Session Program

16–20 Jun 2025

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

Session 5

Wednesday 18 June

09:00

Session 5: Chemical Machine Learning

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

09:00–09:20 **Finite Temperature Crystal Structure Predict**

Speaker
Matt Probert

09:20–09:40
Charting Catalysis: Unveiling Regime Boundaries in Kinetic Phase Diagrams Through Concentration Profiles

Speaker
Maryke Kouyate

09:40–10:00 **ddmo: A Data Driven Model Optimization for Python**

Speaker
Gianmarco Ducci

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

Speaker
Maurits Vuijk

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

Speaker
Charles Percival Warren Pare

10:40

11:00

Session 5: Chemical Machine Learning

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

Speaker
Martin Vondrak

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

Speaker
Elisabeth Keller

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

Speaker
Robert Strothmann

12:00

Thursday 19 June

09:00

Session 5: Chemical Machine Learning

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09:00–09:20

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

Speaker
Andrea Auer

09:20–09:40

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

Speaker
Juan Manuel Lombardi

09:40–10:00

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

Speaker
Damián Baláž

10:00–10:20

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

Speaker
Patricia König

10:40