound and has the advantage of being stored for a long time without toxicity due to the presence of strong Ag-CN-Fe bridges [1]. Designing composite by adding conducting polymers could demonstrate synergistic influences that enhanced structural and electrochemical features. Among conducting polymers, polyaniline (PANI) is one of the most widely used conducting polymers due to easy synthesis, environmental stability [4].

In this study, Ag doped and undoped PB-PANI composites were synthesized using rf rotating plasma modification method. The prepared composites were characterized using Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDS). The Ag doped and undoping PB-PANI composites-based thin film were prepared doctor-blade coating techniques. Electrochemical features of the Ag doped and undoping PB-PANI films were compared with each other.

#### Acknowledgements:

The authors gratefully acknowledge the 2209/A TUBITAK Project for the financial support throughout the research.

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Keyword: Prussian blue, synthesis, characterization, silver nanoparticles

#### ID: 265 - Synthesis and Characterization of Nanomaterials

#### Fabrication and Characterization of Metal Oxide Based Sensing Layers for Mass-sensitive Gas Sensors

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### Introduction

Detection of volatile organic compounds (VOCs) is a big issue for human health and environmental pollution due to their harmful effects. Therefore, there is an increasing interest in highly sensitive, selective, and user-friendly gas sensors for the detection of VOCs day by day. There are many types of gas sensors that have been developed such as optical, electrochemical, mass-sensitive (surface acoustic wave; SAW or quartz crystal microbalance; QCM), etc. for monitoring of VOCs in various application areas. Among them, mass-sensitive type sensors exhibit various unique advantages. Mass-sensitive gas sensors directly detect the mass of gas molecules when the sensor is exposed to target gas molecules [1].

The sensing layer is a significant component of a mass-sensitive gas sensor, and it plays a determinant role in the sensing ability of the sensor [2]. Semiconductor metal oxide materials such as ZnO, WO<sub>3</sub>, and V<sub>2</sub>O5 have been widely used as sensing layers for many years due to their low cost, easy production in nanostructured form, and higher sensor response against a wide range of gases [3].

In this study, nanostructural metal oxide-based sensing materials such as ZnO, V<sub>2</sub>O<sub>5</sub>, and WO3 were fabricated and characterized. Their sensing performances in mass-sensitive gas sensors were also studied against various VOCs.

## **Materials and Method**

Nanostructured ZnO, WO<sub>3</sub> and V<sub>2</sub>O<sub>5</sub> sensing layers were fabricated by hydrothermal technique on various substrates such as glass, Si, FTO (fluorine-doped tin oxide coated glass), and LiNbO<sub>3</sub> (lithium niobate). A scanning electron microscope (SEM) equipped with electron dispersive spectroscopy (EDS) and X-ray diffraction (XRD) was used to characterize the morphology and crystal phase of fabricated samples.

#### **Results and Discussion**

Figure 1 shows the SEM images of hydrothermally fabricated ZnO nanorods. As seen in Figure 1, nanorods are homogeneously covered the entire substrate.

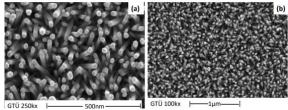


Figure 1. SEM images of ZnO nanorods sensing layer.

Figure 2 shows SEM images of  $V_2O_5$  nanostructures. According to Figure 2, nanostructures homogenously distributed on the surface of the substrate.

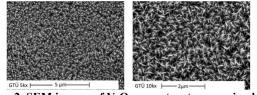


Figure 2. SEM images of V2O5 nanostructure sensing layer.

#### Acknowledgements:

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Keyword: Mass-sensitive, Gas Sensor, Nanostructure, VOCs

## pH-mediated Emission of Boron/Nitrogen co-doped Carbon Quantum Dots

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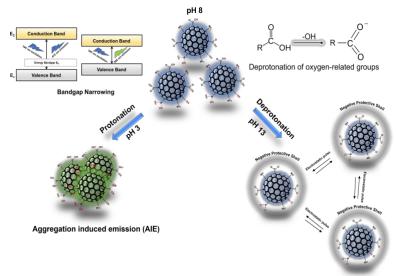
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Carbon quantum dots (CQDs) have been used in many different fields due to their unique physical, chemical, and optical properties. CQDs are fluorescent nanoparticles with very different properties from bulk materials. For the last two decades, many studies have been carried out to evaluate the PL mechanism of CQDs. As a result, different theories have been proposed. PL properties of CQDs are highly dependent on environmental conditions. One of the most crucial environmental conditions is pH. In this study, we synthesized boron/nitrogen co-doped carbon quantum dots (B/N CQDs) via a simple hydrothermal method. To monitor the effect of environmental pH on B/N CQDs, the pH was manipulated from 3 to 13. Changes in the emission of CQDs and their absorption properties were investigated by PL and UV-vis spectroscopy. The surface charge and morphology of nanoparticles were detected by Zeta potential and TEM. For further analysis, three CQDs in natural, acidic, and alkaline environments were selected and analyzed through X-ray photoelectron spectroscopy (XPS). As a result, in highly acidic and alkali conditions excitation-dependent property was lost. Also in acidic conditions, there is a red-shift observed because of aggregation-induced emission(AIE). TEM images and XPS spectra of CQDs revealed that protonation of surface groups disrupts the stability and led to aggregation. This phenomenon resulted in an increase in the size of particles and a narrowing bandgap. Deprotonation of CQDs enhanced oxygen-related groups created an increase in total negative charge. Within the scope of these findings, we observed that protonation or deprotonation of surface groups dramatically tunes the fluorescence properties of CQDs. Also, the change in emission is due to particle aggregation, not because of the change in the surface condition. We determined that the aggregation-induced emission properties may be employed in the design of novel sensor systems.



Scheme. Graphical representation of changes in CQDs at different pHs

Keyword: Carbon Quantum Dots ,Fluorescence, Aggregation Induced Emission, pH

#### Synthesis and Functionalization of Mesoporous Silica Nanoparticles to Fight Breast Cancer

#### İbrahim Egemen Küçük, Doğu Şeyda, Safiye Beyza Kaçar, Hilal Karadayı, Feray Şimşek, Gizem Karaaslan, <u>Yunus</u> Emre Doğan<sup>\*</sup>

Middle East Technical University, Ankara, Turkey

Breast Cancer is the second most common and the fourth most fatal cancer in Turkey (2020). Although conventional treatments such as chemotherapy, radiation and hormone therapy, show considerable success; the survival rate of breast cancer remains small (23%, 5-year). Moreover, these have various side effects. In order to reduce the side effects of treatment and to increase the drug efficacy nanoparticles can be used. Nanoparticles are superior in the field of the drug delivery system due to their availability of tailoring a wide range of properties such as morphology, surface chemistry, and size. Among these nanoparticle systems, Mesoporous Silica nanoparticles(MSNs) have promising properties in terms of ease in their surface functionalization, high drug loading capacity, control of drug release, and biodegradability. In this project, the following characteristics are used for the synthesis: 100-150nm sized, 2-4 nm pore size, and the spherical shape. Furthermore, for the selective targeting of the Breast Cancer cells, the folic acid was conjugated to their surfaces. Then, a potential chemotherapeutic agent, curcumin, was loaded into the mesopores via hydrophobic interactions. In this study, we characterized the size, morphology, structure, and surface charge of the nanoparticles by using Scanning Electron Microscopy, Transmission Electron Microscopy, Selected Area Diffraction, X-Ray Diffraction, Fourier-Transform Infrared Spectroscopy Analysis, Dynamic Light Scattering Analysis, Zeta Potential Measurement. Moreover, their biological activity was evaluated by the Cytotoxicity Analysis via MTT assay.

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Keyword: Mesoporous Silica Nanaoparticle, Drug Delivery, Folic Acid, Curcumin

## The Fabrication of Silver Nanoparticle-decorated Titanium Dioxide Nanoflowers Through Bioinspired Poly(L-DOPA) Thin Film and Their Biological Applications

#### <u>Nuray Serginay</u>\*, Atena Ghosi Gharehaghaji, Hayrunnisa Mazlumoğlu, Mehmet Yılmaz Atatürk University, Erzurum, Turkey

TiO<sub>2</sub> nanostructures represent remarkable advantages in terms of nontoxicity, high biocompatibility, high photochemical and thermal stability, and, low cost. With their unique characteristics, these nanostructures offer numerous capabilities in many biomedical applications. When TiO<sub>2</sub> nanostructures are combined with Ag nanoparticles, the resultant nanosystem can provide improved properties including enhanced antibacterial activity, high biocompatibility, and, reduced cytotoxicity.

Herein, for the first time, we propose the bioinspired poly (L-DOPA)-mediated Ag nanostructure-decorated TiO<sub>2</sub> nanoflowers (NF) (TiO<sub>2</sub> /PLDP/Ag) as an antibacterial agent against antibiotic-resistant Gram-negative (Escherichia coli) and Grampositive bacteria (Staphylococcus aureus). Our main objectives are to control the size, density, and morphology of Ag nanostructures through the experimental parameters and determine their characteristics in the antibacterial test. For this, firstly, TiO<sub>2</sub> NFs were synthesized through the hydrothermal

method. Then, a conformal thin layer of PLDP was created onto the  $TiO_2$  NFs ( $TiO_2$  /PLDP). Finally, by tuning the number of silver ions, the main characteristics of the deposited Ag nanostructures including the size, density, and morphology were manipulated in a well- controlled manner. The resultant colloidal  $TiO_2$  /PLDP/Ag NP system provided unique characteristics as an antibacterial agent in both bacteria strains. We strongly believe that the proposed system paved the way for the application in in-vivo studies for the removal of biofilms and anti-inflammatory effects.

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Keyword: Titanium dioxide nanoflowers, hydrothermal synthesis, L-DOPA, silver nanoparticles

### The Fabrication of Novel Fluorescence dye-loaded PEG-PLA Nanoparticle Systems

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Polyethylene glycol–polylactic acid (PEG–PLA) block copolymers are one of the widely used biomaterials (Zhong Xiao et al., 2010). These polymers can be used as copolymers as well as to form functional groups or to make surface modifications to nanoparticles (Ghasemi et al., 2018). In this study, a PEG-PLA copolymer was synthesized via a ring-opening polymerization method. Then, PEG-PLA nanospheres were obtained by the emulsification solvent evaporation and purification method. We investigated the dye loading potential of the polymer with a novel dye that was produced in our laboratory. This hydrophobic dye creates a high fluorescence at 360 nm. When the PEG-PLA nanosphere system is loaded with dye molecules, a quite low change was detected in optical properties with higher stability. This observation shows that the loading of dye to the polymeric nanosystem increases its stability. The morphological image of the nanospheres loaded with dye was characterized by SEM. Also, their optical properties were evaluated through UV-vis spectrophotometer and fluorescence spectrophotometer. The dye-loaded nanoparticle suspension created blue emission under a 365 nm UV lamp. The dye-loaded polymer nanospheres synthesized in this study can be used in various biomedical applications such as bioimaging and biosensing.

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Keyword: PEG-PLA, fluorescence, blue emission, dye loading

ID: 299 - Synthesis and Characterization of Nanomaterials

## Properties And *In Vitro* Cytotoxicity of Polycaprolacton-Based Nanofibrous Biomaterial Systems Containing Hydroxyl or Carboxylic Acid Modified Multiwalled Carbon Nanotubes

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<sup>2</sup> Gazi University, Ankara, Turkey

In this research, nanofibrous biomaterials were fabricated via the electrospinning method by incorporating multi-walled carbon nanotube (MWCNT) functionalized with hydroxyl (-OH) or carboxyl (-COOH) groups into the polycaprolactone (PCL) biopolymer matrix. The morphological and physicochemical properties of all synthesized biocomposite Nanofibers were investigated by scanning electron microscopy, atomic force microscopy, Fourier transforms infrared spectroscopy, X-ray diffraction, and contact angle (CA) analysis. In addition, *in vitro* cytotoxicity testing was performed to evaluate the toxic effect of composite nanofibrous biomaterials systems on human umbilical vein endothelial cells (HUVECs) and mouse fibroblast cells (L929). According to the results obtained, the addition of (-OH) and (-COOH) functionalized MWCNT reduced the CA of pure PCL from 133.7 degrees  $\pm 0.8$  to 96.1 degrees  $\pm 3.2$  and 82.2 degrees  $\pm 0.8$ , respectively. The addition of functionalized MWCNT increased the surface wettability of PCL-based nanofibrous biomaterials. In addition, all-composite nanofibrous biomaterial systems showed a negligible cytotoxic effect on HUVECs and L929 fibroblast. The results exhibited that MWCNT-COOH was better for PCL than MWCNT-OH in terms of cytocompatibility, surface roughness, and hydrophilicity. It was concluded that PCL/MWCNT-COOH nanofibrous biomaterial systems could have potential use in biomedical applications, especially in bone tissue engineering and orthopedic applications, where load-bearing scaffolds are needed.

Keyword: Polycaprolactone, Biomaterials, Nanofiber, MWCNT

ID: 328 - Synthesis and Characterization of Nanomaterials

## Effect of Calcination Temperature on Structural and Morphological Properties of Nickel ferrite Nanoparticles and Biosensor Application

### Vildan Şanko\*, Ahmet Şenocak, Süreyya Oğuz Tümay, Erhan Demirbaş

Gebze Technical University, KOCAELİ, Turkey

Nickel ferrite nanoparticles, one of the important spinel ferrites, are widely used in electronic, magnetic and electrochemical devices [1]. Their unique magnetic structure, thermal stability, remarkable electrochemical abilities have made them an attractive material for many fields [2]. In this study, nickel ferrite nanoparticles were obtained by co-precipitation method [3]. This method is advantageous to make size of ferrite nanoparticles controllable by temperature or mixing time. However, it is known that the calcination temperature is of great importance for the further stabilization of the synthesized nanoparticles in most cases. Therefore, 500 °C, 750 °C and 1000 °C were used as calcination temperatures to evaluate the properties of nickel ferrite nanoparticles. The three nickel ferrite groups were characterized by Fourier transform infrared (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), transmission electron (TEM) and scanning electron (SEM) microscopes. Increase in the calcination temperature led to rise in crystallinity and morphologically significant differences were also obtained. Nickel ferrite nanoparticles obtained at a calcination temperature of 750 °C were preferred for use in electrochemical biosensor studies. In addition, cyclic (CV) and differential pulse voltammetry (DPV) techniques were used to investigate the biosensor properties against urea analyte with this selected group. The nickel ferrite structure is used for the first time in electrochemical urea detection, bringing a new perspective to its use in enzymatic urea biosensors.

### Acknowledgment

Vildan Sanko thanks TUBITAK for financial support through the TUBITAK 2211-C National Ph.D. program Scholarship Programs in the Priority Fields in Science and Technology. Also, Vildan Sanko thanks YOK 100/2000 doctorate program.

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Keyword: Ferrite nanoparticles, Calcination process, Electrochemical detection

## Design and Characterization of Zinc Ferrite Nanoparticles as Enzyme Immobilization Matrix

## Vildan Şanko<sup>\*</sup>, Ahmet Şenocak, Süreyya Oğuz Tümay, Erhan Demirbaş

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It is known that ferrite nanoparticles show positive effects in the preparation of modern sensors and biosensors in both industrial and biomedical fields [1]. Due to their mesoporous structure, they have a large surface area, which provides space for more enzyme immobilization in biosensor studies [2]. The synthesis methods and conditions used such as co-precipitation, hydrothermal, solvothermal, sol-gel are the main factors that determine the quality of ferrite nanoparticles. Co-precipitation method is preferred in this study as it is one of the simplest and easiest ways of synthesizing options where an environmentally friendly alkaline aqueous solution is widely used for the synthesis of size and morphology controlled nanoparticles [3]. In order to improve the enzymatic detection system, the surfaces of zinc ferrite nanoparticles are modified with tetraethoxysilane and (3-aminopropyl) triethoxysilane to obtain -NH<sub>2</sub> function. Physical, chemical and morphological characterizations of all modified and unmodified zinc ferrites are carried out in detail. Glutaraldehyde crosslinker is used to immobilize the enzyme on the surface of -NH<sub>2</sub> functional ferrite nanoparticles. Although many good properties of zinc ferritin are mentioned in the literature, it has not been used in any enzymatic urea electrochemical biosensor. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) are used to evaluate biosensor performance. The effect of the zinc ferrite-based electrochemical urea system is investigated for the first time, which supports for the positive contribution of ferrite nanoparticles to the sensitive and selective electrochemical biosensor. The contribution of the properties of zinc ferrite to the peak current values of the biosensor has been evaluated, and it is thought that the obtained electrochemical results could create a new perspective for various biosensor studies in the future.

#### Acknowledgment

Vildan Sanko thanks TUBITAK for financial support through the TUBITAK 2211-C National Ph.D. program Scholarship Programs in the Priority Fields in Science and Technology. Also, Vildan Sanko thanks YOK 100/2000 doctorate program.

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Keyword: Zinc ferrite nanoparticles, Enzim immobilization, Electrochemical biosensor

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ID: 350 - Synthesis and Characterization of Nanomaterials

# Effect of Ultrosonic Irradiation and investigation on thermal induced phase development of Bioactive Glass Particles

Not presented.



• GPC (Gel Permeation Chromatography) / SEC Sistemleri

· 5 Dedektöre kadar dedektör kombinasyonu (MALS, Viskometre, DLS, UV, RI)



ID: 352 - Synthesis and Characterization of Nanomaterials

## Smart Thermoresponsive Injectables for Bone and Tissue Regeneration

Not presented.

ID: 358 - Synthesis and Characterization of Nanomaterials

Injectable nano material BioActive Glass for Potential Application in Tissue Regeneration

Not presented.

# ID: 375 - Synthesis and Characterization of Nanomaterials

# Electrochemical Properties of Coumarin 500 Encapsulated in Electrospun Fiber Core

# Derva Bal Altuntas<sup>\* 1</sup>, Atilla Eren Mamuk<sup>2</sup>, Çağdaş Koçak<sup>2</sup>, Sema Aslan<sup>3</sup>

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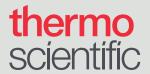
This study coumarin 500 and liquid crystal including polyacrylonitrile Nanofibers in terms of synthesis and characterizations. SEM and FTIR measurements showed that liquid crystal was inserted into the fine polyacrylonitrile Nanofibers successfully. Because it existed a strong molecular interaction between coumarin 500 and liquid crystal, and coumarin 500 was sensitive to polarity of media, the liquid crystal behaved as a guide material for coumarin 500 and it was expected that coumarin 500 was oriented by director of the liquid crystal along the core of fiber. The average polyacrylonitrile nanofiber size was between 0.19  $\mu$ m to 0.25  $\mu$ m and liquid crystal doped and liquid crystal+coumarin 500 doped fibers exhibited similar distribution which is approximately 0.30  $\mu$ m to 0.60  $\mu$ m interval. This proved that the fibers maintained their structure after modifications. Electrochemical evaluation of the different composite Nanofibers showed that there was not a significant current increase upon liquid crystal addition into polyacrylonitrile Nanofibers at voltammograms.

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Keyword: Electrospinning, Liquid crystal, Electrochemistry



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- Her an uyumlu ve görüntüye hazır sistemle veri toplama kolaylığı
- Esnek numune tutucusuyla 10 kg'a kadar numune analizi imkanı
- Mükemmel görüntüleme performansı için geniş dedektör yelpazesi (5 standart dedektör/kamera ve ekstra port girişi)
- Kullanıcı dostu yazılım ve ColorSEM teknolojisiyle sadece 30 saniyede net bir görüntü ve EDS analizi











# Synthesis and Characterization of Magnetic and Conducting Ni-Ferrite/ Chitosan Doped Boric Acid Bio-composites

#### Gökay Karakaya\*, Mehmet Cabuk

Mersin University, Mersin, Turkey

Nowadays, biopolymers are widely used to modify the surface of ferrites since they are highly selective, bio-compatible, ecofriendly and cost-effective. Fe<sub>3</sub>O<sub>4</sub> magnetics offer benefits for integrated chitosan such as incorporation of the functional layer, to reduce aggregation and improve biocompatibility. Magnetic chitosan is applicable in various fields ranging from wastewater treatment, biomedical, food industry, pharmaceutical industries, and electronic screening [1]. Chitosan has poly cationic properties which tend to classify chitosan into dielectric materials [2].

Ferrites are ferrimagnetic materials in which oxygen anions and metal cations arrange themselves into space lattices with different geometric configurations. Among ferrites, spinel ferrites belong to the most promising soft magnetic materials with excellent properties like engineered band gap, high saturation magnetization, coercivity, and better thermal as well as electrical properties. Spinel ferrite has a cubic structure with the chemical formula of MFe<sub>2</sub>O<sub>4</sub>, where M (Ni, Zn, Co, Mg etc.) and Fe cations occupy tetrahedral and octahedral lattice sites, respectively. Among the spinel ferrites, Nickel ferrites are soft, highly magnetic materials that exhibit excellent electrical, magnetic, and optical characteristics [3].

In our study, Ni-ferrite magnetic particles were firstly synthesized by co-precipitation method [4]. The synthesis was performed by considering the calcination temperature of 500 °C. Then the magnetic particles were coated with chitosan (CS) in boric acid (BA) solution. The structures, thermal and morphological properties of Ni-ferrite/CS-BA bio-composite were characterized with ATR-FTIR, TGA, SEM-EDS, TEM and XRD techniques. Some physical properties of materials (density, conductivity, particle size, and magnetic susceptibility) were determined by appropriate methods. These results confirmed the magnetic and conducting Ni-Ferrite/CS-BA structure. After the chitosan coating, the particles exhibited lower particle size (0.997  $\mu$ m) and higher conductivity values than Ni-ferrit particles (1.395  $\mu$ m). The crystalline structures of Ni-ferrit/CS particles were confirmed by XRD patterns. Ni-ferrite/CS bio-composite particles are economically and operationally beneficial as it can be easily separated and controlled with an external magnetic field.

#### Acknowledgments:

The authors would like to thank Mersin University Scientific Research Projects Unit (project number: 2022-1-TP2-4663).

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Keyword: Magnetic chitosan, Ni-ferrite, Bio-composite

# Dual stimuli responsive Boric Acid Doped Chitosan/Zn-Ferrite Bio-composite: Synthesis and Characterization

#### Begüm Perçin Barışan<sup>\*</sup>, Mehmet Çabuk

Mersin University, Mersin, Turkey

Currently, magnetic oxide nanoparticles are attracting significant interest due to their extensive applications, ranging from fundamental research to industrial use. Spinel ferrites have the structure of  $AB_2O_4$  in which A and B display tetrahedral and octahedral cation sites, respectively, and O indicates the oxygen anion site. Metal spinel ferrite nanoparticles have the general molecular formula of MFe<sub>2</sub>O<sub>4</sub> (e.g., M = Zn, Ni, Co, Mn, or Mg). Among the spinel ferrite compounds, zinc ferrite (ZnFe<sub>2</sub>O<sub>4</sub>) has been studied extensively due to its high electromagnetic performance, excellent chemical stability, mechanical hardness, low coercivity, and moderate saturation magnetization, which make it a good contender for applications as soft magnets and low-loss materials at high frequencies [1].

Recently, surface modification of magnetic particles with surfactants and biopolymers has been attractive to many researchers. Chitosan biopolymer, a chitin derivative by N-deacetylation, has improved processability and is soluble in dilute acids by protonation of the primary amines. The biopolymer chitosan, among the other polymers, has excellent film formation, good mechanical properties, biocompatibility, non-toxicity, high water permeability, resistance to chemical modifications, and economic benefits [2]. The magnetic chitosan nanoparticles are promising materials for numerous applications, including target drug delivery and imaging, DNA sequence, adsorption, and electronic screening [3].

In this study, fabrication of colloidally stable magnetic and conducting Zn-ferrite/CS doped boric acid composites are carried out. Co-precipitation method was used in the preparation of the composite due to its simplicity and energy efficiency [4]. In the two-step method, magnetic ZnFe<sub>2</sub>O<sub>4</sub> particles and chitosan-boric acid solution were separately prepared. Then the ZnFe<sub>2</sub>O<sub>4</sub> particles were dispersed in chitosan-boric acid solution and Zn-ferrite/CS-BA was formed via the precipitation and cross-linking, respectively. Characterization of the particles were carried out with ATR-FTIR, TGA, SEM-EDS, TEM and XRD techniques. Some physical properties of the particles such as density, conductivity, particle size, and magnetic susceptibility were determined by the appropriate methods. As a result, ATR-FTIR, SEM and TEM results confirmed the composite structure. XRD results demonstrated the morphology and crystal structure of the particles. According to the physical properties, Zn-ferrite/CS composite was observed to sensitive to external magnetic fields. Chitosan coating was improved the density and conductivity of Zn-ferrite particles. Also, particle size of the Zn-ferrite particles was decreased after chitosan coating (from 1.165 µm to 0.634 µm). In conclusion, Zn-ferrite/CS particles might be suitable and cost effective alternative for various applications since it can be easily separated and controlled with an external magnetic fields.

#### Acknowledgments:

The authors would like to thank Mersin University Scientific Research Projects Unit (project number: 2022-1-TP2-4662).

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Keyword: Zn-ferrite, Biocomposite, Characterization, Boric acid, Magnetic chitosan

ID: 413 - Synthesis and Characterization of Nanomaterials

# Facile Synthesis and Advanced Parameterization of Silver Nanoparticles by Nanosecond Pulsed Laser for SERS Application

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It is possible to create metal nanoparticles (NPs) by nanosecond (ns) pulsed laser ablation synthesis in solution [1,2]. The main advantage of this method is that it requires from 2 to 10 minutes to create these NPs [1,3] and it is possible to control the size distribution [3] by tuning some of the parameters such as laser power, repetition rate, speed of the galvo-scanner head, and process duration. In this study, we characterized silver (Ag) NPs by scanning electron microscopy (SEM) (Figure 1.a), UV-Vis spectroscopy and dark field microscopy to determine the effect of parameter tuning on internal structure and validify our observations about size, shape and orientation of the AgNPs in different solutions.

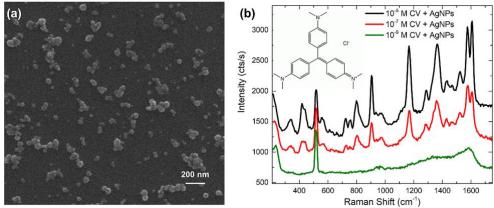


Figure 1: (a) SEM image of AgNPs, (b) Raman spectra of CV molecules mixed with AgNPs solution.

Our work also includes surface-enhanced Raman spectroscopy measurements (Figure 1.b) from different analytes and aging measurements of these NPs. Therefore, the effects of external bonding or oxidation can be classified to select the best solution and ns laser parameters for required application.

# Acknowledgement:

Support from the Scientific and Technological Research Council of Turkey (TÜBİTAK) under grant nr. 119N413 is greatly acknowledged. We thank Prof. Ahmet Oral for giving access to the Raman spectrometer and the microscope, along with METU Central Laboratory and the operators for SEM analysis. D. O. K and B. B. contributed equally to this work.

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Keyword: Plasmonics, Surface-enhanced Raman spectroscopy, Laser ablation

# Preparation of Molecularly Imprinted Polymers for The Solid Phase Extraction of Pyridoxal 5'-Phosphate Prior to Hplc Determination

<u>Ömer Özyurt</u>\* <sup>1</sup>, Elif Gürel Özyurt<sup>1</sup>, Asuman Ünal<sup>2</sup>, Ezel Boyacı<sup>3</sup>, Talal Shahwan<sup>4</sup>, Ahmet Emin Eroğlu<sup>1</sup>

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Three different sorbent materials were prepared for solid phase extraction of pyridoxal phosphate (PLP), namely, carbon sphere nano particle based molecularly imprinted chitosan polymer (MICP) and silica (sol-gel) nano particle based molecularly imprinted polymer (IMIP). The nano size particle based sorbents were characterized by FT-IR, SEM, EDX, XRD, and TGA. The characterization data have shown that, the sorbents were relatively homogeneous distribution of the nano particles, had very fast sorption kinetics and quantitative sorption over a wide range of analyte concentrations (1.0-100.0 mg/L). All the sorbents were found to be selective to PLP in presence of similar compounds; namely, pyridoxamine, nicotinic acid (vitamin B3), pyridoxal and 4-pyridoxic acid. Sorption parameters for each sorbent were optimized. The optimum sorbent amount for 10.0 mL sample volume was found to be 5.0 mg for MICP and 10.0 mg for both MMICP and IMIP. A shaking duration of 30 min was employed in sorption experiments. Among the potential eluents, acetic acid solution (2%, v/v) has shown the best desorption performance for all three sorbents. Method validation was investigated via spike recovery tests on water (ultra-pure, bottled and tap) and artificial serum samples. The recoveries obtained with water samples were greater than 96%, 92%, and 91% for MICP, MMICP, and IMIP, respectively. These results show the potential application of the methodologies for samples with relatively simple matrix. High recoveries (greater than 80%) were also obtained with artificial serum samples, whereas the use of matrix-matched calibration or internal standardization is suggested together with protein precipitation for biological samples with high protein content.

