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

Thursday, 19 June 2025

Poster Session II (16:00 - 18:00)

time	[id] title	presenter
16:00	[65] Towards Extracting Reaction Mechanisms from Automatic Process Exploration	KUMAR, Aditya
16:20	[63] Coupling kinetic Monte-Carlo and Continuum Models with Noise Aware Sparse Grids	HÜLSER, Tobias
16:40	[59] Towards Automated Reaction Control and Inverse Reactivity Reconstruction in Compact Profile Reactors	ZHOU, Jinyi
17:00	[54] Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials	WANG, Yuandong
17:20	[52] Deciphering Electrochemical Barriers: Hammond's Postulate in Electrochemistry	LONNES, Julius
17:40	[61] On the Significance of the Interfacial Capacitance in the Description of Grand-Canonical Energetics	OSCHINSKI, Hedda
17:40	[60] Revisiting the Origins of Electrocatalytic Activity: the Enthalpy-Entropy Compensation in HER	SUMIC, Barbara
17:40	[58] A Solar Battolyzer Approach: On Demand Hydrogen Production and Energy Storage in 2D materials	CHAN, Yu-Te
17:40	[57] Study of Metalloporphyrins Complex Single-Atom Electrocatalyst on Graphene	YUN, Zhe
17:40	[56] Navigating the Latent Space of Chemical Solid State Reactions in Hybrid Battery Interfaces	ZIEGLER, Sina Jennifer
17:40	[55] Designing Novel Intermediate Temperature Proton-conducting Electrolytes for Solid Oxide Fuel Cells	AN, Yun
17:40	[53] Advanced Framework for State of Health Estimation Using Equivalent Circuit Models and Machine Learning	JIN, Limei
17:40	[51] GAP vs. MACE: Efficiency Evaluation in a Liquid Electrolyte System	BEIESDORFER, Anton
17:40	[66] Kinetic Monte Carlo Simulations of Interaction Dynamics: From Prey-Predator Models to Opinion Dynamics	TAVAKKOLI, Fatemeh 'Negin'
17:40	[64] A Framework for Sparse Kinetic Monte-Carlo Models	BAT-ERDENE, Bat-Amgalan
17:40	[62] Predicting the Electronic Structure from Machine Learning	ACH, Maximilian