

6th Erwin Schrödinger Symposium 2023
of the Erwin Schrödinger Society for Nanosciences
„From Nanostructure to Function“

<https://esg-nano.ac.at/>

&

**4th European Conference on Physical Chemistry
(ECPC23)**

of the Division of Physical Chemistry of the
European Chemical Society (EuChemS)

<https://www.euchems.eu/>



October 9-11, 2023
Vorarlberg University of Applied Sciences, Dornbirn
Vorarlberg, Austria

Committee: Oskar Armbruster, Fadi Dohnal, Eva-Kathrin Ehmoser, Wolfgang Kautek,
Aida Naghilou, Sandra Stroj





Foreword

The **6th Erwin Schrödinger Symposium 2023** of the Erwin Schrödinger Society for Nanosciences “**From Nanostructure to Function**” and the **4th European Conference on Physical Chemistry (ECPC23)** held by the Division of Physical Chemistry of the European Chemical Society (EuChemS) aim to stimulate vivid scientific communication and discussion in synthetic, biogenetic, and biomimetic interfacial nanosciences in relation to their fabrication methods, characterization properties, size effects, applications, and modeling of features and structures.

This symposium is organized by the Erwin Schrödinger Society for Nanosciences and the EuChemS Division of Physical Chemistry in a series of successful predecessor events:

- **1st Erwin Schrödinger Symposium 2014**
“**Two Dimensional Nanostructures**”
(November 2014, Vienna, Austria)
- **1st European Conference on Physical and Theoretical Chemistry**
(September 2015, Catania, Italy)
- **2nd Erwin Schrödinger Symposium 2016**
“**Zero Dimensional Nanostructures: Science and Technology of Nanoparticles**”
(May 2016, Vienna, Austria)
- **2nd European Conference on Physical Chemistry - ECPC17**
(September 2017, Borgo, Italy)
- **3rd Erwin Schrödinger Symposium 2018**
“**Progress in Interfacial Nanosciences**”
(July 2018, Dornbirn, Austria)
- **3rd European Conference on Physical Chemistry - ECPC19**
(May/June 2019, Jena, Germany)
- **4th Erwin Schrödinger Symposium 2021**
“**Advanced Materials**”
(January 2021, online)
- **5th Erwin Schrödinger Symposium 2023**
“**Challenges in Nanoscience & Application**”
(March 2023, Mauterndorf, Austria)

International invited experts will illustrate the importance of nanosciences and nanotechnology in future applications. Scientists can contribute their recent research in poster sessions. The conference features active discussions in lecture and poster sessions.

Vienna and Dornbirn; September 2023

The Organizing Committee

Oskar Armbruster
Fadi Dohnal
Eva-Kathrin Ehmoser
Wolfgang Kautek
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Program

Monday, October 9, 2023

09:00 – 09:30 **Registration**

09:30 – 09:45 **Opening and greetings**

09:45 – 10:15 **L01** Anke Weidenkaff (Fraunhofer Society, DE)

Circular Materials, Green Innovations and Biologization for Sustainability

10:15 – 10:45 **L02** Barbara Hribar Lee (University of Ljubljana, SI)

The influence of buffers and other excipients on the mechanism of amyloid fibril formation

10:45 – 11:15 **L03** Mihai Irimia-Vladu (Johannes Kepler University Linz, AT)

The avenue to "Green" in Organic Bioelectronics

11:15 – 12:30 **Poster short lectures**

12:30 – 14:00 **Lunch break & poster session**

14:00 – 14:30 **L04** Alexander Kromka (Czech Academy of Sciences, CZ)

Diamond interfaces for gas and bio sensors

14:30 – 15:00 **L05** Dana Seyringer (Vorarlberg University of Applied Sciences, AT)

Passive optical components for telecom and medical applications

15:00 – 15:30 **L06** Ota Samek (Czech Academy of Sciences, CZ)

The potential of surface-enhanced Raman spectroscopy in clinical setting

15:30 – 16:00 **Coffee**

16:00 – 16:30 **L07** Gavin Macauley (Paul Scherrer Institute, CH)

Artificial Spin Ices: Phase Transitions and Functionality in Arrays of Correlated Nanomagnets

16:30 – 17:00 **L08** Alexander Pogany (Ministry of Climate Action, Environment, Energy, Mobility, Innovation and Technology, AT)

Austrian Research Policy in Nanotechnology

17:00 **Lab tours**





Tuesday, October 10, 2023

- 09:00 – 09:30 **L09** Stefan Willitsch (University of Basel, CH)
Coupling a single trapped ion to a nanomechanical oscillator
- 09:30 – 10:00 **L10** Javier Martín-Sánchez (University of Oviedo, ES)
Nanophotonics in Two-Dimensional Materials
- 10:00 – 10:30 **L11** Moritz Brehm (Johannes Kepler University Linz, AT)
Novel Si-based quantum- and nanoelectronic platforms based on ultra-cold epitaxy
- 10:30 – 11:00 **Coffee**
- 11:00 – 11:30 **L12** Heinz P. Huber (Munich University of Applied Sciences, DE)
Towards an Experimentally Validated Model of Ultrafast Laser Ablation
- 11:30 – 12:00 **L13** Dimitrios Giannakoudakis (Aristotle University of Thessaloniki, GR)
Tuning on demand the physicochemical features of titanium oxide based nanomaterials towards photocatalytic biomass valorization and environmental remediation applications
- 12:00 – 12:30 **L14** Sefik Suzer (Bilkent University, TR)
Local Potential Variations Captured by XPS Provides the Missing Link about Charge Dynamics
- 12:30 – 14:00 **Lunch break & poster session**
- 14:00 – 14:30 **L15** Eckart Rühl (Free University of Berlin, DE)
Label-Free Spectromicroscopy as a Quantitative Probe for Dermal Drug Delivery
- 14:30 – 15:00 **L16** Lars Mohrhusen (Aarhus University, DK)
Nanostructured MoS₂-based catalysts for hydrodeoxygenation of bio-oils: Combining XPS and STM from UHV to operando conditions
- 15:00 – 15:30 **L17** Parvaneh Mokarian (Trinity College Dublin, IE)
Large-area nanopatterning for broadband, quasi-omnidirectional low-reflectance glass
- 15:30 – 16:00 **Coffee**
- 16:00 – 16:30 **L18** Sylvie Choua (University of Strasbourg, FR)
Redox-active metal-organic frameworks in electrode materials for lithium-ion batteries: an EPR study.
- 16:30 – 17:00 **L19** Giovanni Marletta (University of Catania, IT)
Physical-Chemistry at Biointerfaces: From Nanostructures to "Softness"
- 17:00 **Lab tours**



Wednesday, October 11, 2023

- 09:00 – 09:30 **L20** Leonid Zhigilei (University of Virginia, US)
Nanoscale mechanisms of tensile deformation, fracture, and heat transfer in carbon fibers: Insights from large-scale atomistic simulations
- 09:30 – 10:00 **L21** Matthias Domke (Vorarlberg University of Applied Sciences, AT)
Laser-induced generation and transfer of micro and nano particles for electroless deposition of conductive copper structures on textiles
- 10:00 – 10:30 **L22** Noemí Aguiló Aguayo (University of Innsbruck, AT)
Generation of conductive lines and structural coloration on nanostructured-modified textiles
- 10:30 – 11:00 **Coffee**
- 11:00 – 11:30 **L23** Gyözö G. Láng (Eötvös Loránd University, HU)
Impedance analysis of poly(3,4-ethylenedioxythiophene) modified electrodes - stability, thickness distribution and non-stationarity
- 11:30 – 12:00 **L24** Halil İbrahim Okur (Bilkent University, TR)
What can we learn about interfaces from hydration water?
- 12:00 – 12:30 **L25** Wolfgang Kautek (University of Vienna, AT)
Laser diagnostics and interventions in conservation science: historical and synthetic copper patina
- 12:30 – 14:00 **Lunch break & poster session**
- 14:00 – 14:30 **L26** Friedrich Esch (Technical University of Munich, DE)
Monitoring the dynamics of cluster/oxide support systems
- 14:30 – 15:00 **L27** Gabriel Vanko (Slovak Academy of Sciences, SK)
Gallium nitride based heterostructures for sensor applications
- 15:00 – 15:30 **L28** Nina Plankensteiner (Interuniversity Microelectronics Centre, BE)
High surface area 3D nanowire-networks as electrodes for water electrolysis and electrocatalytic CO₂ reduction
- 15:30 – 16:00 **Coffee**
- 16:00 – 16:30 **L29** Juan A. Allegretto (Danube Private University, AT)
Tailoring plasmonics and MOFs: nanostructuring MOF-based SERS substrates towards VOC sensing devices
- 16:30 – 17:00 **L30** Aras Kartouzian (Technical University of Munich, DE)
Unlocking the Hidden Dimension: The Power of Chirality in Scientific Exploration
- 17:00 **Closing & farewell**









Lecture Abstracts



L01

Circular Materials, Green Innovations and Biologization for Sustainability

Anke Weidenkaff

Fraunhofer IWKS and TU Darmstadt

The transformation to a future green circular economy will be based on green materials and ecologic innovations. The development of renewable materials for renewable energy converters requires sustainable large-scale production from secondary raw materials. The decision making for future resilient energy systems has to be based on environmental aspects as well as on performance criteria defined by a holistic life cycle assessment.

In this lecture an efficient circularity of materials with a programmable lifetime and regeneration will be introduced as a suitable approach. The design of circular high performance materials uses theoretical predictions and the criticality analysis of applied elements to improve the cycle life of future energy converters such as thermoelectric generators and refrigerators, batteries, electrolyzers, fuel cells, plasmasplitters, hydrides and solar watersplitting cells.





The influence of buffers and other excipients on the mechanism of amyloid fibril formation

Barbara Hribar-Lee, Sandi Brudar, Matej Jaklin

University of Ljubljana, Faculty of Chemistry and Chemical Technology

Amyloid fibrils are highly ordered protein aggregates that we found to play an important role in the development of various neurological disorders. Although there are a number of experimental studies investigating how and how fast amyloid fibrils form, the exact mechanism of their formation is still unknown. Our recent studies on the fibrillization mechanism of hen egg white lysozyme (HEWL) and β -lactoglobulin (BLG) show that buffer is an important factor determining the fibrillization pathway. HEWL, for example, forms amyloid fibrils in glycine, but not in phosphate buffer. In the case of BLG, glycine acts as a hydrolysis inhibitor, which consequently promotes a very different fibrillization pathway than in water. Here we combine various experimental techniques (AFM, TEM, CD, etc.) with molecular dynamics all atom computer simulations to explain the role of buffer and other excipient molecules on the mechanism of fibril formation in these solutions.