Keyword: Molecularly imprinted polymers, Solid phase extraction, Vitamin B6, Pyridoxal 5'-phosphate, HPLC

# Development of Molecularly Imprinted Solid Phase Extraction Method for The Determination of Vitamin D Derivatives

Hazal Tosun Kurtalan<sup>\* 1</sup>, Yekta Arya Ölçer Altınsoy<sup>1</sup>, Ahmet Emin Eroğlu<sup>1</sup>, Asuman Ünal<sup>2</sup>, Ezel Boyacı<sup>3</sup>,

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Vitamin D is both a micronutrient and a prohormone. There are two structurally different forms of vitamin D2 vitamin D2 (ergocalciferol) and vitamin D3 (cholecalciferol). Both forms can be taken into the body through food or dietary supplements. In addition, cholecalciferol can be synthesized non-enzymatically in the mammalian body as a result of the reaction of the skin precursor 7-dehydrocholesterol with UVB radiation. There are certain factors that affect the level of vitamin D in the human body, causing a deficiency or toxicity. These factors are related to both skin synthesis and supplementation of vitamin D. In case of inadequate or excess vitamin D, various disorders occur in the body. As a result of studies, it has been reported that approximately 1 billion people worldwide<sup>[1]</sup> and almost half of Turkey's population<sup>[2]</sup> have vitamin D deficiency. For all these reasons, it is of great importance that vitamin D determination be performed sensitively and accurately. Molecularly imprinted polymers (MIPs) can be defined as artificial receptors made by mimicking the enzyme-substrate mechanism that works naturally in the body based on the lock-and-key model. Properties such as applicability for various analytes, long shelf life, high mechanical resistance make MIPs applicable as solid phase extraction (SPE) sorbent. In this study, a methodology based on molecular imprinting polymer solid phase extraction (MISPE) is intended prior to the determination of D2 and D3 by HPLC-DAD. In accordance with this purpose, precipitation and sol-gel polymerization methods were used to synthesize molecularly imprinted polymers (MIPs) and non-imprinted polymers (NIPs). Also, different templates, monomers, crosslinkers, and their ratios were tried in the synthesis of MIPs/NIPs by precipitation polymerization. Among all syntheses, MIP, which was synthesized using vitamin D2 as template (T), 4-vinylpyridine (4-VP) as monomer (M), ethylene glycol dimethacrylate (EGDMA) as crosslinker (C) at a molar ratio of 1:6:30 (T:M:C), enabled the co-determination of vitamin D2 and D3. It selectively worked on the vitamin D prohormone group compared to both NIP and commercial SPE sorbents in the presence of other structurally related compounds. The morphologies of the polymers were characterized by SEM and BET. The synthesized MIP particles are spherical in shape, and the average particle size is 1.12 (±0.58) µm. Also, it has a surface area of 6.49  $m^2g^{-1}$ , a pore volume of 0.032 cm<sup>3</sup>g<sup>-1</sup>, and an average pore size of 19.7 nm. The critical experimental parameters of the MISPE method were optimized for the analyte concentration of 1.0 mgL<sup>-1</sup> and determined as follows: 8 hours as the sorption time, 5.0 mg as the sorbent amount, 5.0 mL as the sample solution volume, methanol as the eluent, and 24 hours as the desorption time. A matrix-matched calibration curve with optimized parameters was proposed. The applicability of the developed MISPE method was confirmed by analyzing the sample of liquid vitamin D3 supplementation and overall recovery was found as 95.97% (±1.84) for n=2.

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ID: 417 - Synthesis and Characterization of Nanomaterials

# Synthesis of Palladium(II)-Terpyridine Complex Modified CoFe<sub>2</sub>O<sub>4</sub> Nanoparticles, Investigation of Optical, Thermal and Stimulus-Response Properties

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Terpyridine ligand is a very important functional group for obtaining supramolecular structures and preparing important coordination compounds [1-2]. Numerous important applications such as self-healing materials, shape memory materials, carriers in drug / gene delivery, bioimaging, biodegradable packaging, energy storage, energy conversion, smart polymers and coatings have been realized with molecular architectures prepared using terpyridine ligand structures [1-4]. In addition, multifunctional structures with very important bioactive molecular, magnetic, optical, ferroelectric or catalyst properties have been obtained by combining terpyridine structures and nanostructures [3-5]. In this study, hybrid supramolecular polymeric structures that combine the magnetic properties of the CoFe<sub>2</sub>O<sub>4</sub> structure and the stimulus-response properties of the terpyridine molecule were prepared.

Within the scope of the study, CoFe<sub>2</sub>O<sub>4</sub> nanoparticle structure was prepared using co-precipitation technique. The aminofunctional CoFe<sub>2</sub>O<sub>4</sub> structure was obtained by interacting the surface of the obtained nanoparticles with the aminopropyctriethoxy silane structure. The 4-chloro-terpyridine group was attached to the functional magnetic nanoparticle structure. By interacting the terpyridine functional structures obtained in this way with Pd salts, polymeric systems with supramolecular networks were obtained. The structures obtained at each step were structurally confirmed by FTIR spectrum and X-ray. Morphological and surface properties were determined by SEM analysis. In addition, the thermal properties of the obtained structures were determined by TGA, DTA and DSC thermograms. In addition, the stimulus-response properties of the obtained supramolecular polymers were determined by UV spectrophotometer. The resulting metallo-polymers exhibited magnetic properties and strong double absorption bands around 310 nm and 500 nm, located in  $\pi$ - $\pi$ \* transitions and metalligand charge transfer (MLCT) absorption bands. The resulting hybrid supramolecular structures have potential for applications in smart materials production, electronic, optical, magnetic devices, and catalysts.

## Acknowledgement:

This study was supported by the Scientific Research Projects Unit of İnönü University with the project number FDK-2020-2035.

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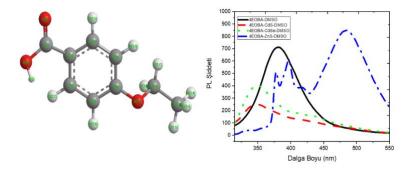
Keyword: Terpyridine ligand, Supramolecular polymers, Nanoparticles, CoFe<sub>2</sub>O<sub>4</sub>

#### ID: 40 - Properties of Nanoscale Materials

# The Possible Interactions between Liquid Crystal and Nanoparticle

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We have done study in which we have examined the fluorescence spectrum by combining the liquid crystals formed between the solid crystal and liquid phases in the phase diagram and the nanoparticles, which exhibit different physicochemical properties, in a solvent environment. Depending on the structure and properties of liquid crystal molecules, they can also interact with nanoparticles and cause their fluorescence to change [1-3]. So, we have studied to determine intra-& intermolecular interactions between 4-Ethoxybenzoic acid(4EOBA), 4-Pentylbenzoic acid(4PentBA), and 4-Pentylphenyl 4-Methylbenzoate (4PP4MetB) liquid crystals and CdS, CdSe with ZnS nanoparticles in DMSO and Methanol. The fluorescence of liquid crystals has been investigated in the shifts between wavelengths of the fluorescence of nanomaterial. It can be said that it has occurred a blue shift at the maximum fluorescence wavelengths of the 4EOBA-CdS-DMSO and 4EOBA-CdSe-DMSO compare to 4EOBA-DMSO. On the other hand, in the 4EOBA-ZnS-DMSO solution occurs red shift in the fluorescence band, while the peaks seen in the fluorescence band can be indicative of the interaction of liquid crystals and nanoparticles.



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Keyword: Liquid Crystals, Nanoparticles, Fluorescence Spectroscopy

# A Mathematical Model for Thin Film Notch Filters

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Demand for optical filters is increasing in various fields such as spectroscopies, glass and defense industries, and medicine. The physics behind the dichroic filters, a type of optical filter, interference. Dichroic filters utilize constructive and destructive interferences of electromagnetic waves that occur by mainly optical path differences from the surfaces, and they are classified according to their filtering shape and working region on the electromagnetic spectrum like high-pass, band-pass, notch, monochromatic, ultraviolet, and near-infrared filters.

Notch filters block to transmit a narrow band of electromagnetic waves on a different part of the spectrum. They have a more complex structure than other types of dichroic filters because of having two cut-off frequencies. A notch filter can be modeled and manufactured by using the features of thin film stacks. Many factors affect the optical behaviors of thin films, but film thickness, the wavelength of incoming light, refractive index, and surface quality are the most outstanding ones.

In this study, multilayer thin film notch filters were modeled according to the optical basis of thin film using Python 3.0 and Jupyter Notebook softwares. Free and expandable materials of the library have been created using the Sellmeier dispersion formulas of the pre-selected dielectric materials TiO<sub>2</sub>, SiO<sub>2</sub>, ZrO<sub>2</sub>, Ga<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, Al2O<sub>3</sub>, AlN, and h-BN as film materials. Constructive and destructive interference behaviors of the single-layer films were investigated using from 10 to 500 nm film thickness, and from 300 to 1200 nm wavelength of light. After single-layer modeling of different thin films, 3 selected materials which are Al<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, and SiO<sub>2</sub>, were deposited on a transparent Corning-glass substrate using electron beam evaporation technique with different film thicknesses. Film thicknesses were measured by the KLA Tencor/P-7 surface profiler. Moreover, the average surface roughness value of the single-layer coatings was measured by Nanomagnetics/ezAFM atomic force microscopy with respect to different deposition rates. Thus, the optimum deposition rate was determined before multilayer modeling and deposition processes.

According to the single-layer examination results, periodic multilayer thin film notch filters were modeled using previously unused materials combinations and their film thicknesses. By controlling the thickness of films, the center wavelength of the notch filters was adjusted in the different regions of the spectrum. Also, mathematical modeling results show numerous thin film notch filters that work on the different parts of the electromagnetic spectrum can be formed using binary material combinations. Even more, notch filters that have two filtering bands or one broadband were modeled by using 3 materials combinations. Also, the effect of the number of periodic binary or triple this film stacks on the transmission of the filter was examined.

Some selected multilayer thin film notch filter models were fabricated to verify the mathematical model with experimental results. The mathematical model and optical measurement results were consistent with each other. Optical measurements of the deposited coatings were performed using Shimadzu/UV-3600 spectrophotometer.

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Keyword: Thin Film, Notch Filter, Python, Electron Beam Evaporation Technique

#### ID: 171 - Properties of Nanoscale Materials

# Characterization of MBE and Magnetron Sputtering grown MgNiO alloys

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In this study, morphological, optical and electrical properties are investigated using Atomic Force Microscopy (AFM), absorption spectroscopy, photoconductivity and current-voltage measurements.  $Mg_xNi_{1-x}O$  samples were grown on strontium titanate (SrTiO3, STO) substrate using the Molecular Beam Epitaxy (MBE) method. Samples grown using Magnetron Sputtering systems were grown on fused silica substrate. At the choice of substrates, high transmission characteristic in UV and VIS regions of electromagnetic spectrum of the substrates are considered [1]. Fused silica has superior transmittance compared to the STO in UV-VIS region. Band gap of the films as a function of elemental concentrations were determined from the analysis of the absorption and photoconductivity measurements. Incorporation of Mg into the lattice of the host material NiO was seen to cause a blue-shift of 12.6% meV/Mg in the bandgap.

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Keyword: Electrooptics, optics, Magnetron Sputtering, Photoconductivity, Optoelectronics, Nickel Oxide, Magnesium Nickel Oxide.

ID: 172 - Properties of Nanoscale Materials

# InGaN/GaN based Top-Hat HELLISH device

Not presented.

#### ID: 236 - Properties of Nanoscale Materials

# Modification and Electrochemical Activity Comparison of Carbon-Based Electrodes

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In last century chemical technologies has advanced in terms of knowledge, materials and techniques. Carbon is a notable chemical element in both organic and inorganic chemistry due to its electronic structure and the presence in the nature [1]. Since carbon structures has been drawn attraction in nanoscience, it is also a widely used in electrochemistry as well [2], [3].

Nanostructures have made possible to use less materials and obtain impressive results which are also used in surface modifications. Thus this has led to acquire more sensitive, reliable, and repeatable results. Aside of the effects of nanomaterials, the substrate choice is also highly important due to achieve inexpensive, reusable and feasible analyses [4].

This study is focused on modification of three carbon-based working electrodes which are glassy carbon, graphite rod, and 3D printed black-carbon/PLA electrodes with silver nanoparticle modified polyethylene glycol. Bare and modified electrode surfaces has been characterized with cyclic voltammetry, scanning electron microscope, atomic force microscope, and water contact angle measurement. All characterization results have pointed that each electrode has surpassing properties on another such as modification ability, recyclability or expenses.

#### Acknowledgments:

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Keyword: 3D printing, carbon working electrode, electrochemical activity, nanostructure, modified surface

ID: 353 - Properties of Nanoscale Materials

# Radiation Effects on Natural and Silicone Rubber used in Medical Applications and Effect of Nanofillers for Self-healing

Not presented.

# Ultra-Sensitive Gas Sensor based Fano Resonance Modes in Periodic and Fibonacci Quasi-Periodic Pt/PtS2 Structures

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Ultra-sensitive greenhouse gas sensors for CO<sub>2</sub>, N<sub>2</sub>O, and CH<sub>4</sub> gases based on Fano resonance modes have been observed through periodic and quasi-periodic phononic crystal structures. We introduced a novel composite based on metal/2D transition metal dichalcogenides (TMDs), namely; platinum/platinum disulfide (Pt/PtS<sub>2</sub>) composite materials. Our gas sensors were built based on the periodic and quasi-periodic phononic crystal structures of simple Fibonacci (F(5)) and generalized Fibonacci (FC(7, 1)) quasi-periodic phononic crystal structures. The FC(7, 1) structure represented the highest sensitivity for CO<sub>2</sub>, N<sub>2</sub>O, and CH<sub>4</sub> gases compared to periodic and F(5) phononic crystal structures. Moreover, very sharp Fano resonance modes were observed for the first time in the investigated gas sensor structures, resulting in high Fano resonance frequency, novel sensitivity, quality factor, and figure of merit values for all gases. The FC(7, 1) quasi-periodic structure introduced the best layer sequences for ultra-sensitive phononic crystal greenhouse gas sensors. The highest sensitivity was introduced by FC(7, 1) quasi-periodic structure for the CH<sub>4</sub> with a value of 2.059 (GHz/m.s<sup>-1</sup>). Further, the temperature effect on the position of Fano resonance modes introduced by FC(7, 1) quasi-periodic PhC gas sensor towards CH<sub>4</sub> gas has been introduced in detail. The results show the highest sensitivity at 70° C with a value of 13.3 (GHz/° C). Moreover, the highest Q and FOM recorded towards CH<sub>4</sub> have values of 7809 and 78.1 (m.s<sup>-1</sup>)<sup>-1</sup> respectively at 100° C.

Keyword: greenhouse gas sensor, fano resonance modes, quasi-periodic phononic crystal, platinum disulfide, simple and generalized Fibonacci

# Ternary Pentagonal BNSi Monolayer: Two-dimensional Structure with Potentially High Carrier Mobility and Strong Excitonic Effects for Photocatalytic Applications

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In recent years many attempts have been made to discover new types of two-dimensional (2D) nanostructures with novel properties beyond the hexagonal crystals. The prediction of pentagraphene has sparked a great deal of research interest to investigate 2D pentagonal systems. In line with these efforts, in this paper, we propose a 2D ternary pentagonal monolayer of BNSi (penta-BNSi) and systematically investigate its structural, vibrational, mechanical, piezoelectric, electronic, photocatalytic, and optical properties by performing first-principles methods. We verify the stability of the penta-BNSi monolayer from the dynamical, thermal, and mechanical aspects based on phonon dispersion, ab initio molecular dynamics, and elastic tensor analysis, respectively. The mechanical properties are examined by calculating in-plane stiffness, Poisson's ratio, and ultimate tensile strength and penta-BNSi is found to be soft and ductile. The electronic structure and electronic transport calculations indicate that the penta-BNSi monolayer possesses a quasidirect band gap and anisotropic, potentially high carrier mobility. Due to the noncentral symmetric character and semiconducting feature, an intrinsic

piezoelectric response emerges in the structure. In addition, penta-BNSi has a suitable band gap as well as proper band edge positions for photocatalytic water splitting within practical pH levels. The analysis of optical properties, including many-body effects, points out strong exciton binding and high light absorption in the visible and near-UV parts of the spectrum. Our findings not only expand the family of 2D pentagonal materials but also uncover an ideal ultrathin material for photocatalytic applications.

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Keyword: Electronic structure, 2-dimensional systems, Density functional theory

# The Synthesis and Characterization of Mo<sub>2</sub>CTx Mxene by Hydrothermal Etching with Different Fluoride Salts for EMI Shielding Applications

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Recently discovered novel two-dimensional materials, Mxenes, attracted the attention of many researchers and are widely studied for the applications of energy storage, catalysis, gas sensing, wastewater treatment etc. More than twenty Mxenes have been successfully synthesized and Mo<sub>2</sub>CT<sub>x</sub> holds great potential due to its theoretically predicted electrochemical, thermoelectric properties and chemical stability. However, the synthesis of Mo<sub>2</sub>CT<sub>x</sub> is challenging due to the strong bonding between Mo-Ga atoms resulting in nearly several days of etching process of Mo<sub>2</sub>Ga<sub>2</sub>C MAX phase. Scientists have overcome this challenge by using hydrothermal etching and decreased the duration of the etching process drastically. In this study, the hydrothermal etching of Mo<sub>2</sub>Ga<sub>2</sub>C to produce Mo<sub>2</sub>CT<sub>x</sub> with different fluoride salts are investigated and the effects of different salts (LiF, BaF<sub>2</sub>, MgF<sub>2</sub> and MnF<sub>4</sub>) are discussed. The fluoride salts are mixed with hydrochloric acid and the hydrothermal etching process is applied at 140 °C and 160 °C for 24 hours. The morphology of synthesized sheets is investigated with SEM and the chemical composition of the materials are reported using EDS analysis. The structural analysis of the Mo<sub>2</sub>CT<sub>x</sub> sheets is analyzed using XRD. After understanding the effects of process parameters such as duration, temperature, and fluoride salt type on the synthesis of  $Mo_2CT_x$  powders, samples are produced to study electromagnetic interference shielding effectiveness. Mo<sub>2</sub>CT<sub>x</sub> powders are hand-mixed with epoxy resin to have different weight percentages. The EMI Shielding properties of Mo<sub>2</sub>C Mxene composite is reported for the first time in this study. EMI Shielding properties of the Mxene composites are reported in accordance with "ASTM D4935 Standard Test Method for Measuring the Electromagnetic Shielding Effectiveness of Planar Materials" using a vector network analyzer in the frequency range of 1.5–10 GHz.

## Acknowledgments:

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ID: 160 - Graphene and 2D Materials

# Two-dimensional Janus GePAs Monolayer: Direct Band Gap Semiconductor with High and Anisotropic Mobility for Efficient Photocatalytic Water Splitting

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The sun is considered an inexhaustible natural energy resource compared to fossil fuels. Regarding the limited amount of fuels such as coal and petroleum and their effect on nature, any application that has the ability to harvest the sunlight and produce energy becomes extremely important. One of the potential mechanisms that can remedy the energy demand in the future is photocatalysis, and two-dimensional (2D) materials with suitable electronic and optical properties offer new possibilities for photocatalytic applications. Although various 2D materials have hitherto been specified as adequate candidates, materials with high photocatalytic efficiency for water splitting are still minimal. In this regard, a novel 2D Janus GePAs monolayer is predicted and its capability for photocatalytic water splitting is examined by performing first-principles density functional theory. The GePAs monolayer is shown to possess robust dynamic and thermal stability. The direct electronic band gap in the visible region and band edge positions of the strain-free and strained monolayers are revealed to be convenient for redox reactions in wide pH ranges. The low recombination probability of charge carriers ensured by high and anisotropic carrier mobility enhances the material's photocatalytic potential. Optical response calculations, including many-body interactions, exhibit significant optical absorption capacity in the UV–visible range. Furthermore, ultra-low exciton binding energy facilitates dissociation into free electrons and holes, promoting photocatalytic reactions. Our study suggests GePAs monolayer is an ideal and remarkably promising material to be utilized in visible-light-driven photocatalytic applications.

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Keyword: ab initio, density functional theory, Janus, photocatalysis, water splitting

# Nail Polish Derived Laser Induced Graphitic Structures

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Graphene, which is a two dimensional material with single layer carbon atoms arranged in a hexagonal lattice, is identified with its outstanding electrical, thermal and mechanical properties. Many different synthesis techniques (CVD; Mechanical or chemical exfoliation; SiC vacuum decomposition, etc.) have been proposed and used related to their advantages and limitations. Recently, laser induced graphene (LIG) has attracted attention due to its ease and low cost. In this study we show that nail polish can be used as a precursor for LIG. Nail polish derived LIG is produced in air using a 405 nm laser and characterized by using SEM, XRD and Raman Spectroscopy.

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Keyword: Laser Induced Graphene

# Electronic and Magnetic Properties of Artificial Triangular Graphene Quantum Dots with Zigzag Edges

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Triangular zigzag graphene quantum dots (TGQD) constitute a subclass of graphene nanostructures with unusual electronic, magnetic and optical properties [1,2]. In particular, their energy spectrum exhibits a shell of degenerate states at the Fermi level due to the broken sublattice symmetry of the two non-equivalent carbon sublattices, leading to spin-polarized edge structure. This property also gives the opportunity of designing an analog system to investigating fractional quantum Hall effect without the need for a magnetic field [3]. However, since natural graphene nanostructures have stability and tunability issues, those properties have not been observed experimentally yet. On the other hand, fabrication of artificial semi-conductor graphene [4] allows better controllability and reliability in terms of structural properties.

In this work, our aim was to examine the electronic and magnetic properties of artificial semi-conductor TGQDs and to design these properties as desired by exactly solving the many-body Hamiltonian using continuum quantum Monte Carlo methods [5] through various trial wave functions. Those many-body trial wave functions were first obtained using tight-binding and mean-field Hubbard orbitals, then optimized by the VMC method, and finally used as a starting point for the diffusion Monte Carlo (DMC) calculations. This allowed us to accurately obtain the many-electron ground state of TGQDs, investigate the effects of system parameters such as dot radius, potential sharpness, and the distance between dots, and show that a antiferromagnetic-metallic phase transition may occur.

#### Acknowledgments:

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Keyword: artificial semi-conductor systems, 2d materials, triangular graphene quantum dots, quantum monte carlo, artificial graphene nanosystems

# Production of N-doped Graphene Reinforced PCL Nanofibers by Electrospinning

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Nanofibers are known as nanometer-sized thin fibers. Nanofibers have a high surface area (high length/volume ratio) and rigidity, so they are used in pure or composite form in a wide range of fields such as spatial and optical applications, defense industry, filtration, agriculture, medical [1]. Among the methods used to obtain Nanofibers, the electrospinning process comes first. Graphene was the first nanomaterial discovered in 2-dimensional form. It is a single atomic layer with a thickness of sp<sup>2</sup> hybridized carbon atoms arranged in a hexagonal (honeycomb) lattice. The electrical properties and high carrier mobility, which are among the unique structural features of graphene, make it a sought-after material [2]. In order to improve the electrical behavior of graphene in composite structures, it is doped with different heteroatoms. Among them, N doping has been widely used to popularize and predict the effect of physicochemical, electrochemical and electrical properties as a method to improve the properties of targeted carbons [3].

The main aim of this study is to obtain Nanofibers by electrospinning by preparing a solution with PCL (Poly e-caprolactone) matrix under appropriate thermodynamic conditions by obtaining modified graphene as a result of adding suitable reagents to ensure the formation of C-N. First, N-doped HNO<sub>3</sub>-modified graphene was obtained by using nitrogen reagents after graphene was modified with HNO<sub>3</sub> to increase its miscibility. Next, the spray solution was prepared by combining the final graphene material and PCL at different weight ratios in dichloromethane (DCM) / DMF, a solvent mixture suitable for electrospinning. Mats knitted from fine fibers were characterized in terms of structure, surface and morphology using FTIR, XRD and SEM.

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[3] Recent Advances in Boron- and Nitrogen-Doped Carbon-Based Materials and Their Various Applications Anukul K. Thakur,Klaudia Kurtyka,Mandira Majumder,Xiaoqin Yang,Huy Q. Ta,Alicja Bachmatiuk,Lijun Liu,Barbara Trzebicka,Mark H. Rummeli

Keyword: Electrospinning, Nanofiber, Graphene.

# **Preparation and Characterization of PVDF-Graphene Nanocomposites**

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Polyvinylidene fluoride (PVDF) is one of the popular membrane materials due to its superior properties such as thermal stability, chemical resistance and excellent mechanical strength. It is a semi-crystalline polymer where the crystalline phase provides mechanical and impact strength while the amorphous phase provides flexibility[1]. The superior properties of graphene are also reflected in polymer/graphene nanocomposites. Polymer/graphene nanocomposites show superior mechanical, thermal, gas barrier, electrical and flame retardant properties when compared to the undoped polymer. In addition, it has been reported that the improvement observed in the mechanical and electrical properties of graphene-containing polymer nanocomposites is much better than that of clay or other carbon-containing polymer nanocomposites [2].

In this study, PVDF, which is frequently encountered in ultrafiltration membrane separation process, was selected as a polymer material to obtain clean water of potable quality. In order to separate hydrophilic species, hydrophilic graphene (HNO<sub>3</sub> modified graphene) was added to the structure of hydrophobic PVDF. PVDF and PVDF/HNO<sub>3</sub> modified graphene nanocomposite Nanofibers were obtained using electrospinning method with two different polymer molecular weights. The effect of the solution properties on the nanofiber diameter was evaluated by measuring the concentration, viscosity, surface tension, electrical conductivity and contact angles.

Morphological and structural characterizations of Nanofibers were performed using various instrumental analysis methods (FT-IR, XRD, TGA, SEM). In addition, contact angle measurements were performed to measure surface hydrophobicity. When the effects of solution parameters on Nanofibers obtained by electrospinning were evaluated, it was observed that the addition of HNO<sub>3</sub> modified graphene to the structure caused a decrease in the viscosity and therefore a decrease in the diameter of the nanofiber as a result of a decrease in the interactions of PVDF molecules. In addition, the decrease in surface tension due to the increase in the amount of HNO<sub>3</sub> modified graphene also caused a decrease in the diameter of the nanofiber. Increasing the amount of HNO<sub>3</sub> modified graphene in the PVDF structure caused a decrease in the contact angle.

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Keyword: Electrospinning, nanofiber, polyvinylidene fluoride, graphene, ultrafiltration.

# Synthesis of Transition Metal Fe2AlB2 MAB Phase via High-Temperature Sintering Method

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In recent years, studies have been carried out on similar MAB phases due to using MAX phases as a leading material in synthesizing 2D structures. Theoretical and experimental studies have proven MAB phases obtained by replacing the carbon and/or nitrogen corresponding to the element X in the MAX phases with boron [1]. MAB phases are layered orthorhombic transition metal borides similar to MAX phases but with higher structural stability. In the MAB phase, M represents the transition metal, A represents the III-A or IV-A group element, and B represents the boron element. In the MAB phases M: Cr, Mo, W, Fe, Mn or solid alloys of these elements (such as FeB, CrB and MnB). Recent studies on MAB phases have mainly focused on single crystal growth and crystal structure determination [1], electronic properties [2], mechanical properties [3] and oxidation resistance [4]. MAB phases can also be produced by methods similar to MAX phases. MAB phases are obtained by sintering at high temperatures (1000-1500°C) in an Ar atmosphere after elemental (Al, B, Cr, W, Mo, Mn, Fe) or alloy (such as FeB, CrB, MnB) precursor materials are mixed and pressed in certain proportions. In this study, the precursor materials (Al, B, and Fe) of the elements used in synthesizing the Fe<sub>2</sub>AlB<sub>2</sub> MAB phase were mixed homogeneously by ball milling at the determined stoichiometric ratios, and cold-pressed 1-inch raw pellets with physical bond were then sintered at certain temperatures.

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#### ID: 244 - Graphene and 2D Materials

# Graphene/SOI-based Self-powered Schottky Barrier Photodiode Array

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Various techniques have been demonstrated to fabricate Graphene/n-type Silicon (G/n-Si) Schottky barrier photodiode on bulk Si substrate. However, it is not possible to obtain a G/n-Si Schottky barrier photodiode array with this device structure due to inevitable electrical and optical leakage. Herein, we reported the fabrication of novel 4-element Graphene/Silicon on Insulator (SOI) based Schottky barrier photodiode array (PDA) and investigated its optoelectronic device performance. In our device design, monolayer graphene is used as common electrode on lithographically defined linear array of n-type Si elements on SOI substrate. As revealed by wavelength resolved photocurrent spectroscopy measurements, each element in the PDA structure exhibited a maximum spectral responsivity of around 0.1 A/W under zero-biased operational mode. Time-dependent photocurrent spectroscopy measurements showed excellent photocurrent reversibility of the device with ~1.36 us and ~1.27 us rise time and decay time, respectively. Each element in the array displayed an average specific detectivity of around  $1.3 \times 10^{\Lambda/12}$  Jones and a substantially small noise equivalent power of ~0.14 pW/Hz<sup>-1/2</sup>. We also analyzed almost almost no crosstalk between neighboring G/n-Si elements in the array for each PD element in the optical cross-talk measurements. This study is expected to offer exciting opportunities in terms of high value-added G/n-Si based PDA device applications such as multiwavelength light measurement, level metering, high-speed photometry, position/motion detection, and more. (See details in the Ref [1].)

