Workshop on Integrating Simulations and Experiments for Advanced Applications

During the meeting, the latest results of research and industrial activities within the EU-funded projects **BLESSED**, **ULTIMATE-I**, and **HIP-2d-QM** will be presented, with a focus on:

- **fuel cells and functional materials**,
- **advanced simulation methods**,
- **textiles for optical and space applications**.

The working language of the meeting is **English**.

The meeting will take place
on **Tuesday, January 13, 2026**, from **9:30 a.m. to 12:30 p.m.**
in **Hall 3, 1st floor, SANU Palace**,
35 Knez Mihailova Street, Belgrade.

Organized by: Dr Miljan Dašić, Dr Igor Stanković, and Dr Jelena Pešić.

time	topic/presenter
9:30	**Registration**
10:00	**Welcome to the Institute of Technical Sciences SASA** *Lidija Mančić*
10:05	ULTIMATE-I project **ReaxFF and classical potentials for modeling the interaction of small molecules with graphene** *Igor Stanković* Institute of Physics Belgrade and Senzor Infiz, Belgrade, Serbia
10:15	2D-HIP-QM project **Engineering Current Paths in MoS_2 Nanonetworks for Thin-Film Electronics** *Jelena Pešić* Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia, and Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben, Austria
10:30	ULTIMATE-I project **Development of Carbon Fiber–Reinforced Polymer Replicated Mirrors for Lightweight Visible–Long-Wave Infrared Optics** *Carlos Garcia* Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
10:45	BLESSED project **Freudenberg Technology Innovation: Advancing Materials and Processes Through Simulation** *Matthias Baldofski[1] and Marcin Rybicki[2]* [1] Freudenberg Technology Innovation SE&Co., Weinheim, Germany, [2] Freudenberg e-Power Systems GmbH, München, Germany

time	topic/presenter
11:00	BLESSED project **Multiscale Modeling of Enzyme-Substrate Interactions** *Dr Miljan Dašić* J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Dolejškova 2155/3, 182 00 Prague 8, Czech Republic Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
11:15	BLESSED project **Understanding Electrode Fabrication and Carbon Degradation in PEMFCs Studies using Density Functional Theory and Discrete Element Method Simulations** Matilde Russo[1,3], Sourab Barath Vijayaraghavan[1,2], Peter Lindstedt [3], Alejandro A. Franco[1,2], Matthias Baldofski[1] [1] Freudenberg Technology Innovation SE & Co. KG, 69469 Weinheim, Germany, [2] Université de Picardie Jules Verne, F - 80039, Amiens Cedex 1, France Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, Hub de l'Energie, 15 rue Baudelocque, 80039, Amiens Cedex, France, [3] Imperial College London, Exhibition Road, South Kensington, London SW72AZ, UK
11:45	BLESSED project **Hydration-Controlled Water Network Formation and Density in Crystalline and Amorphous Nafion Membranes** Mateja Jovanović[1,2,3], Nicolas Bernhard[1], Matthias Baldofski[1], Marcin Rybicki[1,4], Miljan Dašić[3], Igor Stanković[3,5] [1] Freudenberg Technology Innovation SE&Co., Weinheim, Germany, [2]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts(SASA), Belgrade, Serbia, [3] Institute of Physics, University of Belgrade, Zemun, Serbia, [4] Freudenberg e-Power Systems GmbH, München, Germany [5]Departamento de Ingenería Mecánica, Universidad Técnica Federico Santa María, Valparaíso, Chile
12:00	**Concluding remarks and discussion**

ReaxFF and classical potentials for modeling the interaction of small molecules with graphene

Igor Stanković

Institute of Physics Belgrade and Senzor Infiz, Belgrade, Serbia

This presentation delves into the intriguing world of small molecules and their collective dynamics, offering insights into their behaviour in diverse nanoscale systems. Graphite and graphene are two remarkable carbon-based materials that have been at the forefront of a revolution in energy storage and two-dimensional electronics. Graphite, a layered material composed of stacked graphene sheets, has long been used as the anode material in conventional lithium-ion batteries. However, the quest for higher energy density and faster charging capabilities has driven researchers to explore novel electrolytes and modifications of graphite. This talk presents two examples in which molecular dynamics simulations were combined with state-of-the-art experiments to reveal the fascinating diversity of collective interactions of small molecules with carbon-based layered materials.

The first study focuses on the intercalation mechanism of aluminium fluoride (AlF3), a small molecule, into graphite electrodes in rechargeable aluminium batteries [1]. By employing scanning tunneling microscopy, density functional theory calculations, and large-scale molecular dynamics simulations, we unravel the collective dynamics of AlF3 clusters between graphite layers. In the second example, we investigate the role of water molecule dynamics in the ferroelectric response of graphene nanoribbon devices. Our findings demonstrate that the collective dynamics of water molecules stabilize the ferroelectric effect. Using a combination of electrical transport measurements and ReaxFF molecular dynamics simulations, we conclude that water molecules bridging between graphene nanoribbon layers stabilize the formation of water clusters via intermolecular Coulomb interactions, driving a robust ferroelectric behavior and remnant polarization observed at the device level. This work lays the foundations for exploiting water dynamics in next-generation ferroelectric heterostructures, with direct implications for neuromorphic computing and memory devices [2].

