

Session Program

16-20 Jun 2025

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

Session 1

Monday 16 June

16:00

Session 1: Theory of Heat and Charge Transport

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

16:00–16:40

Data-Driven Modelling of Biomolecular Self-Assembly Processes

Speaker

Carlo Camilloni

16:40–17:00

Non-Parametric Solid-State Embedding for NMR Computations using All-Electron DFT

Speaker

Federico Civaia

17:00–17:20

Crossing Boundaries? Probing Ion Conduction across Interfaces in Solid Electrolytes using Computational NMR Spectroscopy

Speaker

Tabea Huss

17:20–17:40

Assessing Dataset Composition and Transferability in Machine Learning-Based NMR Predictions of Solid-State Electrolytes: A Case Study on LLZO and NPS

Speaker

Javier Valenzuela Reina

18:00–18:20

Dinner

18:20