Session Program

22–26 Apr 2024

Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis X

Poster Session

Monday 22 April

20:00

Poster Session

Session | **Location:** Hotel Marena Wellness & Spa Turystyczna 1, 72-415 Międzywodzie, Poland

20:00–22:00

On the pH-Dependent Shift of the „Hupd Peak“ on Polycrystaline Pt-Group Surfaces

Speaker
Ms Hedda Oschinski

20:00–22:00

Bridging the Gap: From EIS to Real-World Battery Performance with Stochastic Pulse Design

Speaker
Ms Limei Jin

20:00–22:00

With Markov Jumps Toward Sustainability – Computational Modeling of Catalytic Reactions

Speaker
Dr Martin Deimel

20:00–22:00

Machine Learning Assisted Realistic Description of Catalytic Centers on M1 Catalyst Surfaces

Speaker
Mr Kyeonghyeon Nam

20:00–22:00

Exploring Dynamic Solvation Effects at the Electrochemical IrO2/Water Interface

Speaker
Mr Nikhil Bapat

20:00–22:00

Excitation Trapping and Polaron Formation in Solar Battery Materials

Speaker
Ms Nóra Kovács

20:00–22:00

Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials

Speaker
Ms Yuandong Wang

20:00–22:00

Incorporation of Preparation Variability Into Reactor Models of Heterogeneous Catalysts

Speaker
Mr Muhammad Zeeshan Ashraf

20:00–22:00

Combining DFTB and Structure Mapping for the Prediction of Transition Paths in the Deactivation of ZnO@Cu Catalysts

Speaker
Dr Artem Samtsevych

20:00–22:00

How the Metal Substrate Affects Oxide Cluster Shapes in Inverse Catalysts

Speaker
Mr Luuk Kempen

20:00–22:00

Realistic Representations of IrO2 Catalyst Surfaces through Extensive Sampling

Speaker
Dr Hao Wan

20:00–22:00

Adaptive Quasi Monte Carlo Quadrature With Possible Application in Bayesian Inference of Chemical Kinetic Models

Speaker
Jinyi Zhou

20:00–22:00

Machine Learning Enhanced Bayesian Inference on Multiscale Kinetic Models

Speaker
Mr Andreas Panagiotopoulos

20:00–22:00

Predicting Atomic Charges in MOFs by Topological Charge Equilibration

Speaker
Mr Babak Farhadi J ahromi

20:00–22:00

Adapting Explainable Machine Learning to Study Mechanical Properties of 2D Hybrid Perovskites

Speaker
Mr Yuxuan Yao

20:00–22:00 **A Fundamentals Study of the Slater-Koster Tables in NiOx Systems**

Speaker
Mr Yihua Song

20:00–22:00 **Exploring Enhanced Sampling Concepts Using Boltzmann Generators**

Speaker
Mr David Greten

20:00–22:00

Classical Force Field Simulations of Electrolytes at Charged Water Surfaces

Speaker
Dr Jakob Filser

20:00–22:00

Charge Mobility Estimation in Amorphous Organic Semiconductors via Machine Learning

Speaker
Dr Ke Chen

20:00–22:00 **A General-Purpose Framework for Kinetic Monte-Carlo Simulations**

Speaker
Dr Roya Ebrahimi Viand

20:00–22:00 **Exploration of Cathode-Stable Hybrid Solid-State Electrolytes**

Speaker
Ms Sina Jennifer Ziegler

20:00–22:00

Li-Ion-Mediated Polaron Formation and UV Energy Storage in NbWO6 Photo-Batteries: An Integrated Experimental and Computational Approach

Speaker
Dr Yu-Te Chan

20:00–22:00

Considerations of Mean Field Microkinetic Modeling: Selective Hydrogenation of C2H2

Speaker
Dr Olga Vinogradova

22:00

Tuesday 23 April

16:00
18:00

Poster Session

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