

HUMBOLDT KOLLEG

2023

Ankara

RECENT ADVANCES IN
INTERDISCIPLINARY MATERIAL
SCIENCE: PERSPECTIVE FROM
PHYSICS, CHEMISTRY AND BIOLOGY

April 12-14, 2023
Ankara University, Ankara / TURKEY



UNTERSTÜTZT VON / SUPPORTED BY

Alexander von
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HUMBOLDT KOLLEG 2023

Recent Advances in Material Science: Perspectives from Physics, Chemistry and Biology

Regarding the German-Turkish Science collaboration, the Kolleg is expected to attract around a hundred participants from all aspects of physics, chemistry, and biology from both countries to discuss the new challenges, new developments in science ranging from material science, solid-state physics to chemical physics, biophysics, from atomic and optics to computational physics and structural biology.

It is expected to cover the full spectrum of the natural sciences and be interdisciplinary in physics, chemistry and biology to give Humboldtians and other senior researchers the opportunity to report on the latest research results.

This Kolleg will also provide a platform where especially young researchers meet together with Alexander von Humboldt award winners and outstanding Humboldt alumni and other professional physicists both from Germany and Turkey. This will enable both country benefits and new establishments of collaborations. As a results, this Kolleg aims to strengthen regional and professional networking between its alumni and junior researchers and promote interest in Alexander von Humboldt Foundation programmes as a career location.

Plenary speakers will present their latest and high-quality research findings in science from physics, chemistry, and biology who are very well-known scientists in these areas and mostly AvH award winners or Humboldt alumni.

The program of the conference will also give the chance to young researchers to present their research in a Poster session and give the opportunity to get a contact with the Alexander von Humboldt family. Additionally, on the second day there will be an excellent round table discussion regarding the German-Turkish Cooperation in general and in science in particular.

Apart from the scientific program, a good social program will be also prepared for the participants to enjoy the city. It is expected that this Kolleg will provide 3 fruitful days with an interesting and beneficial program.

We are looking forward to welcoming you in Ankara.

Prof. Dr. Handan OLĞAR

Humboldt Kolleg 2023 Ankara Organizer

ORGANIZING COMMITTEE

- **Prof. Dr. Handan OLĞAR**
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- **Nijat SHUKUROV**
PhD Student, Faculty of Science, Department of Applied Physics, University of South Bohemia, Czech Republic

PROGRAMM / PROGRAM

12 April 2023		
09:00 – 09:30	Anmeldung / Registration	
09:30 – 10:00	Eröffnung / Opening	
	Begrüßungsworte / Opening Talks	
	<p>Prof. Dr. Handan OLĞAR Humboldt Ambassador Scientist for Turkey</p> <p>Luisa RATH Alexander von Humboldt Foundation, Regional Manager</p> <p>Prof. Dr. Necdet ÜNÜVAR Rector of Ankara University</p> <p>Prof. Dr. Hasan MANDAL President of TÜBİTAK</p> <p>Herr Jürgen SCHULZ German Ambassador for Turkey</p>	
	Chairperson: Prof. Dr. Şinasi ELLİALTIOĞLU (TED University, Director of Basic Sciences Unit, Turkey)	
10:00 – 11:00	Prof. Dr. Ataç İMAMOĞLU (ETH Zürich, Department of Physics, Quantum Electronics Institute, Switzerland)	Magnetism in Moire Materials
11:00 – 11:30	Kaffeepause / Coffee Break	
	Chairperson: Prof. Dr. Burç MISIRLIOĞLU (Sabancı University, Faculty of Engineering and Natural Sciences, Department of Materials Science and Engineering, Turkey)	
11:30 – 12:00	Prof. Dr. Özgür ÖKTEL (Bilkent University, Physics Department, Turkey)	Perpendicular Space Picture for Localized States in Quasicrystals
12:00 – 12:30	Prof. Dr. Lütfi ÖZYÜZER (İzmir Institute of Technology, Department of Physics, Turkey)	Large Area Transparent DMD Thin Film Electrodes Deposited by Magnetron Sputtering
12:30 – 13:00	Dr. Semih ENER (Darmstadt University of Technology, Functional Materials, Department of Material Science, Germany)	Hard Magnetic Materials and Recent Advances on Materials Development
13:00 – 14:30	Mittagessen / Lunch	
	Chairperson: Prof. Dr. Melek YAMAN (Hacettepe University, Faculty of Education, Department of Biology Education, Turkey)	
14:30 – 15:00	Prof. Dr. Ender SUVACI (Eskisehir Technical University, Department of Materials Science and Engineering, Turkey)	MicNo®: New Generation Particle Technology to Improve Lives

15:00 – 15:30	Prof. Dr. Wolfhard JANKE (Leipzig University, Theoretical Physics Institute, Germany)	Critical Behavior of the 3D Ising Model with Power-Law Correlated Defects: Monte Carlo Simulations
15:30-16:00	Kaffeepause / Coffee Break	
Chairperson: Prof. Dr. Murat MANGUOĞLU (Middle East Technical University, Faculty of Engineering, Department of Computer Engineering, Turkey)		
16:00 – 16:30	Prof. Dr. Şefik SÜZER (Bilkent University, Department of Chemistry, Turkey)	Localized X-Ray Photoelectron Impedance Spectroscopy (LoXPIS) for Tapping into the Diffuse Charge Dynamics of Ionic Liquid Electrolytes within Energy Storage Devices
16:30 – 17:00	Prof. Dr. Serim İLDAY (Bilkent University, UNAM National Nanotechnology Research Center, Turkey)	How to Control Far from Equilibrium Self-Assembly of Atoms, Colloids, Microorganisms, and Cells: A Rough Guide
17:00 – 17:30	Kaffeepause / Coffee Break	
Chairperson: Prof. Dr. Ali SINAĞ (Ankara University, Department of Chemistry, Turkey)		
17:30 – 18:00	Assoc. Prof. Dr. Emre ERDEM (Sabancı University, Integrated Manufacturing Technologies Research and Application Center, Turkey)	Defect Controlled Electrodes for High Performance All-in-One Supercapacitors
18:00 – 18:30	Prof. Dr. Saim ÖZKAR (Middle East Technical University, Department of Chemistry, Turkey)	Catalytic Efficiency of Noble Metal Nanocatalysts in Hydrolytic Dehydrogenation of Ammonia Borane
19:00	Empfang / Reception	

13 April 2023

9:30 – 10:00	Prof. Dr. Handan OLĞAR (Humboldt Ambassador Scientist, Ankara University, Department of Physics Engineering)	Opportunities of the Alexander von Humboldt Foundation for International Researchers
10:00 – 10:30	Murat KEMALOĞLU (DAAD IC İstanbul, Turkey)	Opportunities of the DAAD for International Junior Researchers
10:30 – 11:00	Kaffeepause / Coffee Break	
11:00 – 12:00	Diskussion Runder Tisch / Round Table Discussion Deutsche–Türkische Zusammenarbeit in Wissenschaft / German- Turkish Cooperation in Science	