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Keyword: Graphene, Silicon on Insulator, Photodiode Array, 2D Materials, Schottky Barrier Photodiode

# **Growth Graphene by Different CVD Methods**

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Graphene is the two-dimensional honeycomb structure of carbon atoms that each atom is connected to its three nearest carbons by a  $\sigma$ -bond, and share one electron to a conduction band. In generally graphene produces by exfoliation of graphite or cracking hydrocarbon molecules then deposition on substrate. Graphene were grown by three different chemical vapor deposition methods

a) Thermal chemical vapor deposition

b) Plasma enhanced chemical vapor deposition

c) Hot Filament Chemical Vapor Deposition.

Graphene was grown on Cu foil by using Methane, Argon and hydrogen gases. reaction chambers evacuated to 1\*10-6 Torr as bases pressure. substrate temperature varied between 600-1000 0C and gases cracking temperature was between 600-2000 0C and cause to deposition carbon atoms on suitable substrate.

Results analyzed by Raman spectroscopy and it is revealed two peaks centered about on 1580 cm-1 and 2700 cm-1 the origin of which is sp2 hybrid of graphite (G-band) and sp3 hybrid (2D-band). Atomic force microscopy showed roughness, thickness and topography of single layer graphene, scanning electron microscopy revealed surface morphology and an optical microscope used to show size, quality and number of graphene layers. Investigated results revealed which one of the above methods has high yield, low growth temperature and high quality graphene.

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ID: 371 - Graphene and 2D Materials

# Electrochemical Sensor Based on Transition Metal Dichalcogenides for Deoxribonucleic Acid Detection

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Transition metal dichalcogenides (TDMCs) are compounds composed of chalcogen elements and transition metal elements. TDMCs are widely used in biological detection systems for the highly sensitive and selective detection of various biological molecules. The interesting properties of transition metal dichalcogenides (TMDCs) have led to the use of these materials in many applications. TMDCs are frequently used in biological systems due to their optical properties, electronic properties, large surface area, stability in aqueous environments, low toxicity levels and recombinable layered structures [1,2]. For this purpose, the use of TMDCs modified pencil graphite electrode (PGE) for electrochemical deoxribonucleic acid (DNA) detection was summarized in this study. TDMCs modified electrodes were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD) analysis, atomic force microscopy (AFM), and electrochemical techniques. The composition of the detection platform was monitored by energy dispersive X-ray spectroscopy (EDS).

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Keyword: Transition metal dichalcogenides, Electrochemical detection, DNA

ID: 377 - Graphene and 2D Materials

# Electrochemical biosensor for determination of Carcinoembryonic antigen biomarker using human breast ductal adenocarcinoma, human ovarian adenocarcinoma cancer cells

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In this study, an electrochemical biosensor for determination of Carcinoembryonic antigen (CEA) biomarker using human breast ductal adenocarcinoma (MCF-7) and human ovarian adenocarcinoma (SK-OV-3) cancer cells was presented. Disposable pencil graphite electrodes (PGE) has been modifed with Au nanoparticle (Au NP) and nanostructure dispersed chitosan (Cs) matrix. Therefore, the electrochemical interaction between the antibody-electrode surface was facilitated. Experiments were conducted to determine the number of normal cell hGF and cancer cells adhered and attached on immunocytosensor surfaces. CEA-positive MCF-7 cells have shown great potential for adhesion and attachment to immuno-cytosensor surfaces better than CEA-negative cells. The developed cytosensor exhibited very promising results for the future biosensor studies.

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Keyword: Carcinoembriyonic antigen, Nanoparticle, Human breast ductal adenocarcinoma, Human ovarian adenocarcinoma, Immunosensor-cytosensor

# Ballistic thermoelectric transport properties of two-dimensional group III-VI monolayers

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Ballistic transport and thermoelectric properties of group III-VI compounds (XY : X = B, Al, Ga, In, Tl; Y = O, S, Se, Te, Po) are investigated based on first-principles calculations and Landauer formalism. This large family is composed of 25 compounds which stands out with their unique electronic band structures. Mexican hat shaped valence band, which exhibits quartic energy-momentum relation gives rise to a sharp peak in the density of states as well as a steplike electronic transmission spectrum near the valence band edge. The intriguing electronic band structure and transport properties motivate us to explore thermoelectric properties of group III-VI monolayers. We find that, in addition to the stepwise transmission at the band edge, flat bands, valley degeneracy, and band degeneracy are the factors that enhance thermoelectric efficiencies. For heavier compounds, better thermoelectric efficiencies are possible for both n-type and p-type carriers.

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Keyword: 2D Materials, Transport Properties, Thermoelectric Properties

# Post Treatments in Silver Nanowire Networks for Figure-of-Merit Improvement

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Competitive optical transmittance and sheet resistance values as well as low-cost, large scale and reproducible deposition are the main reasons why silver nanowire (Ag NW) networks are considered as one of the most suitable alternative materials to replace commercial indium tin oxide (ITO) transparent electrodes<sup>1</sup>. The produced electrodes have seen use in numerous applications in the fields of optoelectronics<sup>2</sup>, sensing<sup>3</sup> and nanogenerators<sup>4</sup>. As-deposited Ag NW electrodes cannot fully meet the requirements for preparing high performance optoelectronic devices due to the high contact resistance with polyvinyl pyrrolidone (PVP) encapsulating the nanowires<sup>5</sup>. Large surface roughness and poor stability are other evident major problems<sup>6</sup>. Thus, various post treatments are needed for Ag NW network optimization. Previous work in literature<sup>(7-9)</sup> applies to various sets of nanowires with different PVP thicknesses, lengths, and diameters, but the application of the post treatments to the same batch of nanowires and combination of the post treatments and is still incomplete. This study investigates various post treatment methods both in the literature and developed in-house on the same batch of nanowires and aims optimize the Ag NW network electrodes. Moreover, some unique post treatment methods were analyzed and combined to find the best solution to the particular set of Ag NW networks. The combination of the optimal post treatments on the Ag NW networks resulted in the reduction of the sheet resistance from 360  $\Omega$ /sq to 24  $\Omega$ /sq with an optical transmittance of 92% at a wavelength of 550 nm.

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Keyword: Silver nanowires, post treatment, figure of merit improvement



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# Polytryptophan-Based Tubular Micromotors for Dopamine Recognition

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Micro/nanomotors are undoubtedly a groundbreaking development in the field of nanotechnology. Synthetic micro/nanomachines mimic natural motors; hence, they can perform diverse tasks including cargo transport, drug delivery, and environmental remediation [1-2]. In this work, we report the synthesis, characterization, and application of polyamino acid-based catalytic micromotors. Conical-shaped polycarbonate (PC) membrane-assisted polytryptophan functionalized catalytic tubular micromotors were synthesized electrochemically. In order to utilize the micromotors in the detection/recognition of dopamine, which is one of the major neurotransmitters that appear in our central nervous system [3], prepared micromotors were incubated in dopamine solutions of different concentrations. After that, the gradient in the micromotor's velocity in the presence of hydrogen peroxide ( $H_2O_2$ ) was correlated with the recognition of dopamine. For the purpose of examining the effect of fuel concentration on the velocity, hydrogen peroxide concentration was optimized. Synthesized micromotors were characterized by performing electrochemical impedance spectroscopy (EIS) in addition to scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX).

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Keyword: Functionalized micromotor, polytrytophan, dopamine

# The Effect of The Segment Construction on The Motion Ability of Magnetic Motors

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Under the roof of nanotechnology, micromotors have gained strong attention of researchers around the globe in the last decades. A micromotor is a micro-size device that converts the present enery into motion. According to the actutation mechanism of their motion ability they are generally categorised as "fuel-driven" and "fuel-free" micromotors. Usually "fuel-driven" micromotors utilize the decomposition of a "fuel", e.g. hydrogen peroxide and hydrazine, while "fuel-free" micromotors are actuated in the presence of an external force such as light, acoustic field, ultrasound, electrical field or magnetic field [1-2]. Owing to their maneuverability, programmable and fuel-free motion, magnetic micromotors have become a prominent research topic. Though researchers have accomplished tremendous achievements in the field of magnetic micromotors [3-4], the movement ability in unfriendly environment of micromotors is in need of improvement and is worth investigating. Herein we present an investigation on the template-assisted electrochemically synthesized gold (Au) segment containing magnetic micromotors. In order to analyze its effect on the motion ability, iron (Fe) and nickel (Ni) ratio of the deposition solution and deposition time have been studied. The morphologhy of the synthesized micromotors were validated with optical microscopy and scanning electron microscopy (SEM).

#### Acknowledgements:

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Keyword: Micromotors, magnetic micromotors, electrochemical deposition

# Elektrokimya / Enerji





**ID: 49 - Nanoelectronics and Spintronics** 

# Thickness Dependent Electric-Field Controlled Magnetic Anisotropy in Co<sub>2</sub>MnAl/PMN-PT

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Strain mediated magnetoelectric (ME) coupling can be used to modify the magnetization of ferromagnetic/ferroelectric (FM/FE) heterostructures, which play an important role in developing energy efficient and fast memory devices. The manipulating magnetism with an electric field is particularly inspiring from a technical perspective and highlights important fundamental phenomena behind the interfacial coupling mechanism. Beginning with the electric field effect at the interface of ferromagnets and dielectrics to induce changes in magnetic anisotropy, the invention of multiferroics by design suggested the idea of changes in the ferromagnet in a nonvolatile method [1-4]. Because of their electrical and magnetic properties, Co<sub>2</sub>MnAl thin films have the potential to be highly important in such systems as a ferromagnetic layer. However, substrate compatibility is required for the formation of Co<sub>2</sub>MnAl film with defined anisotropy [5]. Forming the anisotropy in the film is incredibly hard due to the high lattice mismatch between crystalline Co<sub>2</sub>MnAl and PMN-PT. However, there are alternative ways of creating magnetic anisotropy, including growth induce anisotropy. In this study, Co<sub>2</sub>MnAl thin films have grown on PMN-PT (011) substrate with various thicknesses by an oblique incidence deposition using DC magnetron sputter system. Since no buffer layer is formed, obtaining a uniaxial magnetic anisotropy is highly dependent on thickness of the film. Five different thicknesses were investigated to find optimum value. Both the magnetization and ferromagnetic resonance measurements show that a 30 nm thick Co<sub>2</sub>MnAl film has ideal magnetization and magnetic anisotropy. The voltage induced anisotropic biaxial strain cause a smooth rotation of magnetic moments in Co<sub>2</sub>MnAl/PMN-PT heterostructure. The piezo-strain induced by applying electric field along the surface normal induces only in-plane strain which leads to rotation of the easy-axis orientation of Co<sub>2</sub>MnAl from [100] to [01-1] direction of the PMN-PT substrate. Due to the anisotropic strain originating from PMN-PT, the remanent magnetization states and coercivity of the Co2MnAl film vary significantly and asymmetrically with the applied voltage. Electrical control of magnetization in the Co<sub>2</sub>MnAl Heusler compound at room temperature will be of interest for developing next generation magnetoelectric random access memory devices.

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Keyword: Voltage-controlled magnetic anisotropy, Thin Film, Multiferroics

# Modelling of Memristive Devices for Neuromorphic Circuit Design and Analysis

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Since its initial conceptualization in 1971 [1], the definition of the memristor has been broadened to include various forms of non-volatile memory that is based on resistance switching, which increases the flow of current in one direction and decreases the flow of current in the opposite direction. Its compelling inherent memory property, nanometric dimensions, low power operation is suitable for bioinspired, neuromorphic circuits. This work will present the modelling efforts of the behavior of devices which are fabricated by our research group. These devices have an active layer (responsible for the resistive switching) of stoichiometric and doped Titanium Oxide of nanometric thickness, electrodes are platinum or gold. Memristive behavior occurs due to the ionic movement within the active layer of the device, modelling aims to shed light to, utilize and simulate the effects of this nanoscale conduction.

The circuit design process relies heavily on circuit simulations. Circuit simulators such as SPICE (Simulation Program with Integrated Circuit Emphasis) and Cadence Spectre use device models to enable accurate circuit analysis. A generalized model of the memristor has not been established yet. Therefore, in order to utilize and benefit from memristive properties in analog circuits, accurate and practical models are required. This work focuses on modelling memristors fabricated by our research group. We used measurement results obtained from our own devices to create phenomenological models through curve fitting, the equations that were derived were then compared to existing memristor models [2]. As a result, we developed a SPICE model of our device.

The modeling effort in this work is particularly geared towards implementing memristors in bioinspired analog circuits. Such circuits (e.g. Central Pattern Generators- neural networks producing autonomous rhythmic activity) have certain requirements in terms memristor specifications. Reliable models enable more flexible design, including but not limited to using networks of memristors to achieve desired behavior. This work will present modelling efforts as well as work on utilizing accurate models in circuit simulations.

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Keyword: Memristor, Complementary Resistive Switching, Neuromorphic, Device model

ID: 344 - Nanoelectronics and Spintronics

Dynamic Laser Speckle Analysis for Detection of Electric Current Flowing in Wires

Not presented.

ID: 12 - Computational Nanoscience

# Size Dependent Change of Mean Square Displacement in Gold Nanocrystals: A Molecular Dynamics Simulation

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Mean square displacements (MSDs) of spherical gold nanocrystals were studied computationally. Using atomistic molecular dynamics (MD) simulations, both size and temperature dependent change of MSDs of nanocrystals were analysed. The structure-property relation was explained based on simulation results. Our analyses show that MSD of spherical gold nanocrystals strongly depends on both temperature and size. While MSD increases linearly with increasing temperature, it decreases with increasing size. Temperature and size-dependence of MSD were attributed to thermal energy and surface-to-volume atom ratio, respectively. In addition, local MSD analyses show that atomic displacements increase radially from the center of the nanocrystals and reach a maximum at the surface layers due to the presence of undercoordinated surface atoms and their relatively unrestricted motions. Results of this work are useful to understand the effect of nanocrystal size on quantifying the amplitude of atomic vibrations and their effects on measured intensities from their x-ray diffraction data.

Keyword: Molecular dynamics simulations, gold nanocrystal, mean square displacement, Debye-Waller factor

# **Computational Investigation of Covalent Organic Frameworks for Urea-Water Separation**

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Covalent organic frameworks (COFs) are an exciting new type of porous organic materials, which are constructed with organic building units *via* strong covalent bonds. COFs are designable and chemically stable materials with large surface areas which make them ideal adsorbents. Although high gas separation performances of COFs have been reported in the literature, their performance for liquid separation is still in its infancy. In this work, as a first time we computationally screened 656 COFs for urea separation from water, which is critical for biological process. First, Grand Canonical Monte Carlo (GCMC) simulations were performed at 310 K and 1bar to compute the saturated urea uptakes of COFs. Many COFs outperformed 62 biocompatible MOFs and several traditional adsorbents including zeolites and well-known MOFs in terms of urea uptake at 310 K. Equilibrium Molecular Dynamics (EMD) simulations were then performed at 310 K to compute the self-diffusion coefficients of urea and water within the pores of COFs. Structure-performance relations were also examined, and pore volume and surface area were found to be highly correlated with the urea uptakes of COFs. Combining GCMC and EMD simulations, we estimated adsorption, diffusion, and membrane selectivities of this study will be useful to guide the future work on the development of efficient COF adsorbents and membranes for urea/water separation.

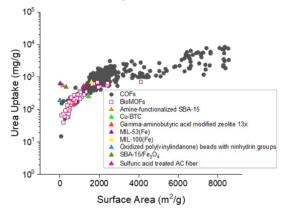


Figure: The comparison of urea uptakes of COFs computed in this work with those of traditional materials reported in the literature [1].



- Savunma Sanayi
- Medikal Sanayi
- Plastik sanayi
- Metal sanayi
- Malzeme bilimleri
- Tekstil sanayi
- Kimya sanayi
- Çevre teknolojileri
- Gıda teknolojileri
- Nano Teknoloji
- İnce film kaplama sistemleri
- Plazma sterilizasyon
- Plasma yüzey hazırlama
- Atmosferik basınç plazma sistemleri
- Endüstriyel corona sistemleri
- Mikrodalga vakum kurutma ve eritme sistemleri
- PECVD ve CVD sistemleri
- Elektromanyetik Fırlatma Sistemi
- Nano Malzeme Üretimi
- Grafen ve elmas üretim sistemleri
- Ozon sistemleri
- Mikrodalga plazma
- Endüstriyel ultra yüksek vakum
- Plazma itkiler
- İyon beam
- Elektron beam
- Dekoratif kaplama sistemleri
- Plazma diagnostik sistemler
- Mikrodalga yakıcılar
- X-ray sistemler

























ID: 121 - Computational Nanoscience

# DFT Investigation of the Electronic Properties of Semiconductor Quantum

Not presented.

ID: 177 - Computational Nanoscience

# Investigation of the Behavior of the Logistic Map Equation in Negative Regime of Rate

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Deterministic chaos and constants such as Feigenbaum offer a chance to uncover predictability in uncertain or unpredictable systems. In literature usually, the growth rate of the logistic map was investigated to find the Feigenbaum constant. However, one can apply the rate in a negative regime which might aid in understanding the degradation of biological materials. The effort is trying to investigate the behavior of the logistic map and find the Feigenbaum constant by applying a negative value of rate to the logistic map. In this work, we construct the bifurcation diagram for negative values of rate, and also, try to find the Feigenbaum constant using the Lyapunov exponent for the bifurcation diagram and compare it to the universal value of the Feigenbaum constant. Finally, we calculated the Feigenbaum constant for the negative regime of the rate in the logistic map and it was in good agreement with the universal value.

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Keyword: Feigenbaum Constant, Logistic Map, Bifurcation Diagram, Lyapunov Exponent

ID: 185 - Computational Nanoscience

# Density Functional Theory Investigations of Rh- & Ir- ZnO(0001) Single Atom Catalysts

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Heterogeneous catalysis constitutes the most significant part of the chemical industry regarding usage prevalence. Heterogeneous catalysts are generally produced using noble metals. However, since noble metals are costly and rare, reducing their amount is of great importance. Achieving this goal while increasing the specific catalytic activity has been made possible by Single-Atom Catalysts(SACs). They consist of a supporting surface and catalytically active sites produced by homogeneously placing the atoms on the surface. Support-metal interaction determines the catalytic properties of SACs. Therefore, it is vital to perform metal-support optimization for effective catalysts. In this work, we present a Density Functional Theory investigation for the catalytic activities of Rh- and Ir- on ZnO(0001) surface by modeling CO oxidation and O2 separation. We also compared the stability of the single-atom surfaces with the double-metal clusters. Further, we examined the effect of noble metal coverage on reactivity by calculating the binding energy of CO on larger supercells. Finally, the effect of the impurities on binding energies for CO2, CO, O2, and O were reported for different surface coverages.

#### Acknowledgments:

This work is financially supported by TÜBITAK, Scientific and Technological Research Council of Turkey (Grant No: 118F355).

Keyword: Density Functional Theory, Single-atom catalysts, Metal Oxides, CO oxidation





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# Plasmonic features of a hybrid system comprising borophene and aluminium

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Recent developments in the synthesis and fabrication of plasmonic nanostructures give us access to unprecedented capabilities for manipulating light-matter interactions at the nanoscale [1,2,3]. In this work, we systematically examine the optical and plasmonic properties of a hybrid system made of borophene and Aluminium film using first-principles time-dependent density functional theory calculations. We discovered that, despite the weak charge transfer between the constituent systems, the borophene plasmon is totally quenched or damped by the proximity to the Al film for a gap distance (dd) below 9 {\AA}, and the Al plasmon dominates the optical response. When the dd value is raised to 9 {\AA} and higher, the borophene plasmon starts to reemerge. This finding is consistent with earlier findings on graphene on metallic film, which demonstrated that the graphene plasmons are quenched by the metallic film's proximity and recovered at high dd values.

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Keyword: Time dependent density functional theory, Plasmons, Photoabsorption spectra

ID: 369 - Computational Nanoscience

Molecular dynamics simulation of iron sputtering by He, Ne, and Ar ions

Not presented.

## ID: 168 - Nanomembranes, Catalytical Nanostructures, and Electrochemical Nanomaterials

# Catalytic Reduction of 4-Nitrophenol Using rGO-Fe<sub>3</sub>O<sub>4</sub>-CuO Nanoparticles

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In this study, a magnetic rGO-Fe<sub>3</sub>O<sub>4</sub>-CuO nanocomposites were successfully synthesized via simple two-step method. Initially, rGO-Fe<sub>3</sub>O<sub>4</sub> nanostructure was prepared with a solvothermal approach. Then, CuO nanoparticles was precipitated on rGO-Fe<sub>3</sub>O<sub>4</sub> with co-precipitation method. The chemical structure and morphology of synthesized rGO-Fe<sub>3</sub>O<sub>4</sub>-CuO nanocomposites were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and Fourier transform infrared (FTIR) spectroscopy. The prepared rGO-Fe<sub>3</sub>O<sub>4</sub>-CuO nanocomposite was utilized as catalyst for reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP). Sodium borohydride (NaBH<sub>4</sub>) were used as reducing agent at room temperature. In addition, the catalytic activities were monitored by UV-Vis. The results showed that total degradation of 4-NP was achieved. The magnetic rGO-Fe<sub>3</sub>O<sub>4</sub>-CuO demonstrated high reaction rate with reusability.

Keyword: graphene, magnetic nanoparticles, metal oxide nanoparticles, nanocomposite, catalytic reduction

# Fabrication and Nanomechanical Analysis of Organic Coatings

### <u>Aslıhan Günsu Özkan</u><sup>\*</sup>, Sena Boydaş, Gülşah Ayadenk, Ayşe Çağıl Kandemir TED University, Ankara, Turkey

The aim of this study to produce defect free biocompatible organic films. To acquire this goal, biocompatible nanocomposite film production was accomplished via spin coating method. Nanomechanical analysis was conducted by colloidal probes of Atomic Force Microscopy (AFM). First, solvent-based production of biocompatible nanocomposites; constituents of which are polyvinylpyrrolidone and Silica (particle size: 50-75 nanometer) was accomplished. Second, spin coating of composites was applied on the glass substrate resulting in homogenous defect free films. AFM analysis revealed the inversely proportional relationship between the spinning rate (increased from 3000 to 10000 rpm) and the arithmetic surface roughness (decreased from 20 nm to 13 nm) for the composite coatings. An AFM with a colloidal probe, having dimensions of 15 micrometers for colloid diameter and 225 micrometers for the cantilever beam length was utilized to conduct nanoindentation test with indentation depth range of 30-80 nm; revealing that the elastic modulus of nanocomposites fits well with Johnson–Kendall–Roberts (JKR) method rather than Hertzian contact model. This is attributed to both the adhesive and soft nature of the polymer.

Keyword: AFM, Organic Coating, Silica

ID: 316 - Organic and Inorganic Nanocomposites

# Encapsulation of Ruthenium Catalysts in Hollow Peanut, Square and Capsule Shaped Silica Gels: New Generation Nano-Reactors

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Hoveyda-Grubbs 2<sup>nd</sup> generation (HG2) catalyst was encapsulated in hollow mesoporous silica gels with different morphologies (peanut, square and capsule) through reducing the pore size of mesoporous shell. The resulting catalytic system efficiently catalyzed the ring-closing metathesis of diethyldiallyl malonate and the ethenolysis reactions of methyl oleate and fatty acid methyl ester mixtures. The interior void in hollow silica gel provided a perfect isolated site for both ruthenium catalyst and olefinic substrates where improved performance and recyclability in metathesis reactions were observed when compared to the homogenous analogs, as well as other reported encapsulated catalysts. The catalyst can be easily recycled and used in ring-closing metathesis of diethyldiallyl malonate up to 10<sup>th</sup> turn. This study demonstrates that hollow silica gels are efficient materials for the encapsulation of homogenous catalysts which improves the stability of the HG2 even under air atmosphere, maintaining its activity up to 6 months on benchtop.

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Keyword: ruthenium, hollow silica gel, nano-reactors, metathesis

# Design and Synthesis of New Random Conjugated Polymers for Photovoltaic Applications

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Nowadays, the dependency on renewable energies has risen tremendously due to global warming and the depletion of fossil fuels which resulted in the climbing demand for solar energy and related research. The branch of organic photovoltaic solar cells (OSCs) is drawing attention as they offer easy processibility, low production cost, flexibility, and lightweight. With the motivation of contributing the improvements in this field of research, a series of new random conjugated polymers have been synthesized consisting of a monomeric donor unit benzodithiophene and monomeric acceptor units benzoxadiazole, thienopyrroledione cores, and a  $\pi$ -bridge selenophene. The strategy which directed the synthesis is the pull and push strategy which is applied by donor-acceptor type polymerization. Benzodithiophene is chosen to be the monomeric donor unit as it promises a very electron-rich structure with its fused structure and it also possesses side benefits like symmetrical and planar conjugated structure to boost  $\pi$ - $\pi$  stacking to enhance electron mobility between intramolecular polymer chains. With the scope of the mentioned approach, thienopyrroledione and benzoxadiazole acceptor units were used as acceptor units in the random polymerization while taking the advantage of their electron-withdrawing groups which exist in the conjugated structures of monomeric acceptor units to succeed in power conversion efficiencies in donor-acceptor type condensation polymerization. All in all, three different new conjugated random polymers were synthesized. Structural, optical, and electronic characterizations of them were completed and in future work, their photovoltaic performances will be studied.

#### Acknowledgement:

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Keyword: Renewable Energy, Photovoltaics, Organic Solar Cells, Conjugated Polymers, Benzoxadiazole

ID: 39 - Polymer Nanotechnology

# Synthesis and Characterization of New Random Conjugated Copolymers for Organic Solar Cell Applications

## <u>Oğuzhan Karakurt</u><sup>\* 1</sup>, Cem Maraşlıoğlu<sup>1</sup>, Levent Kamil Toppare<sup>1</sup>, Ali Çırpan<sup>1</sup>, Şerife Özdemir Hacıoğlu<sup>2</sup>

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The energy demand is the most crucial concern of civilized societies. The resources are limited as most of this demand is satisfied by the non-renewable energy resources. Hence, it is vital to enhance the variety of renewable energy resources to ensure the sustainability of energy-requiring processes which address almost all. Organic photovoltaic solar cells are one of the most promising fields among all those renewable energy resources as they require low production cost and possess features such as flexibility, easy processibility, and lightweight which offer easy commercial applications. In this research, three new random polymers were synthesized by applying donor and acceptor type condensation polymerization consisting of benzodithiophene core as monomeric donor unit and benzoxadiazole and thienopyrroledione as monomeric acceptor units. This research on one hand focuses on the optimizations of equivalencies of monomeric acceptor cores, but it mainly points to the effect of the modification of thiophene as a  $\pi$ -bridge rather than selenophene. The motivation of  $\pi$ -bridge modifications is optimizing the structures to sustain enhanced organic solar cell applications. This motivation directed the research to a comparison of thiophene and selenophene  $\pi$ -bridges. Thiophene is a commonly used  $\pi$ -bridge because of its avoidance to cause solubility issues, and compatible coplanar and conjugated structure, whereas selenophene offers a decrease in aromaticity and an increase in electron delocalization to enhance effective  $\pi$ -conjugation length resulting in a broad absorption spectrum which is one of the most vital indicators of reaching desirable power conversion efficiencies. To sum up, three new random conjugated polymers were synthesized and their structural, electronic, and optical characterizations were completed. In future work, their photovoltaic characterizations will be completed and they will be compared to their selenophene analogs which are also synthesized in our research laboratory.

#### Acknowledgement:

This study is supported by the Scientific and Technological Research Council of TURKEY (TUBITAK) with project number 121C274.

