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Institut für Physik
Fachgebiet Theoretische Festkörperphysik

VORTRAGSANKÜNDIGUNG / SONDERKOLLOQUIUM

Am Mittwoch, dem **6. Oktober 2026**, spricht um **17:15 Uhr** im **Faraday-Hörsaal,**

Herr Prof. Dr. Mark E. Tuckerman

Department of Chemistry, New York University

zum Thema:

"Elucidating anomalous charge transport mechanisms in aqueous and organic electrolyte mixtures for redox-flow battery and alkaline fuel cell applications"

Abstract:

Batteries and fuel cells are important components in a clean energy future; however, challenges remain in ensuring these devices are cost-effective, scalable, and high-performing. Critical to ensuring these key features is the design of electrolytes, which are tasked with transporting charge through the device. Interestingly, while fuel cells have largely relied on a combination of vehicular and structural charge diffusion mechanisms, particularly when aqueous electrolytes are employed, batteries have traditionally operated solely on vehicular charge transport. In this talk, I will discuss models of both types of devices and the design of electrolyte materials for use in each system using first-principles molecular simulation approaches. Specifically, I will describe the structural (Grotthuss) diffusion mechanism operating in the confined aqueous environment of anion exchange membrane (AEM) fuel cells and show that the confinement created by the functionalized polymers leads to an unexpected temperature dependence of the hydroxide diffusion constant. I will discuss pulsed-field gradient NMR experiments that confirm the predictions from the first-principles simulations. Following this, I will discuss a strategy for designing non-aqueous organic concentrated hydrogen-bonded electrolyte solutions for use in redox-flow batteries that can support Grotthuss diffusion. While commonly used organic electrolytes for these systems are ionic liquids whose performance is limited by viscosity considerations, I will discuss a class of electrolytes composed of imidazole (possibly functionalized) and organic acids that can transport charge via mechanisms that are largely independent of viscosity. Due to the complexity of these systems, modeling is performed using a class of machine learning interatomic potentials based on the architecture of transformer networks, such as are used in popular AI platforms such as Claude and ChatGPT and include nuclear quantum effects via the Feynman path integral. I will show that with a strategic choice of electrolyte composition, it is possible to achieve electrical conductivities approaching 0.1 S/cm. I will also discuss the experiments that confirm our findings as well as the underlying mechanisms that lead to these high conductivities.

Wir laden Sie zu diesem Vortrag herzlich ein!

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