	<p>Prof. Dr. Hasan MANDAL Humboldt Fellow, President of the Scientific and Technological Research Council of Turkey</p> <p>Prof. Dr. Ayhan ELMALI Humboldt Fellow, Ankara University, Department of Physics Engineering</p> <p>Prof. Dr. Ece GÖZTEPE-ÇELEBİ Humboldt Fellow, Bilkent University, Dean of the Faculty of Law</p> <p>Prof. Dr. Burhanettin Aykut ARIKAN Türkisch-Deutsche Universität, Dean of the Faculty of Cultural and Social Sciences, İstanbul, Turkey</p>	
12:15 – 12:30	Conference Photo (in front of the building)	
13:00 – 14:00	Mittagessen / Lunch	
<p>Chairperson: Prof. Dr. Kadir PEKMEZ (Hacettepe University, Department of Chemistry, Turkey)</p>		
14:00 – 14:30	<p>Dr. Stefan SCHNABEL (University of Leipzig, Institute of Theoretical Physics, Germany)</p>	Long Lennard-Jones polymers at the Theta-point
14:30 – 15:00	<p>Prof. Dr. Durmuş Ali DEMİR (Humboldt Awardee) (Sabancı University, Faculty of Engineering and Natural Sciences, Turkey)</p>	Quantum Tunneling Time, with Applications to Point Mutations in DNA
15:00 – 15:30	<p>Dr. Ezgi KARACA (Dokuz Eylül University, İzmir International Biomedicine and Genome Institute, Turkey)</p>	Recent Advances in the Computational Structural Biology of Biomolecular Interactions
15:30 – 16:30	Poster Session (Approx. 15-20 poster presentations from Junior Researchers)	
	Kaffeepause / Coffee Break	
<p>Chairperson: Prof. Dr. Hülya ALTUNTAŞ (Eskisehir Technical University, Department of Biology, Turkey)</p>		
16:30-17:00	<p>Dr. Yunus ALAPAN (Georgia Institute of Technology, U.S.A.)</p>	Biohybrid And Synthetic Microrobots with Controlled Navigation in Biological Tissues
17:00 – 17:30	<p>Prof. Dr. Ethem AKTÜRK (Adnan Menderes University, Faculty Of Science, Physics Department, Turkey)</p>	Exotic Two-Dimensional Material: Biphenylene Network
17:30 – 18:00	<p>Prof. Dr. Martin WEIGEL (University of Chemnitz, Department of Physics, Germany)</p>	Magnetic Systems with Quenched Disorder: Results from (Quasi) Exact Ground State
19:30	Feierliches Konferenz Abendessen / Conference Dinner	

14 April 2023

Chairperson: **Prof. Dr. Turgut BAŞTUĞ**
(Hacettepe University, Department of Biophysics, Faculty of Medicine, Turkey)

9:30 – 10:00	Dr. Sezin GALİOĞLU ÖZALTUĞ (Bilkent University, UNAM National Nanotechnology Research Center, Turkey)	Femtosecond Laser Synthesis of Nanoporous Materials
10:00 – 10:30	Prof. Dr. Raşit TURAN (Middle East Technical University, Center for Solar Energy Research and Applications (ODTÜ-GÜNAM), Turkey)	Current Status and Future Perspective of Photovoltaic Solar Cell Technologies
10:30 – 11:00	Prof. Dr. Ayşe KARAKEÇİLİ (Ankara University, Faculty of Engineering, Department of Chemical Engineering, Turkey)	NEW Biomaterials: Crossing Kingdoms
11:00 – 11:30	Kaffeepause / Coffee Break	
Chairperson: Prof. Dr. Emin AÇIKKALP (Eskisehir Technical University, Department of Mechanical Engineering)		
11:30 – 12:00	Prof. Dr. Nimet YILMAZ CANLI (Yıldız Technical University, Faculty of Arts and Sciences, Department of Physics, Turkey)	Liquid Crystals: Structure, Properties and Applications
12:00 – 12:30	Prof. Dr. Ash İŞÇİ YAKAN (Ankara University, Faculty of Engineering, Department of Food Engineering, Department of Food Engineering, Turkey)	Biorenewable Resources and Biofuels
12:30 – 13:00	Prof. Dr. –Ing Markus K. LAKE (Hochschule Niederrhein, Fachbereich Maschinenbau und Verfahrenstechnik, Krefeld)	Design and Synthesis of PVD Coatings for AOP Process for Wastewater Treatment
13:00 – 13:30	Assoc. Prof. Işık SEMERCİ (Ankara University, Faculty of Engineering, Department of Energy Engineering, Turkey)	Ionic liquids and Biomass-Derived Solvents Paving the Way to A Bio-Circular Economy
13:30 – 13:45	Schlussitzung / Closing Session	
13:30 – 14:30	Mittagessen / Lunch	
14:30 – 17:30	Ausflug / Excursion	
	Besichtigung nach der Museum für Anatolische Civilisationen / Visit to The Museum of Anatolian Civilizations	
	Ankara Burg / Ankara Castle	

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April 12-14, 2023
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INVITED PRESENTATIONS

Kinetic Magnetism in Semiconducting Moire Materials

Ataç İmamoğlu

ETH Zürich, Department of Physics, Quantum Electronics Institute, Switzerland

Moire superlattices in two dimensional semiconductors have enabled the observation of a wealth of phenomena driven by strong electronic correlations, ranging from Mott-Wigner states to quantum anomalous Hall effect. In this talk, I will describe magnetic properties of van der Waals heterostructures forming a frustrated triangular lattice in the vicinity of Mott-insulator states of electrons. By directly measuring electronic magnetization through the strength of the polarization-selective attractive polaron resonances, we find that when the Mott state is electron doped, the system exhibits ferromagnetic correlations in agreement with Nagaoka model. Our observations, which are in agreement with DMRG calculations, provide a direct evidence for itinerant magnetism with a kinetic origin.

Strictly Localized States in Quasicrystals

Mehmet Özgür Öktek

Bilkent University, Physics Department, Turkey

Quasicrystals can be described as projections of sections of higher dimensional periodic lattices into real space. The image of the lattice points in the projected-out dimensions, called the perpendicular space, carries valuable information about the local structure of the real space lattice. We use perpendicular space projections to analyze the strictly localized states in four quasicrystal tight-binding models. These zero energy states form a massively degenerate manifold akin to flat bands in periodic systems. For the Penrose lattice, we reproduce the six types of localized states and investigate their overlaps and linear independence. For the Ammann-Beenker and Socolar dodecagonal lattices, an infinite number of localized state types are needed to explain the numerically observed degeneracy. We also consider all pentagonal quasicrystals which have the same projection window as the Penrose lattice and show that the behavior of the zero energy manifold on the two sublattices of the quasicrystal show marked differences.

References

Murod Mirzhalilov ve M. Ö. Oktel, Phys. Rev. B 102, 064213 (2020); M.Ö. Oktel, Phys. Rev. B 104, 014204 (2021); M.Ö. Oktel, Phys. Rev. B 106, 024201 (2022); Akif Keskiner ve M.Ö Oktel, Phys. Rev. B 106, 064207 (2022)

Large Area Transparent DMD Thin Film Electrodes Deposited by Magnetron Sputtering

L. Özyüzer¹, M. Ekmekcioğlu^{1,2}, N. Erdoğan³, S. Özbay⁴, G. Aygün² and M. Özdemir²

¹Department of Physics, Izmir Institute of Technology, Urla 35430, Izmir, Turkey

²Teknoma Technological Materials Inc., Izmir Technology Development Zone, Urla 35430, Izmir, Turkey

³Advanced Material, Process and Energy Technology Center, Turkish Aerospace, 06980 Ankara, Turkey

⁴Department of Chemical Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey

Transparent conductive electrodes (TCEs) such as Indium Tin Oxide (ITO), Indium Zinc Oxide (IZO), and Aluminum Zinc Oxide (AZO), due to their high optical transmittance and good electrical conductivity properties, as well as their stability in the air, they are widely used in many applications such as displays, smart windows, solar cells, photodetectors, electroluminescent devices, organic light emitting diodes (OLEDs) and infrared (IR) reflective coatings. ITO is the most widely used TCEs in commercial devices. However, recently, the increase in the cost of ITO coatings with the increase in indium prices and also the scarcity of indium reserves has led researchers to search for alternative conductive electrode materials with low cost, high optical transmittance, and high electrical conductivity. In some applications, single transparent conductive oxide (TCO) layer is not enough to provide the desired properties. One of the most effective ways to increase optical transmittance and electrical conductivity is to use sandwich-type structures such as dielectric/metal/dielectric (D/M/D) multilayer thin film electrodes. Among the multilayer thin film electrodes, the zinc tin oxide (ZTO or Zn_2SnO_4)/Ag/ZTO (ZAZ) layered structure is promising due to its low surface resistance and high optical transmittance in the visible region of the spectrum. In our studies, ZAZ electrodes were deposited on substrates such as glass, polycarbonate (PC), and acrylic (PMMA) in the form of flat surfaces. The large area magnetron sputtering system were used to coat films. ZAZ multilayer thin films grown on glass, PET, and PC substrates were found to have high optical transmittance and low surface resistance (~8 ohms/square) [1]. In addition, it has been determined that ZTO/Ag/ZTO multilayer thin films grown on polymer substrates improved optical transmittance by causing lower reflection due to the higher absorption originating from the Ag layer in the ZAZ structure. These results show that ZTO/Ag/ZTO multilayer thin films on any substrate can be a promising alternative to ITO thin films as optically transparent and conductive electrodes for various applications. In addition, as a result of electromagnetic designs, it was determined that ZAZ thin films coated on polymer surfaces showed Salisbury-type absorber properties, briefly low radar visibility, and electromagnetic wave shielding.

