Session Program

16–20 Jun 2025

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

Poster Session I

Tuesday 17 June

16:40

Poster Session I

Session |
Location: Haus der bayerischen Landwirtschaft, Rieder Str. 70, 82211 Herrsching am Ammersee, Germany

16:40–17:00
Towards Time-Dependent Electronic Structure Methods for Large Systems

Speaker
Lydia Fichte

17:00–17:20
Superresolution for Real-Time TDDFT, Enabling Spectral Predictions of Large Molecules

Speaker
Alexander Gorfer

17:20–17:40
Beyond Ion Dynamics: Efficient Charge Transport Simulations Including Polarons at the Battery Scale

Speaker
Matteo Rinaldi

17:40–18:00
Predicting Binding Energies at the Electrified Metal-Water Interface

Speaker
Ann-Kathrin Bergmann

17:40–18:00
SISSO-based Screening of Novel Binary Metal Alloys Catalysts for Ammonia Oxidation Reaction

Speaker
Emanuel Colombi Manzi

17:40–18:00
Toward Novel 2D Materials Beyond Nature: Prediction of Phase Stability and Structural Properties

Speaker
Tomoko Yokaichiya

17:40–18:00
Hopping Down the Rabbit Hole: Exploration of the RuO2 Surface Stability

Speaker
Cedric Hannemann

17:40–18:00
From Efficiency to Accuracy: Benchmarking Optimizers on General Purpose Machine-Learned Potential Energy Surfaces

Speaker
David Greten

17:40–18:00 **How Prevalent is Disorder in Computationally Predicted Materials?**

Speaker
Konstantin Jakob

17:40–18:00 **Investigating Photocharged States in Solar Battery Materials**

Speaker
Leon Müller

17:40–18:00 **Accurate Yet Efficient Description of Small and Large Polarons**

Speaker
Daria Ustimchuk

17:40–18:00
Revisiting the Origins of Electrocatalytic Activity: the Enthalpy-Entropy Compensation in HER

Speaker
Andrew Wong

17:40–18:00
Coupling Mass Transport to Surface Kinetics in Models of Electrocatalytic Selectivity

Speaker
Hemanth Pillai

17:40–18:00
Towards The Study of Dissolution of IrO2 Surface During OER Employing MLIP

Speaker
Jimiben Patel

18:00