



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

## XI

Monday, 16 June 2025

**Session 1: Theory of Heat and Charge Transport (16:00 - 18:20)**

time	[id] title	presenter
16:00	[1] Data-Driven Modelling of Biomolecular Self-Assembly Processes	CAMILLONI, Carlo
16:40	[2] Non-Parametric Solid-State Embedding for NMR Computations using All-Electron DFT	CIVAIA, Federico
17:00	[3] Crossing Boundaries? Probing Ion Conduction across Interfaces in Solid Electrolytes using Computational NMR Spectroscopy	HUSS, Tabea
17:20	[4] Assessing Dataset Composition and Transferability in Machine Learning-Based NMR Predictions of Solid-State Electrolytes: A Case Study on LLZO and NPS	VALENZUELA REINA, Javier
18:00	Dinner	