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

Tuesday, 17 June 2025

Poster Session I (16:40 - 18:00)

time	[id] title	presenter
16:40	[38] Towards Time-Dependent Electronic Structure Methods for Large Systems	FICHTE, Lydia
17:00	[39] Superresolution for Real-Time TDDFT, Enabling Spectral Predictions of Large Molecules	GORFER, Alexander
17:20	[41] Beyond Ion Dynamics: Efficient Charge Transport Simulations Including Polarons at the Battery Scale	RINALDI, Matteo
17:40	[40] Accurate Yet Efficient Description of Small and Large Polarons	USTIMCHUK, Daria
17:40	[37] Investigating Photocharged States in Solar Battery Materials	MÜLLER, Leon
17:40	[50] How Prevalent is Disorder in Computationally Predicted Materials?	JAKOB, Konstantin
17:40	[49] From Efficiency to Accuracy: Benchmarking Optimizers on General Purpose Machine-Learned Potential Energy Surfaces	GRETEN, David
17:40	[47] Towards The Study of Dissolution of IrO2 Surface During OER Employing MLIP	PATEL, Jimiben
17:40	[46] Toward Novel 2D Materials Beyond Nature: Prediction of Phase Stability and Structural Properties	YOKAICHIYA, Tomoko
17:40	[45] SISSO-based Screening of Novel Binary Metal Alloys Catalysts for Ammonia Oxidation Reaction	COLOMBI MANZI, Emanuel
17:40	[43] Predicting Binding Energies at the Electrified Metal-Water Interface	BERGMANN, Ann-Kathrin
17:40	[48] Hopping Down the Rabbit Hole: Exploration of the RuO2 Surface Stability	HANNEMANN, Cedric
17:40	[44] Coupling Mass Transport to Surface Kinetics in Models of Electrocatalytic Selectivity	PILLAI, Hemanth
17:40	[42] Revisiting the Origins of Electrocatalytic Activity: the Enthalpy-Entropy Compensation in HER	WONG, Andrew