References

- [1] M. Ekmekcioglu, N. Erdogan, T. Astarlioglu, S. Yigen, G. Aygun, L. Ozyuzer, M. Ozdemir, "High transparent, low surface resistance ZTO/Ag/ZTO multilayer thin film electrodes on glass and polymer substrates", *Vacuum*, **187** (2021) 110100.

Permanent Magnets: Today's Needs and Perspectives For A Carbon Neutral Society

Semih Ener

Functional Materials, Technical University of Darmstadt, Darmstadt/Germany

Magnetic materials can be classified in two different categories: soft and hard. The hard ones retain their magnetism after being magnetized. They are so called permanent magnets. These are materials which possess a persistent magnetic field without the need of an external power source, making them indispensable components for a wide range of technological applications in various fields [1], e.g. electric motors, information storage, renewable energy, biomedical applications, cooling etc. Current permanent magnet market is dominated by two main players which are low-cost, low-performing ferrite-type materials and on the other hand expensive, high-performance rare-earth transition-metal including alloys. In today's reality, the rare-earth transition-metal Nd₂Fe₁₄B-type magnets are the application dominating high performance magnets, but they contain rather critical elements. The rare-earth (RE) supply crisis of approx. ten years ago led to a drastic increase in prices and revealed the dependency on critical RE elements for the production of high-performance permanent magnets. Significant efforts are on-going to find alternative material systems which present magnetic properties similar or superior to those of the Nd₂Fe₁₄B benchmark, but which contain less or no critical elements [2-4]. In this presentation, we will discuss the today's reality on the hard-magnetic materials and also talk about the possible perspectives on the topic including material databases, implementation of combinatorial analysis methods and machine learning models.

References

- [1] O. Gutfleisch, M.A. Willard, E. Brück, C.H. Chen, S.G. Sankar, J.P. Liu., *Advanced Materials* 23 (2011) 821.
- [2] S. Ener, K. Skokov, D. Palanisamy, T. Devillers, J. Fischbacher, G. Gomez Eslava, F. Maccari, L. Schäfer, L.V.B. Diop, I. Radulov, B. Gault, G. Hrkac, N.M. Dempsey, T. Schrefl, D. Raabe, O. Gutfleisch, *Acta Materialia* 214 (2021) 116968.
- [3] D. Palanisamy, S. Ener, F. Maccari, L. Schäfer, K. Skokov, O. Gutfleisch, D. Raabe, B. Gault, *Physical Review Materials* 4 (2020), 054404.
- [4] S. Ener, J. Kroder, K. Skokov, O. Gutfleisch., *Journal of Alloys and Compounds* 683 (2016) 198.

MicNo®: New Generation Particle Technology to Improve Lives

Ender Suvacı

Eskişehir Technical University, Eskişehir, Türkiye

Characteristics of ceramic particles can play a critical role for achieving high performance particulate materials or ceramics. Therefore, tailoring ceramic particles can be utilized to access enhanced properties and performance. Our research group focuses on exploiting this opportunity to improve lives. In this presentation, development of two tailored ceramic particle systems via combining basic understandings in chemistry, physics and biology with the materials science and engineering perspective, and their impact on our lives will be discussed. The first group that will be discussed is our patented novel MicNo® Technology which was developed to overcome the problems of cosmetic formulators. Unique platelet shaped, designed MicNo® particles exhibit only the advantages of micron (safety) and nano (transparent and smooth) particles by mitigating their disadvantages such as whitening effect and potential risks of penetration through the skin, respectively. From toxicological perspective, MicNo® particles demonstrate much better biocompatibility with respect to nano particles; therefore, they can be evaluated as safer form of the nano particles. The second particulate system to be discussed is also our patented technology, called as MicNo-Hyg® that was designed and manufactured to form superior antimicrobial and antiviral coatings over ceramic and textile surfaces. In the presentation, not only MicNo-Hyg® particles' antimicrobial/antiviral performance over ceramic sanitary ware and tile surfaces but also their impact on the appearance and surface roughness of such ceramic surfaces will be discussed.

Critical Behavior of the 3D Ising Model with Power-Law Correlated Defects: Monte Carlo Simulations

Wolfhard Janke

Leipzig University, Theoretical Physics Institute, Germany

We study the critical behavior of the three-dimensional Ising model with long-range correlated point defects whose correlation decays with distance r like to a power law r^{-a} . By applying finite-size scaling techniques to our data of extensive Monte Carlo simulations, we estimate the critical exponents ν, γ, β , and ω in dependence of the correlation exponent $1.5 \leq a \leq 3.5$, based on “global” fits of results for several defect concentrations [1,2]. We briefly show that the estimated exponents ν and γ are compatible with an alternative temperature-scaling analysis [3]. The discussion of the results will be centered on the long-standing theoretical conjecture by Weinrib and Halperin that $\nu = 2/a$.

References

- [1] S. Kazmin and W. Janke, Phys. Rev. B 102, 174206 (2020).
- [2] S. Kazmin and W. Janke, Phys. Rev. B 105, 214111 (2022).
- [3] S. Kazmin and W. Janke, Condens. Matter Phys. 26, 13201 (2023).

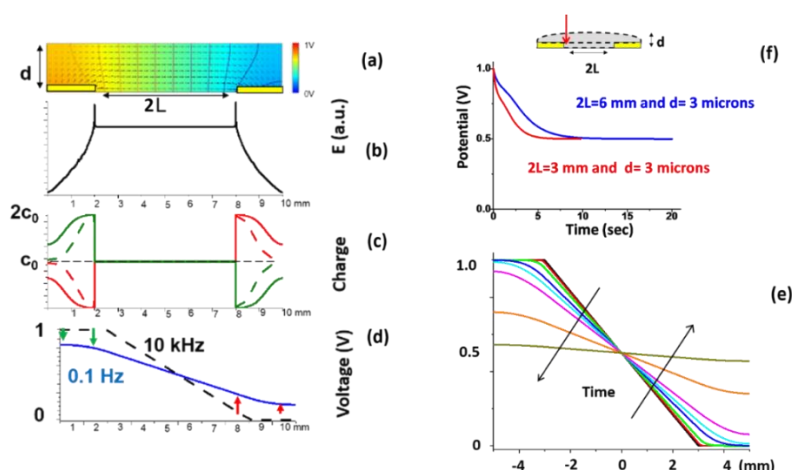
Localized X-Ray Photoelectron Impedance Spectroscopy (Lo-XPIS) for Capturing Charge Dynamics of an Ionic Liquid Electrolyte within an Energy Storage Device

Mustafa Başaran,¹ Erdinc Oz,² Said Ergoktas,³ Coskun Kocabas,³ Burak Ulgut,² Askin Kocabas,¹ and Sefik Süzer^{2,*}

¹Department of Physics, Koç University, 34450, Istanbul, Turkey,

²Department of Chemistry, Bilkent University, 06800, Ankara Turkey,

³Department of Materials, University of Manchester, Manchester M13 9PL, Lancs, England



