

Session Program

22-26 Apr 2024

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

Session V: Catalysis & Multiscale Modeling

Thursday 25 April

09:00

Session V: Catalysis & Multiscale Modeling

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

09:00-09:20

Microkinetic Modelling of CO₂ Hydrogenation to Methanol on Doped ZrO₂(101)

Speaker

Dr Mie Andersen

09:20-09:40

Microkinetic Modeling of Catalytic Reactions With (Fine-Tuned) Machine-Learning Interatomic Potentials

Speaker

Dr Raffaele Cheula

09:40-10:00

Automatic Process Explorer (APE): Potentials and Pitfalls

Speaker

Dr King Chun Lai

10:00-10:20

Coupling Continuum and Microkinetic Models With Multilevel On-The-Fly Sparse Grids

Speaker

Mr Tobias Hülser

10:20

10:40

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10:40-11:10

Broad Yet Narrow: Super-resolution Techniques to Simulate Electronic Spectra of Large Molecular Systems

Speaker

Dr Matthias Kick

11:10-11:30

Exploring O-Dependent Step-Edge Restructuring of Pd with GAP-AKMC

Speaker

Dr Patricia Poths

11:30-11:50

General Purpose Kinetic Monte Carlo Algorithm with Sparse Updating

Speaker

Mr Bat-Amgalan Bat-Erdene

11:50