



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

## Thursday, 25 April 2024

### Session VI: Electrochemical Modeling (15:00 - 16:20)

time	[id] title	presenter
15:00	[33] Exploring the Black Box: Using Explainable ML to Elucidate Elastic Properties of 2D Hybrid Perovskites	Prof. OBERHOFER, Harald
15:30	[34] AI-Driven C2 Catalysis	Dr LI, Haobo
16:00	[35] Methane Activation on the Liquid Copper Catalyst	Dr GAO, Hao

### Session VI: Electrochemical Modeling (16:40 - 18:00)

time	[id] title	presenter
16:40	[36] Modeling Cu Surface Oxidation: From UHV to Electrochemistry	Mr RICCIUS, Felix
17:00	[37] Deciphering Electrochemical AFM Images: Insights from Molecular Dynamics at Electrified Interfaces	Dr EGGERT, Thorben
17:20	[38] The Response of Interfacial Water at an Electrified Pt(111) Surface	Ms LI, Lang
17:40	[39] The Butterfly Effect: Decoding Metal Surfaces with Cyclic Voltammetry	Mr BERGMANN, Nicolas