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Keyword: Solar Energy, Organic Photovoltaics, Conjugated Polymers, Selenophene, Thiophene

# Injectable and Self-Healable Hybrid Hydrogels for Local Cancer Therapy

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Self-healable and pH-sensitive injectable hybrid hydrogels have promising potential for local cancer therapy due to their advantages of the reducing localized drug toxicity in the tumor site. An in-situ injectable gel solution which contains biomolecules, drug molecules etc. can be injected as a liquid at the targeted region and be crosslinked to a gel phase using certain physical or chemical stimuli [1-2]. The gel formation after injection allows introducing the material inside the body in a minimally invasive way and permits the local and sustained delivery therapeutics at the desired site of action while minimizing the side effects often associated with systemic delivery. In this study, we fabricated a novel injectable, selfhealable, pH-sensitive, hybrid hydrogel system for local cancer treatment [3]. The hybrid hydrogel was fabricated by crosslinking of aldehyde functionalized PEG (diBA-PEG) and hydrazide functionalized gelatin (GEL-ADH) polymers using hydrazone bonding without using any toxic crosslinker. In order to enhance the mechanical strength of the gel and to obtain long term controlled drug release as well, doxorubicin (DOX) loaded laponite (LAP) nanodisks were integrated into the gel formation and as a result, Gel-ADH/diBA-PEG/LAP@DOX hybrid hydrogels were fabricated. The gelation time of hybrid hydrogel was observed as to be 80 s. The hybrid hydrogels exhibited pH-sensitive long-term sustained DOX release for over 10 days. The cytotoxicities of the gel precursor components (Gel-ADH, diBA-PEG, and LAP) and the hydrogels were evaluated using the human breast epithelial cell line (SVCT) and endothelial cell line (HUVEC). Gel precursors and hydrogels showed excellent biocompatibility. Moreover, the cytotoxicity of DOX loaded hybrid hydrogels was investigated on human breast cancer cell lines (MCF-7 and MDA-MB-231) and the hybrid gels provided an efficient cell death. In conclusion, this multifunctional Gel-ADH/diBA-PEG/LAP@DOX hybrid hydrogel system has a promising potential for local cancer therapy applications.

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Keyword: hybrid hydrogel, injectable, laponite, pH-sensitive, local cancer therapy

# Development of Multifunctional Nanocomposite Conductive Hydrogels for Flexible and Wearable Sensor Applications

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Hydrogel-based wearable and flexible strain sensors attracted tremendous interest due to their potential application in soft robotics, electronic skins and sensors [1]. In order to convert to the external stimuli such as pressure, strain, temperature into the electrical signals, conductive hybrid hydrogels have a great potential to respond quickly beside excellent conductivity [2]. However, hydrogel-based strain sensors have still many important challenges to need to be overcome such as mechanical properties, self-adhesiveness, self-healing capability and high strain sensitivity [3]. Recently, in order to enhance the mechanical properties of hydrogels nanofillers such as carbon based, clay, silicate are starting to use as reinforcing materials [4]. In this study, we fabricated a novel multifunctional conductive and flexible nanocomposite hydrogel system for strain sensitivity. In conclusion, we believe that this flexible and conductive ionic hydrogel is a promising candidate material for wearable flexible sensors applications.

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Keyword: conductive hydrogel, self-adhesiveness, nanocomposite hydrogel, wearable strain sensors, stretchability

# **Temperature-Responsive P(MEO2-MA) Polymer Brushes for SERS Applications**

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Surface-enhanced Raman spectroscopy (SERS) is a versatile technique which can be utilized in varying fields including environmental protection, medical diagnostic, and homeland security. The enhancement mechanism in SERS mainly relies on the electrical field magnification through the excitation of localized surface plasmon resonances of the underlying SERS-active materials. However, the uncontrolled aggregation of plasmonic nanoparticles lead to inconsistent field enhancement and SERS signals. To overcome this problem, temperature-sensitive polymeric materials have been proposed to control hot-spot formations. Smart polymer brushes exhibit rapid and reversible physicochemical or conformational changes under stimuli [1-4]. In this study, temperature sensitive poly((2-methoxyethoxy)ethyl) methacrylate [P(MEO<sub>2</sub>-MA)] brushes with sulfidryl end group on Si(001) surfaces were synthesized through interface-mediated RAFT polymerization technique. The fabricated platforms were then modified with gold nanoparticles having 20 nm of size. Raman signal enhancement ability of the platforms were evaluated using 10<sup>-3</sup> M aqueous solutions of methylene blue, malachite green and crystal violent dyes at different temperatures (below and above phase transition temperature). The obtained data indicate that SERS ability of the platforms can be manipulated using temperature-responsive polymer brushes.

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# Preparation of Polymer Multilayer Films for Food Technology Applications

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In the recent years, there has been intense research going on to develop new technologies to improve safety and quality of the food. Natural polymers not only reduce the risk to consumer health but also provides less processed and more environment friendly food packages. Alginate and chitosan are suitable polymers for food technology due to their biocompatibility, biodegradability, non-toxicity. In addition to antibacterial properties of chitosan, pH responsive behaviour of alginate and chitosan makes them promising materials for encapsulation and controlled release of functional molecules from surfaces. On the other hand, due to intensive usage of antibiotic drugs, scientists are in the search of substitute strategies. Bacteriophages are strong candidates for this purpose due to being natural predators of bacteria. In this study, layer-by-layer (LbL) films of Chitosan-Alginate are prepared and their encapsulation/release of Salmonella phages from Jerseyvirus genus, which show infectious activity towards *Salmonella enterica* serovar Enteritidis have been examined. The fundamental findings may form a basis for food packaging applications of bacteriophage incorporated polymer thin films.

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Keyword: Layer-by-layer, natural polymers, bacteriophage, antibacterial, food packaging

ID: 356 - Polymer Nanotechnology

Biosynthesis of Silver Nanoparticles from Novel Bischofia Javanoca Plant Loaded Chitosan Hydrogel: As Anti-microbial and Wound Healing Agent

Not presented.

ID: 357 - Polymer Nanotechnology

# Antimicrobial thermosensitive and bioactive hydrogel for regenerative periodontal treatment

Not presented.

### ID: 24 - Nanobiotechnology: Biomaterials and Biosensors

# **Optical Biosensor Studies Using Microfluidic Cartridges**

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Biosensors are defined as analytical devices that convert the reaction between the target molecule and various biological sensors such as antibodies, deoxyribonucleotides (DNA), ribonucleotides (RNA), enzymes, and aptamers into an electrochemical, optical, or mechanical signal [1]. Miniaturization and portability of biosensor platforms have gained popularity, especially lab-on-a-chip (LOC) systems that can analyze biochips. The LOC system allows a reduced amount of analyte for measurement and a shortened time of sample preparation and analysis. Microfluidic systems are used to develop LOC [2]. Using the interferometric imaging system at the ASELSAN Research Center, studies are being conducted to develop immune-based biosensors with single-molecule sensitivity. The capture antibody (IgG) is fixed on the polymer-coated surface of the Si/SiO<sub>2</sub> chip. The antigen that can be captured by the antibody is then incubated on the chip surface. To detect the antigen molecules captured on the surface, the suspension of antibodies bound to the gold nanoparticles is dropped onto the chip surface. The image obtained after incubation is analyzed and the uptake is calculated. A microfluidic cartridge system has been used for a biosensor, which requires fewer samples compared to the conventional method, is inexpensive, consumes little power, is portable and can be used at short notice. For the aforomentioned aims, a unique microfluidic cartridge was developed.

Microfluidic cartridge system, depicted in Figure 1, shows a top view of the cartridge. The system consists of a 1-channel syringe pump (NE -1000), a syringe (BD -1 ml), a syringe connector, the area where the cartridge is placed, and the magnetic holder.



Figure 1: Top view of microfluidic cartridge system

The cartridge system consists of a magnetic pad, a PDMS base, a microscope coverslip, and a magnetic seal (Figure 2). The magnetic pad contains channels for transferring solution from the syringe pump to the surface of a biochip placed in the center of the PDMS base. The microscope cover glass, placed on top of the magnetic pad, holds the solution on the biochip surface. The magnetic seal holds the cartridge system together.



Figure 2 : Magnet holder cartridge system parts in order from left to right: Magnet closure; PDMS mat; Magnet pad

Biosensor development studies continue using the originally designed microfluidic cartridge system with magnetic holder. At this stage, diagnosis can be made within a few minutes and we can capture antigens of concentration of a 1 ng/ml. In the future, efforts will be made to develop user-friendly, rapid diagnostic platforms for home use using this microfluidic cartridge system.

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## Keyword: Microfluidics, optical biosensor

ID: 150 - Nanobiotechnology: Biomaterials and Biosensors

# Preparation of Gold Nanoparticles with Different Geometries and Investigation of their Biophysical Interaction with Model Cell Membranes

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The cellular delivery of drugs and biomolecules is one of the focuses of interest in biomedical and pharmaceutical area. Recently, the development of biocompatible nanocarriers suitable for the cargo delivery into the cells is seen as a challenging yet exciting subject. Inorganic nanoparticles are seen as the promising nanomaterials that can be used for drug delivery due to their high functionality, high cell-targeting potential and adjustable geometry. Among metallic NPs, gold nanoparticles (AuNPs) are widely preferred, especially in biomedical applications due to their biocompatibility and bio-sensing ability [1]. It is well-known that the surface functionality is of vital importance in possible applications where AuNPs will be used. Besides that, even though the studies are very limited about that issue, the geometry of the AuNPs is also a significant parameter which can define the biophysical interaction of NPs with biological environments. Therefore, the effect of particle geometry on AuNP-cell interaction should be well understood, especially for the applications such as delivery of active pharmaceutical agents.

In this study, it's aimed to investigate the biophysical interactions and cellular uptake capacities of AuNPs of different geometries with the model membranes formed by Langmuir-trough. For this purpose, the variation of surface pressure ( $\pi$ ) of lipids at the air-buffer interface with AuNPs injected from the subphase was investigated with time. In addition, the  $\pi$ -Area isotherms were collected and the cellular-uptake capacity of AuNPs into the model membrane was investigated. To get better understanding about the change in  $\pi$ , AuNPs interacting with the monolayer were visualized via AFM and TEM. The results show that AuNP geometry significantly affects its biophysical interaction with model membranes. In addition, the interaction studies were repeated with two different membranes (DPPC/endothelial model membrane) to reveal the role of the compositions of model systems used to mimic the cell membrane.

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Keyword: Gold nanoparticles, Gold nanorods, Gold nanocubes, cellular uptake, endothelial model membrane, biophysical interaction

# Design and Evaluation of Electrospun Nanofibers for Potential Usage as an Antimicrobial Coating

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Electrospinning is a widely-applied technique to produce Nanofibers. Variety of architectures based on electrospun fibers have been realized such as solidified fibers, porous (surface pores or interior pores) fibers, hollow fibers, core-shell fibers, hierarchical structured fibers. Electrospinning afford the multi-functional properties for diverse applications, including nanofiber reinforcement, filtration, catalysis, electronic devices, lithium-ion battery, fuel cells, biomedical field, etc (Xue et al., 2019). A variety of polymeric Nanofibers were prepared using polymers such as synthetic and natural polymers such as polyvinyl alcohol (Unal et al., 2018), poly-E-caprolacton (Kirbay et al., 2018), chitosan and cellulose acetate (Yezer and Demirkol, 2020) etc. Among them, polystyrene (PS) is widely used because of its stiffness, gloss, hardness and biocompatibility (Nitanan et al., 2011).

The aim of this study was to produce antibacterial material with antimicrobial agent incoroporated polystyrene (PS) electrospun nanofibers. The morphology of the PS based electrospun fibers was characterized using a scanning electron microscope (SEM). The average diameter and diameter distribution of electrospun fibers were estimated from the SEM micrographs via Image J program. The contact angle measurements and FTIR analysis of PS Nanofibers were carried out to characterize nanofibers.

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Keyword: Nanobiotechnology, Nanotechnology, Nanomaterials, Nanofibers

# Antibiotic-Resistant Bacteria Biosensor via Quantum Dot and DNA Hybridization on Magnetic Silica Nanoparticles

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Among the pathogenic bacteria, *Staphyloccoccus aureus* (SA), which is one of the most common human pathogens, is particularly prone to resistances to most antibiotics. Due to its severe infection disease burden, SA is a worldwide concern in health care facilities1. In order to screen patients in hospital admission, to analyse the pathways of resistance spread and to administer the appropriate treatment, it is required to develop on-site tests, which are rapid, ultrasensitive, selective, economic and sustainable [2]. In this regard, nanoparticle-enabled techniques provide unique ways to combine the aforementioned properties with the requisite high performance3.

In our study, we aim to design a sandwich DNA hybridization biosensor to detect bacterial infections via genomic DNA by fluorescence. Non-toxic and highly efficient InP/ZnS core/shell QDs and functional porous silica nanoparticles (NPs) are used for signaling and separation process, respectively. InP core QDs are synthesized via amine-derived synthetic approach. The red-shift in the absorption spectra occurs with the ZnS shell, which demonstrates the increase of the size of QDs. After the ZnS shell growth, InP/ZnS core/shell QDs exhibit comparatively narrow PL emission with a 58 nm of full width at half-maximum (FWHM) and 77.5% of photoluminescence quantum yield (PLQY). Time-resolved PL (TRPL) decay measurements show that the average lifetime of the InP/ZnS QDs is 38.33 ns. In order to make the QDs water-soluble, ligand exchange process is performed using MPA.

Porous silica NPs, which possess (a) superparamagnetic or (b) fluorescent properties by incorporating iron oxide or dye molecules such as Rhodamine B, are produced. The MPA-capped InP/ZnS QDs are used as alternative label. The surface of the silica particles is functionalized by a passivating polymer brushes grafting from polymerization. Moreover, to 'catch' complemantary DNA molecules, polymer brushes are functionalized via EDC-NHS chemistry technique. Transmission electron microscopy (TEM), X-ray Photoelectron Spectroscopy (XPS) results confirm the functionalization of silica NPs.

## Acknowledgement:

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Keyword: Staphyloccoccus aureus, DNA Hybridization, nanotechnology

# Developing New Material for Paper-based Diagnostics Using Electrospun Nanofibers

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Electrospun Nanofibers are used in the development of bio-based detection technologies due to their high surface area/volume ratio. Electrospun Nanofibers should be formed bead-free and homogeneous as possible for having a high surface area/volume ratio. To obtain homogeneous nanofibers; polymer concentration, solvent system, polymer viscosity, temperature, humidity, flow rate, applied voltage, distance between collector and needle tip should be optimized (Colangelo et al., 2012; Unal et al., 2019). Electrospun Nanofibers are unique materials that can be used instead of filter paper (Reinholt et al., 2014). In literature, it is mentioned that nanofiber should be as hydrophilic as possible in paper-based sensor applications. This can be achieved by adding a hydrophilic polymer to the hydrophobic polymer used in the production of Nanofibers or by hydrolyzing the produced nanofiber (Yew et al., 2018).

In this study, Nanofibers were prepared with hydrophobic and hydrophilic poylmers for the purpose of developing paper based sensor platforma. Nanofibers were produced via electrospinning technique by using various polymers solution ratios. Performance of the Nanofibers as a sensing platform was tested on U87-MG cells (glioblastoma cell line). For the choosing of appropriate composition for the nanofibers; color measurement experiments were carried out after the color formation using gold nanoparticle bioconjugates.

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Keyword: Nanobiotechnology, Nanotechnology, Nanomaterial, Nanofiber, Paper-based sensors

ID: 280 - Nanobiotechnology: Biomaterials and Biosensors

# Carbon Nanotube Decorated Electrospun Nanofibers as an Immobilization Support for Antibody Conjugation: Electrochemical Detection of CD36

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CD36, a transmembrane glycoprotein, has been reported in studies to be associated with diabetes mellitus and atherosclerosis (Alkhatatbeh et al., 2013; Handberg et al., 2012). Therefore, the sensor system for the detection of CD36 can provide early detection of these diseases in the clinical field. Electrospun Nanofibers (ENs) offer a large surface area and can be used as an immobilization matrix for biological molecules, making them attractive for sensor applications. In the present study, an electrochemical immunosensor was developed using nanocomposite-based ENs for the detection of CD36. Carbon nanotube incorporated electrospun Nanofibers (CNT-ENs) were produced by combining the CNT nanocomposite and polystyrene (PS) polymer solution. The working electrode of the screen-printed carbon electrode (SPCE) was covered with PS/CNT-ENs Nanofibers under determined optimum electrospinning conditions. Then, the bifunctional surface was created with an antibody on the CNT-ENs modified working electrode via carbodiimide chemistry. Validation parameters such as coefficient of variation and percent recovery of the developed antibody-conjugated PS/CNT-ENs were determined. The linear detection (LOD) was calculated as 3.94 ng/mL. In addition, the antibody-conjugated PS/CNT-ENs exhibited a high percent recovery (percent recovery) for artificial blood serum analysis.

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Keyword: Nanobiotechnology, Nanotechnology, Nanomaterials, Nanocomposite-based electrospun nanofiber, Immunosensor

# Graphene Oxide Based Surface Nanomodification Strategies Towards Electrochemical Aptasensing

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Cancer is still the major cause of death despite the "gold standard" screening methods. These techniques are challenging due to lack of sensitivity, ability of screening premalignant tumors and accuracy. Early detection of cancer related molecules is crucial to increase the success of cancer treatment and therefore reduce mortality (Arshad et al., 2022). Vascular endothelial growth factor (VEGF) is a key mediator of tumor angiogenesis thus a potential biomarker for cancer diagnosis and follow-up anti-angiogenic therapy in recurrent cancer cases (Feng et al., 2016). Novel preventive approaches are urgently needed with the respect of reducing the cancer burden. Electrochemical biosensors are powerful analytical tools for rapid, cost-effective, precise and selective diagnosis of various diseases by means of incorporating biological diagnostic probes. Aptamers are emerging artificial nucleic acids known as "chemical antibodies", which possess all advantages of antibodies, but offer significant qualifications such as the in vitro production, less batch-to-batch varieties, high thermal stability and ease of modification (Vandghanooni et al., 2021). Nanomaterials are of great interest in the field of biosensing, since the sensitivity and accuracy of aptamers are highly dependent on the electrochemical surface interface. Graphene oxide (GO) is one of the upper hand two-dimensional (2D) nanomaterial has tremendous chemical and physical properties. Great electrical conductivity, existence of oxygen remaining functional groups, low noise levels and high surface area of graphene oxide meet the key requirements in the development of sensitive biosensors (Justino et al., 2017).

In this study, a label-free aptasensor towards VEGF biomarker was developed using different graphene oxide based surface nanomodification techniques. Two approaches for nanomodification of the sensor surfaces were evaluated based on electrochemical deposition of GO as the reduced graphene oxide (rGO) and direct passive absorption of GO onto disposable graphite electrode surfaces. Electrochemical Impedance Spectroscopy (EIS) was employed to monitor charge transfer resistance (*R*ct) values at the electrode/electrolyte interface. Two nanomodified surfaced were compared in terms of aptamer surface coverage, sensitivity and selectivity towards the target molecule, reaction time and reproducibility by using  $\%\Delta R$ ct calculation. Our aptasensor was successfully able to detect VEGF with a broad target linear range and a high sensitivity and selectivity, markedly.

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Keyword: Graphene oxide, Electrochemical aptasensor, Cancer diagnosis

ID: 284 - Nanobiotechnology: Biomaterials and Biosensors

# Magnetic Nanoparticles-Graphene Oxide Decorated Polydopamine Nanofibers on Screen Printed Electrodes for the Detection of CRP

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The large surface of electrospun Nanofibers (ENFs) offer us attractive properties for biosensor applications (Barati et al., 2020; Smith et al., 2020). In the present study, magnetic nanoparticle and graphene oxide based nanocomposite (MNC) was synthesized, nanocomposite-incorporated ENFs were obtained and it was used as an immobilization platform for antibodies to detect CRP. The surface of screen-printed carbon electrode (SPCE) was covered with nanocomposite-based ENFs (MNC-ENFs) via the electrospinning technique under the determined optimum conditions. Then, antibody immobilization was performed and MNC-ENFs/Anti-CRP based biofunctional surface was obtained directly on SPCE. The analytic characteristics of SPCE/MNC-ENFs/Anti-CRP were determined by electrochemical measurements. The linear detection range was found as 0.5-60 ng/mL and the limit of detection (LOD) was determined as 0.33 ng/mL for CRP. SPCE/MNC-ENFs/Anti-CRP based immunosensor also exhibited good repeatability.

#### Acknowledgement

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Keyword: Nanobiotechnology, Nanomaterials, Nanotechnology;, Electrospun nanofiber, Immunosensor

# Effects of Surface Micro Modification on the Bioactivity of Biomedical Alloys

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Although biomedical alloys are widely preferred materials for orthopedic and dental implant applications due to their superior mechanical properties, their biocompatibility is yet to be improved [1]. One of the most important parameters in terms of biocompatibility in implant applications is the structural and functional integration between the bone tissue and the implant material, which is defined as osseointegration. And since the first interaction between the bone tissue and the implant takes place on the material surface, one of the most critical factors in terms of osseointegration is the surface properties of the material. There are various surface processing methods applied to biomedical alloys for the purpose of improving osseointegration [2]. The commonly applied processes in the literature mainly focus on increasing the roughness and surface energy of metals, however there are very few studies in the literature focusing on the effect of the microstructural mechanisms triggered by the application of these surface modification processes on the surface properties and correlated biocompatibility response [3,4].

With this motivation, in the current study, it is aimed to examine the microstructural mechanisms triggered close to the surface of the metal with the application of a micro-deformation process, and the effect of these mechanisms on the surface properties of the metal, and the effect of the changed surface properties on the bioactivity of the tested biomedical alloy. For this purpose, different controlled micro-deformation areas of various repeating patterns were created on the surface of 316L stainless steel, which is a widely preferred biomedical alloy in orthopedic applications, with the use of a micro-hardness measuring device. After the effects of the applied processes on the microstructure and surface properties of the alloy were characterized by scanning electron microscopy and profilometry, the bioactivity of each surface was examined in via static immersion tests in simulated body fluid environment.

Findings of this study indicated that surface modification via the formation of micro-deformation patterns on the surface of 316L stainless steel positively affected the formation of calcium-phosphate rich structures by altering the roughness and surface energy on the sample surface.

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Keyword: biomedical alloy, surface processing, bioactivity, micro-deformation, 316L stainless steel

# Amino Acid Decorated Fullerenes for Enzyme-like Catalysis and Understanding Natural Enzymes

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Enzymes are the evolutionarily perfected biocatalysts that can increase the reaction rates astonishingly by forming a perfect microenvironment for the substrates. Because of their extreme catalysis performance that does not require any harsh condition, they are the biomolecules which are desired to be mimicked at most. For this purpose, quite different nanomaterials have been examined and among them self-assembling enzyme mimics have placed to a special position since they offer a straightforward way to imitate activities of natural enzymes by spontaneously folding and forming the active sites. Although these self-assembled enzyme mimics are quite advantageous over the other types of enzyme mimic systems, they have not been thus far used to understand the effect of different amino acids on the catalytic activity and why they are evolutionarily preserved for specific catalytic roles. Here, we demonstrated that fullerenes functionalized with catalytically active amino acids, which form multiple active sites via the self-assembly process in the aqueous environment, serve as an effective system to distinguish the catalytic activity differences resulting from single amino acid changes.

By binding the histidine amino acids onto fullerenes from their amino groups, we were able to form a carboxyl-imidazole charge relay system like the one found in catalytic triad, and used this system to mimic different enzyme classes, like hydrolases and lyases that utilizes the catalytic triad to break the covalent bonds of different substrates. In addition to histidine, we added other active site amino acids (serine, tyrosine, glutamine, and arginine) having different chemical characteristics as side groups of our nanocatalysts to understand their effect on the catalysis and why they are selected for certain catalytic roles. Beside of being an effective system for the catalysis of different reactions and determination of the importance of side amino acids on the catalysis, these designed nanocatalysts were also reusable that they protected the initial catalytic efficiency more than 90% for one hour and their catalytic activity occurred under physiological conditions like natural enzymes.

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Keyword: amino acids, biocatalysis, biomimetic synthesis, fullerenes

# A New Approach to Diabetic Wound Healing: Angiogenic Nanorod Doped Biopolymeric Scaffolds

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Diabetic wounds are characterized by delayed acute and chronic wounds resulting from a delayed, incomplete or uncoordinated healing process. One of the main causes of diabetic complications is microvascular dysfunction due to hyperglycemia, which causes ischemia and delayed wound healing (Gianino, Miller ve Gilmore, 2018; Kargozar, Baino, Hamzehlou, Hamblin ve Mozafari, 2020; Rijal ve Narmoneva, 2020). Impaired angiogenesis significantly contributes to the debilitating conditions in diabetic wound healing, which limits the delivery of oxygen and nutrient metabolites to the injured tissue, impairing the wound healing process (Nosrati ve diğerleri, 2021; Kargozar ve diğerleri, 2020; Barui, Nethi, Haque, Basuthakur ve Chitta Ranjan Patra, 2019). In this study, a new biocompatible dressing was developed that supports the continuation of angiogenesis in diabetic wounds. Porous structures were obtained by using biopolymers such as silk fibroin, hyaluronic acid and sodium alginate in the dressing composition. Eu(OH)3 and Tb(OH)3 nanorods, which have the potential to maintain angiogenesis in the diabetic wound environment; Silk fibroin, hyaluronic acid and alginate were added to the scaffold in non-toxic doses. These wound dressings with nanoparticle added were characterized by FT-IR, SEM-EDX, XRD, TGA methods. Also for wound dressings; Some tests were applied to evaluate its mechanical performance such as porosity, swelling and mechanical tests, water holding capacity, degradation test and water vapor permeability. With the addition of Eu(OH)<sub>3</sub> and Tb(OH)<sub>3</sub> nanorods to the tissue scaffolds, the mechanical strength increased, and dose-dependent changes were observed in cell viability. In the L929 fibroblast cell line, wound dressings containing 3 µg/mL Eu(OH)<sub>3</sub> and 1 µg/mL Tb(OH)<sub>3</sub> nanorods were determined to increase cell viability the most, so the prepared wound dressings were determined to have high biocompatibility. At the same time, various tests were performed to evaluate the antimicrobial and biofilm properties of wound dressings and the results were evaluated.

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Keyword: Wound dressing, Diabetic wound, Europium hydroxide, Terbium hydroxide, Nanorod, Antibacterial activity

ID: 310 - Nanobiotechnology: Biomaterials and Biosensors

# Nanomaterial- Based Electrochemical and Optical Sensor Systems for Colorectal Cancer Detection

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Colorectal cancer (CC) is the most common and leading disease after lung cancer. Early diagnosis of the disease is very important for patient survival and proper choice of treatment [2]. Clinical studies have reported that DNA hypermethylation in the V2 promoter region of the Septin 9 gene (SEPT9) in CC [3]. SEPT9 hypermethylation is an important biomarker in cancer diagnosis and treatment and can be detected in tumor tissue as well as in blood, plasma, stool, urine, and other biological samples [1,5]. However, the methods used to determine SEPT9, and other potential markers are usually time-consuming and lead to late diagnoses [4]. Therefore, it is of great importance to develop simple, rapid, and cost-effective Point-of-Care (PoC) systems for cancer diagnosis and prognosis. This study consists of two parts, different PoC tools for the analysis of methylated SEPT9 (mSEPT9) via smartphone in CC patients. In the first part, a screen-printed carbon electrode was used to develop a magnetic nanoparticle (MNP)-based electrochemical biosensor system that selectively detects methylated SEPT9 (mSEPT9) in CC. These electrodes were modified with MNPs and anti-5-methylcytosine antibody (5-mC Ab) [6]. Then, the analyte, consisting of fragments of SEPT9 with different methylation percentages was applied to the surface by hybridization with a ferrocene-labeled peptide nucleic acid (Fc-PNA) probe. Analytical parameters and electrode surface characterization were determined by electrochemical measurements (differential pulse voltammetry (DPV), cycle voltammetry (CV) and impedance spectroscopy (EIS)) after each modification step. Optimization studies and characterization of the developed sensor platform were performed using electrochemical methods. The electrochemical sensor system was integrated into a smartphone for use as a PoC. For this purpose, an electrochemical potentiate was developed and integrated into the smartphone via Bluetooth. CV measurements were performed, and the results were compared. For the second sensor, colorimetric spot tests were developed for both naked eye and fluorescence-based detection. For this, 5-mC Ab was immobilized on a nitrocellulose membrane and mSEPT9 fragments were added. Subsequently, a self-assembled gelatin poly (ethylene glycol)-based nanogel was conjugated with PNA, and the conjugate was dropped onto the test surface. The binding of the PNA conjugate and thus the color intensity on the membrane surface changed according to the methylation percentage. Color analysis was performed using a smartphone. Both systems were applied to clinical plasma samples (CC patients (n =10) and healthy samples (n =10)). The samples were from the CC patients who were accepted to Umraniye Research Hospital, Istanbul, Turkey. In addition, all results were confirmed using a kit for quantification of methylated DNA and the OneStep qMethyl PCR kit. The results show that the analytical performance of the sensor systems is successful and suitable for use in clinical samples. In addition, it was found that it is possible to use the electrochemical and optical sensor system as a diagnostic system for bedside testing.

