Session Program

22–26 Apr 2024

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

Session IV: Chemical Machine Learning

Wednesday 24 April

09:00

Session IV: Chemical Machine Learning

Session | **Location:** Hotel Marena Wellness & Spa Turystyczna 1, 72-415 Międzywodzie, Poland

09:00–09:30 **Materials Search using the Convex Hull Genetic Algorithm and ML**

Speaker
Prof. Matthew Probert

09:30–09:50
Exploring Alternative Dispersion Corrections for the BEEF-vdW Functional

Speaker
Ms Elisabeth Keller

09:50–10:10 **Machine-Learning Driven Exploration of Catalytic Reaction Network**

Speaker
Dr Hyunwook Jung

10:10–10:30 **Charge Equilibration in Machine Learning Potentials**

Speaker
Dr Martin Vondrak

10:30

10:50

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10:50–11:10
Towards Multi-Fidelity Machine Learning Using Robust Density Functional Tight Binding Models

Speaker
Mr Mengnan Cui

11:10–11:30
Improving the Diversity of Transition State Searches With On-The-Fly Learned Biasing Potentials

Speaker
Mr Nils Gönnheimer

11:30–11:50
Learning to Spell Materials - Coordinate-free Discovery with Natural Language Processing

Speaker
Mr Konstantin Jakob

11:50–12:10
AI-Empowered Universal Workflow for Molecular Design of Performant Photoswitches

Speaker
Mr Robert Strothmann

12:10