

XI Conference of Nanotechnology

BOOK OF ABSTRACTS

June 30th to July 5th, 2024
Lublin, Poland



Institute of Physics,
Maria Curie-Skłodowska University in Lublin



Dear Colleagues,

on behalf of the Organizing Committee, we are pleased to invite you to take part in the XI Nanotechnology Conference, NANO2024, which will be held in Lublin, Poland, from June 30th to July 5th, 2024. The conference is a traditional meeting for scientists held every two years in various scientific centres in Poland, and this year is organized by the Institute of Physics, Maria Curie-Skłodowska University (UMCS) in Lublin.

The main goal of the conference is to gather scientists representing various theoretical and experimental disciplines who study nanoscale systems. In this context, the latest achievements and applications in the field of nanotechnology are extremely important. We also plan to organize a special two-day session on one- and two-dimensional systems with the participation of outstanding foreign scientists. We hope that the scientific program of the conference, including a wide array of topics will live to your expectations, and that participation in NANO2024 will be an opportunity to listen to great invited lectures, variety of contributed talks as well as poster presentations, and also meet colleagues and renowned specialists from Poland and all over the world.

We especially encourage young scientists: students and PhD students to participate in the conference by offering them a reduced conference fee. During the conference, we also offer the opportunity to meet with the commercial sector, producers and sellers of equipment, materials and research services related to nanotechnology.

The official language of the conference is English.

We hope you will find NANO2024 valuable, enlightening, and opening horizons of knowledge.

We look forward to seeing you in charming academic town of Lublin.

Organizing Committee

nano2024.umcs.eu

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GENERAL TOPICS

- Chemical and Physical Foundations of Nanotechnology
- Nanobiotechnology, Nanomedicine and Nanosafety
- Nanoelectronics and nanophotonics
- Production and characterization of nanomaterials
- Nano-scale systems
- 1D and 2D systems
- Development of methods and scientific equipment for nanoscale research
- Practical applications of nanotechnology

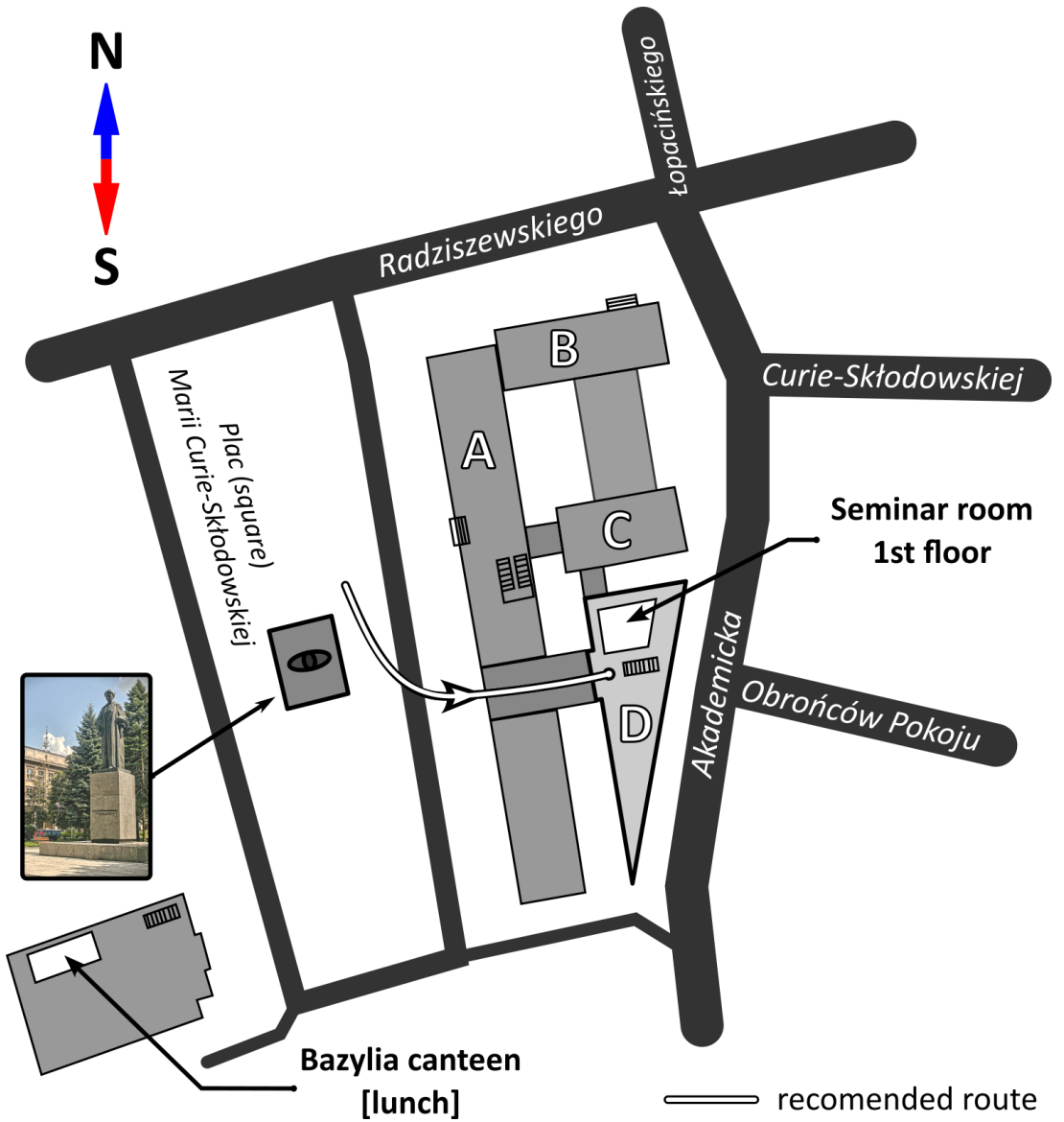
VENUE OF THE CONFERENCE

The XI Conference on Nanotechnology is organized by the Institute of Physics at Maria Curie-Skłodowska University main campus located near the Lublin city centre.

The seminars will take place in **Lecture Hall D104**,
located in **Building D**
of the Institute of Computer Science,
Faculty of Mathematics, Physics and Computer Science,
ul. Radziszewskiego 10, 20-031 Lublin.



Maria Curie-Skłodowska Square



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*Chairman of the Committee of the Development
and Promotion of the Achievements of Young
Scientists, Polish Academy of Sciences, Lublin
Branch*

CONFERENCE PROGRAM

	Monday	Tuesday	Wednesday	Thursday	Friday		
9:00	Opening	Fery	Excursion	Zegrodnik	Tamulevičius		
9:20	Erwin			Jalochowski	Sedlmayr	Szczytko	
9:40		Martin					Drózdź
10:00	Coffee break			Excursion	Coffee break		
10:20	Nowak	Pfnür		Excursion	Olesiak-Bańska	Łapiński	
10:40		Łukasz Piątkowski			Tegenkamp	Szymoński	Majewski
11:10	Osiński		Zaleski				
11:30	Lunch						
11:50	Dawid Piątkowski	Altman	Zandvliet		Godlewski		
12:10			Maćkowski				Esser
12:30	Wojnar	Lewandowski		Skowroński	Dudek		
12:50	Coffee break						
13:15	Dąbrowski	Tringides	De Padova	Kisiel			
13:35							Zaraska
14:15	Wrana	Lutsyk	Dunal	Le Ster			
14:35							<u>Technolutions</u>
15:15	Poster session	20:00	Conference dinner	19:00			
15:35							
15:55	20:00	Conference dinner	19:00				
16:30					Musical theatre		
16:50	20:00	Conference dinner	19:00				
17:10					Musical theatre		
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22:10	20:00	Conference dinner	19:00				
22:30					Musical theatre		
22:50	20:00	Conference dinner	19:00				
23:10					Musical theatre		
23:30	20:00	Conference dinner	19:00				
23:50					Musical theatre		

Sunday, 30th June

18:00	Welcome reception
20:00	

Monday, 1st July

9:00	Opening	
9:20	Erwin	Electron transport in nanocrystal solids: the influence of ligands
10:00	Martin	Dislocations as embedded 1D-nanostructure: controlling dislocations in epitaxial and stacked heterostructures
10:40	Coffee break	
11:10	Nowak	Nanotechnology in cosmetics: opportunities and challenges
11:50	Łukasz Piątkowski	Nanoscale hydration of cell membranes
12:30	Osiński	Designed, Programmable Protein Cages Utilizing Diverse Metal Coordination Geometries Show Reversible pH- Dependent Disassembly
12:50	Lunch	
14:15	Dawid Piątkowski	Hybrid plasmonic nanostructures for non-local luminescence processes
14:55	Maćkowski	Controlling photoswitching of photochromic molecules in hybrid nanostructural assemblies
15:15	Wojnar	Optically active indium selenide crystal phase heterostructures grown by molecular beam epitaxy
15:35	Szkudlarek	Hybrid iron an copper oxides nanoparticles for visible light energy conversion
15:55	Coffee break	
16:30	Dąbrowski	Hybrid van der Waals heterostructures: electronic properties at the nanoscale
17:10	Zaraska	Electrochemically formed nanostructured semiconductors for PEC applications
17:30	Wrana	Ways to get the perovskite structure right
17:50	<u>Technolutions</u>	Research instruments offered by Technolutions- ALD+PVD
18:10	Poster session	
21:00		

Tuesday, 2nd July

9:00	Fery	From bioinspired structure formation to mechanotunable metamaterials
9:40	Jalochowski	The role of predeposited Au on Si(111) in the formation of 2D and 1D nanostructures
10:20	Drózdź	Moiré patterns on Self-twisted β -Sb/ α -Sb Heterostructures
10:40	Coffee break	
11:10	Pfnür	Atomic wires at surfaces: correlations of spin and charge
11:50	Tegenkamp	Electron transport along chiral nanostructures
12:30	Zaleski	Water Confined in 1D channels by Positron Annihilation Lifetime Spectroscopy
12:50	Lunch	
14:15	Altman	Two-dimensional layers for substrate screening and passivation
14:55	Esser	Raman scattering: Vibrational Spectroscopy at Surfaces and 2D layers
15:35	Lewandowski	Structure and magnetic properties of iron oxide nanowires on Cu(410)-O
15:55	Coffee break	
16:30	Tringides	Novel synthesis of 2-d materials: intercalation and the paradox of broad diffraction
17:10	Louerdi	Impact of Boron Doping on the Sputtering Dynamics of Graphene: A Molecular Dynamics Simulation Study
17:30	Lutsyk	Investigation of the electronic structure of graphene/TMDC heterostructures
17:50	Toczek	Synthesis of heterostructure based on epitaxially grown bismuth and van der Waals materials
20:00	Conference dinner	

Wednesday, 3rd July

9:00	Excursion	
12:50	Lunch	
14:15	Zandvliet	The quantum spin Hall effect in germanene
14:55	Palotás	First-principles-based simulation of scanning tunneling microscopy: From magnetic surfaces to molecular structures
15:35	Skowroński	Magnetization switching and dynamics of two-dimensional ferromagnets
15:55	Coffee break	
16:30	De Padova	From 2D $\sqrt{3} \times \sqrt{3}$ R30°-As To 5×5 -Arsenene on Ag(111): A Reversible Phase Transition
17:10	Krok	Characterization at the atomic scale of contact interfaces between thermally self-assembled Au islands and MoS ₂ substrate surfaces
17:30	Dunal	Investigating MoS ₂ /Au interface with the CAFM and local force spectroscopy
17:50	Sovizi	Thickness dependent work function of layered MoO ₃ onto SiO ₂ and MoS ₂ in air

Thursday, 4th July

9:00	Zegrodnik	Topology and superconductivity in 2D materials from theoretical and experimental perspective
9:40	Sedlmayr	A Mach-Zehnder Interferometer Made from the Hinge Modes of Higher Order Topological Insulators
10:20	Rycerz	Quantum transport, thermopower, and incoherent shot-noise in graphene
10:40	Coffee break	
11:10	Olesiak-Bańska	Ultrasmall noble metal nanoparticles as one-photon and multiphoton biomarkers
11:50	Szymoński	AFM-based Nanospectroscopies for Medical Research and Diagnostics
12:30	Piwoński	Investigation of metallic nanostructures on semiconductor substrates for SERS and PIERS applications
12:50	Lunch	
14:15	Godlewski	On-Surface Synthesis of Higher Acenes and Nanographenes
14:55	Szabelski	Theoretical modelling of the structure formation in metal-organic systems on surfaces
15:15	Nieckarz	Towards multicomponent metal-organic Sierpiński triangle fractals on surfaces
15:35	Dudek	Application of nanoparticles to produce multifunctional layers on NiTi shape memory alloys
15:55	Coffee break	
16:30	Kisiel	Detection of the charge and spin state of quantum devices by Atomic Force Microscope
17:10	Weiss	The study of friction versus velocity and load by means of atomic force microscopy
17:30	Le Ster	Nanohighways in α -Bi on graphite
17:50	Payod	Direct-Current Triboelectric Nanogenerator Energy Harvester from Raindrop Impact (DC-TENGEHRI)
19:00	Musical theatre	
21:00		

Friday, 5th July

9:00	Tamulevičius	Templated Self-Assembled Plasmonic Metasurface Platform. From Lasing and Sensing to Photocatalysis
9:40	Szczytko	Tunable band structure in a self-assembled photonic potential
10:20	Hermanowicz	High-performance computing infrastructure for interdisciplinary research
10:40	Coffee break	
11:10	Łapiński	Thermally driven disintegration of the thin metallic films as a manufacturing method of plasmonic nanostructures
11:50	Majewski	Block copolymers as matrices for synthesis of spatially ordered functional nanomaterials
12:30	Closing	
12:50	Lunch	

INVITED SPEAKERS

Electron transport in nanocrystal solids: the influence of ligands

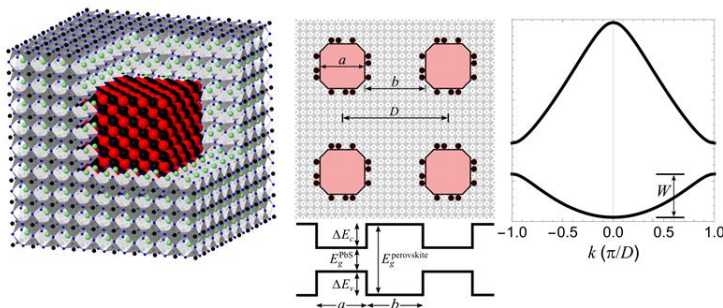
Steve Erwin, Alexander Efros

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The transport of electrons and holes in nanocrystal solids is strongly influenced by the extent to which their quantum-confined wavefunctions overlap. Our research explores the significant impact of ligands, which coat the surface of nanocrystals, on this overlap within two distinct types of nanocrystalline materials: 1) nanocrystal solids consisting of superlattices of CdSe nanocrystals with long organic chain ligands and 2) quantum-dot-in-solids consisting of PbS nanocrystals with inorganic halogen-atom ligands and embedded in a matrix of lead halide perovskite. We use density-functional theory to construct model systems with analytic wave functions. By examining how these wave functions overlap we obtain insights into transport in the solid materials.

In the case of nanocrystal solids with organic ligands, we observe an exponential decay of the wavefunction overlap as a function of ligand length. The characteristic decay length depends mainly on the ligand and is only weakly affected by the size and type of nanocrystal. We derive an analytic expression for the wavefunction overlap and its decay, providing a deeper understanding of band transport mechanisms in these solids [1].

For the quantum-dot-in-solids we find that the halogen ligands are pivotal in establishing the band offset between the quantum dots and the matrix, thereby controlling carrier transport. This insight provides a direct method for tuning transport in these systems. Our approach and analytical framework can also be applied to explore electron transport in a wider array of dot-in-solid materials [2].



Quantum-dot-in-solid perovskite, one-dimensional Kronig-Penney model, width of first subband

- [1] A. Khabibullin, A.L. Efros, and S.C. Erwin. The role of ligands in electron transport in nanocrystal solids. *Nanoscale* 12, 23028 (2020).
- [2] S.C. Erwin and A.L. Efros. Electronic transport in quantum-dot-in-perovskite solids. *Nanoscale* 14, 17725 (2022).

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Dislocations as embedded 1D-nanostructure: controlling dislocations in epitaxial and stacked heterostructures

Jens Martin, Kevin-Peter Gradwohl, Jeremy Maltitz, Jutta Schwarzkopf

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Extended 1D-defects in crystalline materials such as dislocations could alter the local physical properties in a profound way. For example, dislocations result in substantial strain gradients which may cause modifications in band structure or local charge distribution. As such, dislocations affect charge transport and are often best avoided. Yet, dislocations may also be utilized as functional 1D-nanostructure with well-defined atomic arrangement. As such, dislocations have been exploited as nm-sized memristive element in oxide-based perovskites.

In this talk, I will start by recalling some basic principles of dislocation formation during thin film growth. Taking SiGe-heterostructures as an example, I will show under which conditions the formation of misfit dislocations can be suppressed kinetically, and how Monte Carlo simulations can help to understand the formation pattern of misfit dislocation networks. A detailed understanding of misfit dislocations is crucial for the exploitation of SiGe-heterostructures in electronic spin-qubit applications.

As a counter example, I will present a perspective on functional 1D-screw dislocation networks in artificially stacked complex oxide layers. Freestanding oxide membranes have recently emerged as a promising platform, offering new opportunities to design materials with novel properties. In stacked heterostructures, controlling the Moiré superlattices pattern of the two lattices can play a crucial role in creating unique and new electronic, optical, magnetic, and mechanical properties that do not exist in the individual constituent materials or in traditional non-twisted epitaxial heterostructures.

I will present our recent progress in the epitaxy and transfer of freestanding perovskites and our efforts to produce screw dislocation networks in twisted perovskite layers. Current challenges and an outlook on some of the possible future directions of the field will be given.

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Nanotechnology in cosmetics: opportunities and challenges

Izabela Nowak

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The integration of nanotechnology spans across diverse scientific disciplines, encompassing electronics, medicine, and notably, cosmetics. This revolutionary field of science has brought forth a myriad of applications that are reshaping our world. In the realm of cosmetics, nanotechnology is particularly significant as it introduces innovative solutions and enhancements that were previously unattainable. The utilization of engineered nanomaterials has surged in today's society, captivating the attention of cosmetic industries due to their enhanced properties. These properties have led to a rapid evolution in product formulation and efficacy, enabling companies to develop cutting-edge cosmetics that cater to the evolving needs and preferences of consumers.

The extensive adoption of nanotechnology in the cosmetics sector stems from the enhanced properties exhibited by nanoparticles, including improved bioavailability, colour, transparency, and solubility, among others. Bioavailability refers to the ability of active ingredients to be more effectively absorbed by the skin, thereby increasing the potency and effectiveness of cosmetic products. The improved colour and transparency offered by nanoparticles allow for the creation of products with superior aesthetic qualities, such as more vibrant and long-lasting makeup. Additionally, the enhanced solubility of nanoparticles ensures that active ingredients are more uniformly distributed within the formulation, resulting in consistent performance and consumer satisfaction.

Various types of nanomaterials are employed in cosmetics, such as nanosomes, liposomes, fullerenes, silica and solid lipid nanoparticles. Especially solid lipid nanoparticles, on the other hand, provide a stable carrier system for active ingredients, enhancing their stability and prolonging their shelf life. However, recent concerns regarding the safety of nanocosmetics have prompted regulatory actions within the cosmetic industry. In response to these regulatory measures, cosmetic companies are investing in extensive research and development to address safety concerns and meet compliance requirements. The goal is to create a framework that ensures the safe and responsible use of nanotechnology in cosmetics, while still harnessing its remarkable potential to enhance product performance and consumer satisfaction.

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Nanoscale hydration of cell membranes

Łukasz Piątkowski ¹, Emilia Krok ¹, Hanna Orlikowska-Rzeznik ¹,
M. Chattopadhyay ¹, A. Lester ¹, Henri G. Franquelim ², Petra Schuille ³

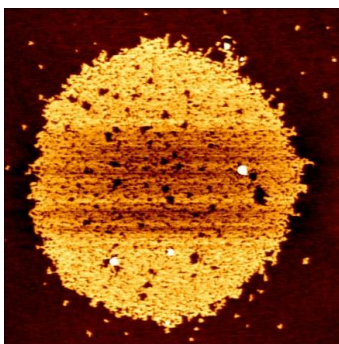
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Although cell membranes exist in excess of water under physiological conditions, there are a number of biochemical processes, such as membrane fusion events, that require partial, transient dehydration of lipid membranes. However, little is known about the structural adaptation of lipid membranes when their interfacial hydration layer is perturbed. We present the study of the nanoscale structural reorganization of phase-separated, supported lipid bilayers (SLBs) under a wide range of hydration conditions. We have shown that as the hydration state of the membrane decreases, there is increased mixing of lipids characteristic of the liquid-disordered (L_d) phase with those forming the liquid-ordered (L_o) phase [1]. This is associated with a 2-fold decrease in the hydrophobic mismatch between the L_d and L_o lipid phases and a 3-fold decrease in the line tension for the fully desiccated membrane. Importantly, the observed changes in the hydrophobic mismatch, line tension, and lipid miscibility are fully reversible upon subsequent rehydration of the membrane. Moreover, a detailed characterization of the influence of membrane hydration on membrane fluidity is provided by the environmentally sensitive fluorescent probe Laurdan [2].

