



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 <i>Lidija Mančić</i>
10:10	ULTIMATE-I project ReaxFF for modeling the interaction of water with graphene edges <i>Igor Stanković</i> Institute of Physics Belgrade and Senzor Infiz, Belgrade, Serbia
10:25	2D-HIP-QM project Engineering Current Paths in MoS₂ Nanonetworks for Thin-Film Electronics <i>Jelena Pešić</i> 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
10:40	ULTIMATE-I project Textile mirrors for space applications <i>Carlos Garcia</i> Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
10:55	Coffee Break

time	topic/presenter
11:00	BLESSED project Multiscale Modeling of Enzyme-Substrate Interactions <i>Dr Miljan Dašić</i> 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 Lindstedt³, Alejandro A. Franco^{1,2}, Matthias Baldofski¹ 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 Bernhard¹, Matthias Baldofski¹, Marcin Rybicki^{1,4}, Miljan Dašić³, Igor Stanković^{3,5} ¹ Freudenberg Technology Innovation SE&Co., Weinheim, Germany, ²Institute 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 ⁵Departamento de Ingeniería Mecánica, Universidad Técnica Federico Santa María, Valparaíso, Chile
12:00	Concluding remarks and discussion