

**Session Program**

**22-26 Apr 2024**

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

**Session VI: Electrochemical Modeling**

# Thursday 25 April

15:00

## Session VI: Electrochemical Modeling

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

15:00–15:30

### Exploring the Black Box: Using Explainable ML to Elucidate Elastic Properties of 2D Hybrid Perovskites

#### Speaker

Prof. Harald Oberhofer

15:30–16:00

### AI-Driven C2 Catalysis

#### Speaker

Dr Haobo Li

16:00–16:20

### Methane Activation on the Liquid Copper Catalyst

#### Speaker

Dr Hao Gao

16:20

16:40

## Session VI: Electrochemical Modeling

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

16:40–17:00

### Modeling Cu Surface Oxidation: From UHV to Electrochemistry

#### Speaker

Mr Felix Riccius

17:00–17:20

### Deciphering Electrochemical AFM Images: Insights from Molecular Dynamics at Electrified Interfaces

#### Speaker

Dr Thorben Eggert

17:20–17:40

### The Response of Interfacial Water at an Electrified Pt(111) Surface

#### Speaker

Ms Lang Li

17:40–18:00

### The Butterfly Effect: Decoding Metal Surfaces with Cyclic Voltammetry

#### Speaker

Mr Nicolas Bergmann

18:00