Acknowledgement: First TEAM (FNP) POIR.04.04.00-00-5D32/18-0;
Project No. 0512/SBAD/6212; Diamond Grant (0042/DIA/2019/48);
NCN-OPUS (2020/37/B/ST4/01785).



"Nanosun" – a nanoscale structure within a lipid cell membrane under conditions of water shortage

- [1] E. Krok, H. G. Franquelim, M. Chattopadhyay, H. Orlikowska, P. Schuille, L. Piątkowski, *Nanoscale* 16, 1, 72-84, (2024)
- [2] H. Orlikowska-Rzeznik, E. Krok, M. Chattopadhyay, A. Batura, L. Piątkowski, *Journal of Physical Chemistry B* 127, 15, 3382–3391 (2023)

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Hybrid plasmonic nanostructures for non-local luminescence processes

Dawid Piątkowski

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The optical properties of metallic nanostructures have fascinated and intrigued researchers for decades. Due to the possibility of strong localization and modification of the optical field, noble metal nanoparticles have found many applications, including controlling photoluminescence and Raman scattering processes, metamaterials engineering, sensorics, high-resolution imaging, and photothermal therapy. However, the optical properties of elongated metallic nanoparticles such as silver nanowires are of particular interest. This is because of surface waves (plasmon polaritons) that can be optically activated on the metal-dielectric interface. Such plasmonic excitations effectively transport the optical energy over distances of several dozen micrometers, keeping the diameter of the waveguide (<100 nm) far below the diffraction limit. This unique property is a promising alternative for further development of highly integrated optoelectronic devices.

This presentation will discuss the process of bidirectional light propagation in a metallic nanowire, which was used for non-local spectroscopy of a model nanoemitter. This process has been investigated in a specially designed nanostructure consisting of a single, tens of micrometers long silver nanowire and a single up-conversion nanocrystal at its end. It was shown that the excitation of such an emitter could be realized remotely via propagating plasmon polaritons, activated by a laser illuminating the opposite end of the nanowire, where the luminescence of the emitter could also be recorded. This presentation will discuss the mechanism of such a bidirectional process, focusing on three fundamental issues: the efficiency of the laser-nanowire interaction, nanowire attenuation, and the strength of the nanocrystal-nanowire coupling. In conclusion, intriguing applications of the observed phenomenon will be discussed, including a new approach to metal-enhanced luminescence analysis.

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Hybrid van der Waals heterostructures: electronic properties at the nanoscale

Pawel Dąbrowski ¹, Przemysław Przybysz ^{1,2}, Iaroslav Lutsyk ¹, Maciej Rogala ¹, Jagoda Sławińska ², Michał Piskorski ¹, Paweł Krukowski ¹, Karol Szalowski ¹, Maxime Le Ster ¹, Witold Kozłowski ¹, Paweł J. Kowalczyk ¹

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Two-dimensional (2D) materials have garnered significant attention due to their unique properties, distinct from those observed in bulk structures. While substantial research has focused on the growth of 2D materials themselves, more complex challenges lie in studying hybrid systems where two or more 2D materials combine through van der Waals interactions. Such heterostructures are not just a simple sum of each separate materials, but they are systems revealing some new and unique properties, which can be observed on the interface between layers. Using scanning tunneling microscopy/spectroscopy (STM/STS) in conjunction with various atomic force microscopy (AFM) modes, as well as global electronic properties (ARPES), chemical analysis (XPS, AES), crystallography (LEED, RHEED), Raman spectroscopy, and work function measurements (UPS), we can obtain complementary information about the electronic and mechanical properties of samples. These results were further supported by density functional theory calculations. Additionally, machine learning algorithms are applied for AFM and STM data analysis, dimensionality reduction, and classification. This approach allows us to precisely describe charge transfer and the evolution of electronic properties resulting from interactions between materials.

This work was financially supported by the National Science Centre, Poland under project 2018/30/E/ST5/00667

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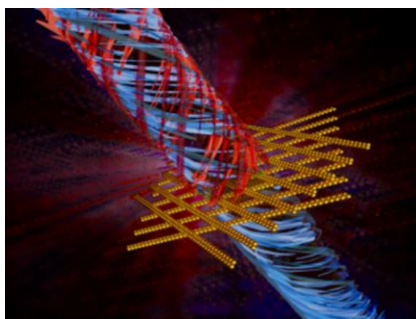
From bioinspired structure formation to mechanotunable metamaterials

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Wrinkling is widely encountered in nature and can even result in submicrometer periodic features e.g. on flower petals. Understanding the physics of wrinkling allows harnessing the process for structure formation in a non-biological context and for metrology of thin film mechanics. The latter is especially interesting for 2D materials and I discuss recent examples including the extension of this work to strain engineering of 2D materials. Controlled wrinkling for structure formation on the other hand offers interesting opportunities for scalable surface patterning. I will discuss the use of wrinkling templates for the formation of particle based metamaterials.



Schematic depiction of a plasmonic metasurface giving rise to giant circular dichroism [1].

- [1] Probst, P. T.; Mayer, M.; Gupta, V.; Steiner, A. M.; Zhou, Z.; Auernhammer, G. K.; König, T. A. F.; Fery, A., Mechano-tunable chiral metasurfaces via colloidal assembly. *Nature Materials* 2021, 20, 1024–1028.

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The role of predeposited Au on Si(111) in the formation of 2D and 1D nanostructures

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The exploding interest in experimental studies of 2D and 1D nanostructures is specifically related to the ability of suitable substrates to control self-assembling processes during the fabrication of these nanostructures. Numerous studies have shown that Si(111) modified by a sub-monolayer of Au fulfils most requirements necessary to form highly ordered nanostructures over large substrate areas. In this lecture, I would like to focus on two early groundbreaking discoveries: 2D metallic quantum wells on Si(111)(6x6)-Au and Si atomic chains formed on vicinal surfaces of Si(111) decorated with Au.

Although the concept of metallic or semi-metallic quantum wells was theoretically predicted [1], its experimental proof was difficult to realize due to the roughness of vacuum-deposited extremely thin films. The problem was overcome by using a Si(111)(6x6) substrate, where a monolayer-by-monolayer growth of Pb was achieved, and clear electrical conductivity oscillations versus thickness of truly 2D layers were observed [2]. The role and importance of the (6x6)-Au interface's electronic roughness and topography in the formation of atomically smooth Pb layers at extremely low temperatures were explained in another publication [3].

Particular 1D nanostructures are relatively common and have been previously investigated using STM and TEM techniques. However, to gain detailed insight into their electronic structure, particularly the electron band structure, a macroscopic-sized sample with matrices of identical 1D structures was desirable. This requirement led us to the concept of Si(111) vicinal surfaces as templates for forming atomic chains on the equidistantly distributed terraces of the Si(111) surface. Inspired by the structural order of the Si(111)(5x2)-Au surface with triple domains of Au atomic chains, we were able to fabricate parallel-aligned and uniformly distributed macroscopic matrices of Au and Si atomic chains [4] on the Si(557) surface. This discovery established a paradigm for the technology of atomic chains on other vicinals of Si(111), including the Si(553)-Au surface, which plays a leading role in the study of the richness of 1D physical phenomena. Some of these peculiarities will be presented and discussed.

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Atomic wires at surfaces: correlations of spin and charge

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Coupling of quasi-one-dimensional systems to a substrate turned out to reveal a rich variety of new physics and to be full of complexity. This is even true for the relatively simple case of single or double atomic chains on semiconductor surfaces of (stepped) Si and Ge, in which the electronic decoration and modification of surface states mostly determine the physical properties of the new systems that are in part quasi-1D. Due to their ultimate limit in one-dimensional confinement they can be considered as prototype examples. As it turns out, neither the formation of even single atomic chains nor the appearance of a quasi-1D Fermi surface are sufficient for the classification as quasi-1D system, as will be shown. It seems more that the occurring phase transitions (or their absence) are better indicators. While the “classical” 1D instabilities such as Peierls, CDW, SDW, superconductivity etc. partly still appear, they are strongly modified or are even replaced by new types of phase transitions due to electronic hybridization in more than 1D and to new electronic correlations, leading, e.g. to metallicity at low temperatures.

Several characteristic examples will be discussed concentrating on Si(553)-Au that forms double-strands of Au atoms on each mini-terrace, and on Si(557)-Pb close to monolayer coverage. While order-disorder type phase transitions can be identified in the Si(553)-Au system, dc conductance shows two maxima as a function of temperature that can be understood as transients between insulating quasi-1D states. Contrary to intuition, most of the current load goes through the Au-modified Si edge states. The Si(557)-Pb system on the other hand, is governed by strong correlations both parallel and perpendicular to the Si-steps, leading to quasi-1D metallic conductance at low temperature and to an insulating spin-orbit density wave in the perpendicular direction with special Fermi nesting conditions.

Since these systems turn out to be electronically highly correlated, the understanding of these correlation phenomena at the borderline between 1D and 2D will be crucial. They are thus opening a wide field of fascinating aspects of correlation physics in strongly anisotropic low-dimensional, but not necessarily purely 1D systems.

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Electron transport along chiral nanostructures

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The transmission properties of electrons through chiral systems attracts currently a lot of attention. In DNA and polypeptides the so-called chiral induced spin selectivity (CISS) effect describes the built-up of an extraordinarily high spin-polarizations upon long-range electron transfer. Moreover, also in chiral carbon nanotubes strong spin-polarizations are reported. This is surprising since heavy-atoms are missing in these carbon-based compounds. It turns out, that also for weakly spin-orbit coupled systems the spin transmissions are strongly amplified by the helicity. Towards these intriguing effects, we studied the transport through various chiral nanostructures.

By means of pre-structured SiC(0001) samples, epitaxial graphene nanoribbons (GNRs) of exceptionally high quality and well-defined edges were prepared [1,2]. The symmetry of the ribbons can be tuned by the SiC substrate, allowing us to fabricate armchair, zigzag and chiral GNRs. The hallmark for ribbons with zigzag and chiral edges is a probe-spacing and temperature independent conductance of e^2/h which strongly indicates fully spin-polarized ballistic transport [3]. The spin-polarized and ballistic transport channel is topologically protected and comes along with asymmetrically coupled edges [4].

In a further example, we performed transport experiments through lysine-doped and cysteine terminated single helical polyalanine molecules (PA). The conductance varies exponentially with the length of the molecules and depend not on temperature, thus electron tunneling is the dominating transport channel. The conductance histograms of all PA molecules investigated revealed characteristic satellite peaks, which correlate to apparent molecule length in multiples of characteristic peptide sequences. We address this effect to ratcheting of interdigitated molecules [6]. Recently, PA molecules adsorbed on surfaces of magnetic $Al_2O_3/Pt/Au/Co/Au$ nanostructures with perpendicular anisotropy were studied. Thereby, a correlation between the PA molecules ordering at the surface with the electron tunneling across this hybrid system as a function of the substrate magnetization orientation as well as the coverage density and helicity was observed. The highest spin polarization values were found for ordered self-assembled monolayers and with a defined chemical coupling of the molecules to the magnetic substrate surface, showing that the current induced spin selectivity is a cooperative effect [7,8].

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Two-dimensional layers for substrate screening and passivation

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Atomically-thin two-dimensional (2D) materials are promising materials for enhancing the performance of or eventually supplanting conventional semiconductor electronic technology. Importantly, the exceptional performance of prototype nano-electronic devices that employ 2D materials could only be achieved using mechanically-exfoliated hexagonal boron nitride (h-BN) for substrate interfacial screening and environmental surface passivation of the active 2D layers. Graphene (gr) has also been shown to passivate germanium (Ge) substrate surfaces against oxidation better than all chemical termination methods studied previously. This may help overcome the drawbacks of Ge for device applications caused by the instability and poor interface quality of the native Ge oxide. This talk will describe (1) our discovery of the potentially scalable process for the fabrication of high-quality h-BN by a novel “2D-distillation” growth (2DDG) mechanism [1], and (2) key insights we have gained about the origins and remaining shortcomings of the passivation provided by graphene grown on Ge by chemical vapor deposition (CVD) [2]. For the former, a metastable h-BN monolayer, formed on Rh(111) by transfer of CVD-grown h-BN with a twist angle, was transformed by 2DDG into a stable untwisted layer upon annealing. 2DDG occurs via BN sublimation from the edge of the metastable layer and its subsequent re-condensation into the stable layer with superior quality. For the latter, the key role in passivation of interfacial hydrogen introduced during CVD growth was revealed by a comparative study of gr/Ge(110) samples with hydrogen intact and after hydrogen was purged (Fig. 1). Our observations also suggest that the disruption of graphene wrinkles during ambient exposure contributes to graphene permeability. The roles of this common feature of CVD-grown graphene and interfacial hydrogen had not been considered before.

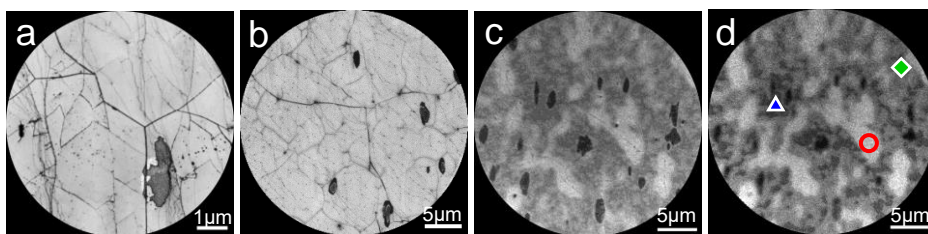


Fig. 1. LEEM images of pristine gr/Ge(110) with interfacial hydrogen present (a) following CVD growth and (b) after 84-day ambient exposure exhibit wrinkles, atomic steps, and multilayers (black islands). (c) LEEM and (d) Ge 3d X-PEEM images of H-purged gr/Ge(110) after ambient exposure exhibit Ge oxide domains (○,◇,△) with different weighting of Ge, GeO, and GeO₂.

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Raman scattering: Vibrational Spectroscopy at Surfaces and 2D layers

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Raman spectroscopy is a standard analytical method to study organic and inorganic material structures. Moreover, Raman spectroscopy can be used to record phonons localized at surfaces, i.e. vibrations of the outermost few atomic planes of a material. This is strongly favoured by surface specific Raman scattering mechanisms and resonance enhancement of the Raman cross section involving surface electronic states. In collaboration with theory groups DFT-based calculations of the structure and electronic bands have revealed the mechanisms of surface Raman Scattering.

Moreover, comparison of theory and experiment have enabled us to conclude on surface structures and their adsorbate induced modifications. As one example I will discuss the structure and metal-semiconductor transition in quasi 1D metallic nanowires like formed by In and Au adsorbates on silicon surfaces. More recently we have also started to investigate d-band metal surfaces (Cu(110)) and d-band 2D-metals (Ti₂C₃T_x-MXene). The termination of the Cu and MXene surfaces with atomic species may change significantly Raman spectra, which in turn allows one to analyse surface structural properties. On conductive samples, Raman scattering by the charge transfer mechanism may play an important role, in addition to deformation potential scattering. This has to be taken into account since Raman scattering intensities and polarization selection rules depend on the scattering mechanism.

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Novel synthesis of 2-d materials: intercalation and the paradox of broad diffraction

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Metal intercalation of graphene is a general way to engineer its electronic band structure and grow novel type of 2-d materials. Examples will be given for rare earth intercalation under graphene grown on SiC (Gr/SiC). The engineering of the band structure depends where the intercalated atoms are bonded under graphene, i.e., between graphene-buffer layer or between buffer layer-SiC. Using surface diffraction, STM and DFT the sub-surface location of Dy was determined as a function of growth temperature. The conclusions were based on quantitative analysis of the diffraction spot intensities, changes of the 6x6 interface Moire observed with STM and DFT energetic stability calculations [1]. STM, STS ARPES and DFT were used to study changes of the band structure of bilayer graphene intercalated with Gd [2,3]. Parabolic bands for pristine graphene change to linear bands with tunable band gap depending on the sub-surface Gd location. These results show that metal intercalation is a routine way to tune the Gr/SiC band structure and generate novel electronic phases.

An equally important question is to characterize the uniformity and homogeneity of pristine graphene and other 2-d materials because the initial morphology can affect the quality of expected electronic phases. A very broad Bell-Shaped-Component (BSC) in surface diffraction was shown paradoxically to be a marker of high quality graphene [4]. Surprisingly it has been observed in all the graphene literature over the last 20 years, but never mentioned. The BSC has been also seen in graphene grown on metals Gr/Ir(111) and in h-BN grown on Ir(111)[5]. Since the BSC is such a strong effect and seen in different 2-d materials its origin must be general and fundamental. Most likely is a manifestation of the uncertainty principle on the mesoscale. Because the wavefunction of the electrons in 2-d materials is confined within a single layer, the wavevector has a large spread as measured with ARPES [6]. This spread is transferred to the diffracted electrons during scattering, generating the BSC and should be a marker of high quality for all 2-d materials.

In collaboration with M. Kolmer, S. Chen, P.A.Thiel (deceased), M. Horn von Hoegen, M. Petrovic, M. Hupalo, A. Kaminski, J.W. Evans, Y. Han, C. Z. Wang.

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The quantum spin Hall effect in germanene

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Germanene, i.e. the germanium analogue of graphene, shares many properties with graphene. Both materials host Dirac fermions, but there are also a few differences: (1) the spin-orbit coupling in germanene is much larger than in graphene and (2) the honeycomb lattice of germanene is not flat, but buckled. The large spin-orbit gap in germanene makes this material the ideal candidate to exhibit the quantum spin Hall effect. We show that germanene is a quantum spin Hall insulator with a gapped interior and topologically protected helical edge states [1]. The buckling of the lattice of the honeycomb allows to tailor the quantum state of matter of germanene. By applying a perpendicular electric field the spin-orbit gap in germanene first closes and then reopens again. The reopening of the gap is accompanied by a topological phase transition of germanene from a two-dimensional topological insulator to a trivial band insulator. This electric field-induced tailoring of the quantum state of matter of germanene allows to controllably switch the topologically protected helical edge states *on* and *off*. The latter makes germanene the material of choice for the realization of a topological field-effect transistor.

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From 2D $\sqrt{3} \times \sqrt{3}$ R30°-As To 5 × 5-Arsenene on Ag(111): A Reversible Phase Transition

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Two dimensional (2D) $\sqrt{3} \times \sqrt{3}$ R30°-As has been obtained on Ag(111) 1×1 surface, by depositing 1 monolayer of As, keeping the silver substrate at temperature of ~ 450 °C, whereas a 2D 5×5 reconstruction, attributed to arsenene, appeared at lower temperature of ~ 350 °C. The two $\sqrt{3} \times \sqrt{3}$ R30°-As and 5×5 -arsenene surface reconstructions were experimentally investigated by means of low electron energy diffraction (LEED), and Auger electron spectroscopy (AES), while the first-principle calculation, by using density functional theory, confirmed their atomic configurations and surface stability. A reversible phase transition, from the 2D $\sqrt{3} \times \sqrt{3}$ R30°-As to the 5×5 -arsenene surface reconstruction, induced by electron-beam irradiation, and recovered to the $\sqrt{3} \times \sqrt{3}$ R30°-As, by applying a high temperature as ~ 450 °C, was observed by LEED, opening a new way to synthesized arsenene.

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Topology and superconductivity in 2D materials from theoretical and experimental perspective

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The talk is composed of two parts. In the first one we focus on the theoretical analysis of unconventional superconductivity as well as quantum anomalous Hall effect (QAHE) in the 2D transition metal dichalcogenide (TMD) moiré systems. Our theoretical results for the twisted WSe₂ bilayer reconstruct the two superconducting domes separated by a Mott insulating state as a function of electron concentration in agreement with the available experimental data [1-3]. According to our calculations the paired state is of highly exotic type characterized by a mixed singlet-triplet symmetry of the gap. Moreover, the superconductivity has non-trivial topology with a non-zero value of the Chern number that could be tuned by the experimentally controllable parameter. Additionally, we analyze the appearance of the magnetically and charge ordered states in selected moiré TMD systems [4]. Our results show that this group of systems are promising candidates for highly tunable materials that can serve as a testing ground for understanding the interplay between strong electronic correlations, topology and various types of symmetry broken states. In the second part we discuss the experimental results concerning the exfoliated flakes (quasi-2D samples) of Bi_{2-x}Te_{3+x} topological insulator (TI) featuring topologically protected conductive surfaces with two spin protected travel directions, meaning all the electrons traveling in one direction are spin up and all the electrons traveling in the other one are spin down. Doping the system with magnetic ions breaks the time reversal symmetry, allowing one travel direction to exist without the other one. Our magnetoresistance and Hall effect measurements at sub-Kelvin temperatures shows that exfoliation does not affect the magnetic properties of the flake and a fractional QAHE can be observed. Moreover, quasi-2D TIs offer exotic forms of superconductivity by exploiting the superconducting proximity effect in a hybrid system, in particular if it is combined with QAHE. The resistance measured versus external magnetic field and current passing across such a hybrid structure will be discussed.