L03

The avenue to “Green” in Organic Bioelectronics

Mihai Irimia-Vladu

Johannes Kepler University Linz, Austria

Through its appealing avenues of processing the component devices at room temperature and from low-cost precursor materials, organic electronics has a tremendous potential for the development of products able to achieve the goals of production sustainability as well as environmental and human friendliness for electronics.

In an effort to stave off the e-waste growth, the presenter and his research group went further down the path opened by organic electronics research and investigated a large number of biomaterials as substrates, dielectrics, semiconductors and smoothing layers for the fabrication of organic field effect transistors, integrated circuits and organic solar cells. The presentation will focus on the highlights of our recent research, especially with respect to materials investigated, devices fabricated and the immense potential for follow up research:

- Flexible natural and biodegradable substrates
- Natural dielectrics
- Bio-origin, H-bonded semiconductors in the families of indigos, anthraquinones and acridones
- Bio-degradation protocols for organic semiconductors

These highlights will be placed in the context of the mountain that one has to climb in order to reach the coveted “green” connotation for electronics, sensors and integrated circuits:

- Biocompatibility issue
- Biodegradability issue
- Compostability issue
- Cost of production / energy expended in production issue
- Materials choice issue (carbon foot print)
- Toxicity and the environmental impact of the synthetic avenue for component materials

The potential of follow-up research in the green electronics field is immense, with large area electronics fabrication, biomedical implants, bio-sensing and smart labeling, representing only the tip of the iceberg of many more immediate possibilities of high interest for our group. Natural and nature-inspired materials have the unrivalled capability to create “safe-first” electronic markets for human and environment, with minimal or even neutral carbon footprint.





Diamond interfaces for gas and bio sensors

Alexander Kromka

Institute of Physics of the Czech Academy of Sciences

The detection and monitoring of harmful gases in the air and the identification of biological events in nature using semiconductor devices play a key role in modern society. A natural consequence of this trend is the increasing demand for the introduction of novel materials that can offer suitable sensitivity and selectivity including new sensing principles, fast and reliable response, biocompatibility and safety, and easy fabrication and use at low cost [1,2]. From a large family of modern materials, much attention has recently been focused on carbon-based materials [3], especially on synthetic diamond films that exhibit an extraordinary combination of advantageous properties in one platform (targeted adjustable functionality, high chemical sensitivity, and stability, semiconductor properties, active optical properties, and transparency, biocompatibility, large-area production, etc.) [4].

In this contribution, the latest advances in chemical vapor deposition and the effects of process conditions (plasma properties, gas composition, process pressure, temperature) on the resulting properties of the diamond coatings and their surfaces for sensing applications will be presented [5]. The hydrogen-terminated diamond film will be shown to be an effective gas-sensing active layer suitable for the detection of mixtures of oxidizing or reducing gases (NO_2 vs. NH_3) at room temperatures [6]. Here, the intrinsic and optically transparent diamond coating is used as an insulating material in which the hydrogen termination induces a surface 2D hole conductivity highly sensitive to the surrounding conditions (gas molecules, pH, biomolecules, or cells). The influence of nano-structured surface morphology on the sensor response will be pointed out. Furthermore, the parameters of the H-diamond layer will be compared with the commercial SnO_2 gas-sensing layer and the differences in their gas sensing principles will be discussed.

Next, the influence of diamond surface chemical terminations and (nano-) structured morphology on the patterned growth of different cell lines will be shown to be a crucial issue for further bioelectronics application of diamond coatings [7]. The use of H-terminated diamond-based field-effect transistors for label-free monitoring of proteins or cells will be discussed in detail [8]. Basic knowledge of real-time monitoring of biomolecules/cells adhered on the diamond surface in terms of sensor sensitivity, stability, and reliability will be critically pointed out. Finally, the new principles of biosensing with diamond devices (impedance, optical, mass, etc.) will be also presented.

- [1] J. Chu et al., *Physical Chemistry Chemical Physics*, 2023, 25, 12668.
- [2] D. Sadighbayan et al., *TrAC Trends in Analytical Chemistry*, 2020, 133, 116067.
- [3] R. Eivazzadeh-Keihan et al., *Chemical Engineering Journal*, 2022, 442, 136183.
- [4] S. Handschuh-Wang et al., *Small*, 2021, 17, 2007529.
- [5] M. Varga et al., *ACS Omega*, 2019, 4, 8441.
- [6] M. Davydova et al., *Beilstein Journal of Nanotechnology*, 2014, 5, 2339.
- [7] A. Broz et al., *Journal of Biomedical Materials Research Part A*, 2017, 105, 1469.
- [8] M. Krátká et al., *Colloids and Surfaces B: Biointerfaces*, 2021, 204, 111689.



L05

Passive optical components for telecom and medical applications

Dana Seyringer

Vorarlberg University of Applied Sciences

This presentation gives a brief overview of passive optical components, in particular optical splitters and optical demultiplexers, that were designed in Research Centre for Microtechnology for telecom and medical applications. Most of the designs were also technologically realized as a part of national and international projects.





The potential of surface-enhanced Raman spectroscopy in clinical setting

Ota Samek

Institute of Scientific Instruments of the Czech Academy of Sciences, Královopolská 147, 612 00 Brno, Czech Republic

The ability to identify and characterize microorganisms from tiny sample volumes in a rapid and reliable way is the first and crucial step in the diagnostics of microbial infections. Ideal analytical techniques would require minimal and low-cost sample preparation, permit automatic analysis of many serial samples, and allow rapid classification of present microorganisms against a stable database.

In this talk, we will focus on the surface-enhanced Raman spectroscopy (SERS) technique which combines nanotechnology with Raman spectroscopy to produce an ultrasensitive and highly specific analytical tool. We will highlight the challenges of the SERS technique which could possibly contribute to the development of the biosensor which would enable quick and convenient point-of-care testing for the clinical diagnostics of body fluids, bacteria, cells, and tissues. Thus, early and accurate infection disease management can be provided at the bedside, outpatient clinics or at remote care centres.



L07

Artificial Spin Ices: Phase Transitions and Functionality in Arrays of Correlated Nanomagnets

Gavin M. Macauley^{1,2}, Luca Berchiolla^{1,2}, Aleksandra Pac^{1,2}, Tianyue Wang^{1,2}, Rhea Stewart^{1,2,†}, Armin Kleibert³, Valerio Scagnoli^{1,2}, Peter M. Derlet^{1,4}, Laura J. Heyderman^{1,2}

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Artificial spin ices are arrays of strongly correlated nanomagnets, which are coupled through the dipolar interaction [1]. While originally envisaged as a two-dimensional analogue to frustrated rare-earth pyrochlores, they are now studied since they exhibit behaviour such as glassiness [2] and charge fragmentation [3], and topologically induced textures such as magnetic ‘monopoles’ [4].

The aspect ratio of the nanomagnets is usually chosen so that they behave as single magnetic domains, which can be described by means of an Ising variable. The long-range dipolar interaction between nanomagnets mixes spin and spatial degrees of freedom. As a result, the physics of these systems is strongly dependent on the exact position and orientation of the nanomagnets.

Unlike in conventional bulk spin ice materials, the microstate of these systems can be imaged in real space using magnetic microscopy techniques. In doing so, we can examine the response of the artificial spin ice to applied field, electrical current, or temperature.

In this talk, I will introduce artificial spin ice and discuss some recent work performed in our group. By way of example, I will discuss how they can be used as a platform to study phase transitions by focusing on the example of the kagome artificial spin ice. This is a highly frustrated system that undergoes two separate ordering transitions. By rotating each nanomagnet in the kagome lattice about its centre, we gain access to a rich phase diagram [5]. Using a combination of magnetic force microscopy to characterise the as-grown states and x-ray photoemission electron microscopy to observe the thermally-active states, we have determined how ordering proceeds in the different arrays. We find that the rotation maps from a spin ice sector near hexagonal geometries to a ferromagnetic phase, and then to a flux closed state.

Finally, I will discuss some proposals about how these artificial spin systems can be functionalized for use in novel computational schemes.

[1] Skjærvø, S.H., Marrows, C.H., Stamps, R.L. and Heyderman, L.J. *Nat. Rev. Phys.* 2, 13–28 (2020).

[2] Morley, S.A., Alba Venero, D., Porro, J.M. et al. *Phys. Rev. B* 95, 104422 (2017).

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[5] In preparation (2023).





Austrian Research Policy in Nanotechnology

Alexander Pogány

BMK

Nanotechnology can contribute to solve the major societal challenges of Europe with regard to energy efficiency, the ageing society, safety and security as well as the European knowledge society. These technologies are Key enabling technologies and the EC makes strong efforts to address these topics under H2020. Austria is well positioned in the photonics and nanotech area. The BMK has initiated platforms with stakeholders from Research and Industry to network and to establish R&D-roadmaps. The BMK runs a big Research programme called "Production of the Future" which includes Nanotechnology and Photonics. Within this programme R&D-projects between research and Industry can be funded. Austria is also taking part in several ERA-Nets in photonics and nanotechnology in order to help research and industry to cooperate with partners abroad. Additionally the BMK has established a strong cooperation with China with the goal to fund R&D-Projects between Austrian counterparts and the Chinese Academy of Science.



L09

Coupling a single trapped ion to a nanomechanical oscillator

M. Weegen, P. Fountas, M. Poggio, S. Willitsch

Departments of Chemistry and Physics, University of Basel, Switzerland

Ultracold trapped ions in radiofrequency traps are well-established and highly controllable quantum systems which find applications in precision spectroscopy, cold chemistry, quantum information and optical clocks. Nanomechanical oscillators play an important role in sensing applications. Their nanoscopic size makes them excellent candidates for the study of physics on the border of classical and quantum regimes and highly susceptible to weak forces. In this talk, we report on the first implementation of an ion-nanowire hybrid system to explore new methods for quantum state preparation, manipulation and readout via the mutual interaction of its constituents. A charged metallic nanowire is positioned in close proximity to a trapped ion such that both systems can be coupled by electrostatic interactions. We demonstrate the resonant coupling between the two systems and characterise the manipulation of the ion motion by the action of the nanooscillator.





