

**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