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A Mach-Zehnder Interferometer Made from the Hinge Modes of Higher Order Topological Insulators

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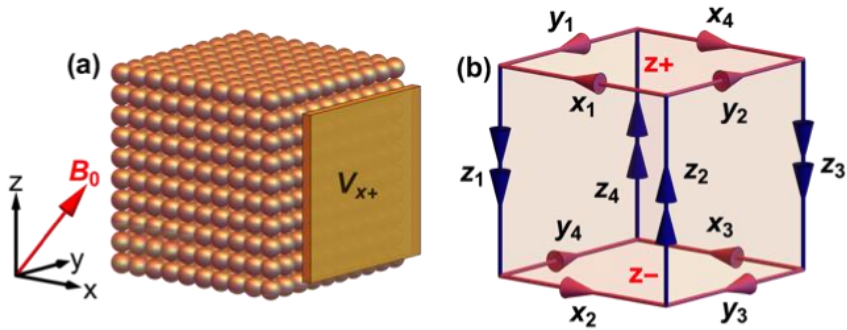
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Three-dimensional higher-order topological insulators can have topologically protected chiral modes propagating on their hinges. Hinges with two copropagating chiral modes can serve as a “beam splitter” between hinges with only a single chiral mode. Here we show how such a crystal, with Ohmic contacts attached to its hinges, can be used to realize a Mach-Zehnder interferometer. We present concrete calculations for a lattice model of a first-order topological insulator in a magnetic field, which, for a suitable choice of parameters, is an extrinsic second-order topological insulator with the required configuration of chiral hinge modes.

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Ultrasmall noble metal nanoparticles as one-photon and multiphoton biomarkers

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Noble metal nanoclusters are ultra-small nanoparticles (diameter <2 nm) with atomically-precise composition and distinct quantum-size effect, which leads to a discrete electronic structure. They present a number of interesting properties like chirality, magnetism, redox chemistry, strong nonlinear optical properties [1, 2]. Moreover, as their composition (number of gold/silver atoms and number of ligands) can be precisely determined and tuned, they serve as a perfect platform for elucidation of structure- physicochemical property relations by theory–experiment investigations. Nanoclusters present multiple advantages in applications such as sensing, imaging and catalysis [3].

Here, we present the studies on linear and nonlinear optical properties of silver and gold nanoclusters as well as alloys with replaced one or multiple gold atoms i.e. Ag_{25-x}Au_x (x=0, 1, 5-10).[4] We discuss how composition and structure influences two-photon absorption cross sections determined in the broad range of wavelengths. Strong nonlinear response of fluorescent nanoclusters in the near infrared wavelengths indicates great potential of nanoclusters in multiphoton bio-imaging, enhanced in case of Au doping to Ag₂₅ nanoclusters. We present also multiphoton chiroptical properties of nanoclusters of various chirality origin: stabilized with chiral ligands (captopril, glutathione, L- and D-arginine) in the first or the second ligand shell stabilizing the surface of nanoclusters. In order to quantitatively describe chiral nonlinear optical properties namely two-photon circular dichroism (TPCD), we introduced two methods: two-photon absorption measurements (with z-scan technique)[5] and two-photon excited luminescence measurements with circularly polarized light (fluorescence-detected TPCD)[6]. Interestingly, both techniques show that TPCD of nanoclusters is ~300 times stronger than their one-photon anisotropy factor.

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AFM-based Nanospectroscopies for Medical Research and Diagnostics

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Typically, AFM is known as a high resolution imaging method providing direct insight into the geometrical structure of various surfaces covering the nanoscale objects. In the context of biology and medicine, it is important that AFM can operate in the liquid environment, thus it offers unprecedented advantage over many other imaging methods. A main difficulty in many applications of the method is related to its lack of chemical specificity. It has been shown, however, that despite imaging, the AFM probe could operate at the nanoscale as a sophisticated tool performing and/or supporting specific spectroscopic measurements providing a wide range of valuable information beyond the geometrical structure of surfaces. In my lecture, I shall review several applications of such spectroscopic methods which were developed over the last decade at the NANOSAM Centre of the Jagiellonian University, demonstrating their potential in medical research and diagnostics. This will include indentation spectroscopy at the nanoscale for “in vitro” endothelial cell research [1-2], force nanospectroscopic imaging for liver endothelium diagnostics and cell pharmacology in “real-time” [3-4], as well as surface-enhanced and tip-enhanced nanoRaman spectroscopies for studies of the damage and repair processes in DNA [5-6]. Finally, an outlook for further development of nanospectroscopic applications in biomedical research shall be presented and discussed in the context of physical and technological limitations of the methods.

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On-Surface Synthesis of Higher Acenes and Nanographenes

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In recent years the on-surface manipulation and chemical reactions created a playground for atomically precise synthesis and development of new atomic and molecular nanostructures. However, the abilities to produce desired systems are limited, among others, by relying on the catalytic role of the substrate in initiating selected reactions. Therefore striving for the generation of desired systems forces the search of new reaction pathways and catalytic transformations. In this talk I will demonstrate our approach based on the application of hydrogen atoms in the on-surface experiments. First, I will discuss the synthesis of the acene series based on the application of “extra” hydrogen atoms. These hydrogen atoms located in the molecular precursors make them air-stable and provide the approach for the efficient synthesis of higher acenes [1,2], with tridecacene [3] being the longest synthesized so far. The application of atomic hydrogen in on-surface transformations will be exemplified by organometallic hybrids [4] and graphene nanoribbons [5]. The potential of atomic hydrogen will be highlighted e.g. by the ability of the reaction byproducts removal, the organometallic phases quenching or heteroatomic substitution. Subsequently the focus will be shifted toward non-metallic substrates. While the surface assisted synthesis approach has proven its effectiveness in the precise formation of new organic compounds on metallic surfaces one of the most challenging limitations arises from the deep dependence on the catalytic activity of the substrate. This makes the direct transfer to the technologically desired non-metallic surfaces extremely challenging. In this talk I will present our pathway for the synthesis of new molecular compounds on non-metallic surfaces [6-9] with prospects for circumventing the need to exploit the catalytic role of metallic substrates [10].

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Detection of the charge and spin state of quantum devices by Atomic Force Microscope

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While the traditional Joule dissipation omnipresent in today's electronics is well understood, the energy loss in nanoscale quantum devices and particularly in the strongly interacting electron systems, remains largely unexplored. Two-dimensional graphene bilayers with twist angles are known to host the series of interaction-driven correlated insulating phases with promising applications for nano-electronics or mechanical engineering [1]. The presence of electron interactions might even lead to the emergence of magnetism as it was recently reported in monolayer MoS₂ [2].

Here, we report on low temperature (5K) nanomechanical detection of charge and spin state on two-dimensional quantum devices, namely: encapsulated twisted bilayer graphene (TBG) and monolayer MoS₂. The measurements are performed with a sharp tip of the pendulum atomic force microscope (pAFM). Ultrasensitive cantilever tip acting as an oscillating gate over the TBG shows dissipation peaks attributed to different fractional filling of the flat energy bands. While conventional transport methods provide quantitative information on correlated insulating states in TBG, they lack spacial resolution. pAFM, on the other hand, provides exquisite spatial resolution and thus allows to determine the twist angle distribution of TBG. In gated monolayer MoS₂ device spontaneous magnetic phase transition is detected with force spectroscopy. An abrupt and reproducible changes of the magnetic force were observed at specific electron concentration and were attributed to ferromagnetic to paramagnetic phase transition. Thus, the magnetism of monolayer MoS₂ might be controlled by gate voltage. The pAFM provides a rich source of information on the dissipative nature of the two-dimensional correlated electronic systems, with implications for coupling a mechanical oscillator to the quantum devices.

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First-principles-based simulation of scanning tunneling microscopy: From magnetic surfaces to molecular structures

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Understanding and engineering scanning tunneling microscopy (STM) image contrasts is of crucial importance in wide areas of surface science and related technologies, ranging from magnetic surfaces to molecular structures. In the talk different STM tip effects on the image contrast are highlighted based on first principles calculations, going beyond the Tersoff-Hamann model, e.g., within 3D-WKB tunneling theory [1]. Examples include highly oriented pyrolytic graphite [2], which is commonly used for STM calibration, and complex surface magnetic structures exhibiting non-collinear magnetic order, like recently much studied skyrmions with topological properties [3]. By comparing STM topographic data between experiment and large scale simulations, a statistical analysis of the tip apex structure is demonstrated for the first time [2]. A combination of STM and X-ray photodiffraction helps the understanding of chirality transfer from molecules to crystal surfaces [4]. Furthermore, two recent developments of electron tunneling theories are presented: (i) an extension of Chen's derivative rule [5] for STM simulations including tip-orbital interference effects with demonstrated importance of such effects on the STM contrast for two surface structures: nitrogen-doped graphene and a magnetic Mn₂H complex on the Ag(111) surface [6]; (ii) a combined tunneling electron charge and vector spin transport theory, which provides the first steps toward the theoretical modeling of high-resolution spin transfer torque imaging [3,7].

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Templated Self-Assembled Plasmonic Metasurface Platform. From Lasing and Sensing to Photocatalysis

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Precise average size control, high monodispersity, and reproducibility of chemically synthesized plasmonic nanoparticles (NPs) enable their applications for photonic devices which were originally made employing top-down methods [1]. Templated NP self-assembly is an established method for the manipulation and deposition of NPs into well-defined traps originating desired photonic coupling or local field enhancements. Arrays of noble metal NPs can diffractively couple the light scattered by individual NP localized surface plasmon resonance (LSPR) into narrow and high-Q resonances termed plasmonic lattices or surface lattice resonances (SLR) [2-3]. The wavelength tailorability of the SLR position rises from the size-dependent LSPR coupling with the NP array pitch determined by Rayleigh's anomaly [4]. It delivers unique bottom-up metasurfaces carrying resonances applicable for nanolasing where scatterer arrays operate as an in-plane resonator [5]. It serves as Raman excitation laser wavelength-tailored absorption surface-enhanced Raman scattering substrates [4]. In combination with semiconducting materials, it ensures effective water splitting at visible wavelengths [6].

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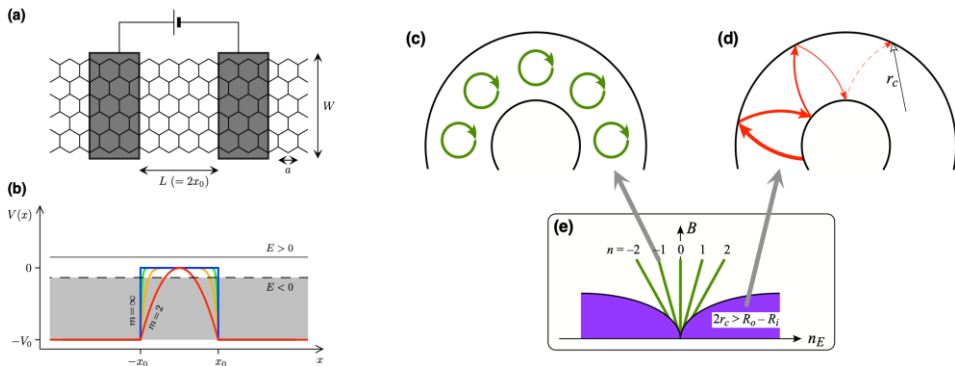
Quantum transport, thermopower, and incoherent shot-noise in graphene

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Soon after the discovery of graphene it becomes clear that several material characteristics of this two-dimensional form of carbon, such as the electrical conductivity, are given by the fundamental constants of nature, including the elementary charge e and the Planck constant \hbar , or even by the dimensionless (universal) factors; these include the visible light absorbance $\approx \pi/136.036$ (related to the fine-structure constant) and the sub-poissonian shot noise for charge neutral samples, quantified by the Fano factor $F = 1/3$. All these features manifest the presence of effective massless spin-1/2 quasiparticles, described the Dirac-Weyl equation in two dimensions. Following this line of approach, we present a few further predictions, partly coinciding with the available experimental results: (i) Away from the charge-neutrality point, ballistic contact in graphene of a width W (see the Figure) is expected to show so-called sub-Sharvin conductance, $G = (\pi/4)G_{Sharvin}$ with $G_{Sharvin} = (4e^2/\hbar)k_F W/\pi$ (k_F denotes the Fermi wavenumber), and the shot-noise $F = 1/8$ [1]. (ii) For the disk (Corbino) geometry, in the limit of $R_o \gg R_i$ (the outer and inner radii, respectively) the conductance approaches $G/G_{Sharvin} = 4 - \pi \approx 0.868$ and $F = (9\pi - 28)/(12 - 3\pi) \approx 0.107$ [2]. (iii) In strong magnetic field B , thermoelectric properties (such as the maximal absolute thermopower) are determined by the separation of Landau levels given by $v_F\sqrt{2e\hbar B}$ (with v_F the Fermi velocity) [3]. (iv) For field and doping adjusted such that the disk conductance is about to vanish, and $R_o \approx R_i$, the noise approaches another universal value of $F \approx 0.55$ [4].



(a) Graphene strip of width W , contacted by two electrodes (dark areas) at a distance L . A voltage source drives a current through the strip. A separate gate electrode (not shown) allows us to tune the carrier concentration around the neutrality point. (b) Electrostatic potential profiles modelling the effect of contact-induced doping. (c–e) Transport regimes for different fields and carrier concentrations n_F . At high fields, the doping can be adjusted to a Landau level $E = E_{nLL}$, $n = 0, \pm 1, \dots$ and resonance occurs (c). At low field but high doping the cyclotron diameter $2r_c > R_o - R_i$, and incoherent scattering along the classical trajectory governs the transport (d).

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We also discuss the robustness of the above-listed properties against the contact-induced doping modelled by smooth potential barriers, for which the discussion in analytic terms is supplemented with computer simulations of quantum transport. We hope that the theoretical results presented herein may serve as a benchmark for the determination of the degree of cleanliness and ballisticity of graphene samples achieved through a given fabrication procedure.

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Tunable band structure in a self-assembled photonic potential

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The properties of polarized electromagnetic waves propagating through one- or two-dimensional structures can be effectively described using a two-mode Hamiltonian, which represents a massive particle with spin 1/2. This approach simplifies theoretical descriptions and facilitates significant advancements in modern photonics by exploiting similarities between equations describing electromagnetic waves and electrons in condensed matter. By applying the Green's function and the k·p perturbation theory, we have obtained results interpretable as effective cavity mode spin-orbit coupling (SOC) and non-Hermitian Hamiltonians [1].

In solid-state systems SOC are crucial for spintronics, topological insulators, and superconductors. Unlike SOC in solid-state materials, which is challenging to manipulate, birefringent optical cavities offer substantial tunability of photonic modes. We have developed a method to electrically control SOC of light using specially designed photonic structures – birefringent microcavities. These consist of a 2-3 μm thin liquid crystal (LC) layer enclosed between two parallel distributed Bragg reflectors deposited on transparent electrodes. This setup has enabled the observation of an optical analog of the spin Hall effect [2]. We discovered Rashba-Dresselhaus SOC in a photonic system and demonstrated control over artificial Zeeman splitting [3] and spatial arrangement of polarization forming half-skyrmions [4]. We observed optical analogs of persistent spin helix, reciprocal Young's, and Stern-Gerlach experiments [5], and a new type of chiral Rashba-Dresselhaus lasing [6]. Our results illustrate an effective strategy for engineering artificial gauge fields and synthetic Hamiltonians with photons to simulate nontrivial condensed matter and quantum phenomena, promising new directions in topological photonics [7-9] and non-Hermitian systems [1,7]. By embedding laser dyes and perovskites within microcavities, we explore light-matter interactions in weak [6] and strong coupling regimes [8,9].

Beyond traditional lithographic methods, our approach using liquid crystal cavities enables the creation of self-organizing macromolecular structures. In the present work, we have developed a self-assembled liquid crystal structure in a planar cavity, which provides a tunable periodic potential and interband SOC between the lattice bands of different parity. We show that doping the LC with dyes allows us to achieve lasing that inherits tunable properties of LC microcavity, including dual and circularly-polarized lasing.

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Thermally driven disintegration of the thin metallic films as a manufacturing method of plasmonic nanostructures

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Metallic thin films can be meta- or unstable after deposited. This leads to disintegration (also so called dewetting, rupture, self-organization, agglomeration) of the continuous layer into isolated nanoislands. That process can be observed at temperature well below the melting point of nanolayer, even at room temperature. The transformation mechanism is driven by thermally accelerated diffusion that leads to the minimalization of surface free energy in the system. Thin films, especially those with nanometer-scale thicknesses, have a relatively high surface energy and a large interfacial area with the substrate. It could create a driving force for the dewetting and form isolated islands. This process is governed by the balance between the energy required to create new surfaces (surface tension) and the energy gained by reducing the total interfacial area (interfacial tension).

The disintegration of metallic thin films could be used for the preparation of the plasmonic structures. Properties of manufactured nanostructures depend not only on its size, but most of all its nanostructure and chemical composition. Therefore, a wide knowledge about kinetics and nanostructures formation parameters play key role from practical applications point of view.

We report the results of our study of the disintegration of the gold, silver and copper mono- and bilayers. Thin metallic films were deposited on both types: silicon and glass substrates. Transformation of the thin film was observed by LEEM and SEM microscopes, as well as manufactured nanostructures were observed by AFM method. Structural investigations were performed by LEED and XPS methods. Plasmonic properties of obtained monometallic and alloyed nanostructures were investigated by UV-VIS spectroscopy method. We show that the manufactured nanostructures can be used for example in sensing applications.

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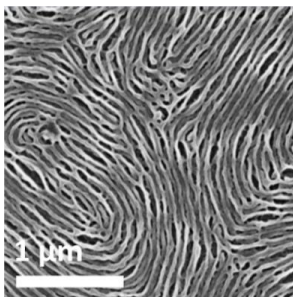
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Block copolymers as matrices for synthesis of spatially ordered functional nanomaterials

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Block copolymers (BCPs), due to chemical incompatibility between the constituent homopolymer chains, undergo microphase separation and self-assemble into a variety of periodic morphologies such as spheres, cylinders, or lamellae. These morphologies, due to their size and heterogeneous chemical makeup, are perfectly tailored to be used as templates for the synthesis of ordered functional nanostructures, such as ordered arrays of metallic nanowires. Although the equilibrium morphologies of the BCP templates are dictated by free-energy minimization principles, in reality, kinetic effects usually prevail, and BCP self-assembly does not reach the thermodynamically prescribed perfectly ordered state. As a result, in the absence of directing biases or other factors that enhance the kinetics of annealing of the trapped defects, BCP morphologies and the resultant nanostructures are poorly ordered. In our work, we investigate how the process of block copolymer self-assembly can be employed as a practical, viable, and large-scale method for the synthesis of spatially ordered functional nanomaterials. We work on the development of synthetic routines in which a BCP matrix is first cast, then photothermally ordered, and finally infused with inorganic precursors and converted to an array of metallic nanowires.[1] More recently, we proposed an alternative single-step synthetic approach in which the BCP self-assembly takes place in a concentrated solution where the polymeric material self-assembles at a much more accelerated rate compared to the melt.[2,3] Additionally, the BCP solution can be blended with a rich group of metal-oxide precursors, enabling single-step synthesis of metal oxide nanowires. We demonstrate the practical utility of this approach in the straightforward fabrication of miniature metal oxide-based volatile organic compound sensors.[4].



Iron (III) oxide gas-sensing nanowires templated by a cylinder-forming BCP .

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CONTRIBUTED TALKS

**Designed, Programmable Protein Cages Utilizing Diverse
Metal Coordination Geometries Show Reversible
pH- Dependent Disassembly**

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Trp RNA-binding attenuation protein (TRAP) is a 74 AA protein that natively forms a ring-like structure consisting of 11 individual subunits. It comes from the bacterial species *Geobacillus stearothermophilus*.

When artificially introduced metal-binding sites are located on the TRAP ring's external rim, the protein gains the ability to form nanometric cage-like structures. We originally demonstrated this using engineered variants of TRAP containing cysteine residues. These proteins formed cages upon addition of Au(I). Preference for other metals can be engineered into the protein based on an understanding of their coordination geometries.

In the current work, two other TRAP mutants were used, namely TRAP S33H K35H and TRAP S33H K35C. The former makes cages with cobalt (II) and zinc (II) ions, the latter with zinc (II) and gold (I) ions. We have characterized these cages both using Cryo-EM and biophysically, showing them to be highly stable. We have found that some cages can be disassembled with addition of EDTA and readily disassembled at pHs below approx. 7.

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Controlling photoswitching of photochromic molecules in hybrid nanostructural assemblies

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The properties of photochromic molecules, including developing ways of external manipulation of the efficiency of photoswitching, have been one of the key aspects in studying these unique systems and considering them for a variety of applications. Such molecules can be used as tuneable molecular switches, as well as attractive materials for sensing and bioimaging. Indeed, coupling photoswitchable molecules with appropriate nanomaterials, such as metallic nanoparticles or up-converting nanocrystals, opens ways for independent control of the conformational state of a molecule, including its fluorescence properties, as well as the efficiency of the photoswitching reaction.

Photochromic molecules DTE-py2 used in this work exhibit two photocyclization states ON (fluorescent) and OFF (non-fluorescent), with the switching facilitated through light illumination. Three approaches are implemented to demonstrate nanostructure-driven tuning of the photoswitching.

In order to modify the efficiency of the photochromic reaction, the DTE-py2 molecules were coupled with silver nanowires. In this case, plasmonic excitation in silver nanowires lead to increased photoswitching upon excitation with wavelengths matching the resonance band. In addition, fluorescence intensity of DTE-py2 molecules is enhanced due to coupling with the nanowires.

The functionality of silver nanowires associated with the ability to transfer energy along the wires via surface plasmon polaritons, provides a way to remotely control the state of the photochromic molecules. Up to 5 photoswitching events have been observed for such an assembly, where a microdroplet of DTE-py2 molecules was precisely deposited on one end of the nanowire.

