Extending First-Principles Calculations to Model Electrochemical Reactions at the Solid-Liquid Interface

S. Surendralal[1] M. Todorova[1] J. Neugebauer[1]

[1]Max-Planck-Institut fuer Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Duesseldorf, Germany

Many of the technological challenges we presently face, such as improving battery materials, electrocatalysis, fuel cells, or corrosion protection, originate from reactions at solid-liquid electrochemical interfaces. Describing and quantifying the underlying fundamental mechanisms is challenging both for experimental and theoretical techniques. Combining concepts from semiconductor physics and corrosion science, we have developed a novel approach that allows us to perform ab initio calculations under controlled potentiostat conditions for electrochemical systems. The proposed approach can be straightforwardly applied in standard density functional theory codes and allows to obtain direct insight into key mechanisms of electrocatalysis and corrosion such as water splitting, H_2 evolution, desorption of surface atoms, solvation etc. To show the performance and the opportunities opened by this approach we discuss several prototypical examples: Corrosion at the water- Mg interface [1], dissolution of Mg under anodic polarization and structure formation at the standard hydrogen electrode.

[1] S. Surendralal, M. Todorova, M. Finnis und J. Neugebauer, *Phys. Rev. Lett.* **120**, 246801 (2018).