

Session Program

22-26 Apr 2024

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

Session I: Selectivity in Catalysis

Monday 22 April

15:00

Session I: Selectivity in Catalysis

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

15:00-15:40

High-Throughput Computational Thermodynamics: What Can We Learn About an Interatomic Potential?

Speaker

Dr Livia Bartók-Pártay

15:40-16:00

Oxygen Adsorption at the Electrochemical Metal/Water Interface: Au(111) vs. Pt(111)

Speaker

Ms Alexandra Dudzinski

16:00-16:20

Free Energy Sampling of Elementary Reaction Barriers for the Oxygen Reduction Reaction

Speaker

Dr Elias Diesen

16:20

16:40

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16:40-17:00

Exploring Pd Subsurface Chemistry During Acetylene Semi-hydrogenation with Adaptive Kinetic Monte Carlo

Speaker

Dr Francesco Cannizzaro

17:00-17:20

Exploring the Relation Between Electrocatalyst Morphology and Product Selectivity from Multiscale Reaction Models

Speaker

Dr Hemanth S. Pillai

17:20