Ultra Thin Magneto Thermal Sensoring

H2020-MSCA-RISE
ULTIMATE-I

HIP-2D-QM

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Argentinian-Serbian Nanotechnology Workshop

Challenges in bridging theory and experiments

Institute of Physics Belgrade, the reading room of the library dr Dragan Popović

Friday, November 22nd, 2024, 10:00-12:30

time	topic/presenter
10:00	**Modeling interaction of small molecules with materials: friction forces, intercalation, and memory effects** *Dr Igor Stankovic* Senzor Infiz / Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
10:35	**Unveiling the Pathways: KPFM and Modeling Insights into MoS_2 Nanosheet Network Behavior in Transistor Devices** *Dr Jelena Pešić* Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben, Austria
11:10	**Low-Energy Ion-Surface Interactions: From Spectral Anomalies to Charge Transfer Mechanisms** *Dr Fernando J. Bonetto* Surface Physics Group, Institute of Physics of Littoral (CONICET-UNL), Güemes 3450, S3000GLN Santa Fe, Argentina.
11:45	**Semi-empirical quantum-mechanical (SQM) methods for modeling molecular interactions** *Dr Miljan Dašić* Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo náměstí 2, 166 10 Prague, Czech Republic Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

organized by: Dr Miljan Dašić, Dr Igor Stanković, Dr Jelena Pešić

Modeling interaction of small molecules with materials: friction forces, intercalation, and memory effects

Dr Igor Stanković

Senzor Infiz / Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Molecular dynamics (MD) simulations have become an invaluable tool for investigating and predicting the behavior of small molecules in complex environments, providing insights into their structural, thermodynamic, and transport properties. This talk will highlight recent advancements in using MD to understand molecular interactions in diverse systems, including phosphonium-based ionic liquids [1], aluminum fluoride intercalation in graphite for battery applications [2], and water clusters in nanoscale geometries [3]. First, we explore the impact of water content on the dynamic properties of phosphonium ionic liquids, revealing how water molecules modulate ion interactions and impact viscosity, diffusion, and thermal stability. Next, we examine the role of AlF_3 in rechargeable aluminum batteries, using MD to uncover the mechanisms behind its intercalation in graphite and implications for energy storage optimization. Finally, we delve into the behavior of water clusters on graphene nanoribbons under varying electric fields, showcasing MD's capability to capture ferroelectric effects relevant to future nanotechnology applications. By illustrating these cases, this talk will emphasize MD's role in elucidating the fundamental mechanisms behind small molecule interactions in complex systems, guiding the design and optimization of materials across energy storage, nanotechnology, and beyond.

[1] I. Stanković, M. Dašić, M. Jovanović, A. Martini, Langmuir 2024, 40, 17, 9049–9058.

[2] S.J. Rodríguez, A.E. Candia, I. Stanković, M.C.G. Passeggi, G.D. Ruano, ACS Appl. Nano Mater. 2023, 6, 18, 16977–16985.

[3] arXiv:2304.09738

Unveiling the Pathways: KPFM and Modeling Insights into MoS$_2$ Nanosheet Network Behavior in Transistor Devices

Dr Jelena Pešić

Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade

Chair of Physics, Department Physics, Mechanics and Electrical Engineering, Montanuniversitaet Leoben

In this talk, we will explore how Kelvin Probe Force Microscopy (KPFM) and a tailored network model reveal the complex behavior of MoS$_2$ nanosheet networks in transistor devices. Using in-operando KPFM, we image the potential distribution across MoS$_2$ networks, isolating potential drops at nanosheet junctions and mapping how these affect current paths. This imaging highlights distinct types of junctions within the network, emphasizing the impact of overlap and trapped impurities on resistance. We develop a model that simulates the formation of current pathways across these nanosheet networks, correlating conductive regions to the overall device morphology and conductivity.