Nanophotonics in Two-Dimensional Materials

Javier Martín-Sánchez

Department of Physics, University of Oviedo, Oviedo, Spain.
Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC–University of Oviedo), El Entrego 33940, Spain.

Two-dimensional materials represent a very rich and promising platform for many applications in nanophotonics. For quantum photonic applications, the development of novel ultra-compact two-dimensional (2D) photonic technologies relies on our ability to fabricate single photon sources (SPS) in 2D van der Waals materials where we are able to control their position as well as their optical emission properties [1]. The challenge still remains to fully understand their physical origin in order to be able to efficiently utilize them and to actively tune their optical properties. One solution is to implement elastic strain engineering through the introduction of a novel class of piezoelectric actuators [2].

On the other hand, controlling light at the nanoscale (nanolight or the so-called polaritons -hybrid light-matter excitation-) play a crucial role in fundamental and applied sciences. Particularly, the recent demonstration of infrared (IR) phonon polaritons (PhPs) – light coupled to lattice vibrations – exhibiting ultra-low losses and sub-diffractive light confinement in van der Waals (vdW) materials [3] set the grounds for an IR nanophotonics. In this regard, anisotropic (hyperbolic) optical materials exhibit numerous distinctive and non-intuitive optical phenomena such as negative refraction, hyper-lensing, focusing, wave-guiding and enhanced quantum radiation [4].

In this work, I will summarize our recent progress about : i) the possibility to reversibly reconfigure the potential landscape leading to formation of site-controlled SPSs upon introduction of in-plane elastic strain fields with controlled magnitude and sign [5]. To do that, we fabricated hybrid piezoelectric devices by transferring a WSe_2 monolayer on top of piezoelectric nanopillars. Moreover, a reversible and robust tuning of the SPSs emission energy (as well as exciton redistribution between individual SPSs) is further shown without affecting the single photon emission purity with relatively large energy shifts. ii) Tuning of the in-plane propagation of nanolight in highly anisotropic MoO_3 2D crystals by using tailored metallic nanoantennas and dielectric environments by means of we demonstrate canalization, refraction and focusing of nanolight [4].

- [1] A. Srivastava et al. *Nat. Nanotechnol.* 10 491 (2015).
- [2] J. Martín-Sánchez et al. *Semicond. Sci. Technol.* 33 013001 (2018); R. Trotta, J. Martín-Sánchez et al. *Nat. Commun.* 7 10375 (2016); O. Iff, D. Tedeschi, J. Martín-Sánchez et al. et al. *Nano Lett.* 19 6931 (2019); J. Martín-Sánchez et al. *Adv. Opt. Mater.* 4 682-687 (2016).
- [3] Ma et al. *Nature* 562, 557–562 (2018) ; Dai et al. *Science* 343, 1125-1129 (2014).
- [4] J. Taboada-Gutiérrez et al. *Nat. Mater.* 19, 964–968 (2020); J. Duan et al. *Nat. Commun.* 12, 4325 (2021); J. Duan et al. *Nat. Mater.* 22, 867-872 (2023); J. Martín-Sánchez et al. *Sci. Adv.* 7, eabj0127 (2021).
- [5] M. Savaresi, A. Martínez-Suárez et al. *arXiv:2301.10273*.



L11

Novel Si-based quantum- and nanoelectronic platforms based on ultra-cold epitaxy

Moritz Brehm

JKU Linz

In this presentation, we will present recent advances in the epitaxial growth of nanostructures in the group-IV system. We demonstrate that molecular beam epitaxy is a suitable tool to overcome limitations in nanostructure fabrication imposed by the inherent lattice mismatch between the group-IV semiconductors silicon and germanium. However, the crystal growth needs to be performed at unconventionally low growth pressures close to the extreme-high-vacuum regime and ultra-low growth temperatures of only 150°C - 350°C.

We report on the growth of high crystal quality layers for which the Ge-rich layers' thickness is vastly supersaturated compared to what common knowledge suggests. We will elaborate on how these layers can be successfully used for up-to-now unattainable optoelectronic devices such as group-IV double hetero-structure diodes or electronic devices such as reconfigurable transistors relying purely on planar nanosheet technology. Further, we demonstrate that ultra-cold epitaxy allows for efficient monolayer position control of Si color centers that are promising candidates for quantum photonics applications.





Towards an Experimentally Validated Model of Ultrafast Laser Ablation

Jan Winter, Maximilian Spellauge, David Redka, Goran Hallum, Heinz P. Huber

Munich University of Applied Sciences

In recent decades, laser-matter interactions in ultrafast laser ablation have been extensively studied. Numerous simulations exist today that combine two-temperature modeling with subsequent lattice response, including phase transitions. These simulations primarily provide a qualitative understanding of laser ablation with single pulses, while the precise quantitative prediction of final state and time-resolved observables remains challenging. Moreover, the majority of experimental approaches to study laser ablation are performed with multiple pulses, making it difficult to experimentally validate single-pulse simulations.

Final state observables that may be predicted by simulations include ablation threshold, depth, volume and morphology [1-3]. Pump probe techniques can measure time-resolved observables for arbitrary delay times, typically ranging from fs [4] to several hundreds of μs [5]. In addition to the quantitative optical response, extensive analysis permits the observation of quantities such as the velocity and disintegration time of spallation layers, the re-solidification time of the surface, and the removal time of the ablation plume [5-8]. When pressure waves become visible in pump-probe microscopy, such as during laser ablation in liquids, pressure amplitudes can also be measured [9,10]. These observables can be used to test theoretical models and gain insight into the laser ablation mechanisms, such as photo-mechanical and photo-thermal processes. They can also help us comprehend how pulse duration, separation, and fluence affect the efficiency of ablation.

Combining simple modeling with time-resolved pump-probe experiments, our group has validated the role of photo-mechanically-induced pressure waves in the ablation process [3,11].

Here, we present a new experimentally validated model of aluminum laser ablation. In addition, we highlight time-resolved studies on the photo-mechanical and –thermal ablation of indium tin oxide thin films [12]. Finally, we emphasize the strong photo-mechanical nature of laser fragmentation of iridium oxide microparticles immersed in water [10].

- [1] J. Winter, M. Spellauge, J. Hermann, C. Eulenkamp, H.P. Huber, and M. Schmidt, "Ultrashort single-pulse laser ablation of stainless steel, aluminium, copper and its dependence on the pulse duration", *Opt. Expr.* 29 (2021)
- [2] D. Redka, C. Gadelmeier, J. Winter, M. Spellauge, C. Eulenkamp, P. Caltà, U. Glatzel, J. Minár, H. P. Huber, "Sub-picosecond single-pulse laser ablation of the CrMnFeCoNi high entropy alloy and comparison to stainless steel AISI 304", *Applied Surface Science* 544 (2021)
- [3] D. Redka, J. Winter, C. Gadelmeier, A. Djuranovic, U. Glatzel, J. Minár, H.P. Huber; "Control of ultrafast laser ablation efficiency by stress confinement due to strong electron localization in high-entropy alloys"; *Applied Surface Science* 594, 153427 (2022)
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L13

Tuning on demand the physicochemical features of titanium oxide based nanomaterials towards photocatalytic biomass valorization and environmental remediation applications

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To design energy and cost-efficient innovative processes with limited environmental footprint, such as the catalytic conversion of biomass to added-value chemicals and products, is of a paramount importance. Another global concern is the elevated levels of pollutions and so modern methods for environmental remediation are still desired. Solar light is the most abundantly available renewable source of power, which can be used as a tool to perform a wide range of catalytic applications/reactions as the above-mentioned. So, photocatalysis is on its infancy towards the global modern goals for sustainable future within the frame of cyclic (bio)economy for as green as possible chemicals and products, as well as for water and air purification.

To take advantage of photocatalysis's unique features, the most vital part is the design and synthesis of novel efficient and environmental-friendly photocatalysts. Titanium oxide based materials have been established as effective photocatalysts, especially for unselective decomposition of organic pollutants. Contrarywise for synthetic applications, such as biomass upgrade, the unselective/uncontrolled photoreactivity is undesired, so tuning on demand the physicochemical properties is essential to accomplish the desired and selective photocatalytic activity.

Our research focus is concentrated on the development and detailed characterize the physicochemical features of a wide range of novel titanium oxide nanomaterials, like nanotubes, nanorods, or anatase nano-core-shells covered with an amorphous phases reach in carbon-containing surface functional groups, obtained following new synthetic protocols. Special emphasis is also given on further elevating their selective photocatalytic performance either by creating nanocomposites with S and N doped (reduced) graphite oxide or by decorate them of substates like activated porous carbon or cotton textiles, depending on the targeted final application. Another approach for boosting the photoreactivity is to make nanostructured mixed metal oxides (n-mMOx) like barium or/and europium titanate oxides.

The herein presented photocatalytic results will be about the selective partial oxidation of the cellulose-derived 5-hydroxymethylfurfural (HMF) to 2,5-diformylfuran (DFF) or the lignin-inspired model aromatic benzyl alcohol. Going a step ahead, the selective cleavage of the β -O-4 linkages of the diaromatic lignin-inspired model compound 2-phenoxy-1-phenylethanol (PP-ol) is also explored. To understand deeper how the material's physicochemical features and especially the surface functional groups affect the selective photoreactivity, theoretical studies are also performed and correlated with the experimental results. Regarding the environmental remediation applications, the experimental photocatalytic results will be focused on the multifunctional media for adsorption/degradation/sense of toxic vapors in air or decompose different kind of organic pollutants in water matrixes.

Last but not least, it will be showcased how sonocatalysis can be utilized as a process intensification tool both for material synthesis as well as by acting synergistically to photochemistry.