The photochromic reaction of DTE-py2 molecules can be also induced via infrared excitation of NaYF₄:Er³⁺/Yb³⁺ up-conversion nanoparticles. Indeed, we can switch DTE-py2 molecules from OFF to ON state by exciting a single NaYF₄:Er³⁺/Yb³⁺ nanoparticle with 980 nm wavelength and observing emission in the visible range. The processes that take place in such a structure can be further enhanced by incorporation of silver nanowires.

The results of comprehensive fluorescence microscopy studies carried out on several experimental architectures involving DTE-py2 photochromic molecules indicate that it is possible to control the spectral dependence of photoswitching dynamics and the efficiency of this process through assembly of plasmonically active or near-infrared active up-converting molecular hybrid nanostructures.

Hybrid iron and copper oxides nanoparticles for visible light energy conversion

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In this study, we investigate hybrid iron and copper oxide nanoparticles, which demonstrate potential for converting visible light into chemical energy without requiring external bias. These materials were chosen for their distinct electronic properties, specifically their optical band gaps within the visible light spectrum and their types of conductivity - 1.58 eV for CuO (p-type) and 2.15 eV for Fe₂O₃ (n-type). The junction's structure creates an electric field that effectively reduces charge-transfer recombination. This enables the carriers to participate in chemical reactions. We characterized the morphology and crystal phase of the nanoparticles using transmission electron microscopy and X-ray absorption with synchrotron radiation. The optical band gaps were determined from reflectance measurements employing the Kubelka-Munk model, while the flat band potential was identified based on Mott-Schottky analysis.

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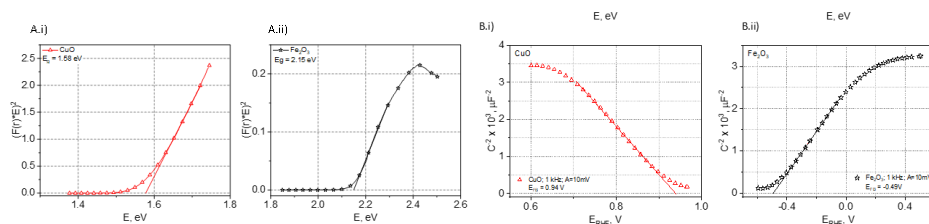


Fig.1. A) Tauc's plots B) and Mott-Schottky plots for i) CuO and ii) Fe₂O₃

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Optically active indium selenide crystal phase heterostructures grown by molecular beam epitaxy

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Indium selenide attracts the great interest due to its outstanding electronic and photonic properties, such as the excellent photo-responsivity, good electron mobility, robust room temperature ferroelectricity, high Seebeck coefficient and the large band gap tunability depending on the thickness. One of the challenges of fabrication indium selenide is the complexity of its phase diagram. Most of indium selenide crystalline phases belong to the family of two-dimensional (2D) semiconductors which are characterized by strong in-plane covalent bonds and weak interlayer van der Waals forces. Different crystalline phases of indium selenide may be characterized by a significantly different value of the band gap, e.g., the band gap of bulk γ -In₂Se₃ amounts to 2.15 eV and that of bulk γ -InSe to 1.32 eV (at cryogenic temperatures).

In this work we report on the growth of crystal phase heterostructures by molecular beam epitaxy (MBE) of indium selenide by changing the indium to selenium flux ratio during the growth. In the case of thin layers grown at 350°C on (111)B-GaAs substrate keeping indium to selenium flux ratio of 0.2 an almost perfect γ -In₂Se₃ crystal phase is obtained. This is confirmed by a comprehensive study involving X-ray diffraction and low temperatures photoluminescence. In the next step, the MBE growth is stopped and the indium to selenium flux ratio risen up to 0.5. After the restart of the growth, indium selenide changes its crystal phase which is monitored *in situ* by a distinct change in the reflection of high energy electron diffraction (RHEED) pattern. This observation is confirmed by transmission electron microscopy which reveals two distinct crystal phases of indium selenide

Interestingly, a quite intense optical emission in the near infrared spectral range appears as effect of the growth of the above described indium selenide crystal phase heterostructures. Moreover, it is found that the emission energy exhibits a distinct change depending on the average thickness of the second layer, from 1.1 eV for layers thicker than 20 nm up to 1.2 eV for a layer with the average thickness of 4 nm, which is consistent with the impact of the quantum size effect. Furthermore, the photoluminescence lines exhibit a distinct blue shift with increasing excitation fluence. Based on the latter effect the observed optical emission is ascribed to the recombination at the type II interface between the two crystalline phases. Consistent with this interpretation is also the fact that the energy of this transition is lower than both: the bandgap of γ -InSe and the bandgap of γ -In₂Se₃. Inhomogeneity of indium selenide thin layers is investigated by spatially resolved cathodoluminescence revealing changes of max.40 meV of the emission energy depending on the spatial position of the excitation spot.

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Electrochemically formed nanostructured semiconductors for PEC applications

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Nanostructured semiconducting metal oxides have been recently considered as very promising materials for various photoelectrochemical (PEC) applications, including the generation of H₂ via photoelectrochemical water splitting. Among various strategies that have been already employed for the fabrication of semiconducting oxide-based nanomaterials, electrochemical methods such as anodic oxidation of metals and alloys, but also cathodic deposition have attracted considerable attention. The most important advantages of electrochemical techniques are their relative simplicity, low cost, and the possibility to control (to some extent) the morphology and composition of the synthesized material by simple adjusting conditions applied during the procedure.

Therefore, this presentation aims to give a brief overview of our most recent achievements in the electrochemical synthesis of various nanostructured semiconductors (e.g., SnO_x [1–3], ZnO [4, 5], Cu₂O [6], Fe₂O₃ [7, 8]) via both, anodic oxidation of metals or alloys [1, 2, 4, 7, 8] as well as cathodic deposition [3, 5, 6]. A special emphasis will be put on the synthesis of semiconductors with precisely designed, complex geometries at the nanoscale, strategies of modifications, properties, and possible applications, especially in photoelectrochemistry and photocatalysis.

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Water Confined in 1D channels by Positron Annihilation Lifetime Spectroscopy

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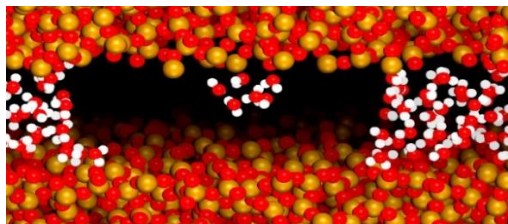
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The properties of water confined in nanochannels play a significant role in the course of various environmental processes, including the creation of life on Earth. Furthermore, the transport of water through nano-channels, which can be derived from the adsorption-desorption behavior, is of great importance in many fields of industry and science. Therefore, ortho-positronium (o-Ps) lifetimes were used to unravel the behavior of water confined in cylindrical silica pores with a diameter of 2 nm at different temperatures and vapor pressures.

In situ, Positron Annihilation Lifetime Spectroscopy study of water-free volumes during successive stages of adsorption [1] indicates the formation of isle-like molecule clusters on the surface of the pore walls. The clusters transform into water plugs that grow and merge (when the distance between them decreases to ca. 1 nm) until complete capillary condensation occurs. Desorption of water from the pores involves the formation of cavities capped with water plugs. The plugs shorten with decreasing pressure, but water trapped in micropores in the pore walls remains until the final stage of desorption. The amount of water in the system can be estimated from the linear dependence between the water volume and the o-Ps intensity.



When cooled, the confined water becomes solid through a viscous state, instead of freezing at 273 K [2]. Reducing the vapor pressure over the water surface allows us to obtain the negative pressure of -164 MPa in liquid water, which changes the temperature range of the viscous state from 225-188 K to 234-189 K. The well-known anomalous temperature dependence of the o-Ps lifetime, which is observed in both bulk and confined water, becomes consistent with the surface tension (as in most liquids) at the negative pressure. This can be explained by assuming that a partial energy transfer to distant water molecules via the OH-stretching modes instead of repelling the molecules surrounding o-Ps is responsible for the anomalous o-Ps lifetimes.

The structures of confined and bulk ice differ significantly. In confined ice, thermally generated defects are accompanied by permanent defects. The volume of both types of defects is 70 Å³. It is much greater than in the most common bulk ice Ih, most likely due to the influence of the silanol groups. Vapor pressure influences ice formation, which results in a greater concentration of permanent defects if the ice is formed under reduced vapor pressure.

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Moiré patterns on Self-twisted β -Sb/ α -Sb Heterostructures

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Two-dimensional van der Waals-like heterostructures, characterized by a twist angle between individual sublayers, offer unique and tunable properties distinct from standalone 2D layers. In such structures, the presence of a twist angle results in the formation of additional long-range lattice period modulation, observed as Moiré superlattice, which typically introduces a realm of exotic quantum phenomena [1].

Using molecular beam epitaxy, we demonstrate the growth of 2D-Sb nanostructures on the W(110) substrate that reveal the adjustable allotropic composition depending on the preparation conditions. Consequently, the composition ranges from isolated islands of α (α -Sb) and β (β -Sb) phases antimonene on the sample surface (Figure 1a) to intriguing self-twisted β -Sb/ α -Sb heterostructures (Figure 1b) [2]. The relatively weak interaction between the individual layers forming the heterostructure allows the twist angle to vary freely. The observed Moiré patterns on β -Sb/ α -Sb heterostructures were compared with a simple model (Figure 1c), revealing satisfactory agreement with the results of experiments. This, combined with the observed quantum size effects and the tracked surface topography during Sb growth, strongly supports the formation of β -Sb/ α -Sb heterostructures. The samples were characterized in-situ using low energy electron microscope and diffraction techniques.

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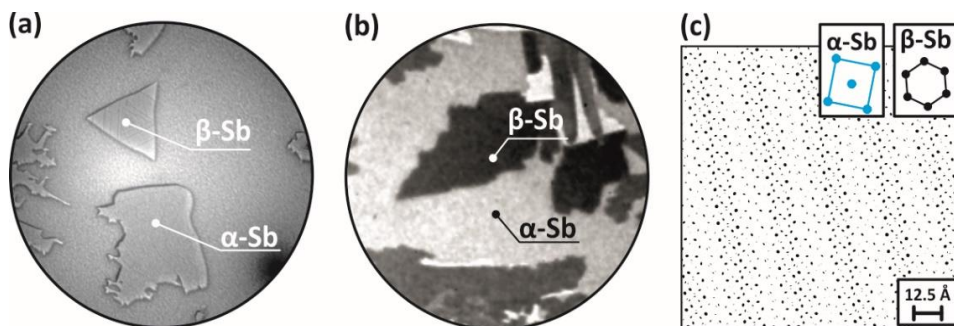


Fig. 1. (a) Isolated islands of α -Sb and β -Sb phases antimonene on the sample surface. (b) Self-twisted β -Sb/ α -Sb heterostructures. (c) Exemplary modelled Moiré pattern resulting from the superposition of α Sb and β Sb sublayers in β Sb/ α Sb heterostructure.

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Theoretical modelling of the structure formation in metal-organic systems on surfaces

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Recently, the surface-assisted synthesis of organic nanostructures has emerged as a valuable technique for producing covalently bonded polymers of adjustable structure and functionality in low dimensions. In this study, we employed Monte Carlo (MC) simulations [1-3] to investigate the formation of metal-organic precursors of covalent polymers through the Ullmann-type coupling reaction of halogenated polyaromatic hydrocarbons (PAHs). We devised a coarse-grained model where the monomers, represented by interconnected segments, and two-coordinate metal atoms (a single segment) were adsorbed on a triangular lattice, simulating a catalytically active crystalline surface oriented along the (111) plane. Various distributions of halogen atoms within the monomer molecules were simulated using directionally assigned interactions, maintaining the resulting metal-organic transient bonds. The simulations predicted the formation of diverse supramolecular assemblies, including linear and cyclic aggregates, ordered and disordered networks, and more intricate structures such as fractal-like patterns, depending on the halogen content and distribution within the molecules. For prochiral monomers, our calculations revealed fundamental structural disparities between enantiopure and racemic assemblies, exhibiting chiral separation and mixing phenomena. Furthermore, the utility of MC modelling will be demonstrated with other adsorbed systems involving trivalent metal atoms and functional molecules of various shapes. The findings of this study offer insights into directing on-surface molecular self-assembly and surface-assisted polymerization reactions towards organic architectures with predetermined size, shape, symmetry, and connectivity.

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Synthesis of heterostructure based on epitaxially grown bismuth and van der Waals materials

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Two-dimensional materials are of growing interest due to their unique chemical, physical, electronic, and optical properties. [1] The less understood ones are in group 15th of the periodic table, and among them are those based on bismuth (Bi). It is a semi metal with minimal radioactivity. 2D-Bi exists in two crystallographic structures - α -Bi (110) with a rectangular unit cell and β -Bi (111) with a hexagonal unit cell. [2]

It has been shown that 2D structures based on bismuth can be fabricated, at the edges of which unusual electron states appear to provide electron flow without electrical resistance, while the interior remains a semiconductor. [2,3] Thus, the fabrication of electronic devices based on Bi could contribute to advances in electronics, optoelectronics, spintronics and catalysis. However, Bi nanostructures are known to degrade rapidly in air. Therefore, it is extremely important to understand the growth and degradation pathways of this new material.

In this work, we will present the properties and morphology of heterostructures based on epitaxially grown bismuth and van der Waals materials - highly oriented pyrolytic graphite (HOPG) and hexagonal boron nitride (hBN).

The growth of bismuth thin films and heterostructures was done in ultra-high vacuum, X-ray photoelectron spectroscopy to analyze the chemical composition of metallic and oxidized surfaces. Raman spectroscopy (in an inert atmosphere) was also used to identify the oxidized phase on the sample surface, and the surface topography of the oxidized layers was also studied in the atmosphere using atomic force microscopy.

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Structure and magnetic properties of iron oxide nanowires on Cu(410)–O

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Islands of magnetic materials with well-defined geometry attract lots of interest due to their potential applications in spintronic and magnetic devices [1]. However, fabrication of such structures usually requires utilizing sophisticated technological processes, such as, e.g., electron lithography. We have developed a direct method for growing well-ordered magnetic iron oxide nanowires through the deposition of Fe under ultra-high vacuum (UHV) onto a vicinal copper surface faceted with molecular oxygen (Cu(410)–O) and post-oxidation at elevated temperatures. The structure of the wires was investigated using scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS) [2]. The studies revealed that the wires grow along the step edges of the substrate, in the [111] direction and represent the ferrimagnetic γ -Fe₂O₃ phase [2,3]. The magnetic properties of fabricated species were determined through magneto-optical Kerr effect (MOKE) measurements under UHV. The results confirmed ferri-/ferromagnetic ordering in the wires at room temperatures, as well as in-plane magnetic anisotropy expected for such nanowires based on micromagnetic simulations [3].

The studies were financially supported at the initial stage by the Foundation for Polish Science (Polish ‘Fundacja na rzecz Nauki Polskiej’) through the First TEAM/2016-2/14 (POIR.04.04.00-00-28CE/16-00) project ‘Multifunctional ultrathin Fe(x)O(y), Fe(x)S(y) and Fe(x)N(y) films with unique electronic, catalytic and magnetic properties’ co-financed by the European Union under the European Regional Development Fund. P. W. additionally acknowledges the European Union for the financial support through the European Social Fund Operational Programme ‘Knowledge Education Development’, Project No. POWR.03.02.00-00-I032/16 ‘Interdisciplinary PhD studies in nanotechnology’.

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Thickness dependent work function of layered MoO₃ onto SiO₂ and MoS₂ in air

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2D MoS₂, MoO₃ and their heterostructures are promising candidates for electronics and catalysis [1,2]. That is why it is interesting to study their electronic properties. In this work, the work function (WF) of thick MoS₂ flakes as well as thickness dependence WF of thin MoO₃ layers on MoS₂ and SiO₂ substrates were measured by Kelvin probe force microscopy in air. As-exfoliated MoS₂ flakes obtained by a tape-exfoliation method had slightly higher WF than pristine counterparts due to tape residues. Regarding MoO₃, two samples were considered: (1) Crystalline MoO₃ layers synthesized by a modified hot plate method and transferred onto SiO₂; (2) Layered amorphous MoO₃ onto MoS₂ synthesized by oxidation of MoS₂ flakes in a humid environment. High-resolution conductive atomic force microscopy (c-AFM) measurements showed that amorphous oxide layers contained some small crystallites of α - or β - MoO₃ (Fig. 1a). In both cases, the WF of oxide increased with thickness (Fig. 1b). This trend was due to interfacial electric field at the MoO₃/substrate interface. SiO₂ (MoS₂) negatively charged the first MoO₃ layer and that charge was screened by subsequent MoO₃ layers. Electron transfer from MoS₂ to MoO₃ and possible interfacial trap states provoked by charged impurities in SiO₂ were responsible for the negative charge in the first MoO₃ layer. A p-n junction based on MoS₂/MoO₃ heterostructure was also fabricated and showed a rectification behavior due to p-type doping of MoS₂ by MoO₃ [3].

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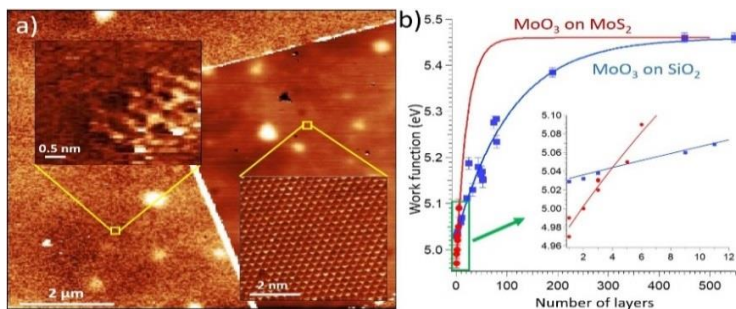


Fig. 1. (a) AFM topography and current images of a synthesized MoS₂/MoO₃ heterostructure. (b) Work function of layered MoO₃ on SiO₂ and MoS₂ vs. number of oxide layers.

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Impact of Boron Doping on the Sputtering Dynamics of Graphene: A Molecular Dynamics Simulation Study

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After years of intensive study, graphene remains a prominent focus in materials science, evolving from fundamental explorations of its exceptional electrical, mechanical, and thermal properties to innovative adaptations in its chemical structure for tailored applications ¹. Recent research has shifted towards graphene-based materials with specialized morphologies and functionalization designed for diverse technological arenas—from energy and sensors to biomedicine and photovoltaics ². Among various modifications, chemical doping has proven crucial, especially with boron and nitrogen, which adjust the electronic characteristics due to their atomic radii compatible with carbon ³. Particularly, boron doping has garnered interest in enhancing p-type conductivity and broadening graphene's use in novel applications ³. One critical aspect of these studies is the precise determination of dopant concentration. This work proposes utilizing laser post-ionization as a method to accomplish the task of detecting emitted boron. In particular, we suggest that secondary neutral mass spectrometry (SNMS) could be used for this purpose.

This study employs molecular dynamics simulations to investigate the sputtering behavior of boron-doped graphene under the bombardment of 10 keV C₆₀ projectile along the surface normal (Figure 1). We explore the influence of the boron concentration across a concentration range of 0-15%, on the sputtering yield, kinetic energy and angular spectra. It has been observed that boron sputtering yield is proportional to the boron concentration, supporting our proposal. However, a detailed examination of the kinetic energy spectra and angular distributions of sputtered boron atoms shows that widespread ejection energies and angles occur, which hinders SNMS's ability to detect boron.

This work was supported by the Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) by providing computer facilities and support within computational grant no. PLG/2024/017104, and by the Narodowe Centrum Nauki Program No. 2019/33/B/ST4/01778.

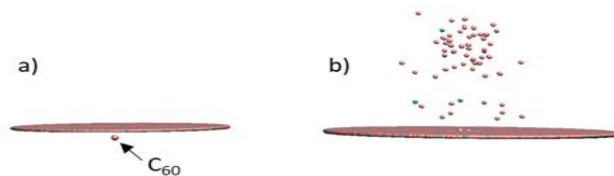


Fig. 1. Visualization of boron-doped graphene before (a) and after (b) impact.

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Ways to get the perovskite structure right

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Tantalate, titanate, and niobate perovskites are regarded as excellent (photo)catalysts, achieving world-record efficiencies e.g. for water splitting [1],[2] yet they are often regarded as unstable. Small external or internal stimuli can change the crystal structure and surface reconstruction, therefore there is a need for a tool that allows for precise tracking of the evolution of atomic structures, best *in situ*. Although there are many possible options, especially SPM-based, they lack out-of-plane resolution to detect small ionic displacements as in the case of ferroelectric materials changes as small as a single pm can lead to dramatic differences in macroscopic properties. This presentation is aimed at showing the way to overcome this challenge, by employing of often forgotten, yet powerful LEED-IV technique, in combination with various SPM methods.

The (001) plane of KTaO_3 is used here as a prototype of a cubic perovskite with cation oxidation states +1/+5. The initial surface is prepared by *in situ* cleaving at room temperature along the (001) plane, resulting in a bulk-terminated surface with equally populated KO and TaO₂ terminations [3]. This picture changes when the surface is annealed, due to the out-of-plane cation diffusion, giving rise to the KO-enrichment at the surface. Changes in morphology are precisely tracked by low-temperature ncAFM measurements using qPlus sensors, whereas evolution in chemical composition are represented by XPS spectra.

