

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

17:40-18:00 **Peeling Back the Layers of M LDH**

Speaker

Dr Juan Manuel Lombardi

18:00

Tuesday 23 April

09:00

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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

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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