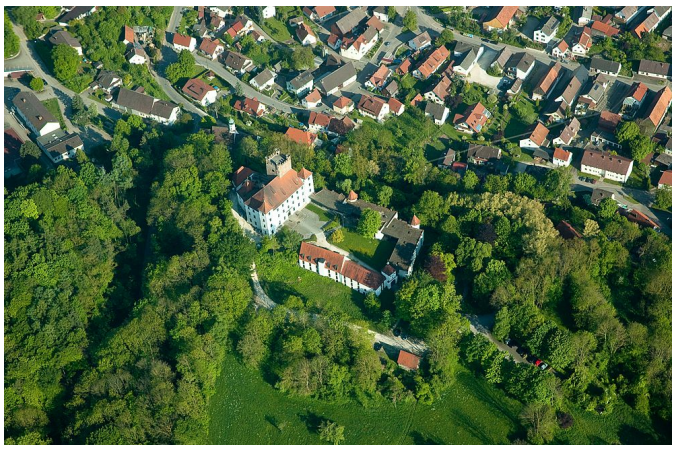
Workshop Program

Computational modelling of batteries: First-principles quantum chemistry meets continuum approaches

Castle Reisensburg near Ulm/Germany

October 23 - 26, 2022

Organizers: Axel Groß (Ulm University, Germany),
Arnulf Latz (Helmholtz Institute Ulm, DLR, Germany)



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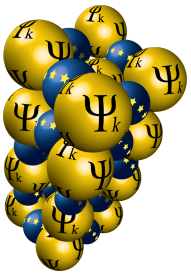
Psi-k Network for Electronic Structure Calculations



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Time table of the workshop

Sunday, October 23, 2022

14:00 - 18:30	Arrival and registration	
18:30 - 20:00	Dinner	
20:00 - 20:15	Axel Groß, Arnulf Latz	Welcome and Introduction
20:15 - 21:00	O. Borodin	Molecular Scale Modeling of Battery Electrolytes and Interfaces

Monday, October 24, 2022

08:00 - 09:00	Breakfast	
09:00 - 12:30	Morning Session	
09:00 - 09:45	Bai-Xiang Xu	Simulation of Solid Interface in Rechargeable Batteries: A Multiscale Perspective
09:45 - 10:30	Ivano Castelli	Autonomous Workflows for an Accelerated Design of Battery Electrodes and Interfaces
10:30 - 11:00	Coffee break	
11:00 - 11:45	Birger Horstmann	Modelling SEI Growth and Function During Battery Operation
11:45 - 12:30	Holger Euchner	Modeling Electrochemical Systems by Density Functional Theory - Batteries and Beyond
12:30 - 14:30	Lunch	
14:30 - 18:00	Afternoon Session	
14:30 - 15:15	Martin Z. Bazant	Ion intercalation in batteries by CIET
15:15 - 16:00	Monica Marinescu	Continuum models for predicting degradation: many opportunities and some caveats
16:00 - 16:30	Coffee break	
16:30 - 18:00		Short Presentation of Posters
18:00 - 20:00	Dinner	
20:00 - 22:00	Poster Session	

Tuesday, October 25, 2022

08:00 - 09:00	Breakfast	
09:00 - 12:30	Morning Session	
09:00 - 09:45	Andreas Heuer	Exploring MD simulations of electrolytes on different scales
09:45 - 10:30	Christoph Scheurer	Towards predictive atomistic modeling of functional and degradation processes at solid/solid interfaces in battery materials.
10:30 - 11:00	Coffee break	
11:00 - 11:30	Jun Huang	Ion Transport in Solid-Electrolyte Interphase: Nonlinearity, Nonmonotonicity, and Impedance
11:30 - 12:00	Max Schammer	From bulk thermodynamics to nano-structuring near electrified interfaces: a holistic continuum approach for battery electrolytes incorporating solvation effects
12:00 - 12:30	Daniel Stottmeister	Understanding electrolyte decomposition at the alkali metal anode interface
12:30 - 14:30	Lunch	
14:30 - 18:00	Afternoon Session	
14:30 - 15:15	Ulrike Krewer	Modeling surface layer growth in batteries with kinetic Monte Carlo and multiscale modeling
15:15 - 16:00	Alessandra Serva	An atomistic modelling view on the role of the electrolyte in electrochemical energy storage devices
16:00 - 16:30	Coffee break	
16:30 - 17:00	Elizabeth Santos	Charge Effects for Lithium Dendrites
17:00 - 17:30	Janina Drews	Continuum Modelling as Tool for Optimizing the Cell Design of Magnesium Batteries
17:30 - 18:00	Martin Werres	Understanding instabilities in lithium based batteries – dual-layer SEI and isolated lithium formation
18:30 - 21:00	Conference Dinner	
21:00 -	Social Event	

Wednesday, October 26, 2022

08:00 - 09:00	Breakfast	
09:00 - 12:30	Morning Session	
09:00 - 09:45	Mohsen Sotoudeh	Understanding ion mobility mechanism through the descriptor and scaling relations in solid crystals
09:45 - 10:30	Matthias Neumann	Random field models for data-driven stochastic 3D microstructure modeling of electrode materials
10:30 - 11:00	Coffee break	
11:00 - 11:45	Christopher Sutton	Identification of the Key Parameters for the Selection of Liquid Electrolytes in Lithium-Sulfur Batteries
11:45 - 12:00	Axel Groß, Arnulf Latz	Concluding remarks
12:00 - 13:00	Lunch	
13:00	Departure	

Poster presentations

Michelle Allion	Coupled Multiscale Simulations of Interfacial Phenomena in Na-Ion Battery Systems
Jafar Azizi	Computational investigation of carbon based anode materials for Li- and post-Li ion batteries
Sebastian Baumgart	First-principles study of charge carrier transport in prussian blue type materials
K. Bhattacharyya	Structure and Reactivity of Transition Metal Oxide Nanoparticles for the Oxygen Evolution Reaction in Electrocatalysis: An Electronic Structure Theory Study
Svenja Both	Effects of microstructural features on the performance of a commercial Ni-rich NMC cathode
Sunel de Kock	Sulfur-containing cathode materials: DFT simulation of XAS and charge carrier interactions
Manuel Dillenz	Detailed structural and electrochemical comparison between high potential layered P2-NaMnNi- and doped P2-NaMnNiMgoxides
Florian Fiesinger	Development of a Mg/O ReaxFF Potential to describe the Passivation Processes in Magnesium-Ion Batteries
Orkun Furat	Methods from machine learning for the structural analysis of Li-ion electrode particles
Katharina Helmbrecht	NASICON with Ca and Mg as charge carriers
Jun Huang	Ion Transport in Solid-Electrolyte Interphase: Nonlinearity, Nonmonotonicity, and Impedance
Lukas Köbbing	How Does the Solid-Electrolyte Interphase Grow? Transport Mechanisms, Mechanics and Interfaces
Huy Sy Nguyen	Effective Model for Sodium Ions Insertion in Hard Carbon
Majid Rezaei	Construction of a Polarizable Force Field for Use in Molecular Dynamics Simulation of Water-In-Salt (WiS) Electrolytes
B. Prifling	Reconstruction of the carbon-binder domain in Li-ion battery cathodes and its influence on the electrochemical performance
Sung Sakong	Modeling Water in Salt Electrolyte from Machine Learning Molecular Dynamics Simulations
Constantin Schwetlick	Modelling Solvation behaviour in highly concentrated Electrolytes
Marcel Weichel	Simulation of the battery electrode drying Process