SPM-based techniques prove therefore to be excellent when it comes to substantial stoichiometry changes related to the ionic or atomic diffusion in the material, yet exact positioning comes with difficulties. Here a homogeneous (2x1) reconstructed surface of $\text{KTaO}_3(001)$ is used to show that by tracking intensities of LEED spots as a function of energy one can get spatial information of ionic positions in all three dimensions. Experimental I-V curves are compared with theoretically calculated by the Vienna package for Erlangen LEED (ViPErLEED) and ultimately cross-correlated with DFT-relaxed crystal structures. The surface of an incipient ferroelectric potassium tantalate causes disturbance of equilibrium positions of ionic species (mostly K and Ta) giving rise to the emergence of a certain degree of ferroelectricity in the subsurface region, down to approx. 10 unit cells. Noteworthy, such a tandem approach, based on the combination of experimentally and theoretically derived structures provides reliable results on surface crystal structure not only for perovskites but for virtually any materials.

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Investigation of the electronic structure of graphene/TMDC heterostructures

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Transition metal dichalcogenides (TMDCs) belong to a class of materials characterized by numerous unprecedented properties not found in other systems, leading to their potential applications in electronics and spintronics. Due to their layered structure, this group of materials can be used as heterostructures with other two-dimensional systems, such as graphene. Consequently, it is expected that such hybrid materials will exhibit new properties associated with complex phenomena occurring at the interface of layers.

The main objective of the presented research was to build graphene/TMDC heterostructures and conduct an analysis of their electronic properties. The key focus was on investigating the mutual interaction of both components and assessing the influence of this interaction on the properties of graphene and TMDC.

For this purpose, two types of TMDC-based heterostructures (1T-TaS₂, T_d-WTe₂) and graphene were constructed and characterized – graphene/TMDC and TMDC/graphene/SiC. For the 1T-TaS₂/graphene/SiC hybrid, an efficient method for identifying 1T-TaS₂ layers using KPFM measurements was developed, enabling the analysis of the oxidation process of 1T-TaS₂. It was also demonstrated that the STM tip allows for selective removal of contaminants from the surface of 1T-TaS₂. LT-STM studies conducted in ultra-high vacuum (UHV) environment enabled the analysis of thin flakes of 1T-TaS₂, including those with single-layer thickness.

On the other hand, the second type of investigated systems, graphene/1T-TaS₂ and graphene/T_d-WTe₂, are unique heterostructures that allowed for measurements at both macro and nanometer scales. For the first time, the electronic structure of such a system was examined using ARPES, demonstrating that TMDC and graphene retain their fundamental properties. Additionally, due to the proximity effect occurring in the heterostructure, p-doping of graphene is observed. This indicates that the interaction within the hybrid should be considered as a factor regulating the properties of the system, rather than destroying them, which was not previously clear for the graphene/TMDC structure. Moreover, such systems have great research potential in the direction of twistrionic effects, as indicated by our preliminary STM studies.

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Investigation of metallic nanostructures on semiconductor substrates for SERS and PIERS applications

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Surface-enhanced Raman spectroscopy (SERS) and photo-induced enhanced Raman spectroscopy (PIERS) require application of advanced metallic nanostructures deposited on a substrate. These nanostructures may be obtained by direct *in-situ* growth on a surface using various methods: electrochemical, hydrothermal, photochemical, chemical reduction, thermal vapor deposition in vacuum, etc. The presentation is devoted to the preparation and characterization of efficient SERS/PIERS platforms created in a two-step process, consisting of deposition of semiconductor coating on silicon substrate in sol-gel dip-coating stage and subsequent photodeposition of metallic nanostructures (NSs). In order to achieve the specified size, quantity and uniform surface coverage of semiconductor by NSs, the key stage affecting the quality of SERS platforms is the control of photoreduction of metal ions and growth of NSs induced by UV radiation. This can be achieved by optimizing such parameters as intensity and wavelength of UV radiation, exposure time, concentration of metal ions and addition of scavengers affecting the separation of photoinduced charge carriers (electrons and holes). The obtained substrates were subjected to microscopic (SEM) and spectroscopic analysis (EDS, UV-Vis, Raman). SERS studies have shown that signal amplification for 4-mercaptobenzoic acid (4-MBA) ranged from 0.6×10^4 to 7.1×10^4 for platforms with gold NSs and from 5.1×10^4 to 1.2×10^6 for platforms with silver NSs. A low detection limit of SERS signal was also obtained for malachite green - 9×10^{-11} M for a substrate with gold NSs. Application of the semiconductor modified with metallic nanostructures gives also the possibility of additional excitation of the system with UV radiation and further signal amplification of 4-MBA from 4.6 to 18.8 times (depending on the sample) in relation to measurement without UV exposure. A TiO₂-AgNSs heterojunctions exhibit a 10-day-long PIERS signal, induced by UVC light illumination of the material, that decreases by ca. 50% only in that time. Photoenhanced spectroscopic properties of nanoplatforms, enables ultrasensitive detection of analytes (pollutants, drugs, explosives) in nanoscale and their multiple use.

Research were conducted in two scientific teams: nanomaterials technology group - having experience in preparation of advanced nanomaterials (*Faculty of Chemistry, University of Lodz*) and in Raman imaging spectroscopy group - highly skilled in investigation of FT-IR and Raman properties of nanomaterials (*Faculty of Chemistry, Jagiellonian University in Krakow*).

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Characterization at the atomic scale of contact interfaces between thermally self-assembled Au islands and MoS₂ substrate surfaces

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The potential for new functionalities in emerging technologies such as optoelectronics and nanoengineering can be realized through the interaction between metal nanoparticles and transition metal dichalcogenides (TMDs). An attractive "bottom-up" approach in this regard involves the process of self-organization during metal deposition on semiconductor surfaces, enabling the formation of nanostructures with desired geometrical and electrical properties. The present study focuses on the growth process of single metallic nanostructures formed by gold deposition on MoS₂ surfaces and synthetically formed MoS₂/SiO₂ bilayers. Structural analysis of the formed Au nanoislands was carried out using scanning tunneling microscopy (STM) under ultra-high vacuum (UHV) conditions and high-resolution scanning electron microscopy (HR-SEM). In addition, high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) was used to visualize the cross-section of the Au/MoS₂/SiO₂ interface. The crystallographic symmetry of the MoS₂ surface contributes to the triangular shape of the planar Au nanoislands, with lateral dimensions ranging from 10 to 50 nm and heights from 2 to 8 nm. The precise size of these nanoislands can be controlled by adjusting the amount of deposited gold and the substrate temperature during the growth process [1]. Detailed investigations using HAADF-STEM microscopy techniques have yielded comprehensive insights into the interface formed between the epitaxial Au nanoislands and the MoS₂ substrate surface, as well as the structure of the MoS₂ layer itself. The atomic-scale resolution obtained through cross-sections of Au/MoS₂/SiO₂ interfaces revealed that the density of lattice sites occupied by Au atoms in the plane constituting the nanoisland/substrate interface is lower than in the Au bulk. This may be responsible for the weak interaction between the nanoislands and the substrate making this system an exemplary system for nanomanipulation [2] or to observe a geometric energy confinement in charge state-dependent sputtering by HCl ions [3].

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Magnetization switching and dynamics of two-dimensional ferromagnets

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Two-dimensional (2D) materials enable unique multilayer system stacking, high interface-to-bulk ratio and unconventional types of symmetry breaking mechanisms. It has been presented, that by using a combination of 2D layer with high spin-orbit coupling (WTe₂) and ferromagnet (Py), the symmetry of spin-orbit torque can be controlled [1]. In addition to transition-metal dichalcogenides ferromagnetic materials can also be synthesized in a form of van der Waals crystals, which are characterized by very high perpendicular magnetic anisotropy and anomalous Hall effect (AHE) [2]. However, determination of other properties of the magnetic materials, such as magnetization damping or saturation magnetization remains challenging, as typically, 2D magnets are fabricated in form of irregular and μm -size flakes.

In the present work, I will summarize the investigation of 2D-materials hybrids using static and dynamical measurement methods. I will show AHE and spin-Hall effect in FeGeTe/Pt bilayer and point out the crucial role of the interface between two layers. I will continue with a FeGeTe-oxide/hBN system where a strong and bias voltage-controlled exchange bias was recently discovered. Next, I will move to the magnetization dynamics measurement of the CrGeTe/Pt using ferromagnetic resonance spectroscopy and spin-diode effect. An update of the spin-pumping effect in CeGeTe exhibiting very low damping will be presented [4]. The talk will be concluded by current challenges and prospects of the magnetization dynamics in van der Waals ferromagnets.

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Investigating MoS₂/Au interface with the CAFM and local force spectroscopy

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The resistive switching effect refers to a material's reversible alteration in electrical conductivity after an electrical stimulation. This effect can be implemented in non-volatile computer memory technology, where different states of conductivity correspond to the logical states within a memory cell. Such memory cells are typically composed of a simple metal/insulator/metal (MIM) structure, with a switchable material placed between two metallic electrodes. By applying an external electric field, the insulating material's resistance can be modified, causing it to switch between states of high and low resistivity. These states can be used to denote the binary logical states "0" and "1," which are essential for encoding the information processed by computer algorithms. A promising category for this application are two-dimensional (2D) materials, which are currently the subject of intense research due to their atomical thickness, outstanding mechanical properties like Young's modulus and strength or electronic properties covering a wide range of applications from insulators to conductors or even superconductors. Transition metal dichalcogenides, a subgroup of 2D materials with the general formula MX₂ (where M represents a transition metal and X is a chalcogen), are particularly noteworthy. Among these, MoS₂ is the most extensively researched for resistive switching applications because of its environmental robustness and the relatively low temperature of chemical vapour deposition.

Due to the enormous surface/volume ratio of 2D materials their performance in a memory cell is greatly influenced by the quality of the interface between the material and the substrate. Therefore, it is vital to explore how the quality of the substrate affects the electronic performance of the devices or the underlying physics of the material-substrate interaction. In our work we investigated the impact of interface quality between MoS₂ and gold electrode in nanoscale using CAFM and local force spectroscopy. Two sets of samples have been prepared one in controlled conditions with sputtering and annealing of gold before the exfoliation and the second in wet air conditions with standard commonly used tape and polymer transfer technique. We will show that there is a significant influence of gold substrate on the electronic structure of MoS₂. In turn, for samples made in the air we observe the influence of the contaminants on the band gap. With the use of force spectroscopy and local conductivity measurements, we will characterize the interface properties and show the possibility of their modifications.

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Towards multicomponent metal-organic Sierpiński triangle fractals on surfaces

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The surface-supported coordination-driven self-assembly of small organic molecules is a convenient method allowing for the precise construction of openwork two-dimensional (2D) crystals with desired porosity, connectivity, and programmed physicochemical properties [1]. However, the design of surface-confined metal-organic fractal crystals is much more challenging, and such exotic supramolecular structures have been achieved so far only in the case of a few conformationally rigid molecular building blocks [2,3]. Therefore, in this communication, we present our latest theoretical findings focused on the rational construction of nitrogen-doped metal-organic Sierpiński triangle (MOST) fractals on surfaces exploiting a conformationally flexible precursor (2,2':6',2''-terpyridine-6,6''-dicarbonitrile) mixed in a 3:2 molar ratio with trivalent metal adatoms M (where M is Fe, Ni, or Co). Moreover, we demonstrate that mixed MOSTs fractals comprising conformationally rigid tecton (4,4''-dicyano-1,1':3',1''-terphenyl), and conformationally flexible precursor (2,2':6',2''-terpyridine-6,6''-dicarbonitrile) are also easily achievable. In our simple lattice model, the aromatic ligands listed above were modeled in a simplified way as a collection of flat, rigid, and interconnected segments with properly encoded short-ranged ligand→metal interactions. Additionally, the ligand→metal coordinate bonds were assumed to be directional, short-ranged (limited to the neighboring adsorption sites on a triangular lattice), and reversible (at relatively high temperature). The single coordinate bond with a potential energy $\varepsilon = -1.0$ was allowed to form only when a linker molecule (connector) and metal adatom M met in a proper configuration on a flat lattice, and interaction directions assigned to them were oppositely directed ($\rightarrow\leftarrow$) and collinear. We found, that the simulated deterministic fractals are not only aesthetically pleasing but also important from a cognitive viewpoint, as nanopores and mononuclear metal centers incorporated into their skeleton create unusual planar tessellations realizing fundamental ideas of Euclidean geometry.

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Application of nanoparticles to produce multifunctional layers on NiTi shape memory alloys

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The work attempts to develop a surface modification technique for NiTi shape memory alloy implants for medical applications. The aim was to produce advanced multifunctional hybrid layers, consisted of chemically synthesized nanometric molecular system of titanium dioxides and silver known for its potent antibacterial attributes, alongside bioactive nanosized hydroxyapatite. This approach not only aimed at improving the biocompatibility and promotion of osseointegration but also antimicrobial performance of the implant, thereby advancing its suitability for long-term implantation.

The layers underwent cathodic deposition using EPD method with a range of deposition parameters such as deposition time (1-5 minutes) and voltage (10-20 V), followed by a subsequent heat treatment process in vacuum conditions. To ascertain the optimal heating temperature ensuring minimal risk of shrinkage and cracking in the layers, precise dilatometric measurements and high-temperature microscopy analyses were conducted.

The study extensively studied the influence of deposition conditions on the quality and morphology of the produced layers, particularly emphasizing the impact of heating conditions on their structural changes. As a result, a new material was obtained with a completely different structure and properties from the starting materials used. Elevated temperatures induced notable alterations, including structural modifications in hydroxyapatite, partial decomposition of silver-containing phases, and the formation of Ag@C structures. However, the most significant changes were observed in the titanium oxide structure, manifesting as pronounced defects. These structural variations significantly heightened the activity of the resultant layers, consequently affecting their properties. The employed procedures facilitated the generation of continuous coatings devoid of cracks and delamination, presenting promising results in the realm of implantation medicine.

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The study of friction versus velocity and load by means of atomic force microscopy

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The atomic force microscope (AFM) operated in lateral force microscopy (LFM) contact mode becomes one of the major tools for studying phenomenon of friction across scales – from the atomic scale to the microscale. The existence of different friction mechanisms and the fact that friction force depends on numerous variables (for instance: loading force, sliding velocity, roughness, contact elasticity, temperature, humidity and many others), as well as on the chemical composition of the friction pair, makes the LFM experiment and data analysis an interesting and challenging task.

The main goal of this research was to study the dry nanoscale friction mechanisms, particularly adhesive friction and stick-slip, for different friction pairs: AFM tip (silicon oxide or single diamond crystal) versus functional nanocoating (selected fluoroalkylsilanes, graphene or single graphene oxide flakes). Determination of the friction force versus the sliding velocity dependencies, obtained for a number of the loading forces (from near zero to a few tens of nanonewtons), facilitates the identification of the friction mechanisms responsible for measured friction force [1].

For near zero (as well as for negative) loads, adhesive friction is dominating (almost independently of the sliding velocity range), while energy-dissipative stick-slip marks its presence for larger loads (from a dozen of nanonewtons and more). This observation is universal for all studied friction pairs in this work.

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Nanohighways in α -Bi on graphite

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Friction emerges from energy dissipation at the contact interface between two materials in relative motion, and it has been estimated that friction takes up to 23% of the world's energy consumption [1]. Structural superlubricity (SS) [2] is a special regime of motion in which two incommensurately coupled crystals are associated with vanishing energy barrier crossing. These frictionless regimes have been so far realized in multilayered graphene and other van der Waals (vdW) contacts with hexagonal or triangular crystalline symmetries leading to isotropic frictionless contacts for a wide range of twist angles. Recently, a new class of SS has been predicted with a 1D, flat directional translational potential energy landscape or *nanohighways* [3] but has not yet been demonstrated in a vdW system. In this talk, I will show low energy electron microscopy (LEEM) results which allow for visualization of the growth of α -bismuthene (α -Bi) islands on highly ordered pyrolytic graphite (HOPG). The spontaneous back-and-forth diffusion over hundreds of nanometers of massive islands (up to 20000 nm²) is a manifestation of directional SS, supported by registry index simulations. Finally, I will show that the islands dynamics follows Lévy flight statistics [4], which have been to date very elusive in solid state systems.

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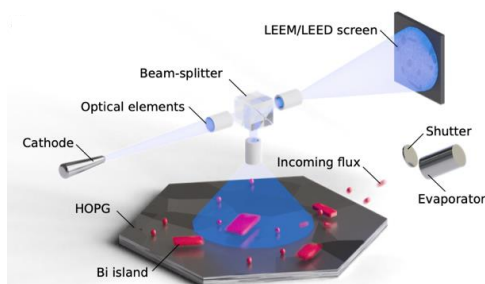


Figure: *in-situ* LEEM/LEED apparatus

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Direct-Current Triboelectric Nanogenerator Energy Harvester from Raindrop Impact (DC-TENGEHRI)

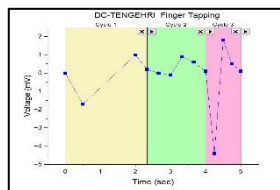
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With the need for sustainable energy solutions in our current energy demand, the triboelectric nanogenerator (TENG) has emerged as a promising alternative, capable of converting randomly distributed, irregular, and wasted low-frequency energy into electric power. This study focuses on the development of a TENG tailored for harvesting raindrop energy and producing a direct current (DC). The proposed DC-TENG features a drum-like structure which generates current through the interaction of triboelectric materials. A previous investigation explored energy harvesting from footfall (DC-TENGEHF) [1]. The results exhibited a peak voltage of 35.0 mV and a generated short circuit current of 0.1 μ A per cycle. This initial experiment aimed to assess device design and fabrication feasibility.

The current study demonstrates peak voltage readings of approximately 3.5 mV and a measured direct current of \sim 0.1 μ A from a single finger tap, aligning with previous findings by Lou et al. (2018) [2] and confirming direct-current output. Furthermore, a shower sprinkler was employed to simulate rainfall, positioning the device flat on the ground directly beneath it. This experiment yielded voltage outputs ranging from 0.5 mV to 2.0 mV and current levels fluctuating between 0.0 μ A to \sim 0.1 μ A. Notably, the fixed shower head's height was approximately 1.5 meters, suggesting the potential for increased voltage output with greater height. This observation is supported by the DC-TENGEHF [1] results, where higher force from footfall resulted in elevated voltage outputs compared to rainfall.

A prototype of a DC-TENGEHRI has been successfully developed and tested as a proof of concept for harvesting raindrop energy using TENG. While it has demonstrated the successful generation of direct current (DC) output, this DC-TENGEHRI remains an initial prototype with the potential for further modification and improvement. With continued development, this device holds promise as a sustainable power source during rainstorms that offers resilience in situations where electricity may be disrupted.



DC-TENGEHRI device (left) and finger tapping voltage vs time graph(right)

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High-performance computing infrastructure for interdisciplinary research

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This contribution introduces the EuroCC2 project, a National Competence Centre (NCC; URL: <https://cc.eurohpc.pl>) in high-performance computing (HPC), operating under the EuroHPC Joint Undertaking – a collaborative effort involving 33 European countries and the European Commission. The Polish NCC aims to facilitate access to computational resources and provide technological and training support to universities, research institutes, industry, and public administration, further promoting the utilization of HPC infrastructure.

Various initiatives of the NCC, focusing on access to national and European supercomputing infrastructure as well as HPC competence development, are presented, showcasing their relevance to the scientific community.

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POSTER SESSION

Novel virus-like particle arrays exhibiting surface lattice resonance for ultrasensitive biodetection

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Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) that causes COVID-19 has stimulated the scientific world to intensify studies aimed at developing quick and safe ways of detecting viruses in human body. Currently, there are two widely used diagnostic methods: molecular diagnostics and serologic test. The first one is considered to be a very sensitive, but time-consuming, whereas the second is fast and simple but cannot be applied for early COVID-19 diagnosis. Thus, there is a need for developing new methods that would provide fast and reliable detection of viruses. Surface-enhanced Raman scattering (SERS) is a powerful analytical technique used in chemistry, pharmacology and biomedicine for studying biological systems, e.g. proteins, tissue, bacteria and viruses. This method, based on the appearance of the so-called localized surface plasmon resonance (LSPR) in noble metal nanostructures that amplifies vibrational signals from the analyte deposited onto them, deserves consideration in biodetection due sensitivity towards even nanomolar concentrations of biomolecules, with the measurements being performed in a label-free way [1]. By utilizing the capillary-assisted particle assembly (CAPA) [2], we have prepared an innovative matrix composed of SARS-CoV-2 virus-like particles (VLPs) characterized by the presence of the LSPR in the gold cores and the surface lattice resonance (SLR) related to the periodic arrangements of particles. The SLR further amplifies the SERS signals originating from molecules specifically binding to VLPs [3], making the fabricated system suitable for applications in ultrasensitive biodetection [4].

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Empowering Environmental Sustainability Functionalized SBA-15 as a Cutting-Edge Solution for Effective Metal Uptake

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One of the most promising and modern solutions to combat environmental pollution is the development of bio-perforated, mesoporous SBA-15 silica. This material boasts an impressive surface area of approximately 800m²/g. It features structurally amorphous properties, forming uniaxially ordered hexagonal channels with a diameter of 5 nm and a length on the order of micrometers. These channels are uniformly distributed throughout the volume, allowing for high capillary properties. SBA-15 also demonstrates a neutral impact on the environment and living organisms, exhibiting no toxic or irritating effects. Furthermore, its physicochemical properties are easily adjustable through various technological processes, offering great flexibility in terms of chemical modification. This high degree of adaptability allows for the functionalization of SBA-15 with a wide range of functional groups, either on its outer or inner walls, while maintaining precise control over their concentration within the material's volume.

