

# Surface Science Discussions 2024 – Programme

Seminar Chairman: Mikołaj Lewandowski

09.01.2024 - SESSION 1		
10:00-10:05 (CET)	05:00 PM in CN, 06:00 PM in JP and KR 04:00 AM in FL, USA, 08:00 PM in NSW, AUS	Welcome word from the Organizers
10:05-10:50	OPENING LECTURE Prof. Dr. Klaus Kern	Atomic Scale Imaging: From Biomolecular Function to Quantum Dynamics
	The catalyst under reaction conditions	
10:50-11:15	Prof. Dr. Günther Rupprechter	In situ Surface Microscopy of Nanostructures and Reactants During Catalysis
11:15-11:40	Prof. Dr. Qiang Fu	Interface Catalysis Over Oxide/Metal and Oxide/Oxide Catalysts
11:40-12:05	Dr. Su-Hyun Yoo	Tailoring Electrocatalyst Performance Through Engineering Dopants and Understanding Dopant Evolution After Hydrogen Oxidation Reaction
12:05-12:20	Coffee break	
09.01.2024 - SESSION 2		
	Hydroxylation and oxidation of surfaces	
12:20-12:45	Prof. Dr. Angelika Kühnle	Water at Mineral Surfaces: Hydration of K-Feldspar Microcline (001)
12:45-13:10	Prof. Dr. Franciszek Krok	The Effect of Reduction and Oxidation Processes on Structural and Electronic Properties of TiO <sub>2</sub> (110)
13:10-13:35	Prof. Dr. Edvin Lundgren	Surface Sensitive Studies of the Electrolyte/Electrode Interface
13:35-14:00	Dr. Baran Eren	Operando X-ray Spectroscopy Study on the Oxidation State of Nickel during the Oxygen Evolution Reaction
14:00-15:00	Lunch break	
09.01.2024 - SESSION 3		
15:00-15:15	nanoscore gmbh (Unisoku EU-representative)	Unisoku Scanning Probe Microscopy Products
	Novel approaches in theoretical studies of catalytic reactions	
15:15-15:40	Dr. Alessandro Fortunelli	ML-Accelerated DFT Sampling of Dynamical Processes in Catalysis & Materials Science
15:40-16:05	Dr. Lucas Foppa	Learning Design Rules for Heterogeneous Catalysts via Artificial Intelligence
16:05-16:30	11:30 PM in CN, 12:30 AM in JP and KR 10:30 AM in FL, USA, 02:30 AM in NSW, AUS	Ab initio Simulation of Surface Reaction in Electrochemical Environment with Hybrid Solvent Model
10.01.2024 - SESSION 1		
	Molecules from different perspectives: Laser-induced processes and magnetic molecular systems	
09:30-09:55 (CET)	03:30 AM in FL, USA, 07:30 PM in NSW, AUS	Prof. Dr. Jennifer MacLeod Design and Characterisation of One-Dimensional Molecular Materials
09:55-10:20	Prof. Dr. Karina Morgenstern Dr. Hiroshi Imada	Single-Molecule Investigation of Laser-Driven Chemistry at Surfaces Single Molecule Laser Nanospectroscopy
10:20-10:45	Prof. Dr. Richard Berndt	Spin Effects in Adsorbed Molecules and Clusters
10:45-11:10	Dr. Martina Corso	Transition Metals Dihalides: From 2D Magnetism to Metal-Organic Hybrids
11:10-11:35	Coffee break	
10.01.2024 - SESSION 2		
	Controlled modification of surfaces	
11:50-12:15	Prof. Dr. Sarp Kaya	Arrangement and Clustering Patterns of Platinum Atoms on the Stepped Copper (211) Surfaces
12:15-12:40	Dr. André Luis Fernandes Cauduro	Cooperative Mechanisms Behind Nanoscale Smoothing on Metal Surfaces: From Adatom Diffusion to Step Nucleation
12:40-13:05	Dr. Maciej Rogala	Exploring Defect Migration Mechanisms in the Context of Resistive Switching at TiO <sub>2</sub> Surfaces
13:05-14:05	Lunch break	
10.01.2024 - SESSION 3		
14:05-14:20	Materials Design	MedeA Computational Software for Atomistic Simulation of Materials
	Growth, structure and properties of molecular layers and 2D materials	
14:20-14:45	Prof. Dr. Grażyna Antczak	Identification of Chiral CoPc+F16CuPc on Ag(100) Domains in Reciprocal Space with the Molecular Structure Factor
14:45-15:10	Prof. Dr. M. Alexander Schneider	Growing Te Containing TMDCs on Metal Substrates in UHV
15:10-15:35	Prof. Dr. Fabian D. Naterer	Lessons Learned from Applying Sparse Sampling and Parallel Spectroscopy for Fast Quasiparticle Interference Imaging
15:35-16:20	CLOSING LECTURE Prof. Dr. Cristiana di Valentin	Architecturing Graphene Interfaces with Metal Surfaces or Molecular Layers For Tailor-Made Nanotechnology
16:20-16:25	11:25 PM in CN, 00:25 AM in JP and KR 10:25 AM in FL, USA, 02:25 AM in NSW, AUS	Concluding remarks by the Organizers