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CHEMIE KOLLOQUIUM
PROGRAMMVORSCHAU

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Dr. Diddo DIDDENS

Helmholtz-Institut Münster

„Modeling of Molecular Processes in Battery Electrolytes”

Vortragsort: Zoom – Lecture

https://jku.zoom.us/j/99628069412?pwd=Z3RDVmY1d3BWNlZMSkdid0hRRGNhZz09

Vortragszeit: 17:15

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Abstract

Due to their relevance as modern energy storages, batteries based on various chemistries (lithium ion, lithium metal, but also beyond-lithium approaches based on e.g. magnesium) are currently under extensive investigation. Besides the optimization of the active material (i.e. the electrodes), also the electrolyte has to meet several demands, such as a sufficiently high conductivity and electrochemical stability, or alternatively, the ability to form passivation layers at the electrode interfaces. In this talk, I will focus on molecular modeling techniques describing these phenomena, and show how they can be employed to rationalize experimental data. The first part of the talk deals with the prediction of electrochemical stabilities via Quantum Chemistry calculations. Here, it turns out that accounting for the intermolecular environment of a given electrolyte compound as well as for putative decomposition reactions is particularly important to yield quantitative agreement with experimental data, thus contrasting standard approaches based on frontier orbitals. In the second part of the talk, I will focus on ion transport properties in polymeric and liquid electrolytes, and discuss different ion transport mechanisms identified from classical Molecular Dynamics simulations within the framework of a simplified analytical ion transport model. Finally, computational results on magnesium-based systems will be presented.

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