Electrochemical devices are based on the fundamental process of ion migration and accumulation on surfaces. Complex interplay of molecular properties of ions and device dimensions control the entire process and define the overall dynamics of the system. Particularly, for ionic liquid-based electrolytes it is often not clear which property and to what extent contributes to the overall performance of the device. Herein we use X-ray photoelectron spectroscopy (XPS), while the device is under electrical bias. Such a procedure reveals localized electrical potential developments, through binding energy shifts of the atomic core levels, in a chemically specific fashion. Combining it with Square-Wave AC Modulation, the information can also be extended to time domain, and investigate devices configured as a coplanar capacitor, having an ionic liquid as the electrolyte, in macro-dimensions. Our analysis reveals that nonlinear voltage profile across the device emerge from spatially nonuniform electrical double layer formation on electrode surfaces. Interestingly coplanar capacitor has extremely slow time response which is particularly controlled by IL film thickness. XPS measurements can capture the ion dynamics in tens of seconds to microseconds range, and reveal that ionic motion is all over the device, including those on metallic electrode regions. This behavior can only be attributed to motion in more than one dimension. The ion dynamics can also be faithfully simulated by using a modified PNP equation, taking into account steric effects, and device dimensions. XPS measurements on two devices with different dimensions corroborated with and validated the simulation results. The present results propose a new experimental approach and provide new insights into the dynamics of ions across electrochemical devices.

References

M. Basaran, E. Oz, S. Ergoktas, C. Kocabas, B. Ulgut, A. Kocabas, S. Süzer (2022), Faraday Discussions **236**, 86.

How to Control Far From Equilibrium Self-Assembly of Atoms, Colloids, Microorganisms, and Cells: A Rough Guide

Serim İlday

Bilkent University, UNAM National Nanotechnology Research Center, Turkey

Systems far from thermodynamic equilibrium operate under highly nonlinear and strongly stochastic conditions, making emergent phenomena difficult or impossible to predict, mimic, or control. In this talk, I will argue that the emergent phenomena far from equilibrium can be steered via the triple mechanism of nonlinearity, fluctuations, and feedback mechanisms. I will support my arguments by showcasing the controlled emergence of various materials, from atoms to cells [1-4].

References

- [1] S. İlday et al., Nano Lett. 16, 1942-1948 (2016)
- [2] S. İlday et al., Nature Commun. 8:14942 (2017)
- [3] G. Makey et al., Nature Phys. 16, 795-801 (2020)
- [4] Ü. S. Nizam et al., J. Phys.: Condens. Matter 33, 304002 (2021)

Defect Controlled Electrodes for High Performance All-In-One Supercapacitors

Emre Erdem

Sabancı University, Faculty of Engineering and Science, Materials Science and Nano Engineering, Orhanli, Istanbul, Turkey

Electron paramagnetic resonance (EPR) spectroscopy is a very powerful method due to its enhanced sensitivity to unpaired electrons. In order to understand the defect structure in functional nano-materials we use multi-frequency EPR spectroscopy. In this presentation i) basics of EPR spectroscopy, ii) quantum confinement effects in ferroelectric nano-materials and iii) EPR and Photoluminescence (PL) investigations of intrinsic defect centers in semiconductor zinc oxide (ZnO) nanoparticles will be given. Starting with the introductory information about EPR spectroscopy; poling, aging, doping and nano-size effects will be discussed for the ferroelectric materials such as, PbTiO_3 , BaTiO_3 , PbZrTiO_3 (PZT) etc. In the last part of the talk, surface and core defects and their reactivity under temperature and light will be presented for ZnO semiconductor nano-materials. Defect models will be discussed. Finally application of such materials as electrode materials and their electrochemical performance test results in the supercapacitor devices will be presented.

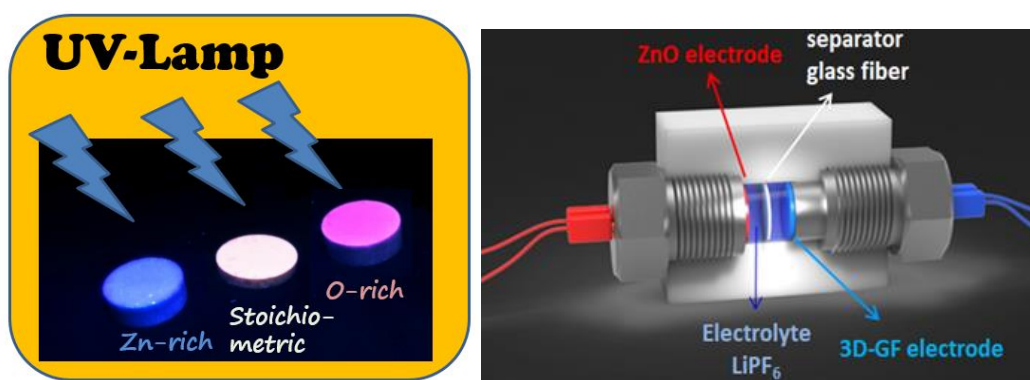


Figure: (left) Defect evolution of non-stoichiometric ZnO. (right) The supercapacitor device based on ZnO and 3D graphene foam electrodes.

Catalytic Efficiency of Noble Metal Nanocatalysts in Hydrolytic Dehydrogenation of Ammonia Borane

Saim Özkar

Department of Chemistry, Middle East Technical University, Ankara

Because of the severe energy crisis and global warming there is an urgent need for replacing the fossil fuels by the environmentally friendly renewable sources on the way towards sustainable energy future. Hydrogen is a green energy carrier and anticipated to play vital role in such a transition. However, its large-scale application has been hampered by the lack of efficient, safe, and controllable hydrogen storage systems. Fortunately, it has been realized that ammonia borane (NH_3BH_3 , AB) can be used for storing hydrogen safely and feasibly due to its nontoxicity, high hydrogen content, long-term stability in aqueous solutions and solid state, and high solubility in water. The most convenient way for releasing hydrogen from AB is its hydrolysis in the presence of suitable catalyst. Significant achievements have been obtained in increasing the rate of releasing H_2 from AB by employing transition metal nanoparticles (NPs) as catalysts. The noble metals are in general much more active than the non-noble metal by a factor of hundreds in hydrogen generation from the hydrolysis of AB. However, high price of noble metals hampers their large-scale applications in catalysis. Achieving high catalytic performance with the smallest amount of metal is critical for any catalytic applications of noble metals. While continuous efforts have been devoted to improve the catalytic activity of non-noble metals, an immense challenge is the enhancement of utilization efficiency and catalytic performance, and thus ultimately lowering the cost of noble metal catalysts. The following ways are available for increasing the catalytic efficacy of noble metal nanocatalysts in hydrolytic dehydrogenation of AB: (i) Reducing the particle size of metal catalysts to nanometer increases the surface area of catalysts and thus, the number of active sites. For example, using the colloidal metal(0) NPs can provide significant enhancement in catalytic activity because of large fraction of surface atoms. However, the putatively naked colloidal NPs are expectedly unstable against agglomeration and tend to aggregate to larger particles, which greatly hampers their recyclability and catalytic performance. Therefore, the colloidal metal NPs need to be stabilized by adding appropriate ligands into solution or by immobilization on materials with large surface area. (ii) Supporting them on materials with large surface area such as carbonaceous materials or metal oxides. The catalytic activity and stability of supported metal NPs depend on the particle size distribution, surface area of support, and strength of metal-support interaction relative to the metal-metal bond. Selecting suitable supports is of paramount importance in obtaining NPs which are stable and yet catalytically active. The strength of metal-support interaction turns to be crucial for catalytic activity and stability of the supported NPs. (iii) The carbonaceous supports provide meager improvements in catalytic activity of noble metal NPs for hydrolytic dehydrogenation of AB and almost no boost in their stability and reusability. (iv) Selecting a suitable oxide support is of critical importance for obtaining highly active and stable NPs with long lifetime. In particular the reduceable oxides may provide a favorable metal-support interaction leading to notable increase in the catalytic activity and stability of noble metal(0) NPs. (v) Downsizing the noble metal NPs and lowering the relative amount of metal can significantly enhance the utilization efficiency of the precious metal nanocatalysts. (vi) Supporting the noble metal NPs on the surface of magnetic powder enables the easy separation of nanocatalysts using an external magnet and thus provides high reusability for noble metal nanocatalysts. Consequently, all these means can enhance the utilization efficiency and ultimately lower the cost of noble metal nanocatalysts in evolution of H_2 from the hydrolysis of AB. The progresses in developing highly efficient noble metal(0) nanocatalysts which have been reported to be active catalysts in releasing H_2 from AB will be discussed along with the available parameters including temperature, particle size, surface area, catalyst to substrate ratio, turnover frequency, and metal support interaction.