Our findings suggest that current flow often follows the path of least resistance, confirming the "winner-takes-all" behavior documented in similar systems. The model further quantifies the likelihood of current pathway formation, supporting a more detailed understanding of connectivity within these networks. Ultimately, this study bridges microscopic KPFM 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, *under review.*

Semi-empirical quantum-mechanical (SQM) methods for modeling molecular interactions

Dr Miljan Dašić

Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo náměstí 2, 166 10 Prague, Czech Republic

Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, Serbia

Semi-empirical quantum mechanical (SQM) methods represent computational techniques used to model molecular interactions implementing a balance of accuracy and computational efficiency [1]. Unlike fully ab-initio methods that exclusively rely on quantum mechanical calculations, SQM methods include empirical data [2], such as: ionization potentials, electron affinities, and orbital energies from experimental sources. These parameters simplify calculations by approximating certain electron interactions, thus providing insights into electronic structure, binding energies, and molecular geometries for larger systems, where purely quantum mechanical treatment would be computationally too expensive, or even prohibitive.

In case of research regarding hydrogen fuel cells, SQM methods provide complementary insights to primary methods, such as Density Functional Theory (DFT), which is often used for detailed studies, especially in catalysis. While DFT provides precise descriptions of chemical processes, SQM is a valuable tool for estimating binding energies in fuel cell catalysts, for studying interaction energies in polymer electrolyte membranes, and for analyzing adsorption on catalytic surfaces where computational speed is a priority. By applying SQM either as a preliminary tool or integrated within hybrid models, it is possible to explore broader molecular configurations and interactions of fuel cell components, hence coupling efficient initial studies with higher-accuracy studies. Such a flexibility makes SQM useful in preliminary screenings, where large datasets and complex systems need to be handled fastly.

As the lecturer Dr Dašić is actively conducting research based on a specific SQM approach, namely the SQM2.20 scoring function which is used in determining Protein-Ligand binding affinity predictions [3], one part of the lecture will cover that topic.
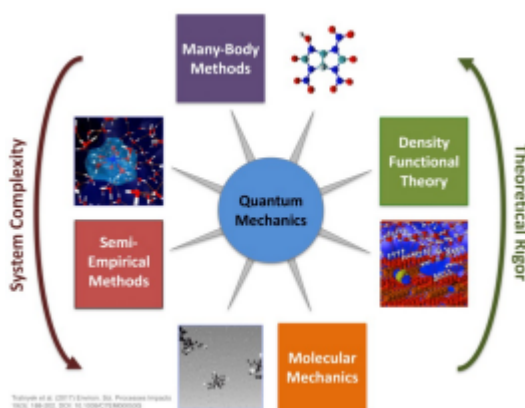
Rerefences
[1] Dral, Pavlo O., ed. Quantum Chemistry in the Age of Machine Learning. Elsevier, **2022**.
[2] Stewart, James JP., Journal of Molecular modeling **2007**, 13, 1173.
[3] Pecina, A.; Fanfrlík, J., Lepšík, M., Řezáč, J., Nature Communications **2024**, 15, 1127.

Low-Energy Ion-Surface Interactions: From Spectral Anomalies to Charge Transfer Mechanisms

Fernando J. Bonetto

Surface Physics Group, Institute of Physics of Littoral (CONICET-UNL), Güemes 3450, S3000GLN Santa Fe, Argentina.

The Surface Physics Group of Santa Fe (Argentina) specializes in characterizing surfaces and 2D materials through advanced techniques, including STM, AFM, AES, EELS, and LEIS, combined with theoretical models. This presentation will focus on three recent studies conducted in our group on low-energy ion interactions with surfaces.

The first study explores unexpected peaks in the LEIS spectra of Ar+ ions scattered from a Cu(111) surface, which cannot be explained by the standard binary collision model. Using molecular dynamics simulations, we show that these spectral features arise from surface defects such as islands or steps, demonstrating the impact of imperfections on LEIS spectra. Next, we investigate charge transfer in collisions between hydrogen ions and C60-based carbon films deposited on Cu(111). The study reveals how substrate atoms and electronic structure of the grown films influence the charge transfer process depending on film thickness.

Finally, we present novel measurements of neutral and ion fractions of Ne+ions backscattered by MoS_2 and metallic Mo surfaces. Despite the distinct electronic properties of the two targets, neutralization rates remain high across various energies and collision angles. Theoretical calculations indicate that resonant charge transfer is more prominent in MoS_2, while Auger neutralization dominates for metallic Mo. The discrepancy between experimental and calculated neutral fractions is attributed to excited states in Ne projectiles. These findings offer new insights into ion-surface interactions and enhance our understanding of charge transfer mechanisms in low-energy collisions.