

INVESTIGATION OF METALLIC LITHIUM ANODES BY MEANS OF REACTIVE MOLECULAR DYNAMICS

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Electrochemical phenomena in a battery can be studied over a wide range of time and length scales, spanning everything from processes at an atomistic scale to visible phenomena at a macroscopic magnitude. Although ab-initio quantum chemistry methods like density functional theory (DFT) excel in accuracy, such methods do not provide the feasibility to embrace neither the relevant time nor length scale for many chemical processes in a battery. Classical molecular dynamics on the other hand facilitates the treatment of much larger systems, but lacks in the simulation of chemical systems. The idea behind reactive force fields like ReaxFF is to bridge the gap between quantum mechanical methods and classical molecular dynamics, by extending a proper description of chemical reactions to larger time and length scales.

An appropriate description for the interatomic interactions in a system within the ReaxFF framework however requires extensive adjustments towards a training set, which is entirely based on ab-initio calculations and comprises the most important properties and stabilities of the system. Starting from the investigation of basic bulk and surface systems by means of quantum mechanical methods for metallic lithium anodes, this work shows the development of a reactive force field for this class of electrodes.

Our ambition is the improvement and development of new battery-materials by revealing and predicting the significant phenomenons at an atomistic level, thus providing a database of obtained reaction rates for even more realistic simulations.