Long Lennard-Jones polymers at the Theta-point

Stefan Schnabel

University of Leipzig, Institute of Theoretical Physics, Germany

Polymers in dilute solution undergo a phase transition from extended random coils to collapsed globules when the solvent changes from good to bad. At the critical (Theta) point the polymer behaves on large enough scales like an ideal chain or a pure random walk. Renormalization group calculations predict logarithmic corrections to scaling which so far have not been confirmed by computer simulation or experiment. The main challenge is that very long chains have to be considered, a feat that has only been possible for systems on lattice geometries.

Recently [1] we devised a Monte Carlo method for the simulation of long off-lattice polymers with untruncated interaction. It allows for the simulation of polymers with ten thousands of fully interacting repeat units. Here, we determine the Theta-temperature and investigate the scaling properties at the critical point of a bead-stick polymer model whose monomers (beads) interact pairwise via a Lennard-Jones potential.

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Quantum Tunneling Time, with Applications to Point Mutations in DNA

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Quantum tunneling is what enables various energetically-forbidden transitions in biological, chemical and physical systems. The shining of the Sun and cold exothermic reactions occur with tunneling, and point mutations in DNA are believed to occur with tunneling, too. Tunneling time delay, measured to be finite in ionization and cold atom experiments, needs be modeled separately due to the non-operator nature of time in quantum theory. In this talk, we shall first discuss tunneling time models and emphasize entropic tunneling time and Bohmian tunneling time as two viable candidates. We shall next exemplify Bohmian tunneling time by the free-fall of cold atoms, and entropic tunneling time by the proton tunneling in intra-base and inter-base transitions in DNA. We will conclude the talk by discussing other potential applications of tunneling time, including the time delay across Josephson junctions in annealing quantum computers.

Recent Advances in the Computational Structural Biology of Biomolecular Interactions

Ezgi Karaca

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Proteins and their interactions are at the mainstay of any cellular process. Studying these interactions at the atomistic scale pave the way for a mechanistic understanding of biological function. It also provides the first essential step toward the development of new drugs. This study field is called structural biology. Since late 2020, thanks to the efficient implementation of AI methods into the structure prediction protocols, we have been witnessing a revolution in the structural biology field. With these developments, we are closer more than ever for interpreting biological data of different resolutions at the structural level. In our lab, we are developing tools and approaches to assist this interpretation, which I will discuss during my presentation.

Biohybrid and Synthetic Microrobots With Controlled Navigation in Biological Tissues

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Control over the microscopic world, at the scale of the smallest organisms, depends on the development of robots and machines that can operate at micro-nanoscales. However, fundamental limitations in the efficient miniaturization of macro-scale robotic technologies require bioinspired/hybrid approaches for actuation, sensing, and control of microrobots. Recent advances in materials, fabrication and actuation technologies have enabled the realization of wireless microrobots powered by external fields, biological organisms, and catalytic reactions. In this talk, I will introduce cell-sized ($<10\ \mu\text{m}$) surface-rolling multifunctional microrobots, inspired by leukocytes in the circulatory system, actuated by external magnetic fields. Microrollers generate unprecedented strong propulsion (up to 100 body lengths per second) enabling their upstream navigation in physiological blood flow and their functionalization with targeting agents and drug molecules allows targeted, on-demand drug delivery to desired cells. I will conclude by highlighting potential strategies toward embodying intelligence to microrobots through physical interactions guided by soft and biological materials and external fields.

Exotic Two-Dimensional Material: Biphenylene Network

Ethem Aktürk

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Following the synthesis of graphene, a planar, freestanding, 2D monolayer of carbon in honeycomb network of perfectly sp^2 – hybridized atoms, several novel nanomaterials constituted from group-IV elements, IV-IV and III-V compounds have been first predicted theoretically, and later majority of them have been synthesized. Unveiling physical and chemical properties of those 2D structures and their possible 3D layered van der Waals solids has dominated the research in nanoscience for the last two decades. Recently, Fan et al. synthesized quasi 1D nanoribbons of carbon in the biphenylene network on Au(111) surface, which consist of the adjacent octagon-(o), hexagon- (h), and square- (s), rings; specified briefly as ohs structure. This is a very important achievement realizing metallic, nonhexagonal, nanosized monolayer of carbon, even if this 2D C-ohs structure has been proposed/ predicted earlier in various theoretical studies.

Motivated with this work, we were carried out an extensive study, not only on carbon in ohs (biphenylene) structure, but also on ohs monolayers of group IV elements (Si, Ge), group IV-IV (SiC, GeC, SnC), III-V (BN, BP, Bas, BSb, AlN, AlP, GaN, InN) and II-VI (ZnSe) compounds, their multilayers (thin films) and MoS_2 , as well as 3D periodic ohs crystals. Investigating the dynamical and thermal stability, mechanical and electronic properties of all these structures and predicting their critical features, we unveiled a new class of materials as a counterpart of those in honeycomb network (like well-known, graphene, silicene, germanene, h-BN, h-GaAs, ZnTe etc... which were treated actively in the last decade). In particular, good metallicity of silicene, germanene and 3D layered crystal of carbon ohs as an analog of graphite have demonstrated new allotropes of the corresponding elements. We believe that 2D metallic character and other associated features of ohs monolayers occurred within an atomically thin width will be a fertile research ground for several theoretical and experimental studies on the fundamental aspects of matter (like quantum conductance, quantum dots, quantum Hall effect etc.) in lower dimensionality.

In my presentation, I will discuss the results of extensive study conducted on various types of biphenylene monolayers and multilayers of materials, including group IV elements, group IV-IV, II-V, II-VII compounds and MoS_2 .

Magnetic systems with quenched disorder: results from (quasi) exact ground states

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Quenched impurities are ubiquitous in laboratory samples of magnetic systems. Depending on the type and strength of disorder, the effects on the type of ordering as well as the persistence and order of the accompanying phase transitions can be dramatic, ranging from shifts in transition temperature in disordered ferromagnets to the replacement of conventional long-range order by a locally frozen state in spin glasses. Due to the presence of excessively large relaxation times and the need to perform an average over disorder (sometimes complicated by a lack of self-averaging), numerical studies of such systems are exceedingly difficult. With the help of mappings of the ground-state problems to well known combinatorial optimization problems as well as, where needed, generalized-ensemble Monte Carlo methods meaningful studies of such systems become feasible.

In this lecture I will illustrate how such problems can be tackled with the help of a combination of Monte Carlo methods as well as exact and heuristic optimization methods, and I will illustrate this approach with a range of results for spin glasses and random-field systems in two and three dimensions.

