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

Wednesday, 18 June 2025

Session 5: Chemical Machine Learning (09:00 - 10:40)

time	[id] title	presenter
09:00	[14] Finite Temperature Crystal Structure Predict	PROBERT, Matt
09:20	[15] Charting Catalysis: Unveiling Regime Boundaries in Kinetic Phase Diagrams Through Concentration Profiles	KOUYATE, Maryke
09:40	[16] ddmo: A Data Driven Model Optimization for Python	DUCCI, Gianmarco
10:00	[17] ESEM Automation - Dual Magnification & Advanced Automation	VUIJK, Maurits
10:20	[18] Innovating Catalytic Feature Engineering for Self-Driving Labs	WARREN PARE, Charles Percival

Session 5: Chemical Machine Learning (11:00 - 12:00)

time	[id] title	presenter
11:00	[19] Charge Equilibration in Machine Learning Potentials	VONDRAK, Martin
11:20	[20] Bayesian Uncertainty Estimates for Spin-Component-Scaled Second-Order Møller-Plesset Perturbation Theory	KELLER, Elisabeth
11:40	[21] Towards Theoretical UV/Vis Spectra with Experimental Accuracy. Benchmarks for Spiropyran Photoswitches	STROTHMANN, Robert

Thursday, 19 June 2025

Session 5: Chemical Machine Learning (09:00 - 10:40)

time	[id] title	presenter
09:00	[22] Surface Nanoclustering of Cu(111) and Cu(100) During CO Electro-Oxidation in Alkaline Electrolytes	AUER, Andrea
09:20	[23] Splitting Water Without Falling Apart: Accelerating the Understanding of NiFeV LDH via Genetic Algorithms	LOMBARDI, Juan Manuel
09:40	[24] Graphene Flakes on Autopilot: Toward Autonomous Growth Control of 2□D Materials with ViT□Based World Models	BALÁŽ, Damián
10:00	[25] From Electron Conductivity to Polaron Hopping in SOEC Interfaces - Using LSM Thin Films on YSZ as a Model System	KÖNIG, Patricia