Session Program

Jun 16 – 20, 2025

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

Session 5

Wed, June 18

9:00 AM

Session 5: Chemical Machine Learning

Session |
Location: Haus der bayerischen Landwirtschaft, Rieder Str. 70, 82211 Herrsching am Ammersee, Germany

9:00 – 9:20 AM **Finite Temperature Crystal Structure Predict**

Speaker
Matt Probert

9:20 – 9:40 AM
Charting Catalysis: Unveiling Regime Boundaries in Kinetic Phase Diagrams Through Concentration Profiles

Speaker
Maryke Kouyate

9:40 – 10:00 AM **ddmo: A Data Driven Model Optimization for Python**

Speaker
Gianmarco Ducci

10:00 – 10:20 AM **ESEM Automation - Dual Magnification & Advanced Automation**

Speaker
Maurits Vuijk

10:20 – 10:40 AM **Innovating Catalytic Feature Engineering for Self-Driving Labs**

Speaker
Charles Percival Warren Pare

10:40 AM

11:00 AM

Session 5: Chemical Machine Learning

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11:00 – 11:20 AM **Charge Equilibration in Machine Learning Potentials**

Speaker
Martin Vondrak

11:20 – 11:40 AM
Bayesian Uncertainty Estimates for Spin-Component-Scaled Second-Order Møller-Plesset Perturbation Theory

Speaker
Elisabeth Keller

11:40 AM – 12:00 PM
Towards Theoretical UV/Vis Spectra with Experimental Accuracy. Benchmarks for Spiropyran Photoswitches

Speaker
Robert Strothmann

12:00 PM

Thu, June 19

9:00 AM

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9:00 – 9:20 AM

Surface Nanoclustering of Cu(111) and Cu(100) During CO Electro-Oxidation in Alkaline Electrolytes

Speaker
Andrea Auer

9:20 – 9:40 AM

Splitting Water Without Falling Apart: Accelerating the Understanding of NiFeV LDH via Genetic Algorithms

Speaker
Juan Manuel Lombardi

9:40 – 10:00 AM

Graphene Flakes on Autopilot: Toward Autonomous Growth Control of 2-D Materials with ViT-Based World Models

Speaker
Damián Baláž

10:00 – 10:20 AM

From Electron Conductivity to Polaron Hopping in SOEC Interfaces - Using LSM Thin Films on YSZ as a Model System

Speaker
Patricia König

10:40 AM