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Femtosecond Laser Synthesis of Nanoporous Materials

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Zeolites are preferred adsorbents, ion-exchangers, and catalysts for many reactions of industrial importance. There is an ongoing effort to develop new synthesis methods to investigate nucleation and growth processes of zeolites. In conventional hydrothermal synthesis, the induction period, defined as the time elapsed until the observation of the first crystal, is long (> 15 h or days). However, as there are more than 40 silica polymerization/depolymerization reactions occurring simultaneously in the zeolite precursor suspension, and these have time scales on the order of femto- and pico-seconds, it is a complex task to investigate the nucleation processes precisely. Ultrafast lasers ensure fast and high-resolution spatiotemporal energy deposition in the time scale of a femtosecond, accelerating induction and growth periods of zeolite synthesis. In this talk, I will argue that ultrafast lasers are the ideal candidates and showcase this by presenting nucleation and growth starting from basic zeolite units of a few membered ring structures (5T to 10T) to MFI-type zeolite precursor structures (22T to 36T), and finally achieving full MFI Silicate-1 zeolite structures. Hereby, I assessed the mechanism of nucleation by various characterization methods. Next, I will show the new synthesis method works equally well for at least three more zeolite types. I will advance by comparing this novel synthesis technique with conventional ones and show how it reduces the time and energy demand for zeolite synthesis, and how future research and industrial applications might benefit from it.

Current Status and Future Perspectives of Crystalline Photovoltaic Solar Cell Technologies

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Crystalline Si photovoltaic (PV) solar cell has reached an extremely well maturity level with well-optimized material and process conditions. Although discovered in 50's, it is overwhelmingly dominating the commercial PV market today with a share exceeding 95%. It is generally expected that Si PV will continue to dominate the PV industry in the coming years. Like in microelectronic where Si crystal is the main and untouchable material, Si crystal will play a central role in the energy conversion technologies in the years ahead.

The conversion efficiency limit reachable with single junction Si solar cell, called Shockley–Queisser limit, is calculated to be around %30. Today, the world record realized at R&D level is already 26.7%, whereas at the industrial production lines, maximum cell efficiencies have reached 23-24 % range. Although the gap between theoretical limit and the technological achievement has narrowed down to a few percent, for an ultimate victory of solar energy over the other energy resources, efforts are still underway with new approaches to reduce cost/performance ratio even further. The performance of a solar cell, which is usually expressed in terms of the conversion efficiency, can be improved by reducing the electrical and optical losses through new material and process approaches. New c-Si PV cell architectures called TOPCon, IBC, HIT been have been demonstrated with higher efficiency values. Also, solar cells with more than one junction made of different materials, namely, tandem solar cells have been shown to be very promising structure for future high efficiency devices.

In this presentation, the current status of the PV technology and its status worldwide and future perspectives will be summarized. Activities of ODTÜ-GÜNAM and its road map in the following years will also be presented.

NEW Biomaterials: Crossing Kingdoms

Ayşe Karakeçili

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Use of various materials in different forms has been an attractive research area, not only in biomedical field but also in environmental technology, food industry and circular economy. Apart from polymers, metals, and traditional composites, there is still more to investigate different types of materials as a biomaterial candidate.

Liquid Crystals: Structure, Properties and Applications

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Liquid crystals (**LCs**) are a unique state of matter between solid (crystalline) and liquid (isotropic) phases; some compounds form a different, distinct intermediate phase, sometimes referred to as the "fourth state of matter" or "mesophase". These compounds exhibit mesophases with optical, electronic, and physical properties have a long-range orientational and/or positional arrangement similar to that of a crystal, but also show liquid-like flow [1]. **LCs** are unique structures with remarkable electronic and optoelectronic properties and have tremendous success in commercial applications [2-5]. They are very sensitive to external fields [6]. Liquid crystal displays are inexpensive and work under low operational voltage and low power consumption: they can also often operate in the presence of sunlight (because they modulate the reflected light including the sunlight itself and thus maintain a good contrast). **LC** mesophases may be classified on the basis of the shape molecules, which give rise to properties of the phase [7]. To date the photovoltaic effect has only been demonstrated with calamitic **LCs** via an ionic mechanism [8, 9]. To date, photovoltaic effects have mostly been studied with commercial liquid crystals we thought it would be interesting to investigate the effect of new synthesized liquid crystals which prepared by our group in P3HT/PCBM based organic solar cells and in dye synthesized solar cells (DSSCs). In our previous studies, the photovoltaic properties of organic solar cells with and without liquid crystal (**LC**) additives were also compared. Especially for future OPV applications, **LCs** may play an important role and more efforts have to be made to realize their full potential.

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Biorenewable Resources and Biofuels

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In today's era, economic stability and national security issues are tightly linked to energy security and energy independency. Besides, depending on other countries' non-renewable energy sources, petroleum consumption brings environmental problems with it. It is necessary to replace the fossil fuels by renewable and sustainable fuels. Lignocellulosic materials such as agricultural residues are widely available in large amounts and can be used for production of biofuels. However, cost-effective, environmentally sound and efficient production processes have to be developed in order to compete with fossil fuels. The conversion of lignocellulosic biomass into biofuels is a complex and multi-stage process. The low digestibility of cellulosic materials is one of the most important obstacle in a bio-refinery. Hence, an effective pretreatment step is required to deconstruct the structure of biomass. Although, different pretreatment approaches are employed to overcome this technological bottleneck, it still remains a serious challenge to break the recalcitrance of biomass through an energetically efficient and environmentally friendly process. Due to their unique and green features, Deep Eutectic Solvents (DES) have emerged among the most promising solvents in bio-refinery processes to achieve that goal. Even though more research is still needed, DES can already be important actors in bio-refinery designs for sustainable development.

Design and Synthesis of PVD Coatings for AOP Process for Wastewater Treatment

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A photocatalytic surface coating with titanium dioxide provides a physical effect that is able to decompose organic deposits by irradiation with ultraviolet light. The UV irradiation initiates an advanced oxidation process (AOP) of the organic substances. Advanced Oxidation Processes are used in wastewater treatment to effectively minimize micro-pollutants, such as drug residues or organics. This type of purification is often used as the fourth purification stage in wastewater treatment plants.

In addition to the further development of oxidative processes, the Niederrhein University of Applied Sciences is engaged in the development of surface systems produced by the Physical Vapor Deposition process. The presentation will focus on the development of photocatalytically active TiO_2 layers in the modification anatase for use in a UV reactor. Another aspect is the development and fabrication of electrically conductive diamond coatings (BDD) for use in a rod bundle reactor.

Starting with a consideration of the requirements for the material systems, the requirements for the magnetron sputter ion plating PVD coating processes are presented. One focus of the work is the avoidance of target poisoning in the reactive MSIP process for the production of anatase. Furthermore, the mechanical-technological coating properties are investigated and evaluated for use in wastewater treatment. First results on water treatment using the example of methylene blue degradation are presented.

Ionic Liquids And Biomass-Derived Solvents Paving the Way to a Bio-Circular Economy

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The use of fossil fuels is being phased out in the modern world in an effort to address the pressing issues of population growth, climate change, and energy security. In this context, renewable energy sources help to create a cleaner and environmentally benign future. Since it is the only source of carbon atoms that stores energy in its chemical bonds, biomass stands out as one of the most promising sources. Biomass can be transformed into fuels and chemicals in a manner similar to how petroleum is currently used.

A biorefinery is primarily a facility that breaks down low-value feedstocks, biomass, into their components, which can then be transformed into a wide variety of fuels, chemicals, and materials. In order to facilitate the widespread production of biomass-derived fuels and chemicals, the compact nature of lignocellulosic biomass must be altered, and the components cellulose, hemicellulose, and lignin must be made available with a view to their maximum utilization. Although majority of current biorefineries employ conventional chemical agents, efforts establishing strategies that promote bio-circular economy has been initiated. Among these strategies, the use of ionic liquids as a significant invention of the modern chemistry and platform chemicals for biomass disintegration have been attractive since they encourage closed-loop operations and quantitative reuse of the solvents.

