

**Session Program**

**22-26 Apr 2024**

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

**Session II: Battery, Materials, and Technology**

## Monday 22 April

17:20

### Session II: Battery, Materials, and Technology

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

17:20–17:40

#### Plane-wave DFT Simulations of Quadrupolar Nuclei NMR

**Speaker**

Mr Javier Valenzuela Reina

18:00

17:40–18:00

#### Peeling Back the Layers of M LDH

**Speaker**

Dr Juan Manuel Lombardi

## Tuesday 23 April

09:00

### Session II: Battery, Materials, and Technology

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

09:00–09:40

#### Predicting the Periodic Hamiltonian and Surface Reactivity of LPS

##### Speaker

Hanna Türk

09:40–10:00

#### Simulating NMR Observables with Machine Learning

##### Speaker

Dr Angela Harper

10:00–10:20

#### “Watt’s Up” With 7Li: Computing NMR Parameters in Battery Materials Using an All-Electron DFT QM/MM Approach

##### Speaker

Mr Federico Civaia

10:20–10:40

#### Spin to Win: Rotational Dynamics in Lithium Thiophosphate Solid Electrolytes

##### Speaker

Ms Tabea Huss

10:40

11:00

### Session II: Battery, Materials, and Technology

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

11:00–11:20

#### GAN-nabis: The Highs and Lows of Structure Generation

##### Speaker

Ms Patricia König

11:20–11:40

#### Computer Vision in Electron Microscopy: Segmentation & Towards Automation

##### Speaker

Mr Maurits Willem Vuijk

11:40–12:00

#### Data-Driven Approach for Networks Reconstruction and Generation

##### Speaker

Dr Gianmarco Ducci

12:00