Modelling electrochemical solid/liquid interfaces by first principles calculations

Mira Todorova, Suhyun Yoo, Sudarsan Surendralal and Jörg Neugebauer

Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237Düsseldorf, Germany

Processes taking place at solid-liquid interfaces are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Describing and quantifying the underlying fundamental mechanisms is equally challenging for experimental and theoretical techniques.

Ab initio modelling using DFT has proven immensely successful in providing atomistic insight into various questions of materials science. A challenge in applying these methods to electrochemical problems is the presence of the solvent or constraints imposed by the periodic boundary conditions common to many DFT codes. Utilising concepts from semiconductor physics allowed us to overcome these obstacles [1, 2]. Key ideas of the underlying methods will be discussed by showing two prototypical applications: Selective stabilisation of polar ZnO(0001) surfaces by an aqueous environment [3] and corrosion on Mg surfaces [4].

References:

[1] M. Todorova and J. Neugebauer, Phys. Rev. Applied **1**, 014001 (2014).
[2] M. Todorova and J. Neugebauer, Faraday Discuss. **180**, 97 (2015).
[3] S. Yoo, M. Todorova und J. Neugebauer, Phys. Rev. Lett. **120**, 066101 (2018).
[4] S. Surendralal, M. Todorova und J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).