Local Potential Variations Captured by XPS Provides the Missing Link about Charge Dynamics

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Electrical response of chemical and biological systems are predominantly determined by ionic motion which is slow, compared to its electronic counterpart. Iontronics is the science involving both electronic and ionic motions for interfacing solid-state-world with bio-, where the crucial role is bestowed to the nm-scale Electrical-Double-Layer(s) (EDLs). However, motion throughout the entire system (i.e. interfaces and the bulk), typically in mm-scales needs to be considered. Current understanding of the role(s) of the materials used and the geometries adopted of such systems using state-of-the-art electrical, spectroscopic and microscopic tools as well as theoretical methodologies are far from complete and calls for a fresh outlook. This is where XPS, a surface sensitive chemical analysis tool, with its additional ability to reveal the localized electrical potential distribution by dissecting the entire device, can make an unprecedented impact. Within the last 2 decades we have coupled XPS with AC-Modulation and turned it to a Chemical-Oscilloscope for capturing both time- (10^{-6} to 10^2 seconds) and position- (0.05 mm to 10 mm) sensitive electrical potential developments. Using this non-invasive methodology, guided by modelling, we recently have investigated charging dynamics of several devices having ionic- and/or dipolar-liquids as the electrolyte, and unveiled, the hitherto unknown, 2-Dimensional character of the phenomenon by incorporating long-advocated steric factors and non-linear coupling(s). We will present our recent work using this methodology on investigation of electrochemical devices with different ionic liquid make-up and geometries.



L15

Label-Free Spectromicroscopy as a Quantitative Probe for Dermal Drug Delivery

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Topical drug delivery is a well-known approach for curing skin diseases. Often, there is no detailed knowledge on the spatial distribution of the drugs and formulations on the nanoscale as a function of exposure time. However, this knowledge is required for optimizing topical therapies. Label-free spectromicroscopy approaches are presented for probing highly dilute molecular and nanoparticulate drugs as well as drug nanocarriers in human skin for intact and barrier-disrupted skin as well as different drug formulations. Label-free spectromicroscopy includes scanning transmission X-ray microscopy (STXM) and atomic force microscopy-based optical near-field microscopy (s-SNOM) and photothermal expansion (AFM-IR). The advantage of these techniques is that they provide high chemical selectivity derived from the tunability of the employed radiation sources, a spatial resolution far below the diffraction limit of optical microscopy, and the results can be quantified. Most advantageous for the identification of dilute drugs is hyperspectral imaging, where the full spectroscopic information is contained in each pixel of the micrographs. The experimental data are analyzed with respect to changes in optical density, singular value decomposition, as well as principal component and cluster analyses. Highly promising are attempts to employ undersampling strategies by taking only a few percent of the data at randomly chosen locations, so that long data acquisition times and radiation damage are avoided. This requires the use of suitable mathematical approaches, such as low-rank matrix reconstruction or compressed sensing.





Nanostructured MoS₂-based catalysts for hydrodeoxygenation of bio-oils: Combining XPS and STM from UHV to operando conditions

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For the technological utilization of sustainable feedstocks such as pyrolysis oils from biomass, oxygen removal via hydrodeoxygenation (HDO) is one of the most essential steps. [1] Metal-promoted MoS₂-based catalysts are well-established for hydrode-sulphurization (HDS) of crude oil components, and thus a promising material for HDO catalysts. [2-4] This is already proven technology for simple feedstocks such as vegetable oils, but more complex compounds with high oxygen content and multiple oxygen functionalities such as bio-oils remain challenging, and thus gain increasing interest.

In contrast to the established use in (virtually oxygen free) HDS, the sulphide catalyst will be exposed to organic oxygenates and water formed in the herein desired HDO process. Thus, in the presence of oxygen, sulphur atoms may be partially exchanged. Thereby, active sites can become blocked, which triggers strong catalyst degradation on the long term. [5,6]

To gain an atomistic understanding of such processes, herein two-dimensional MoS₂ nanoparticles on Au (111) surfaces were investigated combining microscopic (scanning tunneling microscopy (STM)) and spectroscopic insights (photoelectron spectroscopy (XPS)) under various conditions mimicking HDO from UHV level to the near-ambient-pressure regime (few mbar, NAP-STM, NAP-XPS).

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L17

Large-area nanopatterning for broadband, quasi-omnidirectional low-reflectance glass

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Method for producing large-area, broadband, quasi-omnidirectional low-reflectivity glass surfaces is presented. Using block copolymer patterning and inductively coupled plasma etching, near-periodic arrays of pillars are formed in glass. The patterned surface has reflectivity <0.5% - almost an order of magnitude smaller than plain glass - with a bandwidth of ~300 nm. Substrates etched on both sides transmit >99.5% across the wavelength range 850-1200 nm, with >99% down to $\lambda = 650$ nm. The process is demonstrated on a 5 cm diameter fused silica wafer and high transmittance is maintained up to at least 70° incidence. The resulting substrates might find application as lab optics (windows, lenses, etc) display screens for televisions, computers, phones, and as encapsulants for optoelectronic devices.





Redox-active metal-organic frameworks in electrode materials for lithium-ion batteries: an EPR study.

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In recent years, there has been a growing demand for high-performance and sustainable energy storage solutions to meet the increasing needs of various applications, including electric vehicles, portable electronics, and grid-scale energy storage. In this context, the high surface area and ability to host various ions within their pores make MOFs (Metal Organic Framework) attractive for improving energy density and cycling stability, ultimately leading to more efficient and sustainable energy storage systems. In this study, the intrinsic porosity of MOFs was exploited by inserting bioinspired redox-active species to give new species. A non-destructive in situ electron paramagnetic resonance (EPR) approach was used to directly observe the redox reactions and mechanisms that promote dendritic lithium growth during cycling process.



L19

Physical-Chemistry at Biointerfaces: From Nanostructures to "Softness"

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In the last two decades, the concept of Biointerfaces underwent a "state transition" from merely representing "2d-interfaces between synthetic materials and the biological medium" to represent complex, often hybrid, basically dynamics, 3D systems, characterized by peculiar organization and properties and hosting/boosting complex chemical and biochemical transport processes.

Biointerfaces can be viewed either under an applied biomedical perspective, including (somewhat empirically) their role in biomaterials, biosensing, therapeutics, etc..., or can be conceived looking back to the framework of the Physical Chemistry of Interfaces as ruler of their puzzling organization-behavior relationships. This last view is the one here proposed.

In this context, new "lines of sight" emerged recently, as the one considering Biointerfaces as an intriguing sub-domain of the wider class of Soft Interfaces, whose "collective structural and functional reactions to weak stimuli" perfectly suit the peculiar adaptive character of Biointerfaces. In fact, their wide ranges of rearrangement time (fast-medium-slow response times) and space (nano-meso-micro scale) responses allow to define biointerfaces as "soft" systems, sensitively responding to the actions of "topographical" micro- and nano-structuring.

These last factors, in particular, have been recognized as "rulers" of selective adsorption processes, "drivers" of the biomolecule conformational state and promoters of clustering/declustering processes, finally controlling basic aspects of the cell life cycle and suggesting a close relationship between nanostructures and (nanosized) "biomolecular" machinery, i.e., the mechanisms that allows cells to self-adapt to the extracellular stimuli.

In the present lecture, interface nanostructuring, i.e., building suitable nanotopography and nanocurvatures, will be shown to be able to obtain quantitatively adsorption and controlled "local" epitope orientation by means of selective chelation-based processes (providing well-defined anchoring of oriented biomolecules [1,2]), counter-intuitive size-related protein trapping at nanowells [3], and nanocurvature-driven "geometrical" resonances for of adsorption [4] . Finally, a case of "soft" collective behaviours of adsorbed layers of "elastic" peptide systems to the pH changes [5, 6] will be reported and discussed in terms of Molecular Dynamics simulation.

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Nanoscale mechanisms of tensile deformation, fracture, and heat transfer in carbon fibers: Insights from large-scale atomistic simulations

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Carbon fiber is a lightweight, ultra-strong material widely used in aerospace, automotive, defense, sports equipment, and wind energy sectors. The increasing demand for carbon fibers, largely driven by the quest for energy efficiency in transportation and the rapid growth of wind energy industry, are stimulating the exploration of a broader range of molecular precursors, structure-templating agents, and fiber manufacturing procedures aimed at producing high-performance fibers at a reduced cost. This exploration is guided by investigations focused on revealing the relationships between carbon fiber nanostructure and properties. In this presentation, the mechanisms of tensile deformation and heat transfer in carbon fibers are investigated in large-scale molecular dynamics simulations. The key structural features affecting the properties of carbon fibers, such as the relative fractions of graphitic, turbostratic and amorphous microconstituents, degree of alignment, pore size distributions, and chemical cross-linking can be effectively controlled in simulations, thus enabling efficient exploration of structure-properties relationships. The mechanical properties are investigated in the simulations of the deformation and fracture of carbon fibers under axial tensile loading, while the channels of the heat transfer are investigated in nonequilibrium molecular dynamics simulations. The dependence of the tensile strength, fracture strain, Young's modulus, and anisotropic thermal conductivity of carbon fibers on the microstructural characteristics and the presence of a graphitic skin layer are explored in the simulations. The results of the simulations suggest that the design of advanced carbon fiber manufacturing and post-processing methods focused on the elimination of critical mesoscopic structural defects (internal voids, foreign inclusions, and surface flaws) can yield a substantial increase in the strength and fracture strain of carbon fibers.



L21

Laser-induced generation and transfer of micro and nano particles for electroless deposition of conductive copper structures on textiles

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In the present paper we introduce a novel approach that combines a laser-induced forward transfer (LIFT), to generate seed paths of silver micro and nano particles, and electroless copper deposition, to grow conductive structures on textiles. Therby we demonstrate how laser parameters and donor design affect the particle formation, and present different examples for smart textile applications.





Generation of conductive lines and structural coloration on nanostructured-modified textiles

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Current technologies employed for producing conductive lines on textiles often rely on metallic yarns or conductive inks. However, metallic yarns impose constraints on circuit designs, while conductive inks required sintering temperatures above 200°C for creating continuous connectivity, making them unsuitable for heat-sensitive textile materials. In this study, we propose a novel approach involving electroless copper deposition on nanostructured-modified textiles with localized laser-transfer silver nanoparticles to create localized conductive tracks on textiles. We discuss the morphology of the copper coatings, along with their electrical and mechanical properties, and demonstrate the formation of copper conductive patterns on textiles. Furthermore, we explore the differences of hue in the copper deposited textiles attributed to the nanoparticle size and thin-film interference in the formed Cu/Cu₂O core-shell nanoparticles.