The significant advancement in environmental protection, as proposed by our research team, has been achieved by activating the mesopores using specific functional groups tailored for capturing specific types of metals. This functionalization involves the use of various functional groups, such as propyl-carbonate (for metal-binding I, e.g., silver), propyl-phosphate (for metal-binding II, e.g., copper), and cyclam (1,4,9,11 tetraazacyclodecane), which is capable of chelating metal chlorides like copper, chromium, cobalt, nickel, and more. Importantly, this functionalization process ensures the homogeneous distribution of these functional groups within the silica pores.

The potential of metal ion uptake has been rigorously verified using advanced techniques such as SAXS, Positron-Electron annihilation, BET (Brunauer-Emmett-Teller), and spectroscopy methods like UV-VIS spectroscopy. Time-dependent metal uptake curves have been instrumental in estimating the real-time sorption capacity of functionalized SBA-15. Mechanical studies, including Young's modulus parameters at various force levels (ranging from nN to N), have been conducted on individually prepared SBA-15 pellets to assess their stability and mechanical properties. The combined efforts of functionalizing SBA-15 and evaluating its sorption potential through various methodologies aim to pave the way for developing an entirely new class of materials with unique properties for remediating contaminated environments. This research holds the promise of making a significant and positive impact on preserving our environment and protecting human health.

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Semiconducting layers on FeAl alloys – electrochemical synthesis and detailed characterization

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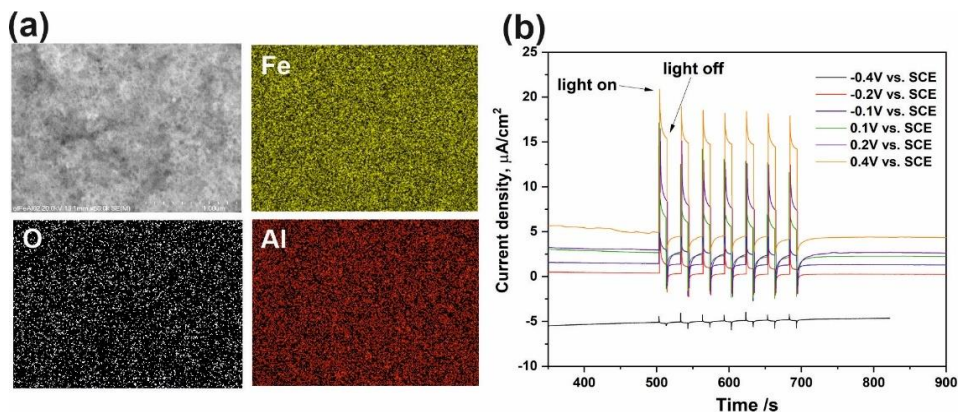
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Iron oxide-based materials, especially hematite (α -Fe₂O₃) are considered as promising candidates for photoelectrochemical applications because of several favorable properties, among which, a narrow band gap allowing the absorption of a wide range of visible light seems to be especially important [1]. Therefore, here we present a new strategy for the fabrication of nanostructured iron oxide-based photocatalysts by a simple one-step anodic oxidation of FeAl alloy followed by its thermal treatment and selective etching [2]. Morphology, composition, optical, and semiconducting properties of the obtained materials were carefully characterized by many complementary techniques including SEM, EDS, XRD, UV-vis spectroscopy, Mott-Schottky analysis, and detailed photoelectrochemical measurements. The results proved that the proposed strategy can be successfully employed for the synthesis of nanostructured photocatalysts.

This work was partially supported by the National Science Centre, Poland (contract no. UMO-2019/35/B/ST5/04215)



SEM image together with EDS mapping of anodic film obtained on FeAl alloy (a) and photocurrents recorded during its sequential illumination with simulated solar light at various potentials (b)

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Early-stage wear of MoS₂ surfaces on the nanoscale

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A clear understanding of friction and wear mechanisms on the nanoscale is essential for finding solutions to reduce energy dissipation in various mechanical systems, as well as the emission of greenhouse gases. In this context, the study of two-dimensional materials belonging to transition-metal dichalcogenide group, such as MoS₂, presents significant research opportunities and potential applications, such as solid lubricants as opposed to conventional liquid ones.

The aim of this study is to understand the complex processes that govern the formation of wear nanostructures on surface interfaces in relation to friction. To this end, we employed nanoindentation and friction force microscopy techniques. By dragging sharp diamond nanotips along the surface of mineral MoS₂ with fixed values of load and velocity, scratches were performed.

The results reveal a rather regular repetition of exfoliated flakes on both sides of the wear tracks and cracks propagated not necessarily along the scan direction. We have also observed a stick-slip behaviour in the lateral force profile recorded during the scratching, that we aim to compare with ongoing molecular dynamics simulations.

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Biological activity examination of Au@Fe₃O₄ nanoparticles with photoactive properties

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Photothermal therapy (PTT) is a targeted anticancer therapy that uses electromagnetic radiation in the NIR range and substances that can absorb such radiation. These substances, called photoactive factors, can convert absorbed radiation energy into thermal energy, and they are usually introduced into cancer cells before starting exposure to radiation within the biological window. An increase in cells temperature after exposure to radiation leads to their death. Current research focuses on the capability of various types of nanoparticles, also those with magnetic properties, as photoactive agents.

The research aimed to synthesize using magnetic NPs modified with gold, i.e., 1:3 Fe₃O₄:Au and 1:4 Fe₃O₄:Au NPs, and evaluate their effectiveness for PTT. The physicochemical properties of such NPs were examined (absorption spectra and hydrodynamic diameter of NPs – DLS). The energy conversion capacity of NPs was also examined by measuring the temperature of NPs solutions after irradiating them with a laser at the wavelength used for the PTT procedure. Tests of the biological activity of the obtained nanoparticles were carried out on four cell lines – two normal (MRC-5, HaCaT) and two cancerous (A549, A375). Based on the MTT viability test, cytotoxicity was examined after 24 h and 48 h of incubation of the cell cultures with NPs solutions. Then, the PTT procedure conducted using NPs as photoactive agents was performed. Significant temperature changes of cell cultures (about 20°C for 1:4 Fe₃O₄:Au NPs) were observed after NPs photoactivation (Fig. 1).

It has been proven that tested NPs have the ability to convert energy and cause a significant reduction in cell viability after photoactivation. Moreover, it was found that both types of magnetic NPs are less toxic to normal cells.

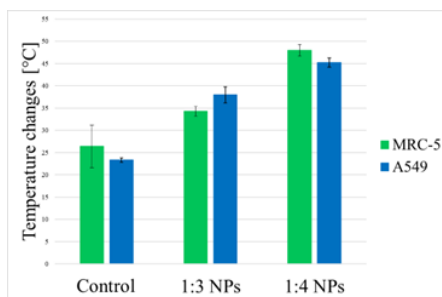


Fig. 1. Temperature changes of cell cultures after NPs photoactivation.

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Examining the impact of surface modification of magnetic nanoparticles on their photoactive properties

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Nanomaterials have already found many applications in biomedicine, including in the development of new diagnostic tools, drug delivery systems and vaccines. There are many potential applications of nanotechnology in biomedicine that are currently being explored, and further research in this area could revolutionize healthcare.

The aim of the research was the synthesis, modification and application of core/shell magnetic nanoparticles in photothermal therapy (PTT). This therapy takes advantage of the ability of photoactive factors to convert the energy of electromagnetic radiation into thermal energy. As a result of irradiation of photoactive factors with near-infrared radiation, there is a short-term and local increase in temperature, which leads to cell death.

In the first stage of the work, cores were obtained - iron (II, III) oxide nanoparticles using the method of controlled oxidation of the Fe(II) precursor. Then, the surface of the cores was covered with gold nanoparticles and coated with a layer of polyethylene glycol, which allowed to obtain two types of nanoparticles: Fe₃O₄@Au@PEG-OH and Fe₃O₄@Au@PEG-NH₂. In the next stage of the research, the physicochemical parameters of the nanoparticles were characterized and cytotoxicity tests were performed. In vitro studies were performed on 4 cell lines: A549 (lung epithelial cancer cell line), MRC-5 (normal lung epithelial cell line), A375 (epidermal cancer cell line) and HaCaT (normal keratinocyte cell line). Based on the results obtained, it was found that in most cases the tested nanoparticles are not toxic to cells. In the next stage of the research, after confirming that the obtained nanoparticles had the ability to convert energy, a photothermal therapy procedure was carried out. It was found that the desired therapeutic effect was achieved, as cell viability was reduced by up to 93%. The highest PTT efficiency was achieved for the A375 cell line using a solution of Fe₃O₄@Au@PEG-NH₂ nanoparticles with a concentration of 75 µg/ml.

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Application of LEEM microscopy in the study of antimonene on W(110)

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LEEM (Low Energy Electron Microscope) was invented by E. Bauer in the 1960s and has been widely used in surface science since the 1980s. LEEM apparatus uses the phenomenon of electron reflection for imaging the surface of samples and has two basic modes of operation – microscopy (LEEM) and diffraction (LEED - Low Energy Electron Diffraction). The former mode enables real-time imaging of samples, which makes it possible to study surface morphology, phase transitions, thin film growth, segregation, diffusion and other phenomena. In this mode there is also the possibility of dark field measurements, which allows to see the domains of the formed structures rotated relative to each other in the plane of the sample. The second mode is for the observation of diffraction patterns of the sample. In addition, selected area aperture, limiting the spot size of incident electrons, enables μ LEED images from a region of several hundred nanometers.

Nowadays, the study of two-dimensional (2D) materials is an important area of scientific research. Among such materials antimonene is of particular interest: it possesses direct band gap which can be tuned by a number of ways and is resistant to ambient conditions. Antimonene was first theoretically predicted in 2015 by Gaoxue Wang et al. [1], shortly after which it was synthesized by exfoliation by Pablo Ares et al. in 2016 [2].

In this report we study basic properties of antimonene film which is grown by means of molecular beam epitaxy method on the W(110) substrate. We track the growth of 2D layers in real time in the bright and dark field LEEM and LEED modes. The experiments were performed in the LEEM laboratory in Institute of Physics at Maria Curie-Skłodowska University.

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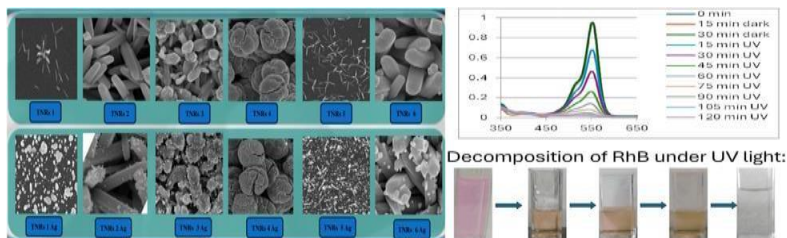
Enhancing Photocatalytic Activity of Titanium Dioxide Nanorods through Silver Nanoparticle Modification

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Nanoparticle-based photocatalysis exhibits potential for diverse applications, such as solar energy conversion, water electrolysis, and environmental pollution remediation. Titanium dioxide (TiO₂) is a potent and chemically unreactive photocatalyst that is commonly employed in both basic scientific investigations and practical business uses. Its non-toxic nature and promising performance make it the preferred option. This study aims to improve the photocatalytic properties of titanium dioxide nanorods (TNRs) by modifying them with silver nanoparticles (AgNPs). This modification is carried out using two different methods: sol-gel combined with dip-coating deposition and the hydrothermal method. The production of AgNPs was achieved through the photoreduction of Ag⁺ ions. The investigation explores the impact of different growth factors on the morphological development of TiO₂ nanorods. In this study, different TiO₂ nanostructures were synthesized by modulating the (i) Chemical composition – water acid ratio and (ii) precursor concentration involved in the hydrothermal process. The nanocomposite morphology was characterised using scanning electron microscope (SEM) and X-ray photoelectron spectroscopy (XPS) techniques, which revealed important structural features that are essential for photocatalytic performance. The results indicate that modifying the parameters causes the different morphologic structure (like thin nanorods, thick nanorods, nanoflower, nanoball). The photocatalytic efficiency of the TNRs and Ag-coated TNRs was assessed by measuring the degradation of the organic dye rhodamine B (RhB) under both ultraviolet (UV) irradiation and visible light. The UV-Vis spectroscopy technique was employed to analyse the changes in the RhB spectrum during photocatalytic processes. The results clearly show that UV light causes the RhB solution to lose its colour, whereas under visible light, RhB changes into rhodamine 110, indicating a successful photocatalytic transformation. The nanoball-like structures modification with the active metal silver (TNRs 4 Ag) exhibited high photocatalytic efficiency in both ultraviolet (UV) and visible light for different chemical composition parameter. For the precursor amount parameter, the TNRs 2 Ag (nanorods structure) are more efficient in UV but in visible light photocatalyst TNRs 6 Ag sample are more effective. The results emphasis the potential of TiO₂-based nanocomposites, specifically TNRs modified with AgNPs, in advancing photo-catalytic technologies for environmental remediation and energy conversion applications.



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Nonlinear optical and chiral properties of DNA-stabilized silver nanoclusters

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New class of chiral materials that can be used in bioimaging or biosensing are atomically precise nanoclusters (NC) [1,2]. Prominent among them are DNA-stabilized silver nanoclusters (Fig. 1(a)), which consist of a few to few tens silver atoms. Oligomers DNA, as ligand influence on strong photostabilities. Depending on the number of silver atoms and the DNA strand used NC exhibit different optical properties. The advantage of Ag-DNA are: narrow-band fluorescence, displaying a wide palette of sequence-selected emission colors that range from visible to near infrared (NIR) wavelengths and high quantum yields in select cases [3].

During conference will be present results of optical and chiral properties NC in both linear and nonlinear regime (Fig. 1(b) (c)), particularly: two-photon absorption cross sections [4], two-photon circularly polarized luminescence (CPL) and fluorescence-detected circular dichroism (FD CD). As optical properties of Ag-DNA excited one-photons are knowing, but 2PA have not been experimentally explored. Due to their near-infrared emission, and chiral properties Ag-DNA are promising fluorophores in bioimaging; strand exchange on-off switches, sensitive specific sensors; background-free fluorescence microscopy and nanophotonics [3].

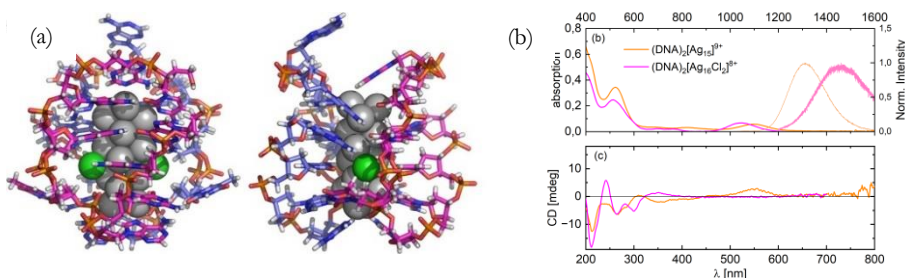


Fig. 1. (a) Overall structure of (DNA)₂[Ag₁₆Cl₂]⁸⁺ [5] (b) Absorbance, emission and (c) CD spectra of (DNA)₂[Ag₁₆Cl₂]⁸⁺ (pink) and (DNA)₂[Ag₁₅]⁹⁺ (orange).

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Significant improvement of conductivity in Na-V-Te-O glass through nanocrystallization

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Vanadate-tellurate glasses are good semiconductors due to their high polaronic conductivity, reaching up to 10^{-5} Scm^{-1} at room temperature. Doping them with sodium ions may have an interesting effect on the structure of these glasses and cause the appearance of the second ionic component of the conductivity. The presented research focused on preparing three $\text{Na}_2\text{O-V}_2\text{O}_5\text{-TeO}_2$ glasses with different sodium contents: 10, 20, and 30 %mol. Two promising compositions with 10 and 20 %mol of Na_2O were subjected to nanocrystallization. The topography and structure of all as-quenched and heat-treated materials were examined using confocal microscopy, scanning electron microscopy, X-ray diffraction, and Fourier transform infrared spectroscopy. The as-quenched glasses were amorphous and homogeneous, while the heat-treated samples contained nanocrystalline phases dispersed within the glass network. IR spectra indicated that the glass network consisted mainly of tellurate and vanadate units. The increase in sodium ion content caused the depolymerization of the glass network. Thermal properties: glass transition temperature, crystallization temperatures, and thermal stability of the glasses were measured using differential scanning calorimetry. The electrical properties were examined using impedance spectroscopy. All glasses were characterized by measurable DC conductivity, the values of which decreased with increasing sodium content. The high conductivity in glasses with the lowest concentration of sodium ions was associated with polaron hopping between the high concentration of vanadium ions. The electrical results were analyzed using Jonscher's law to estimate the DC conductivity part, while the Schnakenberg relation allowed us to estimate the hopping and disorder activation energies for polaron transport. The addition of sodium ions caused the appearance of a second mobile charge carrier. The conductivity reduction effect is related to the mixed conductivity, in which the percolation paths of both carriers intersect. The nanocrystallization process benefitted the conductivity of samples by organizing the vanadium oxide phase. The presented research shows that the nanocrystallization process has a high potential to improve the electronic conductivity in ion-doped $\text{V}_2\text{O}_5\text{-TeO}_2$ glass.

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In search of surface plasmon resonance – properties of luminescent phosphate glasses doped with Ag

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The versatility of amorphous materials is manifested primarily by their wide range of applications - from window glass to laser glass. One of the main reasons for the observed ubiquity of glasses is the ability to introduce various modifications to them with little complexity in the manufacturing process. One implementation of this idea is glassy optical matrices doped with rare earth elements that can serve as phosphors in LEDs. Due to its good chemical resistance, exceptional solubility of rare earth elements and unusual internal structure, phosphate glass stabilized with heavy metal oxides is an excellent candidate for such a matrix. At the same time, it is characterized by relatively lower luminescence efficiency compared to phosphors obtained using other techniques. However, using the advantages of the mentioned material, it is possible to carry out a modification based on the concept described by Malta et al. [1], in which Ag particles are obtained by reduction in glass, exhibiting surface plasmon resonance, which guarantees the enhancement of the luminescence of Eu^{3+} ions. Thus, it is possible to obtain material with significantly improved parameters in an uncomplicated way.

For a series of phosphate glasses with a nominal composition of $\text{P}_2\text{O}_5\text{-Bi}_2\text{O}_3\text{-K}_2\text{O-Nb}_2\text{O}_5$ doped with 0.5 mol% Eu, the method of introducing into the composition and obtaining Ag nanoparticles in the annealing process was investigated. The obtained materials were structurally characterized using XRD and FT-IR spectroscopy. Heat treatment temperatures and the full thermal characteristics of the glasses were determined based on DSC/DTA measurements. Moreover, the optical properties of the obtained materials were determined using UV-Vis absorption spectroscopy and fluorescence spectroscopy.

Based on the conducted research, the impact of the introduced silver on the properties of the glasses and the potential use of the presented phosphor as a matrix for Ag nanoparticles were determined.

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Formation of one dimensional nanostructures in the molecular beam epitaxy of antimony triselenide

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Antimony triselenide belongs to the family of one-dimensional semiconductors, which could be used for downscaling semiconductor channels in transistors even to the limit of a single atomic chain. Its crystal structure consists of one dimensional ribbons held together by weak Se-Se van der Waals interactions. The interest in bulk antimony triselenide has been boasted mainly by its applications in photovoltaic devices leading to the development of Sb₂Se₃-based solar cells with the efficiency exceeding 10%. The advantages of using antimony triselenide for these purposes are the high absorption coefficient, the appropriate value of the band gap that allows the absorption of the solar spectrum, single-phase structure and low toxicity.

In this work, the growth of antimony triselenide by molecular beam epitaxy on GaAs substrates with various crystalline orientations is reported. It is demonstrated that this semiconductor spontaneously forms tiny, monocrystalline, highly anisotropic Sb₂Se₃ nanostructures with the areal density of the order of 10⁹ cm⁻² and the cross-section dimensions of the order of a few nanometers implying a significant contribution of the quantum confinement to their electronic landscape. They lie always in the surface plane and their orientation corresponds to one of <1-10> azimuths of the substrate. With increasing deposition time all three dimensions: the length, the width and the height of these nanostructures increase simultaneously, with the length usually one order of magnitude larger than the two other parameters. The monocrystalline nature of Sb₂Se₃ lattice within a single nanostructure is demonstrated by transmission electron microscopy. Raman scattering and X-ray diffraction confirm its high crystalline quality.

To confirm that there is an epitaxial relationship between the substrate and the nanostructures, and thus the crystalline orientation of the substrate is an important parameter that directly affects the orientation of the nanostructures' growth direction, antimony triselenide is grown on three differently oriented GaAs substrates. It is found that in the case of (111)B oriented GaAs substrate three equivalent growth directions of the nanostructures are preferred corresponding to [1-10], [10-1] and [01-1] crystallographic directions of the substrate. In the case of (100) oriented GaAs substrate, there are only two equivalent growth directions: the [011] and [01-1] directions, while in the case of (110) oriented GaAs substrate, there is only one preferred orientation of the nanostructures: the [1-10] direction.

