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

Thursday, 25 April 2024

Session V: Catalysis & Multiscale Modeling (09:00 - 10:20)

time	[id] title	presenter
09:00	[26] Microkinetic Modelling of CO2 Hydrogenation to Methanol on Doped ZrO2(101)	Dr ANDERSEN, Mie
09:20	[27] Microkinetic Modeling of Catalytic Reactions With (Fine-Tuned) Machine-Learning Interatomic Potentials	Dr CHEULA, Raffaele
09:40	[28] Automatic Process Explorer (APE): Potentials and Pitfalls	Dr LAI, King Chun
10:00	[29] Coupling Continuum and Microkinetic Models With Multilevel On-The-Fly Sparse Grids	Mr HÜLSER, Tobias

Session V: Catalysis & Multiscale Modeling (10:40 - 11:50)

time	[id] title	presenter
10:40	[30] Broad Yet Narrow: Super-resolution Techniques to Simulate Electronic Spectra of Large Molecular Systems	Dr KICK, Matthias
11:10	[31] Exploring O-Dependent Step-Edge Restructuring of Pd with GAP-AKMC	Dr POTHS, Patricia
11:30	[32] General Purpose Kinetic Monte Carlo Algorithm with Sparse Updating	Mr BAT-ERDENE, Bat-Amgalan