L23

Impedance analysis of poly(3,4-ethylenedioxythiophene) modified electrodes - stability, thickness distribution and non-stationarity

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The aim of the present study was the electrochemical preparation and characterization of poly(3,4-ethylenedioxythiophene) (PEDOT) modified electrodes before and after overoxidation. The benefits of using electropolymerization reactions to modify electrode surfaces is the ability to change the properties of the polymer film by changing the experimental conditions, and the ability to tailor the electrodes for specific applications. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were used for the electrochemical characterization of the systems. According to the results, the impedance response of the overoxidized films differ considerably from those measured for freshly prepared films. The decreasing capacitance of the double layer region and the increasing charge transfer resistance suggest that during overoxidation the electrochemical activity of the film decreases and the charge transfer process at the metal/film interface becomes more hindered than in the case of pristine films. In addition, time evolution of the electrochemical properties of the films can be observed after overoxidation, indicating the non-stationarity of the system. The mechanical properties of a PEDOT layer and its resistance against the consequences of overoxidation could be significantly improved by the electrochemical deposition of poly(bisphenol A) (poly(BPA)) on its surface and in its pores, i.e. by the combination of the two polymers. This procedure looks promising in terms of mechanical properties [1,2]. It is known that pure poly(BPA) has low electrochemical conductivity and poor electrochemical activity [3], therefore, it was expected that its presence would not affect considerably the electrochemical properties of the PEDOT layer, even after its overoxidation.

When modeling the impedance response of the polymer modified electrodes, we encountered two difficulties: thickness distribution of the film and time evolution of the system. To reduce the effect of non-stationarity [4], we used the four-dimensional (4D) analysis method for the calculation of the impedances corresponding to different time instants. One of the most important results of the present work is that in case of PEDOT and poly(BPA)/PEDOT modified electrodes the deviations of the impedance responses from the purely capacitive behavior predicted at low frequencies by the theoretical models (i.e. the frequency dispersion of the low frequency capacitance) can be well explained solely by the assumption of uneven film thickness. It has been found that the impedance model, which considers the film thickness distribution (by assuming regions of different film thicknesses on the basis of SEM micrographs) gives a good description of the impedance data, both before and after overoxidation. By using this model reasonable values for the different parameters characterizing the polymer film electrodes could be obtained by CNLS fitting the impedance function to the experimental data.

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What can we learn about interfaces from hydration water?

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Biological and physiological surfaces are essential for life. They serve as a hub for surface chemical reactions, including chemical signaling and transport of substances. Numerous efforts have been directed toward exploring these surfaces from different points of view. In this talk, the focus will be on answering the question of how we can utilize interfacial water molecules to probe processes occurring on macroscopic and nanoscopic surfaces. As a recent example, the ultrasensitive label-free detection of the interaction between perfringolysin O (PFO), a pore forming toxin, and lipid membrane will be demonstrated.



L25

Laser diagnostics and interventions in conservation science: historical and synthetic copper patina

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The history of copper in architecture can be linked to its durability, corrosion resistance, and prestigious appearance. Environmental influences that lead to the formation of patina layers not only affect copper surfaces in architecture but also in microelectronics, medicine and automotive technologies. Corrosion monitoring by the deployment of in-situ nanosecond pulse laser repassivation of protective conversion layers has been addressed in the context [1,2].

In this study, the analysis of destruction and reformation of protecting anodic oxide films such as copper oxides (e.g. cuprite, Cu_2O) and brochantite ($\text{CuSO}_4 \cdot 3\text{Cu}(\text{OH})_2$) on historical copper roofing sheets from the Belvedere Castle, Vienna, allowed insight into the mechanism of long-term protection on objects of cultural heritage. Surface and layer analyses were employed by scanning electron microscopy and energy dispersive X-ray spectroscopy on both artificial [3] and natural patina on original roofing sheets of the Belvedere Palace built by Prince Eugene of Savoy 1723. The possibilities of laser cleaning and laser-induced stratigraphy were explored for the first time on cuprite and brochantite. In order to explore an alternative to conventional cleaning methods of soiling on patina surfaces, the removal of model soiling was investigated. The cleaning thresholds for these contamination layers were determined. They are orders of magnitude smaller than those of the cuprite and brochantite layers. Thus, the possibility of a laser intervention was demonstrated. Through spectroscopic analyses using Laser-Induced Breakdown Spectroscopy (LIBS) [4], the ablation processes of patina films could be quantitatively monitored. Based on these data, physical-chemical strategies were developed to avoid destruction of the metals or oxide layers during a cleaning intervention.

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Monitoring the dynamics of cluster/oxide support systems

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Oxide-supported clusters are pivotal in heterogeneous catalysis. The cluster-support interaction intricately affects structural, diffusion and reaction dynamics of these metastable particles. In this talk I present our recent studies on size-selected Pt clusters supported on magnetite $\text{Fe}_3\text{O}_4(001)$, a reducible oxide that can contribute lattice oxygen to catalytic reactions while maintaining its surface stoichiometry upon reduction, thanks to the high cation mobility. But where does oxidation catalysis take place – at the interface or on the clusters? And what is its impact on support morphology and cluster mobility?

By a combination of high resolution, fast scanning tunneling microscopy (STM), with time resolution down to the 10 ms timescale [1], and a highly sensitive pulsed valve sniffer setup [2], we investigate fundamental aspects of this catalytic system, namely:

- (i) reverse lattice oxygen spillover,
- (ii) size-dependent cluster diffusion and ripening,
- (iii) support restructuring, as well as
- (iv) cluster encapsulation [3, 4].

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L27

Gallium nitride based heterostructures for sensor applications

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Group III-Nitrides (III-N) are very attractive for physical and chemical sensor applications due to their excellent piezoelectric properties [1]. HEMTs but also Schottky diodes and resistors based on AlGaIn/GaN heterostructures are often employed as sensing devices, especially for application in harsh environment or at high temperatures (e.g. the wings of an aircraft, in combustion engine, exhaust etc.) [2]. Recently, the following approaches were reported: (a) a bulk device approach; (b) devices integrated on a bulk substrate cantilevers; (c) devices integrated on membrane structures. The first approach (a) does not require the realization of suspended microstructures. The function is based on the action of hydrostatic pressure which alters Schottky barrier height [3], the internal fields in GaN/AlGaIn/GaN heterostructures [4] and the polarization in AlGaIn/GaN heterostructure [5]. In the second approach (b) AlGaIn/GaN HEMT process technology is performed on a bulk sapphire substrate. The substrate with the integrated HEMT as a strain sensor is then cut out into a bulk cantilever structure. This structure is then exposed to bending [6-11]. The resulting channel resistivity is measured in dependence on applied strain. The interaction between piezoelectric and piezoresistive properties improves the sensitivity of pressure sensors by using AlGaIn/GaN heterostructures with confined 2DEG. The group III-nitrides for sensors based on membrane structures (c) is much less evaluated due to the difficulties to fabricate suspended AlGaIn/GaN heterostructure and only a few reports on membrane test structures are available [1, 12-14].

This work deals with technology of MEMS piezoelectric sensors based on high electron mobility transistors (HEMTs) able to work in harsh environments. The originality of the concept proposal consists in research of new progressive thin layers based on metal oxides and/or their combinations for Schottky gate sensing electrodes and methods of bulk micromachining of the substrate material in order to get free-standing AlGaIn/GaN micromechanic structures. It can work based on two principles. First one is the piezoelectric pressure sensor which reacts to the external pressure load by generating of piezoelectric charge on its electrodes. The second, HEMT principle uses the change of 2DEG channel conductivity with the applied external loading [15-18]. The charge accumulation in the channel is particularly caused by piezoelectric and spontaneous polarization which can be changed by external mechanical load [19]. The model of the sensor has been developed in the 3D finite element method (FEM) software Ansys.

The residual built-in stress suppression seems to be crucial to obtain piezoelectric MEMS pressure sensor with high detection sensitivity. Total accumulated piezoelectric charge depends on the position and area of the sensing electrode. Therefore, optimization of these two input variables is usually performed.

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High surface area 3D nanowire-networks as electrodes for water electrolysis and electrocatalytic CO₂ reduction

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To fulfill the ambitious targets towards a net-zero economy the electrocatalytic conversion of water or CO₂ to H₂, CO, syngas, formic acid, alcohols or even to more complex chemicals through the organic electrosynthesis will be among the key technologies. Although water electrolysis is already a mature technology, widely deployed mass production of green H₂ through electrolysis is still limited due to its high costs associated with use of scarce catalyst materials and costly corrosion-resistant components or low conversion efficiencies. Similar shortcomings are seen for the less mature CO₂ conversion to chemicals in which product selectivity and low catalyst durability introduce even more challenges. Currently a major research focus is directed towards superior (nano)catalyst materials with significant less attention on the electrode architecture itself. Often, ill-defined electrodes with nano-catalysts mixed with ion-conducting polymeric-binders coated on membranes or porous electrodes are investigated, missing fundamental studies on simple well-defined model systems.

Imec has an extensive know-how on nano-patterning, nano-structuring and surface-texturing by techniques such as nano-imprint lithography, lift-off and/or controlled vapor-phase grain growth, electrochemical anodization and plating of metals and metal-oxides. In this talk we show the fabrication of regular-ordered 3D nanowire-networks (nanomeshes) as high surface area porous electrodes applied in water electrolysis and electrocatalytic CO₂ reduction. [1,2] These unique few μm-thin electrodes show compared to planar electrodes a large surface area enhancement up to a factor of ~100x, while providing a high porosity of ~70% together with sufficient mechanical stability, an important aspect towards their practical implementation in electrocatalytic flow cells. Nickel, copper and silver nanomesh electrodes are obtained by electrochemical metal plating in 3D-porous anodic aluminum oxide templates. Nickel nanomesh electrodes applied for water electrolysis in an alkaline membrane-electrode assembly showed pronounced shifts towards lower onset potentials for both H₂ and O₂ evolution reaction due to the high amount of catalytic surface sites available. Electrocatalytic CO₂ reduction was studied on copper and silver nanomesh electrodes. While on Ag nanomesh electrodes the CO₂ reduction to CO was enhanced by the high surface area, on the Cu nanomesh the competing hydrogen evolution reaction was promoted. To conclude, high surface area metal electrodes are a very attractive option for electrocatalytic applications and we show that the extended surface area of our nanomesh electrodes can significantly enhance catalytic reactions.

