



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

## Monday, 22 April 2024

### Session II: Battery, Materials, and Technology (17:20 - 18:00)

time	[id] title	presenter
17:20	[7] Plane-wave DFT Simulations of Quadrupolar Nuclei NMR	Mr VALENZUELA REINA, Javier
17:40	[8] Peeling Back the Layers of M LDH	Dr LOMBARDI, Juan Manuel

# Tuesday, 23 April 2024

## **Session II: Battery, Materials, and Technology (09:00 - 10:40)**

time	[id] title	presenter
09:00	[9] Predicting the Periodic Hamiltonian and Surface Reactivity of LPS	TÜRK, Hanna
09:40	[10] Simulating NMR Observables with Machine Learning	Dr HARPER, Angela
10:00	[11] "Watt's Up" With 7Li: Computing NMR Parameters in Battery Materials Using an All-Electron DFT QM/MM Approach	Mr CIVAIA, Federico
10:20	[12] Spin to Win: Rotational Dynamics in Lithium Thiophosphate Solid Electrolytes	Ms HUSS, Tabea

## **Session II: Battery, Materials, and Technology (11:00 - 12:00)**

time	[id] title	presenter
11:00	[13] GAN-nabis: The Highs and Lows of Structure Generation	Ms KÖNIG, Patricia
11:20	[14] Computer Vision in Electron Microscopy: Segmentation & Towards Automation	Mr VUIJK, Maurits Willem
11:40	[15] Data-Driven Approach for Networks Reconstruction and Generation	Dr DUCCI, Gianmarco