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## Multi-scale Modeling of Growth Processes in Electrochemistry and Battery Research

Monday, November 28, 2022 2:00 PM (15 minutes)

Electrochemistry is at the heart of many important industrial processes or systems, ranging from electrolysis and hydrogen evolution over corrosion, metal deposition up to batteries, fuel cells and photoelectrochemical devices. Here, the interface between the electrolyte and the electrolyte, which can be considered the site where electrocatalytic processes occur, is of particular interest. Due to its complexity and multi-component environment even after many decades of research, our understanding of the properties of this interface is still scarce. In this talk we will discuss how modern theoretical multi-scale methods in conjunction with in-situ experiments on well-defined model systems is capable to unravel the structure and composition of these interfaces as well as the ongoing electrochemical reactions and diffusion processes.

We will concentrate on different interfacial systems, including Li-ion and Mg-ion batteries. In our work we concentrated on realizing and investigating the deposition and growth on model electrodes in order to understand apparent nucleation and growth processes (e.g. dendrite formation/growth). By combining different theoretical methods we could gain insights self-diffusion on transition metal electrodes, battery-relevant materials and finally the dynamics of alloy-based electrocatalysts under operation conditions, showing the importance and urgent need for in-operando experimental studies.

Presenter: Prof. JACOB, T.

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