

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

Tuesday, 17 June 2025

Session 3: Selectivity in Catalysis (10:40 - 12:20)

time	[id] title	presenter
10:40	[8] Advanced Modelling of Catalytic Reactions at the Electrochemical Interface	HONKALA, Katariina
11:20	[9] Grand Canonical Energetics from Canonical Free Energy Sampling of Electrochemical Reactions	DIESEN, Elias
11:40	[10] Diversity-Driven Active Learning of Interatomic Potentials Applied to Automatic Reaction Network Exploration	CANNIZZARO, Francesco
12:00	[11] Some progress toward useful accelerated dynamics methods, but more challenges	HENKELMAN, Graeme