Using ab initio calculations to unravel atomistic processes at electrified solid/liquid interfaces

Mira Todorova, Jing Yang, Sudarsan Surendralal, Suhyun Yoo, Florian Deißenbeck, Stefan Wippermann[1,2], and Jörg Neugebauer

[1] Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
[2] Phillips-Universität Marburg, Germany

Many of the challenges we face today towards achieving a greener economy focus on processes occurring at electrified solid/liquid interfaces. Understanding how the interactions between the solid, the liquid and dissolved species are affected by the applied potential will aid our ability to achieve rational design and targeted optimization of relevant processes. Hereby, ab initio molecular dynamic simulations including explicit modelling of the aqueous environment have proven an indispensable tool to gain insights into reaction mechanisms. More approximate choices to modelling the electrolyte, such as implicit solvent models, are however also popular. The talk will discuss the suitability of approximate models for the aqueous environment to study, e.g., the stability of surface phases in the Mg/H_2O system and incorporation of impurities in nano-aerogels during synthesis [1,2], by coupling DFT calculations with thermodynamic models. Furthermore, insights into reaction mechanism at electrified solid/liquid interfaces enabled by our recent developments of a thermopotentiostat [3,4] will be presented, using the example of Pt[5].

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