

**Session Program**

**16-20 Jun 2025**

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

**Poster Session II**

# Thursday 19 June

16:00

## Poster Session II

**Session** |

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

16:00–16:20

### Towards Extracting Reaction Mechanisms from Automatic Process Exploration

**Speaker**

Aditya Kumar

16:20–16:40

### Coupling kinetic Monte-Carlo and Continuum Models with Noise Aware Sparse Grids

**Speaker**

Tobias Hülser

16:40–17:00

### Towards Automated Reaction Control and Inverse Reactivity Reconstruction in Compact Profile Reactors

**Speaker**

Jinyi Zhou

17:00–17:20

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

**Speaker**

Yuandong Wang

17:20–17:40

### Deciphering Electrochemical Barriers: Hammond's Postulate in Electrochemistry

**Speaker**

Julius Lonnes

17:40–18:00

### Kinetic Monte Carlo Simulations of Interaction Dynamics: From Prey-Predator Models to Opinion Dynamics

**Speaker**

Fatemeh 'Negin' Tavakkoli

17:40–18:00

### A Framework for Sparse Kinetic Monte-Carlo Models

**Speaker**

Bat-Amgalan Bat-Erdene

17:40–18:00

### Predicting the Electronic Structure from Machine Learning

**Speaker**

Maximilian Ach

17:40–18:00

**On the Significance of the Interfacial Capacitance in the Description of Grand-Canonical Energetics****Speaker**

Hedda Oschinski

17:40–18:00

**Revisiting the Origins of Electrocatalytic Activity: the Enthalpy-Entropy Compensation in HER****Speaker**

Barbara Sumic

17:40–18:00

**A Solar Battolyzer Approach: On Demand Hydrogen Production and Energy Storage in 2D materials****Speaker**

Yu-Te Chan

17:40–18:00

**Study of Metalloporphyrins Complex Single-Atom Electrocatalyst on Graphene****Speaker**

Zhe Yun

17:40–18:00

**Navigating the Latent Space of Chemical Solid State Reactions in Hybrid Battery Interfaces****Speaker**

Sina Jennifer Ziegler

17:40–18:00

**Designing Novel Intermediate Temperature Proton-conducting Electrolytes for Solid Oxide Fuel Cells****Speaker**

Yun An

17:40–18:00

**Advanced Framework for State of Health Estimation Using Equivalent Circuit Models and Machine Learning****Speaker**

Limei Jin

17:40–18:00

**GAP vs. MACE: Efficiency Evaluation in a Liquid Electrolyte System****Speaker**

Anton Beiesdorfer

18:00