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Keyword: colorectal cancer, early diagnosis, biosensor, nanoparticle-based electrochemical sensor, nanomaterial-based optical sensor, non-invasive biomarker

ID: 313 - Nanobiotechnology: Biomaterials and Biosensors

# Novel Biosensors for The Detection of Daunomycin-DNA Interaction by Using Graphene Oxide and Zn-based Nanomaterials

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Daunomycin's interaction with calf thymus DNA immobilized on Pencil graphite electrode (PGE) with Graphene Oxide (GO) and Zn-based nanomaterials was investigated utilizing electrochemical techniques such as cyclic voltammetry (CV) and differential pulse voltammetry (DPV). Observing the interaction between DNA and Daunomycin on the electrode surface, It was found that the guanine signal was higher with a bare electrode than with a DNA-modified one. Utilizing CV and DPV, the changes in experimental parameters such as daunomycin concentration and accumulation time were investigated. In addition, the effects of GO and Zn-based nanomaterials were compared. Preliminary results shows that Daunomycin-DNA interaction can be detected with lower detection limit by using nanomaterials modified biosensor than a biosensor that has not been modified.

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 Tadini-Buoninsegni F.; Palchetti I. Label-free bioelectrochemical methods for evaluation of anticancer drug effects at a molecular level, Sensors. 20 (7), 1812, 2020.

Keyword: Electrochemical DNA biosensors, Zn-Based Nanomaterials, Daunomycin, Graphene Oxide based Nanomaterials

## Development of Aptasensor for The Diagnosis of Covid - 19

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The Real-time Polymerase Chain Reaction (RT-PCR) method, which is a lengthy, costly, and specialized method, is used to diagnose the COVID -19 pandemic, that has gripped the entire world today<sup>1</sup>. This project aims to develop a low-cost, rapid, portable, aptasensor platform that can be used without an expert for the diagnosis of COVID -19, a public health problem<sup>2,3</sup> To this end mino-terminated aptamers were synthesized using the SELEX method, and the interaction of the aptamers with the S1 protein of SARS-CoV-2 was investigated by isothermal titration calorimetry (ITC)<sup>4</sup>. Gold electrodes were used for to design the biosensor platform. After the electrode surface was functionalized with cysteamine, the amino-terminated aptamer was conjugated to the surface via a glutaraldehyde crosslinker. Then, the surface characterisation and analytical parameters of the developed sensor platform were determined by adding commercial S1 proteins on the surface using differential pulse voltammetry (DPV), cyclic voltammetry (CV),) and impedance spectroscopy (EIS). To evaluate the working performance of the developed aptasensor assay system, S1 proteins were added to the synthetic serum samples according to the standard addition method and the measurements were repeated. Based on the obtained EIS and CV measurements, the surface characterization of the developed biosensor platform was performed and it was found that the modification was completed. In addition, the DPV results and analytical parameters of the sensor platform (calibration diagram, detection limit, repeatability, coefficient of variation) were determined and the working performance of the developed system was evaluated. In addition, the working performance of the biosensor in patient swab samples and its specificity for COVID -19 were determined by experiments with synthetic serum and influenza A and B proteins. The study demonstrated that the aptasensor system designed according to the findings has the potential to be used for the detection of COVID-19. At the same time, it can be said that the developed system can be quickly adapted to different pandemic situations that might occur in the future, thanks to its ease of use. This device technology, developed to solve a health problem, should help pave the way for rapid diagnosis. The fact that the existing technology can be easily adapted to variants and possible new viruses is also evidence that it is a sustainable technology.

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Keyword: COVID 19, Biosensor, Aptasensor, Electrochemical biosensor, Aptamer

# Electrochemical Preparation of Tungsten Disulfide-Poly(3,4ethylenedioxythiophene:Polystyrene Sulfonate Integrated Surfaces and Their Use for **Epirubicin Detection and as an Actuator**

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Integration of functional materials with electrode surfaces have been one of the important achievements in electrochemical applications. In particular, so-formed electrodes have been utilized in biomedical field to improve the performance of the present researches. These electrodes have been found a special place in cancer based studies by providing good electrochemical activity, stability, sensitivity, selectivity and robosity [1,2]. Among many functional materials, conducting polymers have attracted great attention owing to their favorable features. Poly(3,4-ethylenedioxythiophene:polystyrene sulfonate) (PEDOT:PSS) has been widely used for the preparation of effective electrode materials with excellent mechanical property and good electrical conductivity [3]. Recent works have showed that PEDOT:PSS combined with different nanomaterials had a great potential in the design of novel sensor and actuator platforms. In this context, transition metal dichalcogenides have attracted attention and being helpful. Therefore, in this study tungsten disulfide (WS2) incorporated PEDOT: PSS film modified pencil graphite electrodes (PGEs) were developed and used for epirubicin anticancer drug detection and actuating [2]. In the first part of this study, WS2-PEDOT:PSS coated PGE was used for epirubicin sensing with in a linear concentration range of 0.1 mg/L to 200 mg/L and a detection limit of 0.02 mg/L (35 nM) (n = 3). In the second part of the study, epirubicin was loaded into the WS2-PEDOT:PSS structure during electropolymerization. The actuator property of the resulting electrode was investigated by electrical and pH stimuli. Electrical stimuli showed a good actuator profile when a potential of -0.5 V was applied. Characterization studies of the electrodes were performed by scanning electron microscopy (SEM), X-ray energy dispersive analysis (EDX) and X-ray diffraction (XRD) analysis. In both studies, WS2 combination into the polymeric structure provided improved surface properties.

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Keyword: Poly(3,4-ethylenedioxythiophene:polystyrene sulfonate, tungsten disulfide, epirubicin, electrochemistry

ID: 343 - Nanobiotechnology: Biomaterials and Biosensors

# Modification of titanium with N-halamine by atmospheric cold plasma (CP) and determination of antibacterial activity

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Coating the materials used in implantation with antibacterial materials in order to increase the success of implantation is one of the interesting research areas. One of the frequently preferred materials in implantation is titanium (Ti). Existing coatings on titanium surfaces exhibit a rapid decline in antibacterial efficacy in preventing post-implantation infections. For this reason, renewable, long-lasting anti-bacterial coatings are being researched, and N-Halamine is one of these materials. However, since this type of antibacterial coating method requires advanced chemical analysis methods, its application takes a relatively long time and is costly. In recent years, the atmospheric cold plasma method, which provides surface modification without requiring advanced chemical methods, has come to the fore with its many advantages, thanks to the chemicals known as reactive oxygen and nitrogen species (RONS) in its content. [1].

The aim of this work is to modify surface of Ti material with antibacterial N-Halamine polymer through advantage of CP technology. Ti (Grade 2) was used in the study, with a diameter of 5 mm and a thickness of 3 mm. Argon is used as the plasma gas and used a 15 cm long 3 mm inner diameter (1 mm wall thickness) borosilicate glass material. 6 kV 50 kHz power supply was used for discharge item. Ti surface was exposed to plasma for 20 minutes. Afterwards; Poly (2-(acrylamido)-2-methyl-1-propanesulfonic acid) solution (PAA) was sprayed into the plasma medium for 20 minutes and deposited on the Ti surface. After the final Ti-PAA products were obtained, firstly amination (Ti-PAA-NH) and secondly chlorination (Ti-PAA-NCl) were performed. Surface characterization was determined by SEM-EDX analysis. Antibacterial activity was evaluated using Staphylococcus aureus.

The results show that CP affects the surface properties of titanium and that OH radicals bind to the Ti surface via CP. PAA was deposited on the Ti surface via CP without requiring long chemical reactions. Biofilm was formed by using S.aureus on the coated surface and the adhesion rate of bacteria was investigated. It was determined that the antibacterial activity of the antibacterial polymeric coating obtained via CP was 89.87%.

#### Acknowledgments:

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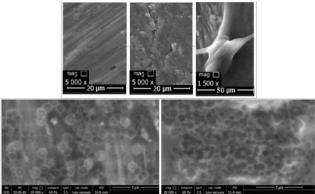


Figure 1. SEM image of Ti surface a) Ti surface b) Ti surface under 20 min plasma exposure (Ti-OH) c) Ti surface coated with PAA under 35 min plasma exposure d) LİVE S.aureus on Ti surface exposed to plasma e) DEAD S.aureus on Ti surface coated with PAA under plasma exposure

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## ID: 360 - Nanobiotechnology: Biomaterials and Biosensors

## **Cortisol Detection by Using Molecularly Imprinted Polymer Modified Electrode**

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Cortisol is one of the steroid hormones produced in the adrenal glands. This hormone controls blood sugar in the human body, regulates metabolism and reduces inflammation. Because it is the body's response to stress, cortisol is also known as the stress hormone [1-3]. Traditional methods such as chromatography have been used for the detection of cortisol hormone. However, due to the complexity and nature of these methods, electrochemical methods come to the fore. Electrochemical methods are preferred because they are sensitive, practical and inexpensive [2]. In this study, cortisol-imprinted surfaces were prepared for the recognition and determination of cortisol. Moleculary imprinted polymer was based on the electropolymerization of cysteine monomer supported with transition-metal dichalcogenide molybdenum disulfide (MoS<sub>2</sub>). The properties of the polymeric structure have been improved by doping MoS<sub>2</sub> that attracted a lot of attention in recent years [4]. Cortisol detection studies were carried out after removing cortisol from the structure by using electrochemical impedance spectroscopy (EIS). In addition, analytical performance was also compared with the poly-L-cysteine/MoS<sub>2</sub> electrode. Molecularly imprinted polymer (MIP)-based electrodes were characterized by scanning electron microscopy (SEM) and electrochemical techniques.

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Keyword: Molecular imprinting, poly-L-cysteine, MoS2, cortisol detection

## **Cancer Cell Detection with Polyamino Acid Coated Nanoelectrodes**

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Cancer is one of the most important health problems. Early diagnosis of cancer is considerable to prevent the fatal outcome of the disease. Various detection platforms have been studied for this purpose [1,2]. Electrochemical detection methods come to the fore since they are simple, fast and inexpensive [3]. In this study, we propose a fast, simple and low-cost electrochemical sensor platform for human breast cancer cell line, MCF-7 detection. In order to increase the sensitivity of the platform, pencil graphite electrode was modified with carbon derivatives: graphene and multi-walled carbon nanotubes. After this step, an amino acid, alanine was electropolymerized on the electrode. Coated electrode was characterized by cyclic voltammetry and electrochemical impedance spectroscopy. So-formed electrode was then modified with anti-Her2 for impedimetric cancer cell detection.

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Keyword: Nanomaterials, polyamino acid, electrochemical detection, MCF-7

# Molecularly imprinted polymer for analysis of glial fibrillary acidic protein in human plasma sample

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Glial fibrillary acidic protein (GFAP) is a protein that is encoded in humans by the GFAP gene [1]. It is a type III intermediate filament (IF) protein that is generated throughout development by a range of central nervous system (CNS) cell types, including astrocytes and ependymal cells [2,3]. GFAP has been recognized as a reliable biomarker of CNS injury [4]. However, due to the absence of rapid and easy-to-use assays for the detection of CNS injury biomarkers, measuring GFAP levels to identify CNS injury has not attained widespread clinical implementation [5]. Herein, a novel electrochemical detection system for glial fibrillary acidic protein (GFAP) using a antibody-free manner based on molecularly imprinted polymer was developed in human plasma sample. The conductivity changes that occurred in the presence of the target analyte were measured using a electrochemical impedance spectroscopy (EIS) in 5.0 [Fe(CN)<sub>6</sub>]<sup>3-/4-</sup> without complicated procedures and expensive equipment. Under the optimal conditions, the developed biosensor exhibited a wide linear concentration range of 10.0-1000.0 fg/mL GFAP and an extremely low detection limit of 5.0 fg/mL (detectable). However, the real concentrations of GFAP protein in the human plasma sample are in the concentration range of our immunosensor, indicating that the developed immunosensor looks potentially compatible with practical applications. Moreover, the developed immunosensor has been applied to the assay of GFAP in human plasma samples with satisfying results, indicating the applicability of the as-fabricated biosensor. This work provides a new sensing platform for GFAP detection in the point-of-care system.

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Keyword: Glial fibrillary acidic protein, Sensing application, Human plasma

#### ID: 401 - Nanobiotechnology: Biomaterials and Biosensors

## Multifunctional Layer by Layer Coatings for Cardiovascular Stent Materials

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Multilayer coatings were deposited on coronary stent alloy surfaces (316L stainless steel and nitinol) via layer-by-layer deposition technique. The substrates were coated with poly(2-ethyl-2-oxazoline)-co-linear polyethyleneimine (PEOX-co-LPEI) stabilized silver nanoparticles and heparin to enhance metal corrosion resistance in physiological conditions, improve the cell and blood compatibility of substrates, and add antibacterial activity to the surfaces. According to the literature, polycationic PEI containing coatings have great potential to enhance the corrosion behavior of metals<sup>1</sup>. However, polycationic macromolecules like PEI are cytotoxic due to their effect on membrane integrity and metabolic activity<sup>2</sup>. In this study, we have suggested a cell compatible coating that enhances corrosion resistance and demonstrates antibacterial activity and hemocompatibility. Partial acidic hydrolysis of PEOX was used to control PEI segments amount and the subsequent charge density on the backbone of the copolymer, thus, decreasing PEI cytotoxicity while keeping its anticorrosive property. MTT assay was performed with HUVEC cells where the relative viability of the coated samples was more than 80%. Tafel plots were obtained via potentiodynamic polarization measurements in PBS solution at 37°C and confirmed a significant improvement in the corrosion resistance. The desired blood compatibility expected from heparin molecules was confirmed with coagulation assay. Silver nanoparticles demonstrated significant antibacterial activity against model gram-positive and gram-negative bacteria, which was confirmed with modified JIS Z 2801 standard.

#### Acknowledgments:

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Keyword: Anticorrosive, Antibacterial, Anticoagulant, Biocompatible, Multifunctional Coating, Layer-by-Layer Deposition

## Ultrasensitive Detection of Brain Metastasis Biomarkers with Quad-Band Metamaterial-Based Perfect Absorber

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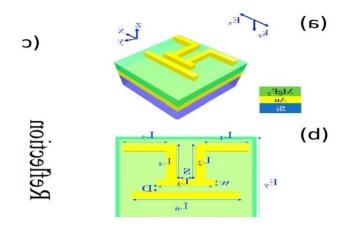
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Recent studies have demonstrated that brain metastatic cancer cells from different primary tumours are induced to highly express S100A9 within the brain microenvironment, which mediates resistance to radiotherapy by downstream activation of NF- $\kappa$ B. Furthermore, it is proposed that S100A9 expression in human brain metastasis from patients with lung cancer, breast cancer or melanoma correlates with benefit from radiotherapy. Because S100A9 expression correlates with poor response to radiotherapy, based on S100A9 expression on surgical specimens or circulating levels detected by point-of-care medical devices (POC-MDs), patients who would benefit from radiotherapy could be selected while patients with high resistance could be spared, thereby avoiding neurocognitive decline.<sup>3</sup> Therefore, generated a POC-MD for ultrasensitive detection of such small biomarkers.

Narrowband features of PAs with high absorption and near-field enhancement make them ideal devices for many light-matter interaction applications such as biosensing, infrared spectroscopy and photodetection. We present a metamaterial-based perfect absorber (PA) that has metal–dielectric–metal layers where a MgF<sub>2</sub> spacer is sandwiched between an optically thick gold film and patterned gold nanoantennas [Fig. (a, b)]. To find out the biosensing capacity of the presented perfect absorber, we experimentally detected the antibody of a common mediator of radioresistance in brain metastasis, "S100A9". Because of its low-molecular-mass, it is hard to detect even when using enzyme-linked immunoassays such as ELISA. Surface functionalization of presented PAs was carried out by photochemical immobilization technique (PIT). In other words, the immobilization of Abs was achieved via utilizing the PIT. This technique is based on forming thiol groups by UV exposure of disulphide bridges presented in Ab, which ensures the irreversible interaction with gold surface in a proper orientation [Fig. (d)]. FTIR measurements were performed on the sensor surface with the same spectroscopic parameters as numerical and experimental measurements before. Fig. (c) indicates the sensing capacity of the PAs, where a clear redshift is indicated for all PAs. Even for such a small molecule, the presented PAs' sensitivity is high enough to detect the change in the resonance frequency with a naked eye. Therefore, these results clearly demonstrate that PIT is a suitable technique for immobilization of Abs on the PA gold surfaces and presented PAs are eligible for ultrasensitive detection of such small biomarkers in POC-MD to potentially personalize the whole-brain radiation therapy (WBRT).

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**Keyword:** perfect absorber, quad-band resonances, refractive index-based sensing, photochemical immobilization technique (PIT), brain metastasis

ID: 407 - Nanobiotechnology: Biomaterials and Biosensors

## Preparation of the Microcrystalline Cellulose Based Polyurethane-MWCNT Composite Modified Electrode as Methotrexate Sensor

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The methotrexate (MTX), known as amethopterine, is an antifolate that acts as an antineoplastic agent [1]. Current clinical applications in cancer therapy include acute lymphoblastic leukaemia, medulloblastoma, osteosarcoma, leptomeningeal metastases, gestational trophoblastic tumours, bladder cancer [1, 2]. Even a low dose of methotrexate is not free from side effects. The most common adverse effects are gastrointestinal manifestations such as nausea, vomiting, mucosal ulcers, and loss of appetite. Due to such side effects, the dose of MTX during chemotherapy is very important. Under-dose is undesirable in cancer treatment. In overdose, side effects from MTX can lead to serious problems. Therefore, determination of MTX is important for both in research activities in cancer chemotheraphy field and in medical diagnosis and treatment.

Polyurethane-multiwall carbon nanotube (PU-MWCNT) membrane-based voltammetric sensors were developed for the rapid, reliable and reproducible measurement of methorotaxate (MTX), an important and widely used chemotherapeutic cancer drug. For voltammetric sensor structures, PU-MWCNT structures in different structures and components were used in the modification of the platinum electrode surface. Firstly, for the synthesis of PU structures, basic polyurethane structures were synthesized from gallic acid, microcrystalline cellulose, PEG-1000 and aliphatic diisocyanate. Different ratios of MWCNT were added to the synthesized basic polyurethane structures. The chemical structures and morphological properties of the obtained PU-MWCNT composite structures were determined by spectroscopic and microscopic analysis methods. Modified electrode structures were prepared by coating these structures on the platinum electrode surface in different film thicknesses. The surface structure and morphology of the modified electrodes were examined in detail by SEM and AFM techniques. The responses of the bare and PU-MWCNT composite film modified electrodes for MTX were compared with square wave stripping voltammetry technique. The sensitivity, linearity, repeatability and deduction limit of modified MTX selective electrodes were also investigated. Modified electrodes showed wide linear detection range (0-10 µmolL<sup>-1</sup>), low detection limit (0.086 µmolL<sup>-1</sup>) and short response time. As a result, the prepared PU-MWCNT electrodes have an important potential to be used for the determination of drug levels in patients undergoing cancer chemotherapy and for the determination of MTX in clinical trials.

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Keyword: Methotrexate, Polyurethane film, Modified electrode, Voltammetric sensor, MWCNT composite

ID: 409 - Nanobiotechnology: Biomaterials and Biosensors

# A highly selective nanostructure enzymatic biosensor based on glutathione peroxidase for determination of glutathione as an antioxidant agent

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Nowadays, enzymatic electrochemical nanobiosensors that act specifically and increase the selectability of the method are highly considered. [1-3]. In this work, an enzymatic biosensor based on glutathione peroxidase (GSH-Px) modified with graphene oxide (GO) and nafion was introduced to electrochemical monitoring of glutathione (GSH) as an important antioxidant in the human body. GO was synthesised by Hummer method [4]. GSH-Px was immobilized covalently via 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) and N-hydroxysuccinimide (NHS) onto modified glassy carbon electrode (GCE) with GO and nafion and successfully used for sensing of GSH in the presence of H2O2 as catalyst with Michaelis-Menten constant about 0.131 mmol/L. Biosensor introduced (GSH-Px/GO/Nafion/GCE) using differential pulse voltammetric (DPV) method detected GSH over the range  $0.003-370.0 \mu$ M, with a detection limit of 1.5 nM. The GSH-Px/GO/Nafion/GCE was successfully applied to the determination of GSH in real samples.

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Keyword: Glutathione peroxidase, Enzymatic nanobiosensor, Glutathione, Graphene oxide, Nafion, Differential pulse voltammetric

## ID: 42 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Vitamin D Loaded Carbon Nanofiber Aerogel Carriers and their Anticancer Activity Against Colon Cancer Cells

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Transport of the drug to the tissue or cell is the key parameter for the treatment of many diseases, especially cancer. Carbonbased nanomaterials are excellent candidates as they have high chemical resistance ability, efficient mechanical properties and weightless characters (1). In recent years, literature data supports the role of vitamin D (VD) in cancer prevention and treatment. Many scientific articles have reported that VD has an important role in the onset, progression, prognosis and treatment of cancer (2,3). Aerogels, on the other hand, stand out with their much larger surface areas and ultra-porous structures compared to other nanomaterials which are important advantages for drug loading capacity (4,5). Developing highly biocompatible and economically inexpensive VD carrier systems were aimed in this study by using carbon Nanofibers in aerogel matrix as carrier materials due to the reasons such as the environmentally friendly, high biocompatibility, absence of cytotoxic effects and easy to handle production protocols.

MTT method was used to determine the antiproliferative and cytotoxic activity of the prepared aerogels. In order to determine the effect of VD-loaded aerogels on the migration of colon cancer cells, wound dehiscence experiment was performed. Biochemical and morphological methods were used to investigate the possible apoptotic mechanism in colon cancer cells. As a result of MTT analysis, it was determined that the aerogel composite drug delivery system containing VD loaded active carbon Nanofibers did not have any cytotoxicity on normal cells, but had a cytotoxic and apoptotic effect on cancer cells. In addition, it was determined that the produced carrier system had an inhibitory effect on cell migration. It is thought that the aerogel containing VD-loaded carbon Nanofibers is effective on colon cancer and a promising new drug delivery system.

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Keyword: Vitamin D, drug delivery system, carbon nanofibers, colon cancer

## ID: 69 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## The Effect of Drug-Loaded Carbon Nanomaterials on Breast Cancer

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Cancer is the second leading cause of death globally, after cardiovascular diseases. Most of the drugs used in the treatment of cancer, despite many great medical developments, are not selective and have a large number of side effects. Doxorubicin (DOX) is a cancer drug that is widely employed in the clinic. Nevertheless, a high concentration of the drug must be administered to achieve the required effect (1). This situation causes toxicity in healthy tissues. Various *in vitro* and *in vivo* preclinic studies illustrate that vitamin D (VD) influences diverse cellular processes in breast cancer (BC) such as proliferation, differentiation, and apoptosis (2). However, supraphysiological concentrations of VD applied to achieve anti-neoplastic activity trigger hypercalcemia. Current literature data suggest the combination of VD with existing cancer therapies which may have more potent anticancer activity for BC (3). Carbon-based nanomaterials are promising in cancer treatment with their high chemical resistance capabilities, intrabody distribution properties and biocompatibility (4-5). In this study, carbon nanofiber in aerogel matrix as a carrier material loaded with DOX was developed to reduce the cytotoxic effect on healthy cells and inhibit BC cells. Moreover, the effect of aerogel carriers loaded with DOX and VD combination was investigated. The antiproliferative and cytotoxic activity of the designed drug delivery system on BC cells was examined by MTT method. The effect of aerogel carriers on cell migration was demonstrated by wound healing assay. Possible apoptotic mechanisms were investigated utilizing biochemical and morphological methods. In view of the results, drug-loaded carbon Nanofibers in aerogels appear to be effective on BC cell lines as promising drug delivery systems.

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Keyword: Breast cancer, carbon nanofiber, Doxorubicin, drug delivery system, vitamin D

## ID: 101 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Modeling and Characterization of Nanomedicine Transport within Tumor Microenvironment across Scales

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Despite significant advances in recent decades, diagnosis and treatment of cancer remain to be a major challenge. Advances in nanotechnology have enabled numerous nanoparticle (NP) formulations for efficient delivery of drugs and diagnostic agents to the target tumor site. The size, shape, charge, and surface characteristics of so-called nanomedicine can be tuned to affect the interactions of the NP with the physiological environment [1]. However, design efforts to develop nanomedicine for efficient delivery to tumor is complicated by a lack of clear understanding of NP transport characteristics. NP delivery is a multistage process that involves the transport of NPs across tissue-tissue interfaces such as the vascular wall as within tumor interstitium where NP transport can be hindered by various physiological barriers posed by the tumor microenvironment such as high interstitial fluid pressure and dense extracellular matrix ECM [2,3]. In particular, the relationships between NP design characteristics, tumor microstructure, and NP advective and diffusive transport across tumor tissue are not widely available and need to be established. To address this challenge, this study adopts an integrative approach that involves computational modeling and characterization of NP transport at two distinct length/time scales [4]. In particular, hydraulic conductivity, effective diffusivity, and retardation of NPs in collagen ECM are estimated for varying NP design characteristics, tissue microstructure, and interstitial flow conditions based on (i) microscale modeling of fluid flow, Brownian dynamics of NPs, and particle-fluid-structure interactions within the fibrous interstitial space, (ii) continuum modeling of fluid and NP transport within porous media and fitting of the model to spatiotemporal NP concentration measured on a microfluidic model of tumor ECM. The transport properties estimated by computational and experimental methodologies are compared for validation of the integrative approach. It is anticipated that the findings of this study will be ultimately useful in advancing rational design of nanomedicine for tumor delivery.

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Keyword: nanoparticle, Brownian dynamics, collagen, diffusivity, hydraulic conductivity

## ID: 104 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## **Development of Polymer-Lipid Hybrid Nanoparticles for Anticancer Drug Delivery**

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The challenge of conventional cancer treatment is the side effects caused by the chemotherapeutic drugs. In order to prevent these side effects, nanocarrier systems can be designed to have functions of controlled and selective drug release. Among these systems, core-shell structured hybrid nanoparticles have been drawing attention in the last decades because of their multifunctional structures. One of the major limitations of these nanocarrier systems is the toxicity related to synthetic surfactants as well as undesired leakage of highly toxic drugs. In this study, we designed a unique nanocarrier system using natural materials devoid of synthetic surfactants for controlled delivery of an anticancer drug. Our nanocarrier system contains a biopolymeric shell and a lipid core which is used to encapsulate Paclitaxel, a hydrophobic anticancer drug. Bovine Serum Albumin (BSA) and Dextran in different molecular weights were covalently conjugated via Maillard reaction to produce shell and used to emulsify lipid core by miniemulsion/solvent evaporation method. Biopolymeric shell acted as a stabilizer to keep the nanoparticle integrity and provided enzyme-sensitive drug release thanks to its protein structure. Besides, undesired drug leakage from the lipid core could be also avoided by the biopolymeric-shell-coating. Shell properties such as concentration of the Maillard conjugate, protein-polysaccharide molar ratio, and polysaccharide molecular weight were systematically investigated to reach optimum nanoparticle features that are size range enabling passive targeting through enhanced permeability and retention (EPR) effect, narrow size distribution, and high stability. Furthermore, zeta potential analysis was performed to evaluate surface charge of the nanoparticles in different conditions such as physiological (pH 7.4) and early endosomal (pH 6.5) mimicking environment. Moreover, the developed nanoparticles were tested in terms of drug loading capacity which is followed by the assessment of in vitro release kinetics of the encapsulated drugs through passive diffusion and enzyme-triggered diffusion. This study can bring new perspectives to the hybrid nanoparticles and has a potential to be a new delivery platform for lipophilic anticancer drugs.

Keyword: Drug delivery systems, Hybrid nanoparticles, Lipophilic drugs, Biopolymer shell, Lipid core

## ID: 133 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Enhancement of Tolvaptan Solubility with Nanofiber and Solid Dispersion Formulations

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Tolvaptan is a vasopressin V2 receptor antagonist active substance that plays a role in the regulation of renal fluid excretion. It is used in the treatment of heart failure due to hyponatremia [1]. Tolvaptan is a BCS Class IV drug and practically insoluble in water and has poor solubility in all pH ranges. It has low bioavailability due to its low solubility. The term "electrospun nanofiber" is used for fibers less than 1 micrometer and produced in the electrical field using various polymers and solvent systems. Thanks to their large surface area and porous structure [2], they can increase the solubility of active substances with low aqueous solubility. Another option for solubility enhancement is solid dispersions, where active substances with low water solubility are dispersed in inert solid hydrophilic polymer matrices [3]. In this study, nanofiber and solid dispersion formulations of tolvaptan with and without cyclodextrin (CD) were prepared to increase the solubility. Nanofibers and solid dispersions were prepared using polyvinyl pyrrolidone (PVP), solubilizers [such as Solutol, Gelucire 44/14, polyethylene oxide (PEO)], and a complexing agent [Hydroxypropyl-B-Cyclodextrin (HPBCD)]. Solid dispersions were prepared by evaporation of the solvent in a rotary evaporator (Büchi Rotavapor R-100). Different polymer solutions [CD-free solid dispersion formulations (S1, S2, S3, S4), CD-containing solid dispersion formulations (CD-S1, CD-S2, CD-S3, CD-S4)] were prepared, and solid dispersions were obtained by evaporating the solvent under a high vacuum (7 mbar) at 50 °C for 1 hour. Nanofibers were produced using an electrospinning device. Polymer solutions [CD-free nanofiber formulations (F1, F2, F3, F4), CDcontaining nanofiber formulations (CD-F1, CD-F2, CD-F3, CD-F4)] were prepared, and electrospun at a flow rate of 4-8 ml/h, a voltage of 16 kV, and a rotation speed of 100 rpm. As a result; the CD-F2 formulation (contains PVP, Solutol, and HPBCD) showed the highest solubility by increasing the solubility 7.96 times compared to the solubility of pure tolvaptan in distilled water and was chosen as the formulation with the highest potential to increase the bioavailability of the drug. The combined use of Nanofibers and CD complexes prepared by hydrophilic polymers is a promising alternative for increasing the solubility of BCS II and BCS IV drugs.