[1] S.J. Rodríguez, A.E. Candia, I. Stanković, M.C.G. Passeggi, and G.D. Ruano, Study of in-plane and interlayer interactions during aluminum fluoride intercalation in graphite: implications for the development of rechargeable batteries, ACS Applied Nano Materials, 6 (18), 16977-16985 (2023).

[2] M. Awais Aslam, I. Stanković, G. Murastov, A. Carl, M. Zubair Khan, Z. Song, K. Watanabe, T. Taniguchi, A. Lugstein, C. Teichert, R. Gorbachev, R. D Rodriguez, A. Matković, Ferroelectricity in graphene nanoribbon devices enabled by collective water molecule dynamics, Nature Communications 16 (1), 10982 (2025).

Engineering Current Paths in MoS_2 Nanonetworks for Thin-Film Electronics

Jelena Pešić

Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia, and Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben, Austria

Solution-processed MoS_2 nanonetworks are attractive for scalable thin-film electronics, yet their performance is frequently constrained by resistive bottlenecks that are difficult to pinpoint. In presented research we combine in-operando Kelvin probe force microscopy with a diagram-based network model to resolve where the voltage actually drops and how current pathways emerge. The nanoscale maps reveal a small number of dominant routes and large potential steps at inter-flake overlaps. Distinct junction classes, set by overlap geometry and trapped residue, govern local resistance and steer percolation. Our model reproduces the observed “winner-takes-all” behaviour, simulates current-path formation across the nanosheet network, quantifies pathway probabilities, and links junction statistics and conductive-region morphology to device-level metrics obtained from Y-function analysis. Together, the imaging and modelling provide a consistent picture in which junction resistance typically exceeds intraflake (basal-plane) resistance, explaining the prevalence of junction-limited transport in these networks. Ultimately, this study bridges microscopic Kelvin probe force observations with macroscopic device properties, helping build strategies for enhancing network connectivity and optimizing device performance in applications of solution-processed 2D materials. [1]

[1] Imaging Junctions in Two-Dimensional Semiconductor Nanosheet Network Transistors, Jelena Pešić, Simon Leitner, Joseph Neilson, Igor Stanković, Muhammad Zubair Khan, Dragana Tizić Matković, Adam G. Kelly, Tian Carey, Jonathan Coleman, Aleksandar Matković, NPJ 2D Materials and Applications 9 (1), 1-9, (2025)

Development of Carbon Fiber–Reinforced Polymer Replicated Mirrors for Lightweight Visible–Long-Wave Infrared Optics

Carlos Garcia

Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile

Carbon fiber–reinforced polymer (CFRP) replicated mirrors offer a route to lightweight, thermally stable, and scalable reflective optics for spaceborne and ground-based instruments. We present an end-to-end replication workflow for spherical, parabolic, and planar elements up to 1 m in diameter, including precision mandrel preparation, CFRP layup and consolidation, vacuum bagging, thermal curing, and deposition of reflective coatings (e.g., gold). Metrology combines classical knife-edge/Ronchi tests with interferometric measurements to quantify surface form and optical quality. Target metrics include visible-band figure accuracy consistent with the Rayleigh λ/4 criterion (~520–550 nm), low microroughness and integrated scatter, and high reflectivity from the visible to long-wave infrared (LWIR, 8–14 μm). We discuss space-relevant considerations such as thermal stability and outgassing, and outline application pathways spanning educational and amateur telescopes, segmented professional optics, solar concentrators, detector systems, and CubeSat-class LWIR Earth-observation payloads. A development roadmap is proposed to further improve mandrel fidelity, coating uniformity, and environmental qualification maturity.

Freudenberg Technology Innovation: Advancing Materials and Processes Through Simulation

Matthias Baldofski[1] and Marcin Rybicki[2]

[1] Freudenberg Technology Innovation SE&Co., Weinheim, Germany,
[2] Freudenberg e-Power Systems GmbH, München, Germany

This presentation provides an overview of Freudenberg, a global technology company with a rich history spanning more than 170 years. We will explore the company's evolution, its diverse product portfolio, and organizational structure, highlighting how innovation has been a cornerstone of its success.

A key focus will be on Freudenberg Technology Innovation (FTI), the central R&D unit that drives cutting-edge research and development across the group. Within FTI, the Digital Modeling department plays a pivotal role in advancing simulation-based approaches to accelerate material and product innovation. We will discuss how computational methods—ranging from atomistic and molecular dynamics simulations to continuum modeling—are integrated into the development process.

Finally, the talk will showcase selected R&D projects that illustrate the synergy between experimental research and digital modeling, demonstrating how these efforts contribute to sustainable solutions and technological leadership in various industries.