In this work, the potentials of ionic liquids and biomass derived solvents; gamma-valerolactone, and levulinic acid to process a variety of lignocellulosic feedstocks including hardwood, softwood, agricultural residues, cellulosic wastes such as paper mill sludge and waste diapers were described for bioenergy applications.

HUMBOLDT KOLLEG 2023 Ankara



RECENT ADVANCES IN
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POSTER PRESENTATIONS

Research at BvK LaB @ TARLA

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BvK LaB at TARLA (Turkish Accelerator and Radiation Laboratory) uses light to unravel the structures and function of biologically important proteins and protein complexes for understanding the mechanisms of biological phenomena. The research in our lab comprises molecular biology, recombinant or native protein production and purification, protein characterization, sample preparation for either crystallography or electron microscopy, structure modeling, biochemical measurements (enzyme kinetics), and complementary techniques such as cross-linking mass spectrometry, SAXS (Small Angle X-ray Scattering), and CD (Circular Dichroism) Spectroscopy. Current projects vary from the structural characterization of mega membrane protein complexes with cryo-EM, cross-linking mass spectrometry, and molecular docking, to the development of peptide based inhibitors with anticancer effects, as well as plant protein characterization from agricultural waste. We will summarize the research activities at BvK LaB related to our current projects.

Smartphone Based Colorimetric Measurement of Glucose via Silver Nanoparticle Formation in a Microchip

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In recent years, colorimetric sensors have been widely used in point-of-care (POC) diagnostic systems due to their ease of use and accessibility. The main advantage of these sensor systems is that they can detect many analytes from biofluids within a certain concentration range using colors visible to the naked eye. However, colorimetric sensors suffer from poor color homogeneity and weak colorimetric signal in detection. To overcome these disadvantages, we developed a microfluidic-based sensor system that enables rapid colorimetric detection of glucose by utilizing the synthesis mechanisms of silver nanoparticles (AgNPs). This work demonstrates, for the first time, the *in-situ* synthesis of AgNPs in a microfluidic platform as a colorimetric nanomaterial for glucose detection. In addition, the proposed microfluidic-based analytical device was integrated with a smartphone-based RGB (Red-Green-Blue) analysis method to improve the visual identification of the colorimetric signal. In this approach, digitized RGB values were collected using pixel-based data point method to obtain color variations of before and after sensor images of analyte exposure. The digitized RGB analysis results showed that the green values represented a significant change in terms of pixel densities compared to red and blue colors ($R^2 = 0.9407$). Furthermore, green pixel densities provide reliable and more accurate quantitative results for the 10-100 mM glucose concentration range. In conclusion, the integration of a microfluidic-based glucose sensor and digitized RGB data as a smartphone readout enables a simple sensing platform for fast and easy point-of-care (POC) glucose monitoring.

A Graphene-Based THz Metamaterial Absorber for Electro-Optic Switching and Chemical Sensing Applications

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Graphene-based THz metamaterial structures have attracted a great deal of interest due to their potential applications as optoelectronic devices, optical modulators and chemical sensors. In this study, a polarization-sensitive graphene-based metamaterial absorber is numerically designed and analyzed for THz switching and refractive index sensing applications by using a commercial 3D full-wave electromagnetic solver [1]. The metamaterial structure is composed of unit cells with nested three splitting resonators (SRRs) on top of a back-side gold-coated 10 μm -thick SiO_2 substrate. Chemical potential, relaxation time and temperature of graphene are set to 0.6 eV, 0.7 ps and 300 K in the design stage. Perfect absorption with 99% absorption ratio is generated at 5.61 THz for TM-polarized waves and at 6.00 THz for TE-polarized waves. Tuning of absorption is demonstrated by changing the chemical potential of graphene by electrostatic biasing. Maximum modulation degrees of ‘on/off’ absorption are found to be 72.0% at 5.3 THz for TM-polarized waves and 65.9% at 6.0 THz for TE-polarized waves. The variation of absorption peak frequency as a function of the refractive indices of various chemical analytes (such as water, ethanol, glycerin, benzene) shows a linearly decreasing trend as the refractive index increases. Sensitivities are calculated to be 0.74 THz/RIU for both TM and TE-polarized waves. Furthermore, the proposed absorber is demonstrated to maintain good absorption properties with the incident angles increasing up to 75° for both TM and TE-wave polarizations.

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Tailoring Optical Properties of $Ag_{1-x}Cu_x$ Alloy Nanoparticles by Laser Ablation and Fragmentation in Ethanol

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Alloy nanoparticles of Silver and Copper alloys were synthesized by femtosecond pulsed laser ablation method in ethanol. Copper and silver alloy targets ($Ag_{1-x}Cu_x$, $X = 15,30,50,70,85$) were produced by pure Ag and Cu targets by arc melting method. Compositions of targets were chosen accordingly to control the nature of the resulting nanoparticles. Our initial results show that core-shell structure appears in all of the compositions in the first synthesis. We have shown that when these nanoparticles are subjected to laser fragmentation process, the structure of the nanoparticles remain as core-shell when copper percentage is higher or change to biphasic type when silver proportion is higher. Absorbance behavior shifts with laser fragmentation time to the region of plasmonic peak of pure silver nanoparticles, resulting in tunable plasmonic absorbance. Therefore, tunable plasmonic absorbance can be achieved by changing the composition of the target or laser fragmentation time. The changing composition also affects the thickness of the shell which shows that thickness of the core-shell structure can be manipulated by altering the composition of the alloy target. Our first data also shows that the photoluminescence behavior of the nanoparticles is also tunable between photoluminescence of pure Ag and pure Cu nanoparticles. In conclusion, our first results indicate that we have synthesized core-shell and biphasic type $Ag_{1-x}Cu_x$ alloy nanoparticles with tunable shell thickness, absorbance and photoluminescence.

Neutrino Oscillation Experiments at CERN

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After the Second World War, European scientists, administrators and educators thought that scientific cooperation was necessary to ensure peace in the world, and for this purpose, the European Center for Nuclear Research (CERN) was established in 1953 with the signature of 12 countries. CERN, which was established to advance the frontiers of human knowledge by offering researchers a unique range of particle accelerator facilities, basically aims to reveal how and what the universe consists of and how it works. One of the most important studies carried out in CERN, which is the largest particle physics laboratory today, is neutrino physics studies. In 1934, Enrico Fermi, who studied beta decay, started the studies of neutrino physics by naming the particle with a small mass as the *neutrino*. The neutrino, first observed by Reines and Cowan in 1956, has now become an even more curious particle. Then, unlike other subatomic particles, it was suggested by Bruno Pontecorvo in 1957 that it has the feature of oscillation. The oscillations of the neutrino particle have been observed in many experiments under different conditions. Today, studies to discover the properties of the neutrino particle continue in many areas, especially CERN. There are many neutrino emission experiments carried out at CERN and still continuing. The results obtained make important contributions to the field of neutrino physics.

Adsorption of Porphine-Based Organic Molecules on Mxene Monolayer Based on First Principles

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In materials science, the unique electronic, optical, and mechanical properties of 2D graphene have led researchers to search for new materials [1,2]. One of these materials is MXenes, which are formed by combining different ions/molecules [3]. MXenes are two-dimensional transition metal carbide nanomaterials. They are 2D hybrid materials that are chemically stable, have good electrical conductivity and are environmentally friendly [4, 5]. In this study, Ti₂C (titanium carbide) was used as MXene substrate and on this substrate; Porphine organic molecule, which is very interesting due to its tunable chemical, electronic, magnetic and optical properties, has been adsorbed [6,7]. This hybrid structure formed by doping bare porphin molecule with Ag, Au, Cu on Ti₂C substrate was investigated with density functional theory based on first principles. The electronic and magnetic properties of all 2D structures obtained were investigated in detail.