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Keyword: Nanofiber, Solid Dispersion, Cyclodextrin, Solubility

## ID: 207 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Preparation and *in Vitro* Release Studies of Mesalazine Loaded Silk Fibroin-based Nanoparticles

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#### Introduction

Silk fibroin(SF) is a natural, protein-based biopolymer. It has features such as, biocompatibility, biodegradability. SF nanoparticles attract attention due to controlled drug release properties and easy preparation [1]. Mesalazine, (MSZ), an amino salicylate drug, is widely used for the treatment inflammatory bowel disease. The aim of this study is to prepare MSZ loaded SF nanoparticles to investigate SF suitability for colon specific drug delivery.

#### Methods

SF solution was prepared previously decribed [2]. SF particles were produced by nanoprecipitation method. For this purpose the SF solution was added dropwisely to acetone/dimethylsulfoxide mixture containing MSZ. Nanoparticles were collected after centrifugation. Particle size, polydispersity index (PDI) and zeta potential values of particles were measured, and encapsulation efficiencies were calculated by indirect method. Drug release studies were performed at pH 1.2, 6.8, and 7.4 separately for 8 h and by changing the medium at specific time points for 24 h using dialysis membrane method.

#### **Results/Conclusions**

Characterization studies for particle formulations were carried out in terms of particle size, polydispersity index (PDI), zeta potential and encapsulation efficiency. Particle size of particles were found as 1771, 1443 and 1277 nm, respectively, PDI of silk fibroin particles were found as 0,71, 0,84 and 0,96, respectively. This may be due to the aggregation tendency of silk nanoparticles. Zeta potential values were found to be -11.46 mV on average and encapsulation efficiency values were found to be 17.74% on average. According to the release studies it was shown that 100% of mesalazine was released at the end of the 4 h. Mesalazine was released more slowly than that of other media at pH 7.4, associated to its pH dependent solubility. The results showed that SF should be combined with different polymers for obtaining appropriate release profile for colon specific drug delivery.

## Acknowledgments:

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Keyword: silk fibroin, nanoparticles

## ID: 210 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Evaluation of the Effect of Nanofiber Formulations on the Expression of IBD Marker TNF-α by Cell Culture Studies

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## Introduction

Hydrocortisone (HC), a corticosteroid drug, is used in the treatment of inflammatory bowel disease (IBD). Methylmethacrylate polymers (Eudragit®) are biocompatible and easily available polymers and suitable for colon targeted drug delivery (1). Electrospun Nanofibers are nano-sized drug delivery systems with large surface area and high viscosity. TNF-alpha is an important cytokine that is a marker for IBD, its expression is increased in case of inflammation (2). The aim of the study is to evaluate TNF- $\alpha$ , which can be considered as a marker gene for IBD, a disease that results in immune system stimulation, on the basis of gene and protein, with cell culture studies.

## **Material and Methods**

Hydrocortisone loaded Eudragit S100 and L100-55 based Nanofibers were produced with electrospinning technology. 6 different formulation was produced. Hydrocortisone free formulations were named as F1 (S100 based), F2 (L100-55 based) and F3 (S100 and L100-55 based), hydrocortisone laoded formulations were named as F4 S100 based), F5 (L100-55 based) and F6 (S100 and L100-55 based). Tnf- $\alpha$  mRNA expression induced by the all formulations in RAW 264.7 cell line was evaluated by qPCR. Protein expression was evaluated by western blot analysis within the scope of cell culture studies.

#### **Results and Discussion**

As a result of previous in vitro characterization studies and in vitro cytotoxicity studies, the all formulations (especially F6 formulation) were found to have IBD treatment potential and were not cytotoxic. In this study, In the evaluation of mRNA expression by qPCR, it was observed that TNF- $\alpha$  gene expression decreased approximately 3 to 4 times in the F2, F3 and F6 formulations applied to the lipopolysaccharide stimulated samples compared to the control group treated with only lipopolysaccharide. Likewise, when the expression change on protein basis was evaluated by western blot analysis, it was determined that there was an increase in expression about 2 times.

#### Conclusion

According to the results, It can be concluded that F6 formulations are potential and promising drug delivery system in the treatment of inflammatory bowel disease.

## Acknowledgements:

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Keyword: Nanofiber, Hydrocortisone, TNF-alpha, Inflammatory Bowel Disease, Cell Culture

## ID: 246 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Plasma Surface Treatment of Polylactic acid-based Thin Matrices for Drug Delivery

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The development of efficient and sustainable polymer-based drug delivery systems through different modification approaches in the field of polymer science and engineering is a contemporary challenge for the researchers and scientists. Among various polymeric systems, bio-based polyesters have attracted more attention of the community as a platform to elaborate their need and importance in the field of drug delivery with controllable release kinetics due to integrate properties. Regarding suitable biodegradable polyester-based materials, polylactic acid have been an extensively investigated renewable polyester in the biomedical field due to non-toxicity, high biocompatibility, and easy processing properties. However, low functionalization capability, and hydrophobicity limits its applications and hence demands for different physical and chemical modifications to overcome these limitations. Here, we report on low temperature argon plasma treatment of polylactic acid-based thin films with different concentration of PLA to study the effect of plasma treatment time of surface properties such as surface energy, hydrophobicity/hydrophilicity, cell adhesion, proliferation, wettability, roughness, swelling ratios, porosity, etc., on PLAbased matrices to compare the drug loading efficiency of un-treated and plasma treated samples. In this context, the effect of plasma treatment for 1, 5, and 10 minutes was studied to determine which physical and chemical processes occur at the PLAbased thin surfaces in order to select more appropriate treatment time. The swelling ratios and wettability characteristics were found to be more effectively increased after 1 minute plasma treatment. Scanning electron microscopy indicates that surface of the thin films was more porous after plasma treatment. Fourier transform infrared spectroscopy indicates the presence of hydrophilic functionalities like hydroxyl group (-OH) on plasma assisted PLA matrices that helps in the hydrophilic drug loading into thin films and chemical kinetics reveals an increase in drug loading efficiency of plasma modified samples.

## Acknowledgments:

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Keyword: biopolymers, drug delivery, cold plasma treatment

#### ID: 263 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Enhancement of Tamoxifen Citrate Solubility By y-Cyclodextrin Metal Organic Frameworks (y-CD MOFs)

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Poor aqueous solubility of drugs presents various challenges in the development of effective drug-delivery systems for various delivery routes. Tremendous research have been done in the area of pharmaceutical technology, on formulation development of poorly soluble drugs particularly for oral delivery.  $\gamma$  -CD-MOFs offer a new platform to overcome solubility, stability and permeability issues owing to their high surface area, high porosity and biocompatibility [1,2]. Tamoxifen citrate (TMX) is a Biopharmaceutical Classification System (BCS) Class II active pharmaceutical ingredient characterized with low water solubility and limited permeability, indicated for treatment of breast cancer orally [3]. Since TMX is a weak base, a predicted rapid dissolution ionization will occur in the gastric environment, possible precipitation is expected due to the elevated pH in the duedonum.

In this study, it was aimed to increase the solubility of tamoxifen citrate by  $\gamma$ -CD-MOFs prepared with two modified methods based on methanol diffusion tecnique. Tamoxifen citrate was encapsulated by impregnation method. Encapsulation was carried out by stirring overnight at 40°C using ethanol and TMX- $\gamma$ -CD-MOFs were obtained as white, sticky powders. Encapsulation efficiency was calculated by dissolving TMX-  $\gamma$ -CD-MOFs in MeOH:H<sub>2</sub>O (1:1) and then analyzing TMX using UV-Vis spectrophotometer. Encapsulation of TMX/CD-MOF prepared by Method 1 (TMX- $\gamma$ -CD-MOFs-1) and Method 2 (TMX- $\gamma$ -CD-MOFs-2) were %22.45 and %18.6 respectively. The prepared formulations were characterized using Malvern zeta sizer, differential scanning calorimetry (DSC), and FT-IR spectroscopy. The formation of the x-CD MOF structure and the encapsulation were successfully confirmed by the FTIR and DSC studies. Mean particle sizes and polydispersity indexes of the blank  $\gamma$ -CD-MOFs-1 and  $\gamma$ -CD-MOFs-2 were found to be 576.5±63.01 nm and 376±41.18 nm, 0.168±0.147 and 0.099±0.061, respectively. An approximately 2-fold increase was observed in particle size by TMX loading.

Solubility studies were performed with TMX- $\gamma$ -CD-MOFs-1 and TMX- $\gamma$ -CD-MOFs-2 comparatively with TMX, and TMX: $\gamma$ -CD (1:1) physical mixture at pH 6.8 and pH 7.4 at 37°C and in water at 25°C for 72 hours. Solubility study showed that the solubility of the TMX is increased successfully in water, pH 6.8 and pH 7.4. TMX solubility at pH 6.8 increased approximately 40 fold and 70 fold with TMX- $\gamma$ -CD-MOFs-1 and TMX- $\gamma$ -CD-MOFs-2,respectively. As shown in the studies,  $\gamma$ -CD-MOFs have been successful in increasing the solubility of TMX. Particularly TMX- $\gamma$ -CD-MOFs-2 was much more successful at enhancing solubility of TMX compared to TMX- $\gamma$ -CD-MOFs-1. As the particle size of the  $\gamma$ -CD-MOFs decreases, the effect on solubility enhancement increases.

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Keyword: y-Cyclodextrin, Tamoxifen Citrate, Metal Organic Frameworks

ID: 406 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

## Theoretical and Experimental calculation of the Adsorption and Release Process of Methotrexate for Dextrin-Base Hydrogels Model Using DFT Methods

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Nowadays, in cancer treatment, surgery, chemotherapy, targeted therapy, radiotherapy and immunotherapy are frequently preferred [1-2]. Among these methods, chemotherapy is one of the most common methods used to kill cancer cells and treat advanced tumors [3]. However, like chemotherapy, traditional cancer treatment approaches are prone to possible systemic side effects such as liver or kidney dysfunction, neurological side effects, and decreased bone marrow activity [4]. For this reason, dose adjustments of drugs used in chemotherapy should be done effectively and clearly. Within the scope of the study, a dextrin-based hydrogel structure was developed for effective, regular and long-term release of methotrexate (MTX), which is an important cancer drug and frequently used in the treatment of autoimmune diseases. Linear dextrin, polyethylene glycol 1000 and epicatechin were used as monomers in the design of this hydrogel. A two-step procedure was applied in the synthesis of the hydrogel structure. In the first step, the polyethyleneglycol 1000 structure was interacted with epichlorohydrin to obtain the poly(ethylene glycol) diglycidyl ether structure. In the second step, cross-linked polymeric network structures in polyether structure were obtained by the reaction of linear dextrin and epicatechin with the obtained poly(ethylene glycol) diglycidyl ether structure. Characterization of the obtained polymeric structures was performed by FTIR, x-ray spectroscopy. Morphological features and pore structure were examined by SEM and AFM techniques. The absorption and desorption properties of the obtained hydrogel structure for MTX and the time dependent drug release properties were investigated experimentally and theoretically. In addition, for the MTX release kinetics, mathematical modelling method was applied on MTX molecule structure, synthesized hydrogel structure, and pore distribution.

In the theoretical calculations, the interaction between MTX and the linear dextrin-based hydrogel was investigated through density functional theory calculation in both vacuum and water environments. The interactions between MTX and the hydrogel model were calculated according to the solvent effect, hydrogel pore structure, polarizability and binding energy. The natural bond orbital (NBO) calculation and the application of the second-order perturbation theory showed strong charge transfer and the presence of hydrogen bonding between the MTX structure and the hydrogel model. In this way, the synthesized hydrogel structure can be recommended as a drug delivery system in long-term treatments, as it will lead to the absorption of MTX into the linear dextrin-based hydrogel structure and prolongation of the release time.

## Acknowledgments:

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Keyword: Chemotherapy drugs, Methotrexate, Dextrin-Base Hydrogels, DFT Method, Mathematical modelling

## ID: 410 - Nanomedicine, Nano Drug Delivery Systems, and Biopharmaceuticals

# Single stranded DNA library screening towards inhibiting Staphylococcus epidermidis related infections on orthopedic implants

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The most important complication of surgical operations involving orthopedic implants is osteomyelitis. These infections can cause bone tissue destruction, removal of the implant by a second surgical operation or life threatening issues due to general sepsis. *Staphylococcus epidermidis* bacterium is the leading cause of implant-induced osteomyelitis<sup>1</sup>. The most important factor that increases the ability to generate infection is the organism's ability to form a biofilm layer. The biofilm layer on the implants or surrounding tissues prevents the body's defense system elements and antibiotics from affecting the area of infection. Therefore, the prevention of biofilm formation will eliminate the risk of infection. It is known that bacteria can survive in biofilm even after high antibiotic concentration in the environment after infection. Thus, it is necessary to develop methods which may be an alternative to antibiotic therapy.

Aptamers are single-stranded RNA or DNA molecules of 20-100 nucleotides in length, capable of binding with high affinity and selectivity to the target molecule based on structural alignment<sup>2</sup>. Aptamers possess the capacity to bind to a wide variety of targets, such as simple inorganic molecules, complex proteins and cells, and because of their low production costs and lack of immune responses; it has become significant to investigate their use in the diagnosis and treatment of diseases and drug development studies. In this context, in order to limit the use of antibiotics in the treatment of biofilm-associated infections, aptamers represent a suitable field for the development of alternative treatment methods.

In this study, aptamers from our designed ssDNA (80 mer) library were selected against *S. epidermidis* using the SELEX (Systemic Ligand with Exponential Development) method, and selected aptamers synthesized with Biotin labels were further verified via ELONA (Enzyme-linked oligonucleotide assay). The data obtained from the study will be the basis of research to design the implant surfaces in order to prevent the formation of biofilm, or studies where the implant surfaces will be modified in a variety of ways with aptamer to increase the interaction of the aptamer and microorganisms. In this way, it will contribute to the reduction of surgical operations and antibiotic use resulting in replacement of the implant due to infection.

#### Acknowledgement:

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Keyword: Aptamer, SELEX, Titanium implants, Biofilm inhibition

## ID: 81 - Nanooptics, Nanophotonics, and Nanoplasmonics

## **Hot-Spot Engineering Through Soft Actuators**

#### Münire Derebaşi<sup>\*</sup>, Görkem Liman, Gökhan Demirel Gazi University, Ankara, Turkey

Surface-enhanced Raman spectroscopy (SERS) is a powerful analytical tool to detect molecular species at ultralow concentrations. However, considering current approaches, controlling and tuning plasmonic hot-spot formations where the Raman signal enhancements maximize are still challenging due to high process cost, complexity, and inability of large-area fabrication. To address these problems, a strategy is demonstrated based on the controlled folding of polymeric materials, which is a new perspective in the field of SERS. Manipulation of hot-spot formations through controlled polymer folding enables a Raman signal enhancement up to 70 folds for the probe methylene blue molecule. Furthermore, sample collection and analysis have been successfully implemented through the magnetic field control of the platform motion and folding manipulation. The results demonstrate that soft actuator platforms can bring new modalities in sensing applications.

## Acknowledgments:

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Keyword: Raman Spectroscopy, SERS, Hot Spot Engineering, Soft Actuator

## Machine Learning Based Classification of Microparticles Using Optical Scattering Simulations

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The exposure to microplastics in our daily life has reached higher levels within the last decade. While they were first found in water resources, microplastics were recently seen in the placenta [1-2]. Single-use plastics, car tyres, detergents, toothpaste, clothing, cosmetics, and many other resources delivered the micrometre-sized particles into the human body, including that of the babies [3-5]. Hitherto, the scattered light is employed to detect the concentration and size of these particles. Nevertheless, distinguishing the particles made of different materials but having the same size and shape using the scattering patterns has not been studied.

Considering the refractive index of different microplastics, even at the same size, the scattering patterns differ, enabling their classification. Although the solutions of Mie Theory for a single particle do not fully correlate with the real-life data due to the multiple scattering events within the sample, it is still possible to benefit from these solutions in dilute samples. As a result, in this regime, the observed scattering patterns can be related to theoretical scattering patterns.

In this work, we extract the information on the particle size, concentration, and particles' refractive index from the scattering pattern data by utilising a random forest learning algorithm. In addition to a simple numerical tool, here we propose a low-cost setup to obtain scattering patterns of melamine and polystyrene particles and investigate the effects of particle size, concentration, and the material (refractive index).

The proposed experimental setup provides scattering images of those particles at different concentrations using blue, green, and red-emitting lasers. After image processing our experiments' results, we can match them with our numerical results. Showing the consistency between them creates an opportunity to work with many other particles numerically by using their refractive index and other physical and optical properties. Integration of machine learning tools into this system would determine the size and material of microplastics and their concentration quickly and easily. We believe that after development, this low-cost setup could be converted into a hand-held device to detect and monitor microplastic presence simultaneously.

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12300-12310 (2019).

Keyword: scattering, microplastics, machine learning, monitoring, sensing

ID: 240 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Investigation Of Defect Structure Of Al(In)Gan/ Gan High Electron Mobility Transistor (Hemt) Structures

Not presented.

ID: 312 - Nanooptics, Nanophotonics, and Nanoplasmonics

## Tunable Plasmonic Hot-Spot Generation for Surface-Enhanced Raman Spectroscopy through Cilia Inspired Magnetic Actuators

#### **Gorkem Liman**<sup>\* 1</sup>, Emrecan Yildiz<sup>1</sup>, Gokhan Demirel<sup>1</sup>, Emre Ergene<sup>2</sup>

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Surface-enhanced Raman spectroscopy (SERS) is a powerful analytical technique providing sensitive, selective, and nondestructive bio-/chemical information. Raman signal enhancement in SERS is mainly originated from two theories; Electromagnetic and Chemical enhancements. Chemical enhancement (CE), which mainly relies on the charge-transfer processes between the chemisorbed analyte molecules and the SERS-active material, can provide unique enhancement and possibilities to design new SERS platforms. However, electromagnetic enhancement (EM), which is based on electric field magnification through excitation of localized surface plasmon resonances of the underlying SERS-active material, is still the dominant effect in SERS application. In EM, the electromagnetic field is enhanced at highly intense local electric field regions called as "hot-spots". The generation of hot-spots in a SERS platform depends on the interparticle distance between plasmonic particles. Controlling the hot-spot formation is a hot topic not only in SERS field but in photonic, and diagnostic areas.

Herein, we propose a simple yet versatile approach to manipulate hot-spot formation through soft actuators. Soft actuators with conical and cylindrical shapes are fabricated using a silicon rubber and magnetic micro particles in designed molds, which are created by a 3D printer. The fabricated platforms were then decorated with gold nanoparticles. Hot-spot generation performances of the platforms were evaluated by SERS using different Raman reporter molecules. Impressively, conical platforms demonstrate about 120 folds larger Raman signal enhancement in the presence of magnetic field compared to unactuated form. We also observed that hot-spot generation can be manipulated by controlling magnetic field force. Finally, inspired by a Turkish centipede, a proof-of-concept demonstration is performed to collect and analyze analyte molecules in a target point.

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Keyword: SERS, Raman Spectroscopy, Soft Actuators, Hot-Spot Engineering

## **Remote Sensing and Measurement by Secondary Speckle Analysis**

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Speckle pattern is produced by the interference of a set of coherent light wavefronts. This phenomenon is commonly referred to as a source of imaging error, but it can contain useful information about the sample. Major advances in this field have been after the invention of the laser. This method can be used as a non-destructive, non-invasive, and non-contact method for remote study, measurement, and sensing of minor changes in different samples. For this reason, in recent years, it has found many applications in several science and technology disciplines, especially in biomedicine and industry. A key advantage of this method is its simple and relatively inexpensive setup. Speckle is a nanoscale pattern that shows the interaction between light and matter. Also, this method is a suitable sensor for measuring and detecting changes at the nanoscale (The reason for the relation between my research and nanooptics and nanophotonics).

One way to use a speckle pattern to examine a sample is to temporarily analyze its changes, which is called dynamic speckle pattern analysis. In this method, the speckle pattern changes with the change and activity of the sample over time. Therefore, using this method, the activity of the sample can be studied over time. This analysis requires a series of numerical and graphical assessments. In this research, we first introduce the speckle pattern and its applications. Then, we explain the mathematics of dynamic speckle pattern analysis. Following that, we present and discuss the application of the dynamic speckle pattern analysis method to the detection of the current flow in the current-carrying wire.

The secondary speckle pattern analysis is an optical method in which a coherent light source illuminates the uneven sample surface and a defocused camera captures the pattern of scattered interfering spots from the surface. If the object is tilted at a slight angle, the speckle pattern will shift instead of changing in density distribution. Therefore, by tracking the movement of the speckle, it is possible to measure the movement of the surface without contact with the object.

In this research, we will implement the optical setup of the secondary speckle pattern analysis. The analysis software package for this method will provide. Then, by using that, several applications will be pursued. For the first application, will use the secondary speckle analysis method for the detection of the charge status of a non-rechargeable battery.

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Keyword: Speckle pattern, Dynamic speckle pattern, Secondary speckle pattern, Remote sensing and measurement

#### ID: 342 - Nanomechanics, Nanotribology, and Nanomanipulation

## **Reconfigurable Optofluidic Structures by Using Speckle Tweezers**

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Optical trapping is one of the most common methods for investigating and manipulating micro objects. In the simplest case optical trapping is performed using a laser beam with a proper Gaussian intensity distribution that is focused by an objective lens with a high numerical aperture. Applying forces in the range of piconewton on microparticles and colloidal particles without mechanical impact, as well as measuring the forces applied to these samples, is an important feature of optical tweezers that has many applications in different kind of fields such as statistical physics, soft matters and life sciences. The basic principle of optical trapping is the existence of intensity gradient. By using the speckle field, which is, indeed the superposition of random intensity distribution of coherent light and contains several regions with high and low intensity that has gradient intensity, we can manipulate and trap many number of microparticles simultaneously. This kind of optical trapping is known as speckle tweezers. Although speckle pattern is apparently random but we can change the distribution of high and low intensity grains and their sizes by means of wavefront engineering. In this research, we are going to create different spatial distributions of speckle patterns. We will use them to create reconfigurable optofluidic structures by to collectively manipulate and trap micro objects.

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Keyword: Optical trapping, Speckle pattern, Optofluidic structures, Speckle tweezers

## Permeate Flux and Antifouling Properties of the PSf Membrane Significantly Enhanced by Incorporation of Carboxylate ZnO/RGO Nanocomposites

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Membrane technology has been extensively performed in drinking water production and wastewater treatment. However, membrane fouling and bio-fouling is a main obstacle which is significantly limiting the whole membrane industry. Therefore, numerous amounts of research works have been done to overcome membrane fouling during water filtration process including the incorporation of hydrophilic and antibacterial components. To address the challenge, membranes are modified by incorporation of nanomaterials to impart properties such as hydrophilicity and antibacterial. In the present study, carboxylate ZnO/RGO nanocomposite was successfully produced, and performed as nanostructured additives to Polysulfone (PSf) membrane. Functionalization of ZnO and RGO nanostructures were carried out through a chemical method using 3mercaptoropionic acid (MPA) and then the particles were added to the costing solution. The modified PSf membranes with different ZnO/RGO concentrations were prepared using phase inversion process in which, dimethylformamide (DMF) was used as the solvent and water as the non-solvent. The concentration of PSf was 17 wt.%. The structural properties of nanocomposites and the modified membranes were evaluated by various characterization techniques including FESEM, EDS, TEM, XRD, FTIR, and contact angel. Structural studies indicated that by adding ZnO/RGO nanocomposite into the PSf membrane, more finger-like pores and channels were formed. The contact angel results showed that adding nanocomposite into the PSf membrane significantly improved hydrophilicity of the membrane. The antibacterial capabilities of the modified membranes were investigated against Escherichia coli (E. coli as a gram-negative bacteria), and Staphylococcus aureus (S. aureus as a gram-positive bacteria). The permeate flux and antifouling properties were significantly improved at the optimum ZnO/RGO concentration (0.05 wt.%). It can be concluded based on the results that adding ZnO/RGO nanocomposite to the PSf membrane reduced the fouling of the membrane by improving hydrophilicity and antibacterial properties of the membrane.

Keyword: ZnO/RGO nanocomposite, PSF membrane, Antifouling

## Development of the Novel Thin-Film Nanocomposite Forward Osmosis Membranes Modified with ZnO/Ag/chitosan Towards Enhanced Water Flux and Antifouling Properties

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The use of membrane technology for the treatment of water and wastewater has been extensively researched owing to its high efficiency, ease of operation, and absence of chemical use. The FO process is designed to overcome energy challenges associated with pressure-driven membrane processes, such as reverse osmosis (RO), and enhance the efficiency treatment process to achieve low membrane fouling resistance. Membrane biofouling, however, is a major obstacle that blocks the membrane pores and decreases the water flux, a key indicator of FO process efficiency due to the concentration polarization effect. As a solution, nanomaterials are incorporated into membranes to impart properties such as hydrophilicity, water permeability and antibacterial activity [1]. In this regard, a new thin-film nanocomposite membrane (TFN), synthesized ZnO/Ag/chitosan(Cs) composite was incorporated into the polyamide (PA) selective layer of FO membranes during the interfacial polymerization process to control membrane fouling and enhance salt rejection [2],[3]. In order to evaluate the performance of these membranes for forward osmosis, NaCl 1M was used as a draw solution and deionized water as a feed solution. The modified PSf membranes (17 wt.%) with different ZnO/Ag/CS concentrations were prepared using phase inversion process in which, 1-methyl-2-pyrrolidinone (NMP) was used as the solvent and Polyvinylpyrrolidone (PVP) as the pore-forming agent [4]. Different methods were employed to characterize the structural properties of nanocomposites, including XRD, FTIR, FESEM and EDS. The antibacterial properties of the nanocomposite were also examined using MIC/MBC assays [5]. For the purpose of assessing the anti-fouling abilities of the ZnO/Ag/Chitosan(CS) composite membrane, BSA was used as a model foulant. besides, the characterization of the synthesized TFN membranes was evaluated by water contact angel measurements as well as surface and cross section FESEM images of TFN membranes in order to observe the modified finger-like channels formed [6]. According to the contact angel results, the addition of nanocomposite to the PSF membrane significantly improved its hydrophilicity due to the presence of an increased hydroxyl group in the membrane selective layer. as a conclusion, It was found that the optimized TFN membrane (0.1 wt.%) showed 87.5% higher water flux than the traditional TFC membrane, owing to the anti-fouling and hydrophilicity characteristics of the novel ZnO/Ag/Chitosan (CS) membrane with a high flux recovery of over 90%.

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Keyword: ZnO/Ag/CS nanocomposite, PSf membrane, water and wastewater treatment, Forward osmosis membrane, antifouling

## Thin Film Nanocomposite Desalination Membranes Using ZIF-67 Nanoparticles for Improved Boron Rejection

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The leading seawater desalination technology is reverse osmosis membrane technology. Although polyamide reverse osmosis membranes have achieved high salt rejections it needs improvement for water permeability and removal of neutral solutes. Boron is one the neutral solutes to be removed from seawater because it is detrimental when it occurs in irrigation and potable water at high levels. The boron content should not exceed 0.5 ppm for irrigation water and 2.4 ppm for drinking water (WHO, 2011).

There are studies showing that metal organic frameworks like ZIF-8, UIO-66, ZIF-67 could adsorb boron from aqueous solutions more than commercial adsorbents (Lyu 2017, Liu 2019). Zhang et. al. (2019) also studied different nanomaterials especially MOFs for adsorption of boron and find out that ZIF-67 has the highest boron adsorption capacity among other adsorbents. There is one recent study uses ZIF-67 to prepare thin film composite membrane for desalination by Zhao et. al. (2021) and it interprets that TFN membrane prepared using ZIF-67 has 53% higher water permeability than pristine membrane.

Hence, using ZIF-67 in polyamide reverse osmosis membrane could increase permeability and selectivity of boron at the same time. To do this, we synthesize ZIF-67 nanoparticles having 250 nm average particle size by optimizing synthesis conditions such as mole ratio of reactants, reaction medium, mixing speed and reaction time. We characterize ZIF-67 by using XRD, DLS Zetasizer. TGA and BET analyses.

