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

Monday, 22 April 2024

Poster Session (20:00 - 22:00)

time	[id] title	presenter
20:00	[67] Considerations of Mean Field Microkinetic Modeling: Selective Hydrogenation of C2H2	Dr VINOGRADOVA, Olga
20:00	[65] Exploration of Cathode-Stable Hybrid Solid-State Electrolytes	Ms ZIEGLER, Sina Jennifer
20:00	[61] Exploring Enhanced Sampling Concepts Using Boltzmann Generators	Mr GRETEN, David
20:00	[55] Incorporation of Preparation Variability Into Reactor Models of Heterogeneous Catalysts	Mr ASHRAF, Muhammad Zeeshan
20:00	[50] How the Metal Substrate Affects Oxide Cluster Shapes in Inverse Catalysts	Mr KEMPEN, Luuk
20:00	[46] Bridging the Gap: From EIS to Real-World Battery Performance with Stochastic Pulse Design	Ms JIN, Limei
20:00	[66] Li-Ion-Mediated Polaron Formation and UV Energy Storage in NbWO6 Photo-Batteries: An Integrated Experimental and Computational Approach	Dr CHAN, Yu-Te
20:00	[64] A General-Purpose Framework for Kinetic Monte-Carlo Simulations	Dr VIAND, Roya Ebrahimi
20:00	[63] Charge Mobility Estimation in Amorphous Organic Semiconductors via Machine Learning	Dr CHEN, Ke
20:00	[62] Classical Force Field Simulations of Electrolytes at Charged Water Surfaces	Dr FILSER, Jakob
20:00	[60] Machine Learning Enhanced Bayesian Inference on Multiscale Kinetic Models	Mr PANAGIOTOPOULOS, Andreas
20:00	[59] A Fundamentals Study of the Slater-Koster Tables in NiOx Systems	Mr SONG, Yihua
20:00	[58] Adaptive Quasi Monte Carlo Quadrature With Possible Application in Bayesian Inference of Chemical Kinetic Models	ZHOU, Jinyi
20:00	[57] Realistic Representations of IrO2 Catalyst Surfaces through Extensive Sampling	Dr WAN, Hao
20:00	[56] Combining DFTB and Structure Mapping for the Prediction of Transition Paths in the Deactivation of ZnO@Cu Catalysts	Dr SAMTSEVYCH, Artem
20:00	[54] Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials	Ms WANG, Yuandong
20:00	[53] Adapting Explainable Machine Learning to Study Mechanical Properties of 2D Hybrid Perovskites	Mr YAO, Yuxuan
20:00	[51] Predicting Atomic Charges in MOFs by Topological Charge Equilibration	Mr AHROMI, Babak Farhadi J
20:00	[49] Exploring Dynamic Solvation Effects at the Electrochemical IrO2/Water Interface	Mr BAPAT, Nikhil
20:00	[48] Machine Learning Assisted Realistic Description of Catalytic Centers on M1 Catalyst Surfaces	Mr NAM, Kyeonghyeon

20:00	[47] With Markov Jumps Toward Sustainability – Computational Modeling of Catalytic Reactions	Dr DEIMEL, Martin
20:00	[45] On the pH-Dependent Shift of the „Hupd Peak“ on Polycrystaline Pt-Group Surfaces	Ms OSCHINSKI, Hedda
20:00	[52] Excitation Trapping and Polaron Formation in Solar Battery Materials	Ms KOVÁCS, Nóra

Tuesday, 23 April 2024

Poster Session (16:00 - 18:00)