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L29

Tailoring plasmonics and MOFs: nanostructuring MOF-based SERS substrates towards VOC sensing devices

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Volatile Organic Compounds (VOCs) encompass a diverse group of carbon-based chemicals that are present as gases or vapors at ambient temperatures. They originate from a broad range of sources, including natural processes and human activities, permeating our immediate surroundings. [1] The analysis of VOCs has considerable significance across multiple domains, such as industrial operations, and air quality and odor pollution. VOCs also play pivotal roles in bioanalytical applications, with a strong focus on cancer detection through breath analysis, [2] as well as in contributing to the organoleptic characteristics and overall sensory perception of various substances, including food. [3,4] Identification and quantification of VOCs is a paramount task, which requires the initial capture of these compounds subsequently followed by their analysis. In that line of thought, porous materials and particularly Metal-Organic Frameworks (MOFs) come to mind.

MOFs are attractive materials that emerged at the end of the '90s [5] and utilize an elegant principle of coordination of metallic centers by a bi- or multidentate ligand. Each of the coordination points interacts with a different metallic unit instead of chelating the initial metal, which then propagates a network of coordinative bonds and creates extended ordered structures. Besides their unusually large surface, they also offer the advantage of chemical versatility, [6] that allowed their facile implementations in the form of powders, membranes, and thin films. [7,8] MOF films can be grown on different surfaces properly modified. Surface modification typically involves Self-Assembled Monolayers, [9,10] but film growth can be also achieved by polymer brushes as nucleation points. [11,12] Interestingly the growth dynamics will impact the final structural properties of the MOF films and determine their applicability. [13]

Among different analytical tools, Surface-Enhanced Raman Spectroscopy (SERS) has positioned itself as a powerful and versatile tool providing the means for direct fingerprinting of target molecules with fast detection times, in-situ sampling, and the possibility of implementations to miniature portable devices. [14,15] Even further, nanostructuring techniques can render SERS substrates with ad-hoc tunable plasmonic features. [16-18] However, SERS requires the docking of the target analyte near the SERS active surface, and, indeed, MOFs represent an important type of material that can serve on SERS substrates and provide an efficient scaffold for collecting target analytes on its surface. [19]

Here, we analyze the impact of modifying nanostructured plasmonic surfaces with MOF thin films on SERS applications. We aim to address how their growth and structure influence the SERS readout and performance toward the detection of selected VOC analytes.

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Unlocking the Hidden Dimension: The Power of Chirality in Scientific Exploration

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In recent years, there has been an increasing realization of the significant role that chirality plays in scientific investigations across various disciplines. Understanding and manipulating chirality provide insights into molecular interactions, stereochemistry, and the underlying mechanisms that govern processes in fields such as chemistry, biology, pharmacology, and materials science. This contribution emphasizes the added value of including chirality in scientific investigations and based on specific examples demonstrates that by incorporating chirality, we can unlock a deeper understanding of molecular behavior and material properties. Chirality opens up new avenues for discovery and innovation, enabling scientists to tackle complex scientific challenges and make breakthroughs across diverse fields.





Poster Abstracts



P01

Towards the design of an immersible NMR probe for solution reaction monitoring

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NMR spectroscopy has been employed to simplify and enhance the monitoring of reactions. Even though advanced technical tools exist to withdraw aliquots of solution or loop the reaction medium to an external NMR spectrometer, they come with their own issues: temperature drift-induced biases over reaction kinetics, obstruction of the flow tube solid in suspension, flow and sample magnetization optimization. These limitations are leading to the development of a new integrated NMR system. The project involves creating an integrated low-field NMR spectrometer primarily for monitoring reactions while immersing the device into the reaction mixture (called Dip-NMR). In other terms, Dip-NMR's mission is to set a device capable of monitoring reactions within the reaction medium, allowing us to observe and measure reaction progress. This collaborative endeavour includes three academic partners. Endowed with the following tasks: design custom solution-based electromagnets, create the RF coil, control circuit, receiver circuit, optimized microfabrication and B0 field inhomogeneity assessment. The impact of B0 field inhomogeneity on the ideal NMR spectra has been demonstrated using an efficient simulator. A model of the intended magnet structure was created, and the resulting magnetic field was simulated to generate an inhomogeneity map. The probable shape of each peak in the actual NMR spectrum was assessed in the effect of this non-uniform magnetic field. This study involves acquiring signals, processing them in degraded magnetic fields, and monitoring reactions using prototypes. selection of suitable chemical reactions that can be monitored using a high-field NMR spectrometer to establish a standard dataset. The chosen reaction was used for analysis by the built NMR-probe prototype. A suitable statistical method has been adopted to encash the reaction information from the NMR spectra recoded using the built prototype.





Identification of Tumor Tissue in Thin Pathological Samples via Femtosecond Laser-Induced Breakdown Spectroscopy and Machine Learning

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The problem of differentiating cancerous tissue from a healthy one is currently solved in the diagnostic process through microscopic imaging of stained biopsy sections by pathologists. During surgical removal of tissue, oncological safety margins must be established to ensure the complete removal of the tumor without affecting much of the neighbouring healthy tissue. For this purpose, on-site pathological analysis is done on freshly frozen, stained cuts, which is time consuming. We investigate a new approach to minimise the time of discrimination between malign and benign tissue by an in situ, non-contact spectroscopic analysis.



P03

Breakdown of optical selection rules in a rolled-up quantum well

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Optical resonators emerging from rolled-up semiconductor membranes constitute a class of 3D self-assembled micro- and nano-objects for future applications in optoelectronics [1]. Such structures are obtained by integrating optical emitters like quantum wells and quantum dots into a strained layer system, which is released from its original substrate and forms the rolled-up micro- or nanotube by strain relaxation of the layer [2]. Even so, the optical emission of the integrated structure can be easily controlled by the appropriate strain distribution of the rolled-up tubes, little advantage has been taken of this in the past.

In this work [3], we demonstrate how we can tune the properties of an InGaAs quantum well by the rolling up of the structure. We succeed to engineer the band structure allowing to change the electron-hole recombination process from a fundamental electron-heavy hole to an unusual electron-light hole optical emission. Therefore, we deliberately tune the quantum well position inside the microtube wall out of the strain neutral point. We carry out structural and optical characterization as well as band structure calculation to fully characterize its properties. X-ray diffraction allows a complete determination of the strain distribution, which is feed into $k \cdot p$ calculations to predict the band structure of the flat, unrolled structure as well as the rolled-up tube. Comparing photoluminescence and photoluminescence excitation spectra of a rolled-up GaAs quantum well and the rolled-up InGaAs quantum well, we can optically probe the changes of the emission characterization. We find good agreement with our band structure calculations, which predict an inversion of the light-hole and heavy-hole state for the InGaAs quantum well. Circularly polarized photoluminescence excitation spectra show clearly strong valence band mixing effect indicating a breakdown of the selection rules for the hole-electron recombination of the bulk material. The results demonstrate a powerful way to tune the emission characteristics of a quantum well by passive means solely using geometry.

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Engineering UiO-66 Metal-Organic Framework: Amino Functionalization for Aldehyde Conjugation

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Metal-Organic Frameworks (MOFs) have emerged as a versatile class of porous materials with numerous applications ranging from gas storage to catalysis and drug delivery. [1,2] Among MOFs, UiO-66 stands out for its exceptional stability and high surface area, making it an ideal platform for functionalization and customization. [3–5] In this study, we explore the engineering of UiO-66 MOF through amino functionalization to enable covalent binding of aldehydes via Schiff reactions. The amino-functionalized UiO-66 MOF represents a novel class of materials that combines the intrinsic properties of UiO-66 with the reactivity of amino groups. [6] Amino groups introduce functionality and reactivity to the MOF structure, providing a platform for a wide range of applications.

In particular, we focus on their ability to covalently conjugate aldehydes via Schiff reaction. Aldehydes are one kind of Volatile Organic Compounds produced by our bodies through metabolic processes and they can be an indication of our health status. This is particularly true in the case of Cancer diagnosis, especially for Lung Cancer (LC), and the presence of VOCs in exhaled breath are promising candidates towards noninvasive diagnostics of LC and it has motivated an intensive research activity over the last few years. [7,8] Thus obtaining materials suitable for selective capture of aldehydes from gas phase that allows further identification and quantification, is of significant interest. [9,10]

The synthesis of amino-functionalized UiO-66 MOF involved the replacement of the traditional 1,4-benzenedicarboxylate (BDC) linker with an amino-functionalized BDC linker. By carefully controlling the concentration of the amino-functionalized linker, we achieved tunable amino group densities within the MOF structure. This level of control over amino group incorporation allowed us to tailor the material's reactivity and surface functionality. Characterization of the resulting MOFs was carried out using powder X-ray diffraction (PXRD), nitrogen adsorption-desorption isotherms, and Raman Spectroscopy. The key highlight of this research lies in the unique combination of UiO-66's robustness with the versatility of amino groups.

In conclusion, our study showcases the successful engineering of UiO-66 MOF through amino functionalization, offering a versatile and customizable platform for aldehyde conjugation and various other applications. This work underscores the potential of MOFs as adaptable materials in the field of materials science and chemistry, with promising prospects for a wide range of practical applications.

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P05

Femtosecond laser generation of binary metallic oxide nanoparticles for applications in medical imaging diagnosis

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Liquid-Assisted Pulsed Laser Ablation (LA-PLA) is as a promising alternative top-down method to directly synthesize colloidal dispersions of nanoparticles (NPs), because of its low cost, simplicity, and environmental friendliness [1,2]. LA-PLA is particularly attractive for medical applications since the use of stabilizing toxic molecules can be avoided and chemical precursors are replaced by less costly bulk raw materials [3]. Contrast enhanced digital mammography and magnetic resonance imaging in combination with X-ray film mammography in breast cancer screening are complementary. A multimodal approach can be performed without significant delay during the same imaging session. It requires the development of multimodal imaging contrast agents (MCAs) capable of responding to both X-ray radiation and magnetic fields [3-7]. The presented work was to design and optimize the fabrication of nanoparticles for MCA applications with sub-30 fs LA-PLA. The laser targets were ceramic samples combining a magnetic iron oxide, such as Fe₂O₃ or Fe₃O₄, and an oxide phase of a radiopaque metallic element with high atomic weight, such as W, Ta and Bi.