Multiscale Modeling of Enzyme-Substrate Interactions

Dr Miljan Dašić

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Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Enzyme activity arises from molecular processes spanning multiple spatial and temporal scales, from substrate binding at the active site to large-scale conformational motions of the protein. In this talk, we present a multiscale modeling approach based on molecular dynamics and coarse-grained simulations to study how enzymes recognize, bind, and process their substrates. By combining atomistic simulations with enhanced sampling and coarse-grained descriptions, we capture both local interaction patterns and long-time conformational dynamics that control binding affinity and catalytic efficiency. This framework provides a unified view of enzyme–substrate interactions and offers quantitative insight into how molecular structure, flexibility, and environment shape enzymatic function.

Understanding Electrode Fabrication and Carbon Degradation in PEMFCs Studies using Density Functional Theory and Discrete Element Method Simulations

Matilde Russo[1,3], Sourab Barath Vijayaraghavan[1,2], Peter Lindstedt [3], Alejandro A. Franco[1,2], Matthias Baldofski[1]

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A 90% reduction in transport emissions by 2050 is one of the goals of the European Green Deal on climate neutrality. It is accordingly of fundamental importance to introduce environmentally acceptable power generation devices to the automotive sector. PEM fuel cells are poised for widespread adoption in the transition towards a hydrogen economy; contingent on approaching competitive unit costs.

To understand the performance of electrodes in PEMFCs it is imperative that we study the fabrication and degradation of the catalyst layer. In this talk we will present the effect of ink formulation on the CL structure and the degradation the CL due to the oxidation of carbonaceous supports. Some of the challenges relate to the catalyst layer (CL), which is composed of carbonaceous supports with Pt particles sitting on it, that are surrounded by several species in aqueous environment. To improve efficiency, durability and commercialization of PEMFCs, it is crucial to minimize the Pt content as well as the degradation of the carbonaceous material.

In the CL the carbon support undergoes oxidation (i.e., carbon corrosion), even though temperatures are below 100 °C, and that is due to the electrocatalytic aqueous environment, high applied potentials (0.60 – 1.4 V) and presence of Pt. When oxidising species (e.g. O_2, H_2O, H_2O_2, OH-, OH radicals) contact the carbon structure, CO and CO_2 are formed and released, resulting in structural vacancies in the layer. This process causes the progressive degradation of the carbonaceous support and the detachment and agglomeration of Pt particles leading to a loss in catalyst surface area.

In current literature, carbon corrosion is described through global reactions models featuring water and carbon support, e.g. $C(s) + 2\ H_2O \rightarrow CO_2 + 4\ H+ + 4\ e–$. These global reactions are simplifying a phenomenon that is much more complex and composed by several interconnected electrochemical reactions. The carbon support is made of both amorphous and graphitised areas. Soot has been chosen as model compound, in particular naphthalene. Further developments of this work may include the study of corrosion of a defected graphene layer. Several possible reaction pathways have been analysed for the oxidation of naphthalene, reaction enthalpies and activation barriers have been calculated with Density Functional Theory (DFT) using Gaussian 16 with M06-2X method and SMD to address water solvation. Once known the energies of the structures, it is possible to evaluate the rate constants of reactions, also considering the applied potential. The current work is formulating a reaction mechanism that includes such interconnected electrochemical reactions and their energy barriers in order to identify the rate determining steps in the overall

carbon degradation process.

The elementary-step based mechanism obtained from this work can be implemented in a multi-scale model that simulate the functioning of PEMFCs. The work is expected to lead to a better understanding of the critical parts of the fuel cells and facilitate an increase in the lifetime of PEMFCs through improved designs (operating conditions, materials).

We will also present our work on a novel Discrete Element Method (DEM) model to capture the aggregation dynamics of the carbon catalyst in the fabrication of the PEMFC electrode. Since the catalyst ink is a colloidal dispersion, the inter-particle interactions can be rationalised via the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory. Our model simulates the formation of the electrode microstructure from dispersion to drying. The microstructure is then digitally characterised to obtain statistical descriptors such as pore size distribution, fractal dimension, tortuosity factor, and two-point correlations to validate the model against microstructural data obtained from tomographic studies.

We will present the ability of the model to explicitly capture the co-aggregation of ionomer and carbon and present empirical trends on the effect of the spatial distribution of the ionomer and carbon phases on the electrochemical behaviour of the catalyst layer. Results from the simulations will be discussed for different water: alcohol compositions and their effect on ionomer-carbon co-aggregation. This will be followed by discussions of experimental data validating the observations from the model and work done to correlate the outputs from the model against experimental observations.

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Hydration-Controlled Water Network Formation and Density in Crystalline and Amorphous Nafion Membranes

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Proton Exchange Membrane Fuel Cells rely on hydrated polymer membranes such as Nafion, whose density and transport properties are governed by nanoscale structural ordering. Using molecular simulations, we investigate density–hydration relationships in amorphous and crystalline Nafion membranes. Water clustering analysis reveals a clear hydration-driven transition from isolated water domains to percolating and fully connected networks, with crystalline systems exhibiting earlier percolation and higher densities at all hydration levels. This behavior arises from enhanced molecular packing enabled by ordered polymer backbones and aligned water channels, as confirmed by Voronoi analysis. To improve the molecular-level description of protonated environments, we additionally reparametrise the hydronium force field using density functional theory reference data, ensuring consistency with the employed water model and realistic local solvation structure.