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Supercapacitors Prepared Entirely from Waste Fabric

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Energy is one of the most important requirements for the continuation of life. Over the last century, world-wide overpopulation growth has increased the amount of energy needed enormously. Fossil fuels have been the main energy source since the industrial revolution to provide the necessary energy. But fossil fuels have limited sources and their environmentally destructive effects have increased the interest in the production of energy from renewable sources. Renewable energy is clean, environmentally friendly and sustainable. However, they are not always accessible. Regardless of its source, energy storage is an essential phenomenon. Supercapacitors are one of the energy storage devices that store energy easily, clean and cheap. They consist of four different parts which are current collector, electrode material, separator and electrolyte. The current collectors are electrically conductive materials and mostly made by metals, carbon cloths and carbon papers. The most common electrode materials are carbon-based materials, metals or metal oxides. Polymer, biomaterial and polymer-ceramic based materials are used as separator. Finally, various electrolytes are available for the supercapacitors such as aqueous, organic and gel electrolytes and ionic liquids. All the parts are made of different type of materials and have different characteristics. In terms of sustainability, fabrication of a supercapacitor cell from waste materials are possible. This study represents a supercapacitor cell prepared entirely from the waste textile materials. Carbonised fabrics were used as the current collector and separator, the carbonised/activated fabrics as the electrode material and waste fabrics extracted cellulose were utilised to obtain a hydrogel electrolyte.

First-Principles Investigation of 2-Dimensional Tetrahexagonal InN Alloys: Anisotropic Mechanical, Electronic, and Charge Carrier Transport Properties for Photocatalytic Water Splitting

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Two-dimensional (2D) materials with unique physical properties lead to new possibilities in future nanomaterial-based applications. Among them, 2D structures which are suitable to be the solar-driven catalyst for water splitting reactions have become excessively important since the demand for clean energy sources increases in conjunction with the environmental harm of fossil fuels. Apart from the conventional crystals with well-known symmetries, recent studies showed that materials that have exotic decorations could possess superior features. In this respect, we investigate novel 2D tetrahexagonal (*th*-) InN crystal and its ordered alloys In_{0.33}X_{0.67}N (X=Al, Ga) that can be utilized as effective catalysts for water splitting reactions. Proposed structures possess robust energetic, dynamical, thermal, and mechanical stability with a versatile mechanical response. After a critical tensile strain value, all monolayers exhibit strain-induced Negative Poisson's ratio in a particular crystal direction, making them half-auxetic materials. The examined materials are indirect semiconductors with desired bandgaps and band edge positions for water splitting applications. Due to their structural anisotropy, they have direction-dependent mobility that can keep the photogenerated charge carriers separated by reducing their recombination probability, which boosts the photocatalytic process. Relatively high absorption capacity in the wide spectral range underlines their potential performance. The versatile mechanical, electronic, and optical properties of 2D *th*-InN and its alloys In_{0.33}X_{0.67}N (X=Al, Ga), together with their remarkable structural stability, indicate that they can appropriately be exploited in the future for water splitting applications.

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Biomolecule Adsorption on Blue AsP Monolayer Surface, A DFT Study

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2D materials attract the attention of researchers due to their unique chemical and physical properties¹. However, some handicaps of these materials limit their applications². These disadvantages can be overcome by combining 2D materials with biomolecules³. In this study, adsorption of Glycine, Serine and Dopamine biomolecules, which have great potential for use in industry and biomedicine⁴⁻⁶, on ultra-thin single-layer blue AsP, which is promising in technological applications and has wide band gap^{7,8}, was investigated by the DFT as a preliminary study in order to understand its biofilm forming properties. Different geometric models of these biomolecules on pristine and vacancy single layer blue AsP were created and studied in terms of structural and electronic properties.

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DFT+U Simulations for the Adsorption of Pr Atom on the Anatase TiO₂ (101) Surface: Effect of U Parameter

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In this study, the effect of U values on the results obtained in DFT+U (Density Functional Theory) calculations was investigated. It is known that the U parameter significantly changes the results, especially for atoms with d- and f-electrons. In order to examine this effect in detail, Pr adsorption on the anatase TiO₂(101) surface was chosen as an example and the structural, electronic and optical properties of different geometric adsorption possibilities were calculated according to various U parameters. By comparing the obtained data, it has been revealed how the varying U values affect the calculated properties of the Pr/TiO₂(101) surface. This study can be useful in selecting the input parameters that can be used in DFT calculations to provide insight for experimental research.

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Tooth Enamel as Retrospective and Accidental EPR Dosimetric Material

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Radioactive accidents have become fact of our lives since discovery of radioactivity. Numerous accidents have occurred, including Turkey (IAEA, 2000; TAEK, 2017). Determining the exposed dose is important in helping authorities to take necessary precautions. Although, there are human-made dosimetric materials, the absence of these materials at the accident site is very possible. Therefore, human tissues that can be used for dosimetric purposes have been the subject of many researches. Thus, it has been determined in the literature that the human tooth-enamel is sensitive to radiation (Brady et al., 1968; IAEA, 2002). There has been increasing scientific interest of researchers in field of tooth-enamel since discovering usability of tooth-enamel by Brady et al. (1968).

Tooth enamel EPR dosimetry were used in many radiologic accidents like; atomic bomb survivors in Japan (Ikea et al., 1984), Techa River (Russia, Southern Urals) nuclear pollution in 1950 (Romanyukha et al., 1994), Chernobyl (Ishii et al., 1990), Fukushima Daiichi (Inoue et al., 2020) and many others. Therefore, the aim of this work is to present and to give information about the EPR properties and dosimetric features of tooth enamel.

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PEG-based Antimicrobial/Antifouling PECVD Coatings

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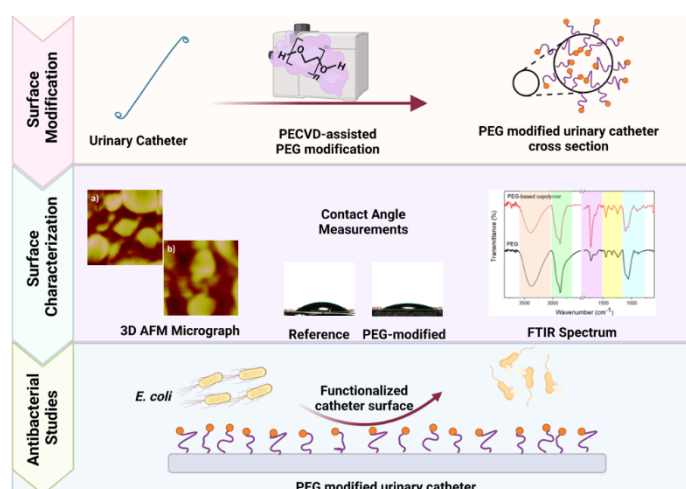
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More than 65% of Healthcare-associated infections are associated with implants or medical devices since such materials in the body possess conducive surfaces for pathogens (bacteria, viruses, fungi etc.) migration, attachment, and proliferation. In addition, HCAs cause death to a large extent. Therefore, anti-microbial coatings have received significant attention from doctors and scientists to minimize bacterial growth and/or prevent biofilm formation on the implant surfaces. Effective anti-microbial coatings are based either on the prevention of microbial attachment (anti-fouling), or on killing pathogens either before or after contact with the surface. Applying both mechanisms in a single coating combines the benefits of each and increases the inhibition of microbial colonization. The aim of this study is to develop polyethylene glycol (PEG)-based copolymer antimicrobial coatings for the inhibition of bacterial contamination on catheters. PEG-based copolymer thin films were synthesized via plasma enhanced chemical vapor deposition (PECVD) technique. The antimicrobial/antifouling activity of PEG-based copolymer coatings against *Escherichia coli* (gram-negative bacteria) was investigated. Concentrations of adherent and non-adherent live bacteria were also investigated to examine the surface behavior. The aim of this approach was to determine, which can either kill the bacteria upon contact (contact-killing) or limit their ability to adhere through the substrate surface (bacteria-repellent). According to the results, PEG surface modification prevented biofilm formation via contact-killing behavior compared to the reference substrates.

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