Then, we prepared thin film nanocomposite membranes by interfacial polymerization using m-phenylenediamine (MPD) in DI water and trimesoyl chloride in hexane. ZIF-67 is dispersed in aqueous solution and then introduced on the top of a support membrane. After that, MPD/ZIF-67 embedded support membrane is exposed to TMC solution. Finally, thin film nanocomposite membrane is dried at 50°C. The membrane preparation parameters such as reaction time, monomer concentrations and nanoparticle amount is optimized. All membranes are characterized to determine the surface properties by using SEM, EDX, and contact angle measurements. Membranes are tested for water permeability, salt and boron selectivity by using cross flow RO test system. The feed concentration was 2000 ppm NaCl and 5 ppm boron while temperature and pressure are 25°C and 15.5 bars respectively. ZIF-67 TFN membrane has a pure water permeability of 47 LMH which is three times that of the thin film composite membrane. This membrane also has maintained high salt and boron rejection.

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Keyword: MOF, ZIF-67, thin film nanocomposite membrane, desalination

ID: 261 - Nanomaterials in Food, Agriculture and Water Purification

## Production of Bimetallic Nanomotors and Investigation of Sensor Properties for Evaluation of Food Freshness

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The increasing commercial rate of quality control sensor applications in the food industry is very interesting. Although many techniques have been commercialized to monitor food freshness quality, high cost, long analysis time, low sensitivity and selectivity are still critical issues (Malhotra et al., 2021). This study is aimed to develop a bimetallic nanomotor-based sensor for xanthine detection, which is one of the chemical analyses applied to detect microbial spoilage in meat products. Bimetallic nanomotors are nano-scale materials that can be produced easily and uniformly by electrochemical methods and convert chemical energy into force and motion. They can be produced in different configurations and different motion mechanisms (Molinero-Ferna et al., 2017; Moo et al., 2017). In the study, which aims to develop sensors that help reduce food waste for supermarkets and consumers in order to evaluate the freshness in the food industry, the rational design of bimetallic nanostructures is optimized for the synthesis of the most suitable properties, the structure, and morphology.

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Keyword: Nanomotor, sensor, xanthine detection, evaluation of food freshness

## **Tungsten-doped Vanadium Dioxide Cathodes for Aqueous Zinc Ion Batteries**

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Aqueous zinc ion batteries (AZIBs) have attracted great interest due to their high theoretical capacity, low-cost, safety, and being environmental friendly. The energy storage capacity of AZIBs is highly dependent on the cathode, and it is difficult to find a suitable cathode material for the AZIBs because of the high polarization of multivalent zinc ions ( $Zn^{2+}$ ). Here, we present a tungsten-doped vanadium dioxide (W-VO<sub>2</sub>) cathode for AZIBs. W-VO<sub>2</sub> with a open tunnel-like framework is a promising cathode material due to its large openings, which facilitates the rapid ion movement and high charge accumulation. W-VO<sub>2</sub> was fabricated by hydrothermal method and the W doping was systematically investigated. Electrochemical performance and the kinetics, such as specific capacity and rate capability of AZIBs were investigated through cyclic voltammetry (CV), galvanostatic charge discharge (GCD), and galvanostatic intermittent titration technique (GITT). The fabricated W-VO<sub>2</sub> cathodes showed a high initial capacity (150 mAh g<sup>-1</sup> at 0.1 A g<sup>-1</sup>), good rate capability and excellent cycling stability (80 % after 10000 GCD cycles at 1.0 A g<sup>-1</sup>).

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Keyword: Vanadium dioxide, cathode, zinc ion battery, energy storage

## Molybdenum-doped VO<sub>2</sub> Cathodes for Aqueous Zinc Ion Batteries

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Among the rechargeable batteries, aqueous zinc-ion batteries (AZIBs) have attracted colossal interest because of its high theoretical specific capacity, low redox potential, abundance of zinc metal, safety, and low cost. Although Zn-based batteries were commercialized long ago, aqueous Zn-ion batteries with mild acidic electrolytes are recently discovered. A suitable cathode material for AZIBs with high theoretical capacity and long cyclability is still under investigation. In this work, we present a molybdenum-doped vanadium dioxide (Mo-VO<sub>2</sub>) cathode for AZIBs. Hydrothermally synthesized Mo-VO<sub>2</sub> cathodes with well-tuned galleries create high capacity and long cycle life for AZIBs. The fabricated Mo-VO<sub>2</sub> cathodes showed a high specific capacity of 180 mAh g-1 at 0.1 A g-1 and a capacity retention of % 84 after 10000 galvanostatic charge-discharge cycles at 1.0 A g-1.

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Keyword: vanadium dioxide, cathode, zinc ion battery, energy storage

## c-ZIF-8/rGO nanocomposite host for Li-S Batteries

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Lithium-sulfur (Li-S) batteries are considered as one of the most promising energy storage devices due to their high theoretical specific capacity of 1675 mAh/g with an average voltage of 2.1 V. Although Li-S batteries possess a high theoretical capacity, they suffer from cathode-related problems. Li-S batteries have multiple electron redox reactions between Li and S, resulting in a series of lithium polysulfide intermediates (Li2Sn,  $2 \le n \le 8$ ). The soluble intermediates (n = 4, 6, and 8) can migrate to the anode side from the cathode, producing insoluble Li2S2/LiS through the reaction with lithium ions. This unwanted process is called as the "shuttle effect," and it exacerbates the Li dendrite growth, permanent lithium loss, and also causes safety issues. Moreover, the insulating nature of S is another reason for the low specific capacity. Therefore, we present a nanocomposite host material from the metal-organic framework (MOF) derived carbon polyhedrons and two-dimensional reduced graphene oxide (rGO) for S in the cathode in the Li–S batteries. c-ZIF-8/rGO is a promising material due to its lightweight, high conductivity, and good electrochemical stability. c-ZIF-8/rGO nanocomposite will be loaded with S using melt-fusion, and then Li-S battery cell will be assembled in the coin cell. The fabricated c-ZIF-8/rGO/S cathodes showed a high specific capacity of 780 mAh g-1 at 0.1 C-rate and capacity retention of % 80 after 100 galvanostatic charge-discharge cycles at 1.0 C-rate.

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Keyword: metal-organic framework, graphene oxide, cathode, lithium-sulfur battery, energy storage

## ZIF-67/MXene nanocomposite cathodes for Li-S Batteries

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Lithium-sulfur (Li-S) batteries are promising energy storage systems due to their very high energy density (2,600 Wh kg<sup>-1</sup>) and outstanding specific capacity (1,675 mAh g<sup>-1</sup>). Li-S batteries are also light-weight and cheaper than the other metal-ion batteries such as Li-, Na- and K-ion batteries. However, several problems including the shuttle effect and insulating nature of sulfur prevent its large-scale integration and commercialization. In this work, cobalt coordinated zeolitic imidazole framework (ZIF-67) nanoparticles will be synthesized on the two-dimensional Ti3C2Tx MXene nanosheets to form nanocomposite structure and then this nanocomposite will be carbonized under Ar gas to form ZIF-67 derived carbon-Ti3C2Tx nanocomposite. After sulfur loading, the fabricated nanocomposite will be used as a host material for Li-S batteries. The fabricated c-ZIF-67/Ti3C2Tx/S cathodes showed a high specific capacity of 840 mAh g<sup>-1</sup> at 0.1 C-rate and capacity retention of % 76 after 100 galvanostatic charge-discharge cycles at 1.0 C-rate.

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Keyword: Energy storage, cathode, metal organic framework, MXene, lithium-sulfur battery

## Effect of Surface Functionalization of Metal Oxide on Capacitive Performance of Manganese Oxide/Reduced Graphene Oxide (MnO<sub>2</sub>/RGO) Composite Electrode Materials

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Among energy storage systems, supercapacitors are considered as promising candidates owing to their high power density, long cycling life and fast charge-discharge process. According to the energy storage mechanism, supercapacitors are classified as electrical double layer capacitors (EDLCs) and pseudocapacitors. The charge accumulation in EDLCs is due to non-Faradaic process at the electrode/electrolyte interface. On the other hand, the capacitance in the pseudocapacitors originates from the reversible Faradaic reactions taking place at the surface of an electrode material [1].

The electrode materials play a critical role in the properties of supercapacitors. In this regard, transition metal oxides have been widely investigated as promising electrode materials for pseuducapacitors due to their abundance, environmental friendliness, low cost and excellent theoretical capacitances as well as multiple oxidation states. However, their low electrical conductivities and poor ion transport abilities significantly hinder the charge transfer rates. To overcome this critical issue, intensive studies have been focused on preparation of composite metal oxides with carbon materials such as graphene [2].

The pseudocapacitive performance of transition metal oxides is highly dependent on the coordination environment of metal atoms, and therefore surface engineering is particularly important for metal oxides. However, there are still very few reports on surface functionalization of metal oxide materials to obtain the desired surface for highly efficient and reversible faradaic reactions [3,4].

In this study, we aim to synthesis of surface-functionalized manganese oxide nanoparticles/reduced graphene oxide (MnO<sub>2</sub>-Ph-R/RGO) nanocomposite materials and investigate their applications in energy storage systems. For this purpose, the surface of MnO<sub>2</sub> transition metal oxides was first functionalized with substituted benzene rings by using diazonium modification method. Then, the surface of the RGO nanosheets was decorated with metal oxide nanoparticles through the self-assembly approach.

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Keyword: Metal oxides, Diazonium modification method, Reduced graphene oxide, supercapacitors

ID: 183 - Nanotechnology for Energy

Nano Si-rGO Composite Anodes for Lithium-Ion Batteries

Not presented.

## Ternary MoS<sub>2</sub>-rGO Based Polymeric Nanocomposites for the Design of Flexible Electrodes with High Cyclic Performance

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Flexible electronic devices, such as sensors, flexible displays, electronic skin, etc., have attracted great interest due to their integration into multifunctional platforms [1,2]. For energy conversion and storage systems, flexible micro-supercapacitors are a promising solution for the next-generation energy demands.

In this study, MoS<sub>2</sub>-rGO-AMPS nanocomposites have been modified directly on flexible carbon fiber (CF) via hydrothermal synthesis. The morphology of the surface and chemical structure of prepared samples are characterized using FESEM, XRD, DRIFT, and XPS techniques. The synthesized electrode supported on CF is directly used as a positive electrode while the plain graphite sheet is used as a negative electrode for the pseudocapacitor (PC) device. The electrochemical performance of the PC device has been evaluated using cyclic voltammetry (CV), and galvanostatic charge-discharge (GCD) techniques in aqueous electrolyte. For the scan rate of 25 mVs<sup>-1</sup>, the energy density has been calculated as 105 Whkg<sup>-1</sup> while the power density has been found as 4.9 kWkg-1. The PC device has shown a 2 V operational potential window and high cyclic stability (~99%) after 20000 dynamic CV cycles.

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Keyword: Flexible, energy storage, MoS<sub>2</sub>, carbon fiber

## Development and Characterization of Binder-free and Sandwich-like Tungten Oxide based Supercapasitor

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Supercapacitors are widely used as a promising energy storage system with their properties such as high power density, fast charge/discharge rates, long cycle stability and lifetime, and low cost. To date, studies have focused on the research of nanostructured materials in terms of gaining the desired properties such as optimum pore size and large surface area in such energy storage systems. In addition, one of the important issues to be improved in supercapacitors is their low energy densities although their power densities are high compared to batteries as energy storage systems (Maitiy et al, 2020).

Metal oxides are widely used in supercapacitors. Tungsten oxide (WO<sub>3</sub>), one of these metal oxides WO<sub>3</sub> transition metal oxides, has been extensively studied and still continues to be investigated due to its outstanding optical, electrical, and chemical properties for wide applications in anti-reflective and electrochromic coatings, chemical sensors, and photocatalysts. It is also used in lithium-ion battery applications due to its high theoretical capacity of 700 mAhg<sup>-1</sup> (Yang et al., 2020).

On the other hand, silica  $(SiO_2)$  has recently attracted the attention of researchers as an electrode material for supercapacitor applications due to its ease of manufacture and combination for the production of composite material. In addition, it is seen that  $SiO_2$  is used in energy storage applications in terms of gaining mechanical strength and reducing resistance (Kariper et al., 2021; Sajjad, 2021).

In this study, binder-free supercapacitor electrode thin films were produced by sandwich-like WO<sub>3</sub>/SiO<sub>2</sub>/WO<sub>3</sub> thin film radio frequency magnetron sputtering production method, and their electrochemical analysis, morphological and structural characterizations were investigated.

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Keyword: Keywords: Supercapasitor, binder-free, sandwich-like, tunsten oxide, thin film

#### **Cobalt Nitrogen Doped Carbon Catalyst for Use in Fuel Cells**

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Platinum (Pt), cathode catalyst exhibits the highest oxygen reduction reaction (ORR) activity, but has disadvantages due to its high cost and susceptibility to electrode poisoning. Therefore, large-scale applications of fuel cells have been limited in development due to the high costs and low energy conversion efficiencies of catalysts. It is imperative to seek alternatives [1]. Recently, doped carbon materials have been extensively investigated due to their excellent electrocatalytic performance. Transition metal and nitrogen doped carbon materials have likewise been investigated for their ORR activities [2]. It is a transition metal that has only just begun to be tested from existing research with cobalt. In this study, a cobalt nitrogen doped carbon catalyst was prepared for use in fuel cells. Activated carbon and cobalt were added by precipitation method in ethanol medium and mixed under nitrogen gas. After the mixing time is over, sodium hydroxide is added. The purpose of adding sodium hydroxide is to precipitate cobalt nanoparticles formed by reduction of cobalt to activated carbon. The materials were subjected to carbonization-activation process under inert atmosphere conditions under different temperatures(400,600,800). It was observed that the BET surface area was the highest at 800 degrees with 591,462 m2/g. Cobalt doping was confirmed with XRD, the form of the material was determined with FTIR, and the oxygen reduction reaction of materials at different temperatures was investigated with LSV.

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Keyword: Fuel cells, activated carbon, activated carbon catalyst, cobalt doped activated carbon, fuel cell catalyst

#### Effect of Fluorination Strategy and Side Chain Engineering

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Due to its low cost, ease of fabrication, applicability on flexible substrates, good film-forming properties, high morphological stability, and light weight, many scientists have been studying organic thin-film photovoltaics (PV) over the past two decades.<sup>1–5</sup> Three random D-A copolymers containing thieno[3,4-*c*] pyrrole-4,6-dione (TPD) and benzodithiophene (BDT) named as P-HTBDT, P-FTBDT and P-FBDT were synthesized. The effect of side chains on BDT and fluorination to benzothiadiazole on photovoltaic performances of fabricated solar cells was investigated. Moderate molecular weights have been obtained for all polymers from the highest P-FBDT Mn:59 kDa to the lowest P-HTBDT Mn:44 kDa. The HOMO levels of the polymers were -5.57, -5.51, and -5.65 eV for P-HTBDT, P-FTBDT, and P-FBDT, respectively, suggesting low-lying HOMO energy levels. The optimized weight ratios of the polymer to PC<sub>71</sub>BM were determined to be 1:2 for all polymers, and the maximum PCEs of the devices were 7.35%, 7.76%, and 9.21% for P-HTBDT, P-FTBDT, and P-FBDT, respectively, after optimizations with 1,8-diiodooctane (DIO) and 1-Chloronaphthalene (CN). The morphologic and topographic investigations were carried out by the images from Transmission electron microscopy (TEM) and Atomic Force Microscopy (AFM). The best performing device was P-FBDT because of its deeper HOMO level, high molecular weight, and exhibits better morphology.

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Keyword: benzodithiophene, fluorine effect, organic solar cell, bulk heterojunction, polymer solar cell

#### Highly Compressible Sponge Supercapacitor Electrode

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Herein, we present the preparation of a compressible supercapacitor electrode using a sponge and electrically active material. The sponge was constructed by infiltrating and cross-linking polydimethylsiloxane into a sugar cube and using it as a template (PDMS). Electroactive material was deposited on the PDMS sponge to generate a substantial amount of interface, resulting in a high specific capacitance and excellent flexibility. The suggested system has capacitance retention over 10.000 cycles and great cycling stability. According to our research, this electrode is a strong contender for use in flexible electronics. Additionally, this study may guide the preparation of flexible, high-performance electrodes that are helpful for wearable energy storage systems.

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Keyword: Compressible, Sponge, Supercapacitor Electrode

#### Investigation of Nucleation Kinetics in Supersaturated Solutions in a Droplet-based Microfluidic System

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The effects of thermodynamic conditions on the kinetics of nucleation from supersaturated solutions has been of great interest in controlling the synthesis of nano/micro particles with advanced physical, chemical, and optical properties. Droplet-based microfluidics provide a controlled platform with minimal consumption of materials for investigation of reaction processes confined in picoliter reactors for faster transfer of heat and mass and, thus, better precision in the desired temperature and concentration. Controlled crystallization of particles in microfluidic systems has particular significance for active pharmaceutical ingredients, proteins, fine chemicals, micro and nanoparticles, and crystals with superlattice structures and intermediate phases. The conventional models for nucleation in liquid solute-solvent systems may not predict the nucleation kinetics precisely for complex systems at high supersaturations.

In this study, we used a transparent thermo-fluidic device on an inverted microscope to observe the solidification kinetics in monodisperse micro-droplets of a supersaturated solution. The device has a flow focusing design for uniform droplet production and a serpentine section integrated with a transparent ITO heater, micro-thermocouples, and a power supply with a PID temperature controller. The device was fabricated using standard soft lithography techniques and a transparent polymer, polydimethylsiloxane (PDMS). A fast digital camera attached to the microscope and a computer program was used to collect and analyze the quantitative data on droplet size and interdroplet distance starting from the point of formation of droplets, followed by their progression in the channel, entrance to the heated serpentine section, where nucleation starts, and exit. We used precursor solutions involving a zirconium chloride salt, organic ligands, and a solvent as the dispersed phase to form monodispersed droplets with picoliter volumes in a continuous phase of silicon oil. Such micro capsules work as homogenous reaction environments with a high ratio of surface area to volume reducing gravitational effects while enhancing surface effects and the control over heat and mass transfer. We optimized the microfluidic flow conditions by varying the ratio of the flow rate of the dispersed phase to the continuous phase, Qd/Qc, in the limits of droplet flow to generate micro reactors with the desired volume and pre-determined concentrations. Data collected from the system was used to calculate the concentration of the ingredients in the droplets at any time during their voyage in the micro channels. Nucleation experiments were conducted at three different temperatures, 50, 80, and 100 °C. Microfluidic flow conditions were adjusted to form droplets of the same size and concentration in each experiment. Visually distinguishable stages of solidification were identified by a change in color and form in the droplets indicating a phase change in the precursor solution. This enabled determination of the residence time required to start the nucleation process at each temperature. Shorter residence times were achieved with increasing temperatures indicating faster nucleation kinetics. Mass transfer data collected at three different temperatures was used to derive an Arrhenius relation to describe the shrinking behavior of droplets and the diffusion of the solvent into the carrier fluid enabling the calculation of the desired initial precursor solution. We showed that miniaturization of the reaction environment and the power of observation and control over the system in microfluidic systems serves them as an effective tool to understand the phenomena related to phase transitions in supersaturated solutions and to optimize the precursor recipes for desired products.

#### Acknowledgments:

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Keyword: Solidification, Nucleation Kinetics, Microfluidics

ID: 368 - Nanophysics

Capillary Pumping between Droplets on Superhydrophobic Surface

Not presented.

#### ID: 60 - Novel Applications of Nanostructured Materials

#### **Fabrication of Highly Transparent and Robust Slippery Coatings**

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Transparent and mechanically durable superhydrophobic coatings have enormous application potential such as solar cells, lenses, windshields and so forth. Superhydrophobic surfaces have been fabricated by the inspiration of lotus leaf. effect. The superhydrophobic surfaces are fabricated by mimicking the lotus effect for self-cleaning behavior with low water droplet adhesion [1,2]. However, this superhydrophobic surfaces have still certain problems such as adhesion of proteins or bacteria, the limited cushion against liquids with low surface tension and the weak mechanical strength for practical applications [3]. In this context, the Slippery liquid infused porous surfaces (SLIPS) have a great attention to overcome the limitation of superhydrophobic surfaces. SLIPS are fabricated by the infusion of slippery lubricant into the porous structures of surface to provide water-repellent coatings with low sliding angles. In this study, we fabricated transparent and robust SLIPS via step-by-step deposition strategy. We tested SLIPS through a mechanical durability test, chemical stability test, and long-term storage in the air. Our results showed that this facile and feasible SLIPS coating exhibited mechanical durability and stability for industrial applications.

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Keyword: SLIPs, superhydrophobic, nanoparticles, transparent, liquid repellency

#### Metallic Nanomaterials Integrated Printed Electronics for Wearable Sensing

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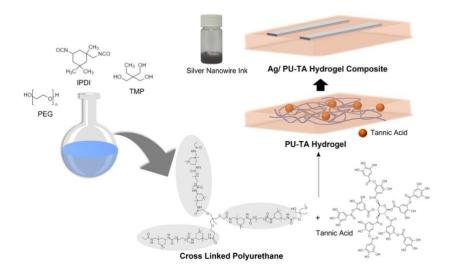
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The advancements in wearable and implantable technologies contributed immensely to the development of medical devices with greater capabilities. Use of such devices in wearable applications require certain characteristics such as flexibility, stretchability, air permeability, wettability, and biocompatibility for a comfortable and efficient utilization. These wearable systems comprise two main parts which are: a conductive component and a base substrate [1]. The choice of a suitable substrate material to meet the desired characteristics listed above for a special type of application is very crucial. Different types of materials are available to be utilized as flexible substrates in wearable electronics. It is possible to categorize these materials into three groups: paper-based, textile-based, and polymer-based. Foams, plastics, elastomers, and hydrogels can be listed as suitable substrate materials.

In this study, we propose a flexible and stretchable polyurethane-tannic acid (PU-TA) hydrogel substrate material integrated with gold (Au) nanorod and/or silver (Ag) nanowire based conductive ink. The proposed PU-TA based substrate is obtained by reacting polyethylene glycol (PEG) and isophorone diisocyanate (IPDI) following a crosslinking by trimethylolpropane (TMP) [2]. Accordingly, the hydrogels are swollen in TA solution to introduce reversible crosslink points and increase the crosslink density. The resulting structure is tough, stretchable, and biocompatible. In order to enhance the conductivity of the system, Au and/or Ag metal nanoparticle-based ink was deposited on the hydrogel via direct printing [3] [4]. This advanced material system is envisaged as promising material for flexible antenna design to be used in wearable electronics.



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#### ID: 86 - Novel Applications of Nanostructured Materials

#### **Electrically Conductive, Transparent and Superhydrophobic Surfaces**

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Fully transparent, electrically conductive and superhydrophobic surfaces show great promise in many applications, such as aircraft windows, automotive windshields, solar panels, and building windows [1,2,3]. Superhydrophobicity, transparency and electrical conductivity are usually mutually exclusive, and it is challenging to combine these different functionalities in one platform. In this study, a fully transparent, electrically conductive and superhydrophobic surface is fabricated in two steps: grafting of poly(ethylene glycol) to the indium-tin oxide (ITO)-coated surface and deposition of hydrophobic nanoparticles on the surface. Here we show that the end-grafted polymers provide an excellent interface for self-assembly of hydrophobic nanoparticles resulting in a transparent and water impact resistant superhydrophobic coatings with high levels of water repellency. The fabricated surfaces had a high contact angle (>160°) and low sliding angle (<5°). The superhydrophobicity and conductivity of the surfaces were retained after exposure to stream of the water jet for 10 minutes, 100,000 drops of water, and 60 minutes of heating and cooling cycles. The self-assembly of hydrophobic nanoparticles on end-grafted polymer resulted in 2% increase in the transparency of the underlying substrate, thanks to the anti-reflective property of the surfaces. The fabrication of multi-functional coatings with the presented approach appears to be promising for self-cleaning, anti-fogging, and anti-icing coatings.

#### Acknowledgment

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Keyword: Superhydrophobic, Transparent, Electrically conductive

ID: 137 - Novel Applications of Nanostructured Materials

#### Development of Electrospun Fiber Coated Thin Film Microextraction Devices for Rapid Mass Spectrometric Determination of Polar Cancer Biomarkers

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Solid Phase Microextraction (SPME) is well known as a sample preparation technique. Flexibility in design, low matrix effect in complex matrices, and in vivo applicability are among the outstanding features of SPME. Moreover, its thin film geometry (TFME) provides higher sensitivity in the analytical method due to the larger extractive phase used. However, the extraction of polar analytes with SPME based techniques still has limitations due to the low affinity of the analytes to the present SPME sorbents<sup>[1]</sup>. One of the ways to improve the sensitivity of the SPME for the polar analytes is to use nanostructured extractive phases, which provide fast sorption kinetics. In this study, a nanostructured extractive phase with polar moieties was prepared using an electrospinning approach followed by hydrolysis of the polymer and tested to extract polar metabolites identified as cancer biomarkers<sup>[2]</sup>. For this purpose, polyacrylonitrile (PAN) was used as the base polymer for the electrospinning process due to its suitability for structural modification and biocompatibility. Our electrospinning results indicated that as the applied voltage is increased from 14 kV to 20 kV, the diameter of electrospun fibers increases. Additionally, it was found that the solution flow rate significantly impacted fiber diameter, with average fiber diameters increasing from about 200 nm to 800 nm when the flow rate was increased. In the optimization of the electrospinning process, the most homogenous coating was obtained when 10% (w/w) PAN solution (in dimethylformamide) with a 15 cm distance syringe-collector was used with 20 kV applied voltage. The electrospun PAN mat was chemically treated with an alkali to convert the nitrile group to the carboxylate functional group with primary purpose of improving its affinity toward polar analytes. Fourier-transform infrared spectroscopy (FTIR) was used to characterize hydrolyzed electrospun PAN. The O-H bending peak at 1459 cm<sup>-1</sup> and the OH stretching peaks at 3500-3200 cm<sup>-1</sup> suggest that carboxylic acid was formed. Finally, blades coated with nanofiber were used to extract selected cancer biomarkers from synthetic urine samples. As probe analytes, phenylalanine, tryptophan, serotonin, and the urinary metabolite of serotonin 5-hydroxindol acetic acid were used. The parameters that could affect the extraction efficiency of the analytes were optimized. The results indicated that the extraction of the selected analytes is strongly affected from the pH and ionic strength of the sample while extraction time reached to its maximum value within 10 min, illustrating the advantage of using nanostructured extractive phase. As increasing the pH had positive effect on sorption, pH 7.0 was selected as sample pH for the study. Following the extraction optimization, the electrospun coated TFME blades were coupled with mass spectrometry for rapid analysis in which the TFME device acts as an electrospray ionization (ESI) source. Optimization of TFME as an ESI source showed that a 10 µl mixture of ACN:MeOH:H<sub>2</sub>O:FA (40:40:20:0.1% FA) as a desorption solvent with 15 seconds of desorption time and 5 kV of the applied voltage to the blade provides the best sensitivity. proving that the analytes can be analyzed in 10 min total including sample preparation and analysis.

#### Acknowledgement:

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Keyword: cancer biomarkers, electrospinning, polar metabolites, solid phase microextraction

ID: 138 - Novel Applications of Nanostructured Materials

#### Preparation of Electrospun Coated Thin Film Microextraction Devices for Rapid Determination of Steroid Hormones with Direct to Mass Spectrometry

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Changes in the plasma concentration of various endogenous compounds such as cholesterol and steroid hormones have important consequences including cancer, atherosclerosis, psychological problems, or metabolic disorders which threaten human life [1]. For this reason, rapid clinical determination of these molecules in human blood plasma has of great importance. In this context, thin film microextraction (TFME), which is a technique based on solid phase microextraction (SPME) has an important advantage in terms of being capable of combining the sample preparation with direct to mass spectrometric analysis [2]. This integration reduces the total analysis time to a few minutes and allows sensitive analysis of droplet-sized samples. However, the current TFME coatings are made by bulk immobilization of extractive particles in PAN glue which offsets some of the advantages stated above by slowing down the extraction and desorption kinetics.

In this study, a novel electrospun based TFME coating was developed with the primary purpose to overcome the slow kinetic with the existing TFME devices. As a first step poly(divinylbenzene) (PDVB) nanoparticles were synthesized as extractive phase and then immobilized into polyacrylonitrile (PAN) by electrospinning method. To obtain PDVB nanoparticles completely embed in a continuous PAN nanofibrous phase various electrospinning parameters were tested. Optimized conditions for electrospinning were 15 cm distance between needle tip and collector plate, 2.4 mL/h feed rate of the polymer mixture and 20 kV applied voltage. Upon preparation of electrospun coated TFME devices, sample preparation conditions were optimized for the extraction of various hormones first from PBS (binding free matrix) then from synthetic serum (binding matrix) with 30  $\mu$ L of sample volume to show its applicability for extracted plasma spot analysis. Since the devices are designed to function as electrospray ionization (ESI) source for mass spectrometry, the effect of various solvent on desorption and electrospray efficiency were tested. The most suitable desorption solvent was determined as isopropyl alcohol with 60 second of desorption time. In the final method, only 15  $\mu$ L of the solvent was sufficient for detecting the analytes when 5 kV of voltage was applied to the blade. Our results showed that compared to dip coating method the electrospun coated TFME devices have superior kinetic of sorption (Fig 1) and can be used for sensitive and fast analyses with direct to MS approach.

