

Modelling Panel Abstract & Speaker Biography

Solvation and Solubility Effects in Lithium-Sulfur Batteries

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The demand for electrochemical storage technology with high energy density increased rapidly in recent years. A major driving force is the electrification of the mobility sector. High expectations rest on the development of beyond Li-Ion battery systems [1]. Especially, lithium-sulfur batteries (Li-S) are believed to be a promising candidate already in the near future. However, degradation mechanisms like the polysulfide shuttle hinder a commercial breakthrough. A thorough understanding of the fundamental processes will be a key factor for future developments and the overall success of Li-S batteries.

In this talk we will present simulation results based on continuum models of Li-S batteries which were recently developed in our group [2], [3]. Our models describe the reaction and transport of solid and dissolved sulfur species in a single S/C particle as well as on cell level. A focus is set on the redistribution of the solid end-products S_8 and Li_2S upon cycling which includes a comprehensive study of the polysulfide shuttle in Li/S batteries with a composite cathode consisting of micro-porous particles.

An effect which is often neglected in battery modelling is the desolvation of ions prior to the electron transfer reaction. Recently, we developed a generic theory for charge and electron transfer reactions at electrified interfaces, which is able to describe charge accumulation at the electrode-electrolyte interface [4]. The model is derived from fundamental thermodynamic and electrostatic laws without any assumptions on structural properties of the double-layer. This concept is now transferred to the conversion reactions in Li-S batteries. This approach allows us to include surface effects, like adsorption and desolvation in our simulations. During discharge the overall concentration of charged species increases and raises the viscosity and cell resistance [5]. Therefore, surface effects are expected to be even more important in the case of Li-S batteries.

Our simulations provide mechanistic insights for the operation of Li-S batteries and will contribute to the understanding and, therefore, improvement of next-generation Li-S batteries.

References

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Speaker Biography:

For the German Aerospace Center (DLR) Jessica Lück works at the Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU) in the field of fundamental battery research based on mathematical modelling in the group of Prof. Arnulf Latz.

Unlike any other research institute in Germany, the HIU brings together virtually all areas of battery research in one organization, combining excellent fundamental research with applications. To acquire a more detailed understanding of the underlying physical, chemical and fluid mechanical processes, the group of Prof. Latz develops multiscale and multiphysical models for intercalation, conversion and all-solid-state batteries.



Gaining an M.Sc. degree in Physics from the University of Kiel (Germany), Jessica Lück was concerned with electrodeposition, correlated surface dynamics and electronically non-adiabatic surface processes on an atomistic scale within the framework of density functional theory. In her current research on conversion and intercalation batteries, she uses her background to study fundamental aspects of charged interfaces in electrochemical systems. Based on continuum mechanics, interfacial reaction and transport processes and the influence of solvation and surface effects on the overall performance of lithium sulfur cells are in focus.