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Reduction to metallic tellurium upon Ar⁺ bombarding of V₂O₅-TeO₂ glass.

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Our experimental procedures, including cleaning and depth profiling with Ar⁺ bombardment, are meticulous and standard in X-ray photoelectron spectroscopy (XPS) analysis. In most materials, Ar⁺ bombardment allows the study of the internal structure of the material, avoiding the oxidized and often carbon-contaminated surface. However, there are a few known examples of oxides whose reduction upon Ar⁺ bombardment is significant enough to change the material structure. During previous extensive studies of the reduction of various binary oxides upon high-energy noble gas ions, only two candidates showed an extraordinary oxygen loss and metallic phase increase higher than a few at. %, namely ZrO₂ and HfO₂ [1].

For the first time, this work shows a significant reduction of tellurium oxide in a glass matrix. XPS studies are accompanied by detailed confocal microscopy and atomic force microscopy (AFM) analysis of the surface. Ar⁺ bombardment influenced the surface of the V₂O₅-TeO₂ glass, removing the oxygen from both oxides and leading to the creation of isolated islands and dendrites. The reduction to metallic tellurium upon Ar⁺ bombardment of V₂O₅-TeO₂ glass is a significant finding that could have far-reaching implications in the field of materials science and nanotechnology.

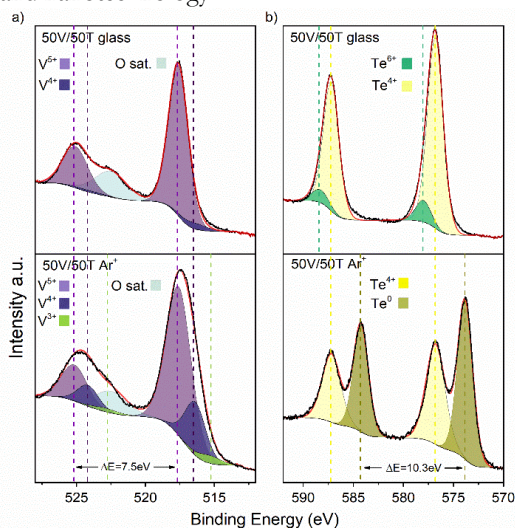


Fig. 1. XPS spectra of a) V2p_{3/2} and b) Te3d_{5/2} of the glass before (top) and after (bottom) Ar⁺ bombardment.

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Nanostructured cerium oxide as an extremely effective adsorbent of arsenic species from water

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Arsenic and inorganic arsenic compounds are the number one among hazardous chemicals on the Priority List of Hazardous Substances by the Agency for Toxic Substances and Disease Registry (USA). This is because long-term exposure to arsenic through food and drinking water has been linked to various types of cancers and vascular diseases. The maximum concentration of arsenic in drinking water, as set by WHO, is only $10 \mu\text{g L}^{-1}$ [1]. This value is significantly lower than the reported quantities of arsenic compounds found in many parts of the world. As a result, it's crucial to develop efficient methods and technologies for monitoring and removing excess arsenic from water on an ongoing basis. Adsorption-based methods allow the removal and/or recovery of arsenic compounds from an aqueous environment. These technologies are relatively cheap and easy to use if the adsorbents used exhibit high arsenic-binding capacity and can be easily adjusted to a wide pH range. Among various types of materials, cerium oxide has recently attracted much attention as an adsorbent of arsenic species. However, recent research has shown that its effectiveness depends on the size of primary particles that make up the cerium oxide. While, the structure of CeO_2 at the nano level is influenced by the synthesis method used.

The presented study provides a clever and simple one-step hard template method to prepare nanostructured cerium oxide [2] and demonstrates its practical application as an adsorbent for removing arsenic species from water [3]. The study reveals that cerium oxide beads have a highly developed internal structure ($S_{\text{BET}} > 170 \text{ m}^2 \text{ g}^{-1}$). They are composed of CeO_2 nanoparticles with a diameter of less than 10 nm, on the surface of which an atomic content of Ce(III), as determined by the XPS method, is 26%. The point of zero charge of this cerium oxide reaches 10 (the highest among already reported). The results also underline the exceptional performance of cerium oxide beads in the adsorption of arsenic species. At $\text{pH} = 7$, they demonstrate superior adsorption capacities for As(III) and As(V) species, with values of 230 mg g^{-1} and 111 mg g^{-1} , respectively, surpassing those of most reported adsorbents. The research also reveals that more than 50% of As(III) is oxidised to As(V) on the ceria surface, while Ce(IV) on the surface is reduced, leading to an increase in the atomic percentage of Ce(III) by about 9%.

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Nanostructured cerium oxide as a catalyst support for ethanol steam reforming for hydrogen production

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The catalytic steam reforming of ethanol (SRE) combined with carbon capture and storage is one of the promising processes for meeting all the requirements as a cost-effective and clean source of hydrogen. Over the past decade, significant progress has been made in the identification of the reaction pathways taking place in ethanol conversion towards hydrogen. From the recent findings, it follows that the improvement of ethanol reforming catalyst formulations should focus on the formation of active phase particles in the nano-size range [1]. It has been shown that the size of metal crystallites enhances both the activity and selectivity of catalysts and improves their long-term stability. Conversely, previous research has shown that the pore diameter of supports, regardless of their type, significantly impacts the active phase's average crystallite size [2]. Thus, employing a support for the active phase with a well-developed internal structure, favourably cerium oxide, is a highly promising approach and should facilitate the formation of tiny, well-dispersed crystallites of the active phase within the pores.

This study presents the high suitability of nanostructured cerium oxide beads as a support for the preparation of cobalt catalysts for ethanol steam reforming for hydrogen production. Comprehensive studies of the catalyst before and after ethanol steam reforming using a wide range of characterization techniques are presented. Cerium oxide was prepared *via* the one-step hard template method using resin Amberlite® XAD7HP as a template. The interior of the CeO₂ beads is hierarchically structured, with free volumes with dimensions on the nanoscale. These confined spaces favor the formation of nanosized, uniformly dispersed highly defective metal oxide crystallites in the non-reduced catalyst regardless of their preparation method. Moreover, in the case of a cobalt catalyst, the support promotes the formation of cobalt oxide species, which interact with them to varying degrees. Also, the smaller Co₃O₄ particles tend to transform into smaller Co particles.

The Co catalyst supported on the nanostructured cerium oxide is has high catalytic activity in SRE since it exhibits almost 100 % ethanol conversion at the early stage of the catalytic process. A well-developed internal surface of the catalyst and highly defective particles of support ensure the greater resistance of the Co catalyst supported on the templated cerium oxide to deactivation despite the formation of a carbon deposit.

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Synthesis and characterisation of mixed metal oxides obtained via a one-step hard template method, employed as catalytic supports

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Metal oxides are widely used in many industrial applications, including catalysis and adsorption. When used as a catalyst support, they provide a surface on which the (metal) active phase crystallites are deposited. Evenly dispersed metal nanoparticles play a pivotal role since they influence catalyst activity, selectivity and stability in various catalytic processes [1]. It has already been presented that the internal structure of supports, including the presence of small pores, significantly affects the size of the active phase crystallites and their dispersion [2]. Therefore, continuous efforts are being made to optimise existing synthesis methods to obtain nanocrystalline metal oxides with well-developed internal surfaces and small pore diameters. One of the effective methods for the synthesis of various metal oxides is the one-step hard template method. This method allows obtaining oxides in the form of spherical grains with a characteristic hierarchical structure, regardless of the synthesis conditions [3]. Cerium oxide is essential due to its specific properties. It is known that the reduction in the size and increase in the number of edges and corner atoms of crystallites of cerium oxide lead to an increase in the content of the Ce³⁺ species concerning Ce⁴⁺. The ability to switch between oxidation states, i.e., redox properties and the ability to store oxygen (OSC), is a key feature of this material and finds wide-ranging applications, including various catalytic processes [3]. Moreover, nanostructured, mesoporous cerium oxide favours deposition of the active phase nanocrystallites. Therefore, the synthesis of the nanocrystalline cerium oxide with well-developed internal surface is highly desired. Modifying this material by introducing an additional metal oxide, such as praseodymium oxide or zirconium oxide, expands the range of CeO₂ applications.

This work presents mixed oxides of Pr_xCe_{1-x}O₂ and Zr_xCe_{1-x}O₂ and corresponding monometallic oxides, namely CeO₂, PrO₂ and ZrO₂. These materials were obtained *via* the one-step hard template method using a porous non-ionic polymer resin Amberlite® XAD7HP as a template. The template microspheres were soaked in appropriate precursor solutions and calcinated to obtain porous oxides. The obtained materials were subjected to physicochemical analysis. The results indicate that the one-step hard template method is a suitable synthesis method for the formation of nanocrystalline products, including mixed oxides.

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Investigating ferroelectricity in perovskite oxides: implications for on-surface reactions and photocatalysis

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Perovskite oxides are well known for their diverse physical and chemical properties. Many of them exhibit excellent performance in photocatalysis and piezocatalysis. One of the reasons for this behaviour is their ferroelectricity [1],[2]. It was already shown that the ferroelectricity of a perovskite has an impact on the surface structure and its reactivity and this issue is currently widely researched [3]. Despite this, the origin of such properties remains insufficiently understood and awaits further research. To address this issue, this poster aims to unravel the connection between the ferroelectric properties of the perovskite oxides and on-surface reactions.

This work examines the differences in morphology and ferroelectric polarization at surfaces of paraelectric $\text{KTaO}_3(001)$ and ferroelectric $\text{KNbO}_3(001)$ and $\text{BaTiO}_3(001)$ crystals after *in-situ* and *ex-situ* cleaving. Initially, the cleaved perovskite surfaces exhibit (1x1) bulk-termination which transforms into (2x1) reconstruction after exposure to vapour water in ultra-high vacuum conditions (UHV). Nanoscale changes in the surface reconstruction were observed with AFM and STM microscopy together with LEED diffraction, while SEM microscopy and polarization camera were used to examine the large-scale ferroelectric domains structures. Furthermore, open-circuit photocurrent measurements were conducted on powdered perovskite crystals, both paraelectric and ferroelectric, to assess their photocatalytic abilities under ambient conditions. The temperature of the electrolyte during the measurements was raised to observe the influence of phase transition on the final photocurrents signal.

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Photocatalytic system for decomposition of non-CO₂ greenhouse gases

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Methane is a greenhouse gas the emission of which has a significant contribution to global warming. For many years the highest emission originated from anthropogenic sources – agriculture and wastes – and the rate of CH₄ production is still increasing [1]. Another gas emitted from livestock is ammonia, which can be toxic and harmful to our health. Many researchers now put effort into finding an efficient, low-cost method to reduce the concentration of greenhouse and toxic gases in the atmosphere.

One of the promising approaches to lower the anthropogenic emissions of CH₄ and NH₃ is to convert them to other non-harmful chemical compounds using catalysis [2,3]. In this work, we aimed to develop a photocatalytic system based on commercially available TiO₂ nanoparticles and synthesized CuO/ZnO composites, which could convert CH₄ and NH₃ under irradiation. Different CuO/ZnO powders were obtained using the most common synthesis methods – precipitation, sintering and photodeposition. The morphology and optical properties were characterized using Scanning Electron Microscopy and UV-Vis spectroscopy. The photocatalytic activity was evaluated in monitoring the degradation of methyl orange (MO) – the model pollutant. Photocatalysts deposited on the polypropylene support were irradiated with the UVA fluorescent blacklight lamp in the presence of the aqueous solution of the pollutant. The bleaching of the pollutant was monitored with UV-Vis spectroscopy. The most efficient photocatalysts were selected for the gas-phase tests under ambient conditions in our custom gas chamber, which contained a model volatile organic pollutant (HCOOH). The photocatalysts were deposited on a polypropylene net and irradiated with different light sources, both UV and visible. Changes in the pollutant concentrations were constantly monitored together with humidity, temperature and CO₂ concentration (Figure). The results of air purification will be presented and discussed.

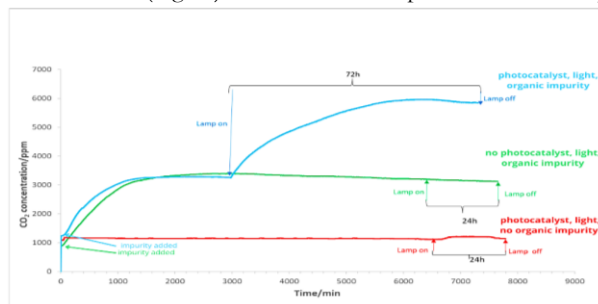


Figure. Photocatalytic degradation of HCOOH in the gas phase (observed as generation of CO₂) in the presence of TiO₂-based photocatalyst under UV-A light.

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Two-dimensional heterostructures of graphene and transition metal oxides for applications in optoelectronics

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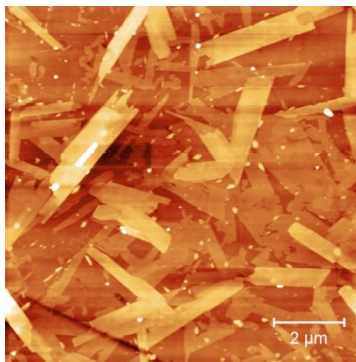
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Since the breakthrough discovery of graphene, two-dimensional (2D) materials have attracted a lot of attention due to their extraordinary properties in comparison with bulk counterparts. In particular, due to its high electrical conductivity, transparency in the visible range of electromagnetic radiation and flexibility, graphene can be considered as an electrode in the construction of an organic light-emitting diode (OLED). However, pristine, undoped graphene is not suitable for use as an electrode because the work function of graphene is not matched to the energy levels of the organic layers used for OLED fabrication.

Here we show that work function of graphene can be modified with transition metal oxides (TMO) such as: MoO₃, Re₂O₇ and heterostructures obtained meets the basic requirements for use as a transparent anode in OLED application. Additionally, we reveal that crystallinity of 2D materials is a key factor for efficient work function modification.

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AFM image of MoO₃/graphene heterostructure.

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Thermal behaviour of Ag-SiO₂-TiO₂ nanocomposites

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Nanomaterials with unique attributes for potential applications in regenerative medicine remains a focal point of scientific inquiry. Notably, titanium oxides are applied for surface modification of metallic implants due to their ability to enhance tissue integration and cell adhesion, critical for successful implantation. These surfaces also facilitate modifications with antibacterial elements like silver, further enhancing their utility [1,2]. Additionally, silica has found application in regenerative medicine by promoting bone structure formation and supporting fracture regeneration. Silica nanoparticles, with their high surface area, facile functionalization, and biocompatibility, are utilized in drug delivery and as anti-biofilm coatings on implants [3,4].

However, employing nanomaterials for implant surface modification often involves advanced surface engineering techniques that necessitate exposure to elevated temperatures. Thus, it becomes imperative to comprehensively characterize the structural changes, morphology, and properties of these materials under such conditions.

In this study, chemically synthesized Ag-SiO₂-TiO₂ nanocomposites were subjected to elevated temperatures for testing. High-temperature X-ray diffraction (HT-XRD) was utilized to analyze phase transformations within the nanocomposites, focusing particularly on changes in titanium oxide phases and alterations in unit cell parameters. Raman spectroscopy provided insights into the molecular and structural composition of the nanocomposites, complemented by thermogravimetry measurements. Characterizing the functional properties of the nanocomposites involved determining their sintering temperature and dimensional changes during heating. Research employing high-temperature microscopy and dilatometry revealed that the maximum annealing temperature should not exceed 900°C to preserve the desired properties of the nanocomposites. This comprehensive analysis gave valuable insights into the behavior of Ag-SiO₂-TiO₂ nanocomposites under elevated temperatures.

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The effect of modification of graphene oxide and reduced graphene oxide films with self-assembled monolayers on their wettability and tribological properties.

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The main goal of this work was to reveal the effect of modification of graphene-related materials (GRMs) by perfluoroalkylsilane and define the role of oxygen-functional groups located in graphene-related materials (GRMs) in modification by perfluoroalkylsilane on achieved wettability and tribological properties. The dip-coating technique was applied for graphene oxide (GO) deposition on silicon substrate. Ascorbic acid was used to reduce graphene oxide, leading to reduced graphene oxide (RGO). Scanning electron microscopy (SEM), Raman spectroscopy, and Fourier transformed infrared spectroscopy (FTIR) confirmed the morphology and structural differences of received graphene films. Modification of GO and RGO films were performed with the use of used for modification by perfluoroalkylsilane (1H,1H,2H,2H-perfluorodecyltrichlorosilane – FDTS) using chemical vapour phase deposition (VPD) method. Analysis and characterization of the obtained films were carried out using infrared spectroscopy (FT-IR), contact angle, surface energy, atomic force microscopy (AFM), and a microtribometer. Based on performed studies, it was found that oxygen functional groups localized on graphene surfaces determine the effectiveness of perfluoroalkylsilane deposition. It was found that the presence of the oxygen-functional groups enhances the self-organization of silane molecules. Therefore, in consequence, the modified GO film exhibits more hydrophobic properties and higher wear resistance.

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Effect of the Si stepped surface anisotropy on Si-Au structures

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Silicene is a two-dimensional material consisting of silicon atoms arranged in a honeycomb lattice [1]. This material is gaining significant interest as it shows potential as a promising alternative for current electronic technologies due to its expected high level of integration [2]. Similar to its precursor, graphene, silicene exhibits linear band dispersion forming Dirac cones, which endow it with unique properties [3].

A key difference between silicene and graphene is that silicene does not exist as a free-standing single layer. So far, silicene has been synthesized in an epitaxial form, predominantly using metal surfaces [4]. However, the presence of a metallic substrate can notably alter the electronic structure of silicene. On the other hand, the substrate serves as an excellent tool for the functionalization of silicene [5]. Strong interactions between silicene and the substrate can lead to the formation of new energy bands and, consequently, to novel exotic properties in complex silicene heterostructures, which are not found in the individual components.

The findings presented here refer to measurements of silicon structures on one-dimensional ordered substrates—specifically, stepped silicon surfaces coated with gold layers. The structures have been obtained in the process of surface segregation in Au thin films grown on Si substrates at annealing temperatures well below the Au-Si eutectic temperature. The surface exhibits plethora of various local phases, and loses its orderly, one-dimensional characteristics, leading to the appearance of broad, irregular terraces, as revealed by scanning tunneling microscopy (STM). Nonetheless, even on these altered structures, planar silicene was still observed alongside structures characteristic of silicon-gold compounds.

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Examining ferroelectricity on surfaces of oxide perovskites

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A tremendous interest towards perovskite materials has been shown in recent years due to their unique electronic and optical properties [1]. To fully understand the origin of those properties it is necessary to investigate not only bulk materials, but their surfaces as well. Processes bound to the surface are vital for large quantity of interactions with the material. Nowadays, one of the most intriguing topics connected with perovskite surfaces is their high (photo)catalytic efficiency, which is linked with the presence of surface charges that can be controlled by allowing atoms to reconstruct [2] or by tuning their ferroelectric state, which was utilized in the presented research.

This poster aims to present behavior of ferroelectric and incipient ferroelectric perovskite single crystalline materials. (001) surfaces of KNbO_3 (KNO), BaTiO_3 (BTO) and KTaO_3 (KTO) crystals were studied by the means of Scanning Electron Microscopy (SEM), under optical microscopy employing polarized light and various techniques based on Atomic Force Microscopy, e.g. Lateral Force Microscopy (LFM) or Piezoresponse Force Microscopy (PFM). SEM data provided lateral information on ferroelectric domain walls structure. Back-scattered electrons imaging proved to be especially sensitive to the orientation of ferroelectric phases, giving rise to a strong contrast dependence on the tilt angle. To provide information about the real potential of perovskite ferroelectrics, AFM measurements were conducted in ambient air and room temperature conditions. Friction signal in contact AFM provided information on the structure of 180° domain walls. Interestingly enough, results show that interactions between the scanning probe and domains are strong enough to not be disrupted by topographical traits such as multi-terraces. Presence of periodic modulation of optoelectronic and structural properties measured at normal conditions indicates that perovskite oxides' surfaces are promising for real-life applications, like piezo- and photocatalysis.

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Magnetic properties of antimonene/Co heterostructure formed by molecular beam epitaxy

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Antimonene is a mono-elemental two-dimensional material exhibiting unique properties distinguishing it from other monolayer representatives. These include the potential properties of a topological insulator [1], extremely low thermal conductivity [2], controlled displacement of Dirac cones [3] and very high stability in air [4]. Its excellent selective adsorption properties have recently resulted in the implementation of this material for sensing devices [5,6]. Despite the considerable knowledge accumulated since the discovery of this material, still less is known about its potential magnetic properties and practical ways to induce them. The purpose of the present study was to investigate the possibility of a magnetic proximity effect between a single layer of antimonene and a cobalt film.

The apparatus used both for preparation and study was a SPLEEM (Spin Polarized Low Energy Electron Microscope) equipped with a GaAs cathode enabling the emission of spin-polarized electrons for magnetic domains imaging. In addition to this unique technique, the standard modes of the microscope were used complementarily in real time: LEEM to study the surface morphology during preparation, and LEED to explore the crystallographic structure of the formed layers.

