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

Wednesday, 24 April 2024

Session IV: Chemical Machine Learning (09:00 - 10:30)

time	[id] title	presenter
09:00	[18] Materials Search using the Convex Hull Genetic Algorithm and ML	Prof. PROBERT, Matthew
09:30	[19] Exploring Alternative Dispersion Corrections for the BEEF-vdW Functional	Ms KELLER, Elisabeth
09:50	[20] Machine-Learning Driven Exploration of Catalytic Reaction Network	Dr JUNG, Hyunwook
10:10	[21] Charge Equilibration in Machine Learning Potentials	Dr VONDRAK, Martin

Session IV: Chemical Machine Learning (10:50 - 12:10)

time	[id] title	presenter
10:50	[22] Towards Multi-Fidelity Machine Learning Using Robust Density Functional Tight Binding Models	Mr CUI, Mengnan
11:10	[23] Improving the Diversity of Transition State Searches With On-The-Fly Learned Biasing Potentials	Mr GÖNNHEIMER, Nils
11:30	[24] Learning to Spell Materials - Coordinate-free Discovery with Natural Language Processing	Mr JAKOB, Konstantin
11:50	[25] AI-Empowered Universal Workflow for Molecular Design of Performant Photoswitches	Mr STROTHMANN, Robert