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

Monday, 22 April 2024

Session I: Selectivity in Catalysis (15:00 - 16:20)

time	[id] title	presenter
15:00	[2] High-Throughput Computational Thermodynamics: What Can We Learn About an Interatomic Potential?	Dr BARTÓK-PÁRTAY, Livia
15:40	[3] Oxygen Adsorption at the Electrochemical Metal/Water Interface: Au(111) vs. Pt(111)	Ms DUDZINSKI, Alexandra
16:00	[4] Free Energy Sampling of Elementary Reaction Barriers for the Oxygen Reduction Reaction	Dr DIESEN, Elias

Session I: Selectivity in Catalysis (16:40 - 17:20)

time	[id] title	presenter
16:40	[5] Exploring Pd Subsurface Chemistry During Acetylene Semi-hydrogenation with Adaptive Kinetic Monte Carlo	Dr CANNIZZARO, Francesco
17:00	[6] Exploring the Relation Between Electrocatalyst Morphology and Product Selectivity from Multiscale Reaction Models	Dr PILLAI, Hemanth S.