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Surface characterization and photochemistry of Austrian historical daguerreotypes

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The first photographic process was published by Louis Jacques Mandé Daguerre in 1839. Due to the insufficient sensitivity of the silver-plated copper substrates, the process could not be used for recording moving scenes. A crucial combination of new technologies had already been developed in Vienna around 1840 [1,2]. The breakthrough came from increased sensitivity by photochemical means and a photographic camera specially constructed by the Viennese optician Voigtländer, which was equipped with the first portrait lens mathematically calculated by Petzval.

The surface morphology and surface chemistry of daguerreotypes are the most important sources of information regarding their production methods and the corrosion and aging processes affecting their long-term preservation. Three non-destructive and non-contact examination methods were used for the analysis of daguerreotypes in this project, digital optical microscopy, scanning electron microscopy and micro X-ray fluorescence. This allowed detailed insights into the photographic process technology of the pioneering Austrian era.

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P07

DRIFTS studies of adsorption sites on bimetallic gold-platinum nanoparticles

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Nanoparticles have been widely explored and are an active research field due to their unique properties and various applications in heterogeneous catalysis, drug delivery systems or the food industry. [1,2] The challenge is to develop reproducible syntheses with precise shape and size control. Bimetallic systems are of particular interest as they exhibit more interesting properties than their monometallic components and offer a variety of compositional optimization for tailored properties. [3] Gold nanoparticles possess unique optoelectronic properties due to plasmon resonances apparent as a pronounced, size dependant absorption band in the visible range of light while platinum is known for its catalytic properties. [1,2] The goal is to combine both noble metals in bimetallic nanoparticles to obtain a multifunctional catalyst with new application possibilities.

Different bimetallic particles consisting of noble metals such as Pt-Au and transition metals such as Pt-Sn have already been investigated and show in some cases an enhanced catalytic activity depending on the composition. [4,5] Other works showed that the ligand influences the adsorption sites and thus the catalytic properties of monometallic platinum nanoparticles. [6]

The synthesis for the amine stabilized bimetallic nanoparticles was optimized based on the work of M. Osmić. In dependence on the approach started with either gold or platinum as seeds the growth mechanism leads to alloyed or phase-segregated nanoparticles. [7] In this work bimetallic gold-platinum nanoparticles were synthesized and characterized by (High resolution)-Transmission electron microscopy (HR TEM) and Energy-dispersive-X-ray-spectroscopy (EDX). To identify and characterize possible adsorption sites Diffuse Reflectance Infrared Fourier transform Spectroscopy (DRIFTS) with CO adsorption was used for bimetallic nanoparticles at P25-TiO₂. For comparison, monometallic platinum and gold particles were also examined separately.

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Investigating Electrochemical Properties of of Metal Electrode/Ionic Liquid Mixture Interfaces Using Operando XPS by Incorporating Additional Circuit Elements

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X-Ray Photoelectron Spectroscopy (XPS) has been utilized to extract local electrical potential profiles by recording core level binding energy shifts upon application of a DC and/or AC [Square Wave (SQW)] bias with different frequencies. In this work, to carry out these measurements, a coplanar capacitor with a polyethylene membrane (PEM) coated with a 1:1 by volume mixture of Ionic Liquids (ILs) N,N-Diethyl-N-methyl-N-(2-methoxyethyl) ammonium bis(trifluoromethanesulfonyl) imide (DEME-TFSI) and N,N-Diethyl-2-methoxy-N-methylethanaminium tetrafluoroborate (DEME-BF₄) was used. Analyses were carried out in-operando; such that XPS measurements were done simultaneously with current measurements. ILs have complex charging/discharging processes and they induce formation of the Electrical Double Layer (EDL) at the interface of the electrode. Certain properties of this process can be extracted via AC modulation under appropriate time windows of observation. Here, two frequencies, 10 kHz and 0.1 Hz, were selected to investigate the effects of fast polarization and the slow migratory currents, respectively. Local electrical potential developments were extracted at different locations of the device, from the variations in binding energies before and after adding two equivalent resistors in series to the device. This modification of the circuit allows us to quantify the AC currents passing through the device as well as the system's resistance and capacitance under particular conditions. With this non-invasive methodology, XPS becomes a useful tool for extracting localized electrochemical information and may be of great importance in better understanding of energy harvesting and storage systems.



P09

Highly-Sensitive Single-Step Detection of Levodopa Using Swellable Microneedle-Mounted Nanogap Sensors

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Microneedle (MN) technology for biomarker detection in interstitial fluid (ISF) offers a promising solution to the challenges associated with self-diagnosis in patients, eliminating the need for invasive blood sampling, complicated handling procedures, and subsequent measurement analysis.

In this study, we introduce an innovative approach utilizing swellable MN-mounted nanogap sensors. These sensors can be effortlessly inserted into skin tissue, rapidly absorbing ISF, and conducting on-the-spot biomarker measurements. This is achieved by enhancing measurement signals through redox cycling within the nanogap electrodes. Our findings demonstrate the capability of the MN-nanogap sensor to detect levodopa (LDA), a medication for Parkinson's disease, with remarkable sensitivity—achieving detection limits of 100 nM in aqueous solutions and 1 μ M in both gelatin phantoms mimicking skin properties and actual porcine skin.





Interaction effects of selected oxidic supports on amine capped nanoscale platinum networks

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Nanoscale transition metal structures are commonly known for their excellent catalytic activity. Especially the platinum-based derivatives are frequently investigated, for example for catalysing hydrogenation and oxidation reactions. [1,2] In this context, a direct dependence of the catalytic activity on the morphological properties of different ligand stabilised nanostructures has been observed. [1,3] Regarding morphological adjustment colloidal approaches offer promising possibilities through ligand variation. In contrast to the typically used long hydrocarbon chain ligands, it has already been reported that the usage of ligands with shorter and branched alkyl chains results in increasing catalytic activity. This was attributed to the individually reduced shielding ability due to the sterically less demanding capping agents. [2,4] By using the short and branched ligand tert-butylamine we obtained highly crystalline porous platinum networks based on small platinum nanoparticles (2.1 ± 0.2 nm) and short nanowires. Besides morphological characterisation via electron microscopy these were investigated by X-ray photoelectron spectroscopy to analyse the ligand surface species. The tert-butylamine stabilised nanostructures were subsequently deposited on various oxidic support materials including TiO₂ (P25), MgO and SnO₂. In addition to the stabilising ligands different oxidic materials may affect the catalytic properties of the resulting catalyst due to metal support interactions. [5,6] To gain further insights into these effects in combination with the amine capping agent we used diffuse reflectance infrared Fourier transform spectroscopy with CO as a probe molecule. CO adsorption can be utilised to characterise the catalytically important surface adsorption sites based on surface sensitive vibrational frequency changes. [6,7]

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P11

Development of a Method for Systematic Classification of Nanocarrier Systems

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According to the EU recommendation, nanomaterials are defined by dimensions, ranging from 1-100 nm. Regulators and scientists have been discussing for a long time whether nanocarriers count as a nano-form, although their diameters may often be larger than 100 nm in one dimension. The reason for this ambiguity is that nanocarriers are often based on complex nanoformulations to release active substances into the environment (controlled release), which in turn can be in the nanoscale and the carrier itself not. As these nanoformulations can be very complex, it is a major analytical challenge to determine the particle size of the nanocarrier and the release rates of the ingredients. In addition, it is difficult to assess their mobility and fate in the environment. With regard to environmental risk assessment, we like to present a novel approach to group and characterize nanocarriers through a systematic review and structuring of current technologies. Based on this review, we aim to identify undetected risks and challenges for chemical regulation. On behalf of the German Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection, a working definition and systematic categorisation of nanocarrier systems will be elaborated. For this purpose, a review of the state of development based on literature data and patents as well as expert discussions will be conducted. From the resulting categorisation (e.g., inorganic/organic or hybrid liposomal carrier systems for medical products, cosmetics or agriculture), three representative nanocarrier types will be selected with respect to potential challenges in environmental risk assessment. These “critical” types will be used to elaborate analytical methods for nanomaterial characterization. The guiding question here is whether the current test protocols (e.g., OECD guidelines) are suitable for assessing the environmental behaviour of nanocarrier types, given their specific characteristics. In this way, the influence of nanocarriers on the change in the environmental behaviour of active substances should be determined as an example. At the end, the implications for an appropriate safety assessment should be described in more detail based on the selected types, to adapt the current environmental risk assessment procedure of these advanced materials, if necessary.





Glass dicing with Temporal Airy Pulses

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Ultrashort pulse laser sources are useful tools for micro- and nano-processing of large band gap dielectric materials. Previous studies have shown that temporally modulated femtosecond laser pulses can produce holes with small diameters and large depths [1,2]. In this work, we present preliminary results that implement three types of pulses: bandwidth-limited (30 fs at 785 nm), positive, and negative Temporal Airy Pulses (TAP), as precursors for glass dicing. The material of choice was 170 μm thick soda-lime glass, inscribed at 1 kHz repetition rate using 20x and 50x objectives, for different laser energies and scanning speeds. After laser processing, the glass was diced by mechanical stress, with a four-point bending stage. We analyzed the quality of the scribed line at the surface and in cross-section after breaking, as well as the necessary breaking force for all three types of laser pulses. We report that positive TAP produced a neat, flat-cut edge on the glass samples compared with the other implemented pulses.

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P13

Acoustofluidic Lab-on-a-Chip Sample Manipulation

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The poster is a brief summary of our intended endeavors within the recently started Deep 11 project. Surface acoustic waves (SAW) are highly interesting in the field of microfluidic sample handling. We will investigate the fabrication of SAW transducers and the acoustic interplay with acoustic black holes in the micrometer scale.





