FHI Poster Sessions 2024

Monday, 25 November 2024

TH Poster Session (14:00 - 16:00)

time	[id] title	presenter
14:00	[122] 1.TH.05 Coupling Mass Transport to Surface Kinetics in Models of Electrocatalytic Selectivity	PILLAI, H.S.
14:00	[121] 1.TH.04 Disentangling Transport and Kinetics in Complex Reaction Chambers by Novel Reduced Order Modeling Approaches	HUELSER, T.
14:00	[120] 1.TH.03 Smart Experimentation: Adaptive Strategies for Efficient Kinetic Learning in Catalytic Reactors	ABIBATA KOUYATE, M.
14:00	[135] 1.TH.18 Enhanced 2D and 3D Structure-Property Sampling with Generative Models for Inverse Materials Design	KÖNIG, P.
14:00	[137] 1.TH.20 Machine Learning Driven Design of Spiropyran Photoswitches	STROTHMANN, R.
14:00	[136] 1.TH.19 Universally Accurate or Specifically Inadequate? Stress-Testing General Purpose Machine Learning Potentials	JAKOB, K.
14:00	[134] 1.TH.17 Excited States Methods for Large and Largest Systems	KICK, M.
14:00	[133] 1.TH.16 High-Throughput Modelling of Phonon Polaritons	GELŽINYTĖ, E.
14:00	[132] 1.TH.15 The SolBat Project: Electron, Phonon, and Polaron Dynamics in Solar Batteries	CHAN, Y.T.
14:00	[130] 1.TH.13 A Complete Picture on Correlated Conduction Mechanisms in Amorphous Lithium Thiophosphate using Long Timescale Molecular Dynamics Simulations	HUSS, T.
14:00	[131] 1.TH.14 Computational Methods for Solid-State NMR of Battery Materials	VALENZUELA REINA, J.
14:00	[129] 1.TH.12 Automated Process Exploration Driven by Diversity in Local Atomic Environments	LAI, K.C.
14:00	[128] 1.TH.11 Automatic Exploration of Surface Reaction Networks	JUNG, H.
14:00	[127] 1.TH.10 IrO2 Surface Evolution from Parallel Tempering Simulations	WAN, H.
14:00	[126] 1.TH.09 Out of the Crystalline Comfort Zone: Sampling the Initial Oxide Formation at Cu(111)	RICCIUS, F.
14:00	[125] 1.TH.08 Machine Learning Work Functions for Metal-Water Interfaces	BERGMANN, N.
14:00	[124] 1.TH.07 Unraveling the Electric Double Layer: Bridging Theoretical Insights and Experimental Observations	LI, L.
14:00	[123] 1.TH.06 Electrocatalytic Selectivity of the Oxygen Reduction Reaction from Ab Initio Free Energy Simulations	DIESEN, E.
14:00	[119] 1.TH.02 Autonomous Microscopy through Computer Vision and Agent Oriented Programming	VUIJK, M.
14:00	[118] 1.TH.01 Digital Catalysis: Accelerated Discovery through the Human in the Loop	PARE, C. W.