

Session Program

16-20 Jun 2025

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

Session 3

Tuesday 17 June

10:40

Session 3: Selectivity in Catalysis

Session |

Location: Haus der bayerischen Landwirtschaft, Rieder Str. 70, 82211 Herrsching am Ammersee, Germany

10:40-11:20

Advanced Modelling of Catalytic Reactions at the Electrochemical Interface

Speaker

Katariina Honkala

11:20-11:40

Grand Canonical Energetics from Canonical Free Energy Sampling of Electrochemical Reactions

Speaker

Elias Diesen

11:40-12:00

Diversity-Driven Active Learning of Interatomic Potentials Applied to Automatic Reaction Network Exploration

Speaker

Francesco Cannizzaro

12:00-12:20

Some progress toward useful accelerated dynamics methods, but more challenges

Speaker

Graeme Henkelman

12:20