A ferromagnetic cobalt film (5 monolayers) was prepared using molecular beam epitaxy (MBE) on a monocrystalline W(110) substrate. Preparation was realized directly in the ultra high vacuum (UHV) (base pressure $3 \cdot 10^{-10}$ mbar) chamber of SPLEEM. In the next step antimonene layer was grown on a top of Co. The LEEM mode provided information on the mechanism of growth and enabled optimization of the preparation process. Using the LEED mode, the formation of alpha phase antimonene was confirmed. The size of its rectangular unit cell was determined as $4.43 (\pm 0.05)$ Å and $4.36 (\pm 0.05)$ Å. These values are consistent with literature data (4.48 Å and 4.31 Å [7]). It is worth noting that α -Sb unit cell on cobalt is almost square. SPLEEM studies revealed that after creation of antimonene, the heterostructure retains its ferromagnetic properties.

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Adsorption of organic dyes on TiO₂ nanoparticles

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Titanium dioxide in the form of nanoparticles is the most commonly used electron transport material in dye sensitized photovoltaic cells. However, the ultraviolet absorption ability of TiO₂ is not sufficient in solar cells, therefore dyes capable of using the visible light have to be employed as sensitizers. The adsorption of a sensitizing compound on the mesoporous semiconductor coating of an illuminated electrode leads to an extension of the absorption range of solar radiation [1]. Controlling the adsorption process of dye molecules is crucial to enhance charge transfer from the photoexcited dye molecule to the conduction band of TiO₂ [2].

The presented work includes scanning electron microscopy analysis of the photoanode coverage composed with TiO₂ nanoparticles, UV-Vis spectroscopic measurements of dye absorption in both free and adsorbed forms as well as characterization of photoelectrodes by electrochemical impedance spectroscopy, X-ray photoelectron spectroscopy and X-ray absorption spectroscopy. Metal-free organic dyes were tested, such as phenylfluorone and alizarin, and additionally, popular N719 ruthenium complex was used as a reference dye [3]. Adsorption of dye molecules was performed by immersing the TiO₂ layer in the dye solution, and the optimal combination of solution concentration and soaking time was established for each dye. Photocells were assembled and tested in the sunlight simulator to determine the photovoltaic parameters. The performance of the cells was improved by introducing a BaSO₄ back reflective layer and cell ageing, which facilitated electrolyte penetration between the sensitized nanoparticles.

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Charge density oscillations in topological Su-Schrieffer-Heeger chain

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Spatial charge oscillations in low-dimensional structures arise from the wave nature of electrons. In one-dimensional (1D) systems, these oscillations are known as Friedel oscillations and occur in confined structures with perturbed spatial potential due to lattice imperfections, impurities, dislocations, and boundary effects [1]. Even in perfectly ordered systems, electrons can form charge density waves (CDW) whose modulations are correlated with the atomic lattice constant.

In 1D regular chains, charge waves can have various oscillation periods, depending on the system's Fermi energy and chain parameters such as hopping integrals and on-site electron energies. A general analytical relation for these charge oscillations has been derived for such chains [2]. However, in topological chains which are characterized by an energy gap across the entire system, the presence of charge waves along the chain is not expected.

In this study, we demonstrate that under specific conditions (beyond chiral symmetry), charge density oscillations can indeed emerge in topological systems. These oscillations are attributed to the energy sidebands of the topological chain. Furthermore, we analyze the oscillation periods of these topological charge waves, which are determined by the average electron occupancy of the chain sites. Note that standing charge wave patterns along the chain or oscillations in the local density of states can be readily observed using Scanning Tunneling Microscopy (STM) techniques [3].

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Formation of plasmonically active nanostructures in bimetallic Ag-Cu thin films

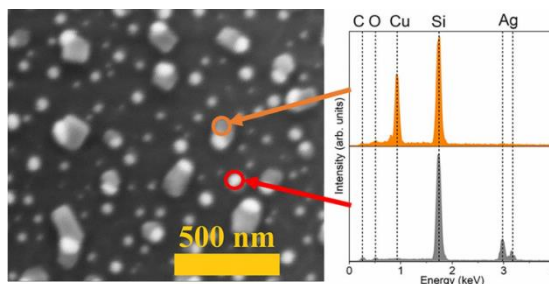
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Formation of plasmonically active silver, copper and composite silver-copper nanostructures were studied. Metallic nanostructures were fabricated by thermal disintegration, so called dewetting, of the thin films in an argon atmosphere. The formation process of the nanostructures was in-situ observed by a novel method, based on resistance measurements. The influence of the material and thickness of the initial thin film on temperature of their disintegration was investigated. Electrical measurements were validated by scanning electron microscopy observations, while metallic the behavior of nanostructures was studied by XPS method. The formation of silver-copper nanocomposite structures was confirmed by UV-vis spectroscopy. Plasmon resonance with two characteristic peaks for nanocomposite structures was observed.



Results of the EDS analysis in a selected two regions of nanostructures obtained by annealing of the 8 nm Ag-Cu bilayer at 800 K.

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The impact of gallic and rosmarinic acid on the physicochemical and biological properties of selected metal nanoparticles

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Gallic acid and rosmarinic acid, belonging to the class of low-molecular-weight polyphenols, display remarkable biological activity. Both polyphenols exhibit antioxidant properties and possess antibacterial and antiviral effects. Some literature reports have also suggested their potential in inhibiting cancer development. It has been established that gallic acid demonstrates anti-amyloidogenic activity against A β in buffered solutions and within cell membrane-like environments. Furthermore, these polyphenols have the ability to inhibit the aggregation of amyloid beta (A β) peptides and/or disassemble mature fibrils, making them promising candidates for Alzheimer's disease (AD) therapy.

However, there is limited understanding regarding the properties of nanoparticles synthesized using these polyphenols. It appears plausible that functionalizing metal nanoparticles with these polyphenols could result in the formation of nanoscale structures with desirable biological properties. Hence, the objective of this study was to synthesize and characterize the physicochemical and biological properties of silver nanoparticles (AgNPs) and platinum nanoparticles (PtNPs) stabilized by gallic and rosmarinic acid.

The metal nanoparticles were synthesized using a chemical reduction method employing sodium borohydride, followed by functionalization with the polyphenols. It was observed that by controlling the reaction conditions, nanoparticles of various sizes could be produced. TEM imaging revealed that the average size of quasi-spherical AgNPs and PtNPs ranged between 5 and 30 nm. Analysis using SERS confirmed effective functionalization of the nanoparticles by these polyphenols. It was noted that each type of gallic and rosmarinic acid-stabilized metal nanoparticles exhibited a negative surface charge over a wide range of ionic strengths and pH levels. However, the stability of the nanoparticles decreased under acidic conditions and at high ionic strengths (> 0.03 M). Changes in mitochondrial activity and secretion of inflammatory and apoptotic mediators were studied following exposure of human promyelocytic (HL-60) and neuroblastoma (SK-N-SH) cells to AgNPs and PtNPs, aiming to determine the impact of polyphenols on the biological activity of nanoparticles. It was observed that for given size and mass concentration, the toxicity of AgNPs was higher than that of PtNPs. Both types of nanoparticles exhibited a strong reduction in mitochondrial activity and induced secretion of interleukin-6 (IL-6), tumor necrosis factor- α , and caspase 9. The addition of pure polyphenols to the metal nanoparticle suspensions was found to influence their biological activity. The results suggest that the presence of polyphenols on the surface of metal nanoparticles is the primary factor shaping their toxicity. However, the toxic effect can also be modulated by the introduction of free polyphenols into the metal nanoparticle suspensions.

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Dynamically reconfigurable helical nanofilaments entwined with liquid crystalline gold nanobipyramids

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The 20th century witnessed remarkable advancements in electricity-based technologies. In the 21st century, technologies predicated on the manipulation and processing of light are anticipated to play an equally pivotal role, enabling access to devices with extraordinary properties not found in nature (metamaterials), ultra-sensitive detectors (plasmonic sensors), ultrafast computational systems (optical computers), and light-mediated reactions (hot electron chemistry). Theoretical studies indicate that one approach to realizing these ambitions involves constructing devices predicated on nanoparticles with strong light interaction capabilities. Consequently, scientists and engineers are confronted with the challenge of synthesizing materials with precisely and dynamically controlled structural parameters, particularly the spatial arrangement of nanoparticles.

In the realm of metamaterials and biosensor technology, materials exhibiting optical chirality in the UV-Visible spectrum are of significant interest. Chirality, a ubiquitous phenomenon in nature, serves as a source of artistic inspiration and is a crucial factor in the advancement of photonic technologies. Additionally, chirality holds substantial importance for the future of optoelectronic technologies. Chiral systems, such as those based on metallic nanoparticles (e.g., helical configurations), are of particular interest [1,2].

In this project, three primary objectives were accomplished. The first objective involved the phase transfer of nanobipyramids, with dimensions up to 54x18 nm, from an aqueous to a hydrophobic environment without altering their morphology. The second objective was to achieve chemical compatibility between the bipyramids and the organic matrix, facilitating the helical alignment of the nanoparticles. The final objective entailed optimizing the system to attain the maximal chiral response in the plasmonic range. Structural analyses were conducted using transmission electron microscopy, while functional evaluations were performed using circular dichroism and UV-Vis spectroscopy.

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Thermal treatment of ultrathin silicene-gold heterostructures – STM study

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The famous discovery of graphene opened a whole branch of material science, intensifying research of two-dimensional materials. Since then, much focus has been pointed at ultrathin materials such as 2D-Xenes or transition metal dichalcogenides, thanks to their unique properties and appearance of uncommon phenomena (e.g. quantum spin Hall effect). Among other two-dimensional materials, thanks to compatibility with current silicon electronics, gather silicene – silicon analogue of graphene.

In contrast to other planar structures, silicene does not appear in free-standing form – it requires support. There are already a multitude substrates reported as suitable for silicene growth [1]. In particular note, silicon Si(111) – one of the most widely utilized substrates in modern electronics – is among them. After deposition of ultrathin metal films on Si(111) it is possible to synthesize silicene, with lead [2] and gold [3] as already reported examples. In the latter case, several possible phases are possible to obtain [4]. On the negative side of this process, this process is highly sensitive to temperature, and multiple phases appear in narrow temperature window, with multilayer structure or complete lack of silicene being probable outcomes.

The results of preliminary studies on different silicon-gold heterostructures, including silicene, will be presented. Special focus will be pointed towards the significant influence of the synthesis temperature. Structures were examined using scanning tunneling microscope (STM) and reflection high-energy electron diffraction (RHEED). Results reveal the crystal structure of the obtained heterostructures and establish a point towards optimization of silicene synthesis and application-oriented studies.

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Insights into the mechanism of the photoactivity of titanium dioxide decorated with plasmonic nanostructures

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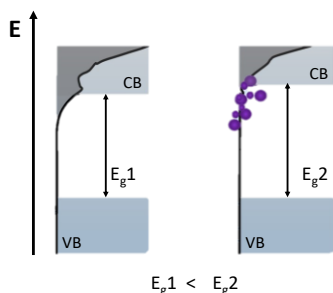
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Heterogeneous plasmonic photocatalysis is a widely developing field nowadays. Metallic nanostructures exhibit the phenomenon of localized surface plasmon resonance (LSPR) which is considered to be responsible for the photoactivity of plasmonic photocatalysts under visible light irradiation. A lot of scientists reports the advantageous influence of LSPR on the modified photocatalysts activity [1-3]. Nevertheless, despite the fact that the presence of metallic nanostructures can be advantageous, the mechanisms of activity increment still remain unclear. Hot-electrons injection or plasmon induced resonance energy transfer processes are mostly acknowledged for the visible light activity. Although these mechanisms are physically possible and their existence has been proven, they are not very efficient at a significant scale. Moreover, these mechanisms may not be prevalent in the case of particular photocatalyst. Therefore, the substantial activity initiation in plasmonic photocatalysts under visible light irradiation driven via mentioned mechanisms is disputable. Another issue is the explanation of changes in the activity in UV range which are often neglected in the era of the activity range extension towards visible light. These changes may be also significant, *e.g.* in the case of full-spectrum irradiation (*i.e.* solar or simulated solar light utilization), and can even influence the photocatalyst activity much more than the plasmonic effect.

During presented research, the influence of plasmonic nanostructures presence on the activity of titanium dioxide was examined. Metallic nanostructures were photodeposited at the TiO₂ surface and the photocatalytic activity was assessed with terephthalic acid hydroxylation reaction or hydrogen evolution reaction. For further understanding, investigation of spectral, photoelectrochemical and spectroelectrochemical properties of modified materials were performed.

Received results indicate that the influence of metals, serving as the electron sinks, and the changes in the electronic structure of modified materials are the most important in terms of activity, whereas the presence of SPR phenomenon is not. Therefore, implementing of SPR in every mechanism of activity of photocatalytic materials decorated with metallic nanostructures should be reconsidered. Authors would like to acknowledge National Science Centre in Poland for financial support within Solar-Driven Chemistry project (2019/01/Y/ST5/00027).



Scheme with the results of spectroelectrochemical measurements depicting the changes in the electronic structure of the TiO₂ before and after deposition of metallic nanostructures.

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The effect of the laser wavelength on the ablation of the (Cd,Cr)Te and CrTe material

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The two-dimensional magnetically anisotropic materials show tremendous potential in the development of next-generation scalable devices, based on the spin transport in atomically thin layers. Chromium telluride compounds are currently considered very perspective types of 2D magnets because of their chemical stability in ambient conditions and ability to retain magnetic ordering at RT down to the monolayer [1]. To date, Cr-Te phases were obtained in the form of atomically thin layers by molecular beam epitaxy and, mainly, by ambient pressure chemical vapor deposition utilizing Te powder and Cr powder or chromium chlorides as the precursors [1].

In this work, we report the first attempt to obtain chromium telluride layers by the pulse laser deposition technique. The first ($\lambda=1064$ nm) and the fourth ($\lambda=266$ nm) harmonics of the YAG Nd³⁺ laser were used to deposit the targets in the form of the pressed pellets of Cr₂Te₃ powder or mixture of Cd and Cr₂Te₃ powder onto the KCl single crystalline substrate. Scanning electron microscopy and energy-dispersive X-ray analysis were performed to evaluate the alteration of the target morphology and composition caused by the laser ablation. Selected area electron diffraction, high-resolution X-ray photoemission spectroscopy, high-resolution transmission electron microscopy and high-angle-annular dark-field scanning transmission electron microscopy methods were utilized for the comprehensive characterization of the deposited layers. CdTe films with zinc blende structure were obtained by infrared irradiation of the Cd+Cr₂Te₃ pellets and pure polycrystalline Te films were obtained by IR irradiation of the Cr₂Te₃ pellets, with no detectable chromium in both cases. Ultra-nanocrystalline films composed of elemental Cd, Te and Cr having high chromium content were deposited by ultraviolet irradiation independently for used targets. The observed difference is explained by different types of laser beam-target interaction. IR laser pulses cause photo-thermal ablation in consequence of the target's heating. As a result, Cr₂Te₃ decomposition due to the thermal instability of this compound [2] and subsequent evaporation of more volatile Cd and Te occurred, but not Cr, whose partial pressure is quite low at the temperature of the experiment [3]. Contrary, the energy of UV quanta is high enough to break the bonds between the atoms in Cr₂Te₃ resulting in photochemical ablation mode and sputtering of all the elements from the targets. The presented results clearly indicated that UV laser is preferred for the PLD of Cr-Te compounds. The experiments to determine the conditions providing the formation of the high-quality thin layer of these compounds on the substrate are now in progress.

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Endophytes and silver nanoparticles: Promising anti-phytopathogens agent

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Endophytic fungi are plant-associated microorganisms that colonize the internal tissues of the host without inducing disease symptoms. The great ability of adaptation to different environments and the expression of high amounts of biological compounds make endophytes to be considered for biotechnological applications. Their properties apply to different areas and are highly useful in different sectors of industries. In the aim of protect biodiversity and reduce environmental pollution caused by chemical pesticides, there is growing interest by researchers all over the world in bioprospecting alternative methods in plant protection. Nanotechnology presents itself as one of the promising technology that can be employed to overcome these challenges. A number of reports are available on the biological synthesis of nanoparticles, but the potential of endophytic fungi in this respect has not yet been fully explored. The aim of studies were mycosynthesis of AgNPs performed by using *Arcopilus aureus*, *Boeremia exigua* var. *exigua* and *Fusarium* sp. as an endophytic fungi, characteristic of synthesized AgNPs and their antifungal assay towards *Boeremia strasserii*, *Colletotrichum fuscum* and *Sclerotinia sclerotiorum*. Morphological features of endophytes were integrated with sequencing of relevant DNA markers, namely ITS, *tef-1*, the RNA polymerase II (*rpb2*) and β -tubulin (*tub*) genes. The synthesis of the AgNPs was initiated by adding 30 mM AgNO₃ in 100 mL of mycelium cell-free filtrate and the reaction mixture was incubated in shaking incubator at 27°C for 96 hrs. with 180 rpm per minute in dark. The primary detection of AgNPs was carried out by visual observation of color change after treatment of fungal extract with AgNO₃. X-ray diffraction and scanning electron microscope (SEM) with detector for transmission revealed the formation of different shapes AgNPs, mainly hexagonal and triangular with sizes in the range of 10–100 nm. The findings of inhibition zone test showed a desirable antifungal activity of AgNPs against tested phytopathogens.

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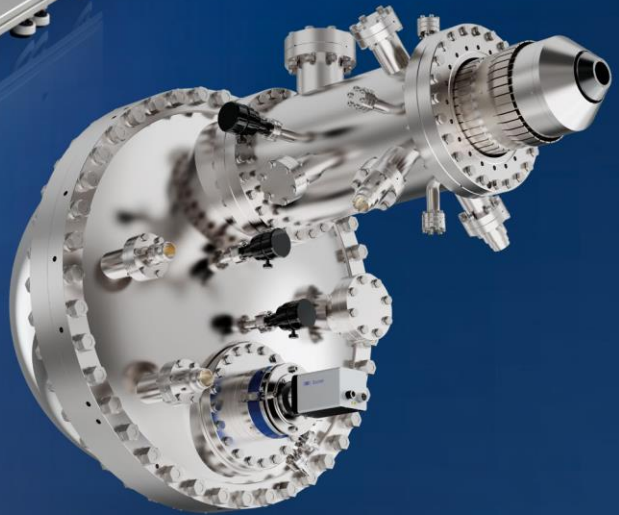


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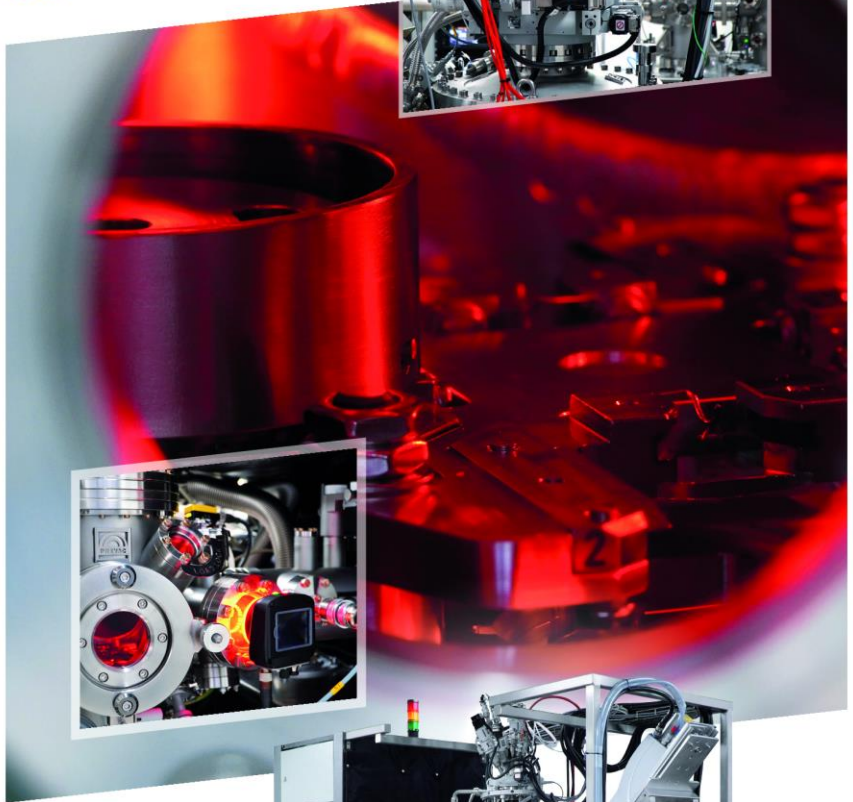
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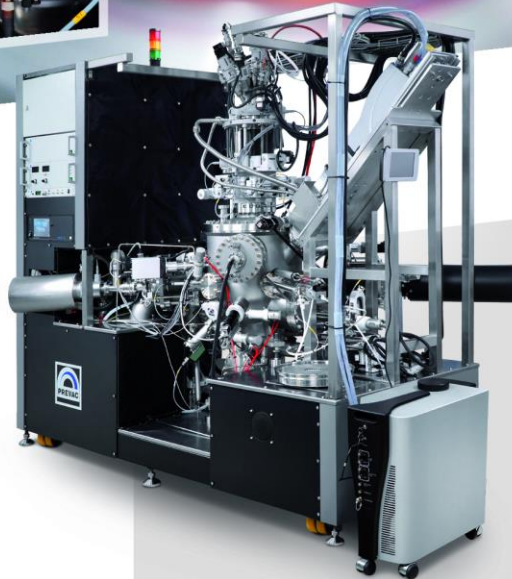


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