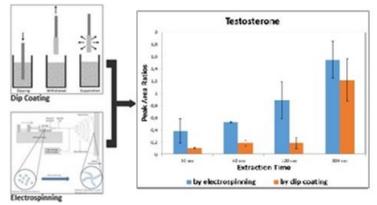


Figure 1. Comparison of extraction kinetics of PDVB coated TFME devices prepared by dip coating and electrospinning methods.

#### Acknowledgement:

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Keyword: PDVB, Electrospinning, Solid Phase Micro Extraction, Thin Film Micro Extraction, Mass Spectrometry

#### **Multicolor Physical Unclonable Functions**

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In today's world, counterfeiting is a major problem. Increasing counterfiting cause economic loss, health risks, and social issues. For this reason, academic and industrial circles have focused on the development of new generation of security labels/barcodes to provide effective anticounterfeiting measures. Physical encoding systems called "physically unclonable functions" (PUFs) have attracted great attention in last decade, due to the potential to provide unique encoding for each object/application that even the manufacturers cannot repeat thanks to randomness of process. Therefore, in order to use this advantage of PUFs effectively, it is essential to develop multiplexed PUFs fabricated by versatile and cost effective fabrication techniques.

In this study, an unique approach that reinforces the advantages of PUFs with a versatile fabrication method is presented. Our approach is based on the practical fabrication of patterns consisting of polymeric features deposited at spatially random positions using the electrospraying. Here, electrohydrodynamic instabilities during electrospraying provide the formation of completely random and complex polymeric structures. The additive nature of the process enables sequential deposition of multiple materials on the same substrate. Furthermore, the solution processing-based fabrication allows incorporation of functional materials into polymeric features and enables the formation of additional security layers. By taking advantage of the advantages mentioned earlier and enriching the technique, multicolor PUFs with multi-layered security measures have been fabricated. Specifically, PUFs containing layered security measures from many different polymer systems such as polystyrene, polymethyl methacrylate, polyethylene oxide, and polyvinylpyrrolidone have been produced and their practical applications have been demonstrated. Furthermore, systematic examination of the process parameters, the condition-structure relationship was revealed where electrosprayed PUF structures display a wide variety of distinct morphologies as well as extend in range from micro to nanoscale. It is demonstrated that security keys extracted from the response of the resulting features exhibit close to ideal values when tested for quantitative metrics (randomness, uniqueness, uniformity, reliability) that are widely used for assessing PUF performance. Electrospraved PUFs, which stand out with their performance and characteristics, can be taken further and cooperated with fluorescent molecules directly during the process. The resulting multicolor PUFs can be authenticated at different levels, which can be performed independently. Here, the random distribution of features forms the first level of security, which can be verified by conventional optical microscopy imaging, and unique morphology of features forms the second security layer, which can be authenticated by advanced techniques (SEM, AFM, etc.), and lastly, the multiple responses from unique fluorescence from randomly located photoluminescent molecules form a third layer of security that can be authenticated with fluorescence imaging. Finally, the high coding capacity was determined and the impenetrable layers of security defined procedurally, and the multicolor PUFs are applied directly as security label on the goods. The images taken from the application/good to be authenticated are verified by comparing the keys obtained with the binaryization and subsequent 256-bit code extraction procedures with those in the database. In addition to this common authentication method, much more practical and faster authentication mechanisms have been developed within the scope of our study, where many limitations are eliminated thanks to the direct implantation of image feature matching algorithms into PUF applications.

#### Acknowledgements:

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Keywords: physically unclonable functions, anti-counterfeiting, electrospraying, fluorescent materials

#### ID: 182 - Novel Applications of Nanostructured Materials

#### Physically Unclonable Functions using fluorescent organic semiconductors

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Anti-counterfeiting and data security applications require design and development of novel materials and methods for encoding information. [1] Physically unclonable functions (PUFs) has been introduced as a new approach in fabrication of encoded surfaces. PUFs are composed of complex structures embodied by stochastic mechanisms. The inherently random responses of PUFs makes the replication of encoded surfaces impossible by third parties or even by the manufacturer itself [2,3]. Fluorescent compounds attract great attention, because of the simple and fast authentication [4].

In this study, we will present fabrication of organic light-emitting physically unclonable functions (OLE-PUFs) using fluorescent organic semiconductors (f-OSCs). The formation of random domains via surface dewetting of thin films of f-OSCs is the basis of our approach. The OLE-PUF fabrication process consists of deposition of f-OSC and thermal annealing as short as 5 minutes at a modest temperature (120 to 170 C). Depending on annealing temperature and film thickness, bright and hemispherical random features with different properties are formed on the surface by various transport mechanisms. Thanks to unique photoluminescence and chemical properties of the *f*-OSC molecule and the random positions of these hemispherical features, multi-layered security measures are established. Multiple-security layer can be incorporated to OLE-PUFs using unique fluorescence profile, excited-state decay dynamics, and Raman spectrum. The OLE-PUFs can be formed on substrates of different chemistry, surface wetting property and rigidity. The drop-casting enables direct deposition on goods with minimal material consumption. OLE-PUFs are highly stable against external effects such as water, sand, UV-light and temperature [5].

#### Acknowledgment

This work was supported by the Research Fund of the Erciyes University (Project Number FDS-2020-9706). M.S.O. and H.U. acknowledge partial support from The Science Academy, Turkey through the Young Scientist Award Program.

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Keyword: Anti-counterfeiting, Organic semiconductor, Physically unclonable functions

#### ID: 205 - Novel Applications of Nanostructured Materials

#### Investigation of Using Titanium Dioxide Nanoparticles on Gear Oils

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Titanium dioxide is a part of green tribology and also a food grade molecule. In this study we have been investigated to improve oil solubility and oil stability of titanium dioxide nanoparticles in gear oils. We have been formulated three different types of gear oils: commercial type gear oil (gear oil with group 1 base oil), gear oil with synthetic type base oil and gear oil with food grade base oil. Stabilities, anti wear and extreme pressure properties of lubricants have been investigated and reported. We have been investigated and reported also particle size effect of titanium dioxide on wear performances of lubricants.

Keyword: Titanium dioxide, Nanoparticles, Gear oils, Tribology, Particle size

#### ID: 291 - Novel Applications of Nanostructured Materials

#### Enhancement of the Second Harmonic Generation Signal at Epsilon Near Zero Metamaterial

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Materials with the near-zero real part of the permittivity function have been utilized in several application fields, including the enhancement of the fluorescence, enhancement of the high harmonic generation efficiency and localized heating. In this numerical study, we investigate the enhancement of the Second Harmonic Generation (SHG) signal of a metal nano-particle on the titanium nitride (TiN) thin film. The effects of coupling plasmon modes of metal nano-particle with localized field modes that are supported by the TiN thin film were demonstrated. The computational 3D-FDTD calculations showed that thin-film metamaterials could be used to enhance nonlinear processes in the vicinity of the epsilon near zero (ENZ) wavelength.

Keyword: Epsilon Near Zero, Second Harmonic Generation, Metamaterials

#### ID: 303 - Novel Applications of Nanostructured Materials

#### **Recycling of Rare Earth Elements from End-of-Life Devices**

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The rare earth elements, which are utilized in practically all modern equipment in the world, are tremendously valuable to the industry and have the power to influence the future. China is known for owning the majority of the reserve, 55%, as well as 90% of the world production. Nearly monopolistic market created embargoes, export restrictions, and unfavorable pricing increases that are directed against consumers worldwide. The devastation that rare earth elements causes to the environment during extraction from the mining areas is another concern and must be resolved. Thus, the consumer's access to rare earth elements. In the contemporary age, technology offers unparalleled convenience. Many of the technological devices used every day have magnets containing considerable amount of rare earth elements. Every year, almost all rare earth element containing- devices are discarded, which leads to a significant loss for the industry. With a proper recycling technique, rare earth elements may be recycled for use in industry.

NANOTerial Technology Co. was founded in July 2021. Among the company's primary pursuits are the recycling of rare earth elements-based magnets and the manufacture of specialized permanent magnets. Various rare earth elements-containing scraps were obtained from the recycling centers, the parts containing the magnets were separated and the remaining parts were recycled again. The magnets obtained were sent to various analyzes (XRD, SEM, VSM) and data were obtained. Data and the future perspectives of the startup and its technology will be presented.

ID: 339 - Novel Applications of Nanostructured Materials

#### Atomic Layer Deposition-Grown Zinc Oxide Film on Disposable Graphite Electrode for Deoxribonucleic Acid Quantification

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Nanomaterials have attracted considerable interest in materials science and different life sciences such as chemistry and biology. Their unique chemical, mechanical and physical properties have made them fascinating for real-life applications. Zinc oxide (ZnO) synthesized at nanoscale is highly worth researching due to its unique electrical, structural and optical properties. Resulting ZnO thin-film coated substrates have been widely preferred in sensors, electronics, transistors, photonics and light-emitting diodes. Atomic layer deposition (ALD) is one of the important techniques for ZnO thin-film formation and has a high importance since it provides precise thickness control and homogeneous growing of the structures [1-3]. This work describes the fabrication of ALD-grown zinc oxide film on pencil graphite electrode and use of the fabricated electrode for double-stranded DNA (dsDNA) quantification. Detection of dsDNA is important to realize effective diagnostic platforms and drug interaction systems [4]. In order to investigate the advantage of ZnO coated electrodes, deposition cycles were optimized. Fabricated electrodes were characterized by scanning electron microscopy (SEM), X-ray diffraction analysis (XRD) and X-ray photoelectron spectroscopy (XPS). Electroactive DNA base guanine was used to determine dsDNA by using differential pulse voltammetry (DPV). In addition, impedimetric detection was carried out. Both results showed that the ZnO-based electrochemical sensing platform had good sensitivity for dsDNA.

#### Acknowledgments:

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Keyword: Zinc oxide, atomic layer deposition, electrochemical DNA detection

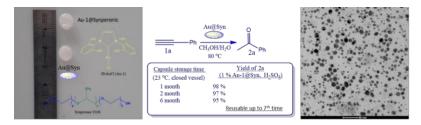
#### ID: 362 - Novel Applications of Nanostructured Materials

#### New Generation Nano-Sized Micellar Catalysts: Gold-NHC Catalyst Tablets for Alkyne Hydration Reactions

#### Zeynep Tunalı<sup>\*</sup>, Bengi Özgün Öztürk

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Organometallic catalysts based on transition metals such as palladium, ruthenium, iridium and gold are the key constituents in synthetic organic chemistry.<sup>1</sup> Although most of these catalysts exhibit high performance in various organic transformation reactions, moisture-free inert atmospheres are required and their usability is limited in water-based organic reactions due to the stability and solubility issues.<sup>2</sup> To address the stability issue, paraffin-based wax capsules were developed to conduct airsensitive catalytic reactions on benchtops.<sup>3</sup> Up to date, wax-capsule strategy for the dosage-delivery of air-sensitive reagents was employed to several different organometallic catalysts based on Pd, Ni, Cr and Ru. The wax-capsules are also used for the delivery of air-sensitive inorganic reagents such as potassium hydride.



Scheme 1. Au-1@Synperonic®F108 catalyst tablet

Herein, we report the encapsulation of IPrAuCl (Au-1) in Synperonic®F108 (Syn), a triblock non-ionic polymeric surfactant, acting as both a catalyst tablet medium and surfactant for dispersion of hydrophobic alkyne substrates and gold–NHC complexes in aqueous media(Scheme 1). The catalyst tablets (Au-1@Syn) formed stable nano-sized micelle structures in a water/methanol mixture and can be easily recycled as aqueous micelles and can be reused up to 7 times without any significant activity loss in the alkyne hydration reaction.

#### Acknowledgments:

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Keyword: Micellar Catalysis, Gold-NHC, Alkyne Hydration, Nano-reactors

ID: 405 - Novel Applications of Nanostructured Materials

#### Development of POSS-doped sol-gel film-coated BOPP film structures, investigation of gas barrier and morphological properties

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Flexible packaging plays an important role in the packaging and protection of food products. By product protection, it is meant to provide a moisture and oxygen barrier, as well as preventing the external contact of the product. In addition, the contact of light with the product should be prevented, and the protection of food from the effect of light is provided by the use of different types of packaging. Flexible packaging, the use of which has increased in recent years with its high efficiency and sustainability in the packaging market; polyester, bidirectional stretched polypropylene (BOPP) film and cellulosic packaging materials [1]. However, it is necessary to increase the protective properties of such food packages in order to increase the storage life of foods and to keep them for a longer period of time without spoiling. For this purpose, many studies have been carried out for the preparation of polymeric films with low gas permeability. In this study, sol-gel surface coatings containing polyhedral oligomeric silsesquioxane (POSS) groups were applied with a film applicator. These coating structures were examined by FTIR and x-ray techniques. Surface properties were determined by SEM, AFM and liquid contact angle measurements. The change in optical properties of the obtained film structures was evaluated by UV spectroscopy. Delamination tests were applied after the surface was coated with ormoser structures suitable for the sol-gel system and the structural characterization parameters were determined. Oxygen permeability was measured with the ASTM D3695 test at 23 °C and zero humidity. The WVTR value was determined according to the ASTM F-1249 standard at 23°C in an 80-90% humidity environment. Optimization studies were performed by comparing OTR and WVTR values with the values before lamination. The gloss, haze and optical transmittance properties of the obtained ormoser coated BOPP films were determined as well as their oxygen, moisture and gas permeability properties. As a result, the obtained POSS-doped sol-gel film-coated BOPP film structures are homogeneous, smooth and smooth. In addition, the positive effects of POSS groups used in the coating structure in reducing the gas and moisture permeability of the BOPP film were observed.

#### Acknowledgments:

This study was supported by the Scientific Research Projects Unit of İnönü University with the project number FYL-2019-1775.

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Keyword: BOPP film, Polypropylene, Sol-Gel Chemistry, POSS nanostructure, Sol-Gel coating

#### Energy Storage Application of PVC Wastes that Electrical Conductivity Imparted by Functionalized with Quantum Dots

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Polyvinyl chloride (PVC) is one of the most widely used plastic types which is the most harmful to the environment among all plastics. In addition to the use of hazardous materials such as vinyl chloride monomer and ethylene dichloride other additives in its production also increase the toxic effect and create another waste industry. While PVC contaminants were annihilated by burning in the oceans prelusively, the disposal process is eventualized in open areas via using special vehicles recently. This situation is also another drawback of PVC usage [1-2]. Although, with the developing technology there are promising studies for the use of this material in different areas the necessity of using harmful gases such as CO<sub>2</sub> in the applied processes another issues has to be considered from the environmental point of view. In this study, unlike some previous studies, the carbonization process was applied to PVC wastes in Argon atmosphere by using quantum dots without the requirement of CO2 gas in the carbonization stage. Thereby, with an innovative, environmental, and cost-effective approach we ably increased electrical conductivity of cleaning material waste PVC. When the resistance of pristine material was 13 k  $\Omega$ , the PVC contaminant functionalized with quantum dots has  $0.9\,\Omega$  ohms. Thereafter, we utilized these quantum dots functionalized PVC waste as an alternative carbon source to activated carbon in energy storage applications. As it is known, activated carbon studies mostly focused on research for the evaluation of waste biomass. However, harmful gases emitted to the environment at these stages, unfortunately, increase ozone pollution. Thanks to this technology we have developed, quantum dots functionalized PVC has gained almost 10<sup>4</sup> times more electrical conductivity than pristine PVC without causing any harmful gas emission to the environment, and an innovative material with better results has been developed as an alternative to activated carbon in energy storage studies.

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Keyword: Quantum Dots, Energy Storage, Supercapacitor

ID: 422 - Nanomaterials in Food, Agriculture and Water Purification

#### Novel Selective Adsorption and Photodegradation of BPA by Molecularly Imprinted Modified Titanium Dioxide Particles in Water Samples

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Titanium dioxide (TiO<sub>2</sub>) nanomaterials have caused widespread concern in the past several decades for their bulk characteristics and potential applications in many different areas. Lately, the combination between molecularly imprinted polymers (MIPs) and TiO<sub>2</sub> nanomaterials has been proven to improve the relative adsorption capacity, selectivity, and accelerate the rate of mass transfer of analyte which is not possible using TiO<sub>2</sub> alone. In this work, MIP was synthesized and can be efficiently applied in the removal of bisphenol A (BPA) in aqueous solutions via selective photodegradation. Firstly, TiO<sub>2</sub> particles were synthesized, then the MIP layers loaded on the surface, and finally, MIPs modified TiO<sub>2</sub> nanomaterials were got after the template molecule was removed. FTIR, SEM, and XRD analyses were employed to characterize materials. The prepared material can be a significant candidate for the treatment of pollutants in wastewater.

Keyword: Photodegradation, Molecularly Imprinted Polymers, Surface Imprinting, Photocataylsis, Spectroscopy, Wastewater Treatment

#### ID: 424 - Nanomembranes, Catalytical Nanostructures, and Electrochemical Nanomaterials

## Development of carbon nanotube and nano-NiFe2O4 -based electrodes for the detection of azathioprine by electrochemical method

#### Fatma Bilge Emre<sup>\*</sup>, İmren Özcan, Gizem Aslan, Süleyman Köytepe

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Compared to traditional methods, electrochemical sensors are very advantageous in many applications due to their short detection time, portability, no need for high-cost devices, high sensitivity, and simple sample determination procedure. Therefore, electrochemical sensors, in particular, are receiving more attention in drug detection and analysis. [1]. Preparing sensitive and selective drug sensors, especially conductive carbon structures and nanoparticles is of great importance [2]. Today, the importance and success of electrochemical sensors powered by carbon-based nanomaterials increase the number and type of commercial electrodes used in the clinic and in the biomedical field. In this study, multiwall carbon nanotube (MWCNT)-based electrodes were developed for the determination of azathioprine, which are used to prevent rejection in immunosuppressive Rheumatoid arthritis, polyangiitis granulomatosis, Crohn's disease, ulcerative colitis, and systemic lupus erythematosus and kidney transplants. In this electrode structure, nano-NiFe2O4 was added to increase the efficiency of MWCNT. Modified electrode structures were obtained by coating the obtained MWCNT-NiFe<sub>2</sub>O<sub>4</sub> structures on the glassy carbon electrode. Azathioprine sensitivity of the obtained electrode was confirmed by experimental and theoretical calculations. In addition, the NiFe2O4 size distribution and morphology on the electrode surface were investigated by theoretical calculations. FTIR, X-ray, and EDX techniques examined the chemical structure of the prepared modified electrodes. Surface morphology and surface roughness were investigated in detail by SEM and AFM techniques. The prepared nanoparticle-loaded carbon-based electrodes exhibited good reproducibility, wide linear range, and selectivity for Azathioprine determination. It is thought that such carbon-based structures may increase selectivity and sensitivity, especially in the determination of azathioprine in body fluids such as blood.

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Keyword: Azathioprine, Functional carbon structures, nano-NiFe2O4, voltammetry

## Combining down and up conversion: Making hybrid structures from quantum dots and upconverting nanoparticles

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Quantum dots (QD) have been employed tremendously in various scopes. Their well-known small down conversion and high quantum yield features has recently become a focus in their combination with upconverting nanoparticles (UCNP) which earned reputation with their large up conversion behaviour. When the two particles come together, upon the excitement of UCNPs, a chain is triggered and due to the emission of UCNPs, QDs are excited and emit light thereby. This, in return provides a strong photoluminescence (PL) event actuated by a low-energy light (908 nm). In this study, CdSe QDs were synthesized using a one-step fast and facile method. They were found to exhibit spherical shape with 4 nm diameter. The absorbance of the particles was determined as 535 nm. Their stabilization through oleate groups was approved via FTIR analysis. NaYF<sub>4</sub>:Yb,Er UCNPs were synthesized in a Teflon autoclave at relatively low temperature of 180°C. The shape of UCNPs were found to be cubic with uniform size of 10 nm each. Their XRD spectrum showed that they were in a-phase. The two particles were combined employing two different methods: in the first one they were forced to approach one another in the presence of an anionic surfactant, namely sodium dodecyl sulfate, and form a bundle covered by the polar headgroup of the surfactant. In the second one, surfaces of both particles were functionalized by ligand exchange using different molecules with different functional groups, particularly with amine and carboxyl groups, followed by their covalent attachment with carbodiimide crosslinking process. The PL and emission behaviours of the two hybrid, i.e., combined, particles were examined and compared. Although the first method provides a rather easy synthesis, the presence of SDS may lead to complications in the application of biosensors. Consequently, the second method allows the attachment of further molecules through its free functional groups. These hybrid particles allow tuning the visible light and can be used in applications including but not limited to photoelectrochemical sensors, imaging, smart optical agents (with appropriate functionalization), etc.

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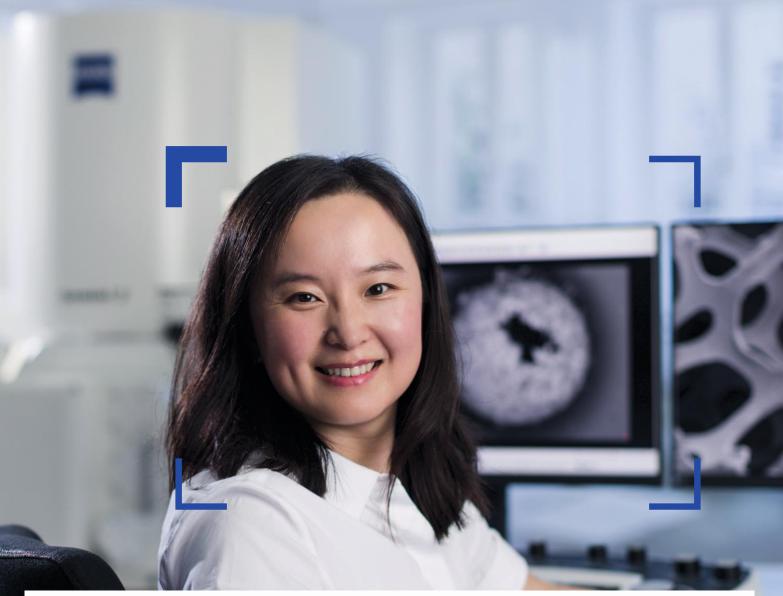
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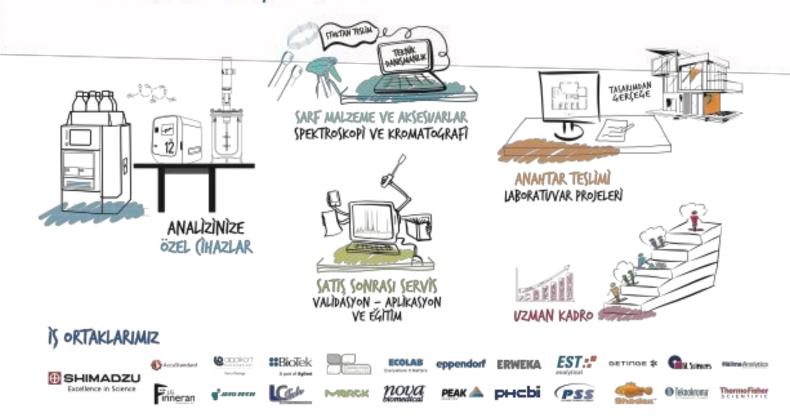
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Tasarımı, teknolojisi güçlü fikirlere dayalı geniş bir ürün yelpazesi sunmakla kalmıyor, hizmet anlayışımızla farklı endüstrilerin ar-ge ve üretim aşamalarının, kamu ve araştırma laboratuvarlarının verimliliğini arttırıyoruz. Sizi dinliyor, analiz ihtiyaçlarınızı en iyi karşılayacak ürün ve hizmetlere odaklanıyor, laboratuvarlarınız için aradığınız çözümleri ister tek tek isterseniz anahtar teslimi olarak sunuyoruz.

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## NAN TR-16



16.NANO BİLİM & NANOTEKNOLOJİ KONFERANSI

## SkyScan 2214



Nano Ölçekte 3D X-ışını Mikroskobu

Yeni çok amaçlı X-ışını Nano Tomografi SKYSCAN 2214, tek bir cihazda en geniş nesne boyutları ve uzamsal çözünürlükleri kapsar. Jeoloji, Petrol ve Gaz Araştırmaları, Polimerler, Kompozitler, Fiber, CFPR, Piller ve Yakıt hücreleri, Yaşam Bilimlerinde, yumuşak dokular, kemik osteositleri ve dentin tübülleri, bitkiler, böcekler, paleontolojik örnekler vb. dahil olmak üzere her tür örneğin 3D görüntüleme ve tam modellemesi için benzersiz olanaklar sunar.

PREKLİNİK MİKRO-CT SKYSCAN 1276 CMOS SÜRÜMÜ



Yüksek Çözünürlüklü, Hızlı In-Vivo Masaüstü Mikro-CT

SKYSCAN 1276 CMOS Sürümü, küçük laboratuvar hayvanlarını (fareler, sıçanlar, ...) ve biyolojik örnekleri taramak için sürekli değişken büyütmeye sahip, yüksek performanslı, bağımsız, hızlı, masaüstü bir in vivo microCT'dir. Sistemin tavşanlar dahil büyük hayvanları da monte etmesini sağlayan isteğe bağlı bir Büyük Hayvan Taşıma Sistemi (LATS) mevcuttur.



#### SKYSCAN 1273

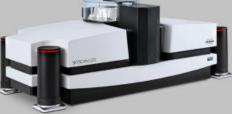
Yüksek Kapasiteli 3D X-ray Mikroskobu

SKYSCAN 1273, tezgah üstü cihazlarla tahribatsız muayene (NDT) için yeni bir standart belirleyerek daha önce yalnızca zeminde duran sistemlerle elde edilen bir performans sağlar. 500 mm uzunluğa, 300 mm çapa ve maksimum 20 kg ağırlığa kadar numuneler tarayabilir.

## SKYSCAN 1272 CMOS SÜRÜMÜ

Yüksek çözünürlüklü 3D X-ray Mikroskobu

Masaüstü SKYSCAN 1272 CMOS, mikro bilgisayarlı tomografi (mikro-CT) teknolojisine dayanan yenilikçi bir yüksek çözünürlüklü 3D X-ray mikroskobudur ve en son X-ışını teknolojilerini entegre etmek için güvenilir SKYSCAN 1272 platformu üzerine kuruludur.



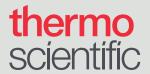


## RS 2000 Küçük Hayvan İşınlayıcı

Eşsiz %95 veya daha yüksek doz homojenliğine sahip endüstri standardı küçük hayvan x-ışını kaynağı.

Rad Source ışınlayıcılar, bilim insanlarına yüksek doz homojenliği ve doz oranları için birçok avantajlı konfigürasyon için araştırma araçları ve uygulama esnekliği sağlayan yaşam bilimleri için tasarlanmıştır.

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## Axia ChemiSEM

En verimli SEM-EDS kullanıcı deneyimi için yeni nesil ColorSEM teknolojisi ile tanışın...

Thermo Fisher Scientific tarafından geliştirilen yeni nesil taramalı elektron mikroskobu Axia ChemiSEM ile yapabileceklerinizin sınırı yok.

- Eşsiz ve canlı kantitatif kompozisyon görüntüleme ile element analizinde çığır açan hız
- Her an uyumlu ve görüntüye hazır sistemle veri toplama kolaylığı
- Esnek numune tutucusuyla 10 kg'a kadar numune analizi imkanı
- Mükemmel görüntüleme performansı için geniş dedektör yelpazesi (5 standart dedektör/kamera ve ekstra port girişi)
- Kullanıcı dostu yazılım ve ColorSEM teknolojisiyle sadece 30 saniyede net bir görüntü ve EDS analizi

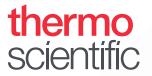












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## Thermo Scientific Phenom Pharos

Dünyanın ilk ve tek masaüstü FEG (Field Emission Gun) Elektron Kaynaklı Taramalı Elektron Mikroskobu.



Akademik ve Endüstriyel araştırmalar için; hızlı analiz imkanı, kompakt yapısı, uzun ömürlü FEG elektron kaynağı ve düşük servis maliyetiyle Phenom Pharos'un başlıca özellikleri;

30 saniyede elektron görüntüsü	2nm'den düşük çözünürlük	2.000.000 x büyütme	Uzun ömürlü Schottky FEG elektron kaynaklı masaüstü #SEM
1,0 kV ile 20,0 kV arası ayarlanabilir voltaj	27-160 x büyütmeli renkli navigasyon kamera	Özelleştirilmiş yazılımlar ve numune tutucuları	X-Y eksenlerinde Standart Motorize Numune Tutucusu
3 düzey vakum seçeneği (yüksek – orta – düşük)	Standart BSD detektör	Opsiyonel SED ve EDS dedektörler	Maksimum numune boyutu 35 mm çap, 100 mm yükseklik



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