3D 1x4 Splitter Based on MMI Approach

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The paper presents the design, simulation, optimization, and fabrication of a 3D optical splitter utilizing multimode interference with four S-Bend outputs. The waveguide channel profile in the splitter design uses polymer IP-Dip, and it is fabricated using 3D laser lithography based on the direct laser writing process. The structure was designed for operation at a telecommunication wavelength of 1.55 μm . The optimal size of the multimode interference splitter and the optimal length of the outputs were determined based on minimum insertion losses and minimum non-uniformity. To demonstrate the 1x4 splitting, the output characteristics were investigated by near-field measurement.



P15

High wetting-contrast glass surfaces fabricated by femtosecond laser structuring for open microfluidics and biological applications

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FH Vorarlberg, Spectra Physics Rankweil

In our work, we combine laser structuring with a coating step to fabricate functional surfaces with high wetting-contrast. The use of laser structuring for wetting applications is advantageous because the generation of “hierarchical” structures, which usually enable superhydrophobic behavior, is possible with an easy and fast direct writing step.





In-Situ Synthesis and In-Operando XPS Characterization of Gold and Silver Nanoparticles within Liquid Electrolytes

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Metal nanoparticles have several applications due to their unique properties that differ from bulk material. Due to their different chemical, physical and biological properties, NP's used in optical sensors, diagnostics, electronics, health care, cosmetics, textile, pharmaceutical industry and cancer treatment, which makes synthesis of nanoparticles also important. In this project, Silver, Gold and Platinum NP's were synthesized in situ electrochemically. Via XPS, NP's can be determined by application of positive and negative voltages. In first experiment, for the synthesis of silver nanoparticles ionic liquid (DEME-TFSI), PEG and HAuCl₄ salt mixture was used. Second experiment conducted via silver electrodes and ionic liquid DEME-TFSI for synthesis of silver NP'S. In third experiment, gold NPs were synthesized with PEG and HAuCl₄ mixture. Another experiment done for synthesis of gold NPs with ionic liquid. DEME-TFSI + HAuCl₄ mixture and UV-Visible Spectroscopy was used for characterization. In another experiment, for synthesis of Platinum NPs, Pt electrode, Pt wire and PEG was used. As a last experiment, silver NPs synthesized with Pt electrode, silver wire and PEG- HAuCl₄ mixture. For characterization of NP's, shifts under the applied voltage bias in C 1s and O1s, which correspond to PEG, F1 for IL and Pt 4f, Au 4f and Ag 3d binding energies that were obtained from XPS are compared. Similar shifts refers to being in the same medium, therefore when BE's of metals shifts along with their medium (IL or PEG), it can be deduced that metal NP's were produced within the existing liquid medium.



P17

Laser-tissue interaction of pump-probe elastography and teeth

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Pump-probe elastography (PPE) provides an all-optical approach to examine mechanical properties of samples. The PPE microscope setup consists of a femtosecond laser source (with 1040 nm wavelength, 380 fs pulse-duration, 100 MHz repetition rate and up to 30 uJ pulse energy), an optical delay line (half-motorized, delaying 0 to 25 ns) and an epi-illumination microscope. The acoustic waves are generated by focusing a pump-pulse through a microscope objective onto the sample. To image the propagation of the generated waves, a second pulse ($\lambda = 520$ nm) with temporal delay of up to 25 ns is used for Köhler illumination, while imaging the surface with a sCMOS camera. With the adjustable delay line different propagation of the waves can be detected and therefore a possible change in the wave's propagation speed may be observed. Earlier work has shown that pump-probe microscope can be used with glass and water as sample. There the homogeneous structure of the samples resulted in perfectly round acoustic waves with uniform speed in all direction. It was also possible to produce waves not only on the glass surface but by focusing the beam into the sample, only body waves within the glass were produced.

A possible area of operation, the microscope could be used with teeth. A hard biological sample with different structural layers and growth directions. To test the microscope with this sort of samples artificial dentin (mainly used in art designs as substitution of elephant ivory) and thawed mammoth ivory were used. As the artificial dentin has a homogeneous structure, only roundly shaped waves were observed. For the mammoth ivory different cuts were used and within the longitudinal cut the faster growth direction were possible to observe. Therefore, the acoustic waves occurred oval shaped with two propagation axis with different speeds.





On the electrochemical production of ferrate ions - in-situ detection of the product using dual dynamic voltammetry

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Ferrate salts are materials consisting of ferrate ion, which is the +6 oxidation state of iron. The use of ferrate salts is increasingly recommended for water treatment [1]. They have several advantages: at neutral and acidic pH they are stronger oxidants than chlorine and ozone, are better disinfectant than both ozone and chlorine, and there is no known resistant bacteria or virus to ferrate ion. In addition, ferrates are considered “green chemicals” since the reduction products of ferrate ions are non-toxic Fe(III) compounds (ferric oxide or hydroxide) that can be used as flocculants in the water treatment process. The electrochemical ferrate synthesis is mostly carried out through the anodic dissolution of an Iron-containing electrode in highly alkaline media [2,3]. This method does not require expensive reagents and can yield a very pure product [4].

Despite the great interest in electrochemical ferrate synthesis, there are several contradictions in the literature concerning the optimum conditions and no clear information on the exact mechanism of the process. One of the most important questions is the applied potential during electrochemical ferrate synthesis: at insufficiently positive potentials the rate of ferrate production is small, while at too positive potentials the rate of the parasitic oxygen production is too high, decreasing the current efficiency of the ferrate production. A special-made cell was constructed, that made possible not only the electrochemical synthesis of ferrate but also the accurate examination of the processes leading to it [5]. Dual Dynamic Voltammetry (DDV) [6], a unique technique was used for the investigation of the ferrate production mechanism. DDV made the precise, high-resolution examination of the ferrate production possible. Using this technique, the overlapping oxygen and ferrate production reactions could be separated, and the optimum potential for ferrate synthesis could be determined.

The results show that Dual Dynamic Voltammetry is a capable electroanalytical method for the examination of otherwise problematic systems. The result also can be used for the optimization of the industrial scale ferrate synthesis.

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P19

Optimizing Ultrasound Dispersion for (not only) Spider Silk in Distilled Water: A Comparative Study of Bombyx Mori and Trichonephila Tubuliformis and Major Ampullate Gland Silk

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Universität für Bodenkultur, Institut für Physik und Materialwissenschaften

This study optimizes silk dissolution in aqua bidest, comparing Bombyx Mori silk to spider silk (Trichonephila Tubuliformis and Major Ampullate Gland Silk). Reduced silk quantities enhance resource efficiency. Precision-tuned ultrasonic dispersion improves dissolution effectiveness. Our ongoing work targets minimal energy input near the cavitation limit. This research promises sustainable and efficient silk dissolution. Presentation of first results.





Laser stratigraphy and laser cleaning of historical and synthetic copper patina in conservation science

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Environmental influences that lead to the formation of patina layers not only affect copper surfaces in architecture but also in microelectronics, medicine and automotive technologies. In this study, the analysis of destruction and reformation of protecting anodic oxide films such as copper oxides (e.g. cuprite, Cu_2O) and brochantite ($\text{CuSO}_4 \cdot 3\text{Cu}(\text{OH})_2$) on historical copper roofing sheets from the Belvedere Palace, built by Prince Eugene of Savoy 1723, allowed insight into the mechanism of long-term protection on objects of cultural heritage.

Scanning electron microscopy and energy dispersive X-ray spectroscopy on both artificial [1] and natural patina on original roofing sheets. The possibilities of laser cleaning and laser-induced stratigraphy were explored for the first time on cuprite and brochantite. In order to explore an alternative to conventional cleaning methods of soiling on patina surfaces, the removal of model soiling was investigated. The cleaning thresholds for these contamination layers were orders of magnitude smaller than those of the cuprite and brochantite layers. Through spectroscopic analyses using Laser-Induced Breakdown Spectroscopy (LIBS) [2], the ablation processes of patina films could be quantitatively monitored. Based on these data, physical-chemical strategies were developed to avoid destruction of the protective conversion layers during a laser cleaning intervention.

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	Monday, October 9, 2023	Tuesday, October 10, 2023	Wednesday, October 11, 2023
09:00 - 09:15		L09	L20
09:15 - 09:30	Registration	Stefan Willitsch	Leonid V. Zhigilei
09:30 - 09:45	Opening and greetings	L10	L21
09:45 - 10:00	L01	Javier Martín-Sánchez	Matthias Domke
10:00 - 10:15	Anke Weidenkaff	L11	L22
10:15 - 10:30	L02	Moritz Brehm	Noemí Aguiló Aguayo
10:30 - 10:45	Barbara Hribar-Lee	Coffee	Coffee
10:45 - 11:00	L03		
11:00 - 11:15	Mihai Irimia-Vladu	L12	L23
11:15 - 11:30		Heinz P. Huber	Gyöző G. Láng
11:30 - 11:45		L13	L24
11:45 - 12:00	Poster short lectures	Dimitrios Giannakoudakis	Halil I. Okur
12:00 - 12:15		L14	L25
12:15 - 12:30		Sefik Suzer	Wolfgang Kautek
12:30 - 12:45			
12:45 - 13:00			
13:00 - 13:15	Lunch break & poster session	Lunch break & poster session	Lunch break & poster session
13:15 - 13:30			
13:30 - 13:45			
13:45 - 14:00			
14:00 - 14:15	L04	L15	L26
14:15 - 14:30	Alexander Kromka	Eckart Rühl	Friedrich Esch
14:30 - 14:45	L05	L16	L27
14:45 - 15:00	Dana Seyringer	Lars Mohrhusen	Gabriel Vanko
15:00 - 15:15	L06	L17	L28
15:15 - 15:30	Ota Samek	Parvaneh Mokarian-Tabari	Nina Plankensteiner
15:30 - 15:45	Coffee	Coffee	Coffee
15:45 - 16:00			
16:00 - 16:15	L07	L18	L29
16:15 - 16:30	Gavin Macauley	Sylvie Choua	Juan A. Allegretto
16:30 - 16:45	L08	L19	L30
16:45 - 17:00	Alexander Pogany	Giovanni Marletta	Aras Kartouzian
17:00	Lab tours	Lab tours	Closing & farewell

