

# Mira Todorova



*Max-Planck-Institut für Eisenforschung GmbH  
Computational Materials Design,  
Düsseldorf/Germany*

**Tuesday, 10<sup>th</sup> April 2018, 16:00 s.t.**

TU Wien, Institut für Angewandte Physik, E134  
1040 Wien, Wiedner Hauptstraße 8-10  
Yellow Tower „B“, 5<sup>th</sup> floor, SEM.R. DB gelb 05 B



## Atomistic insights into surface stability and reactivity at solid/liquid interfaces from first principles calculations

Solid/liquid interfaces are at the heart of many problems of practical importance, be it battery materials, electrocatalysis or corrosion. A systematic improvement of any of these processes requires understanding of the processes occurring at such interfaces. Central to such an understanding is the identification of the structures forming at the surface of the solid immersed in an aqueous electrolyte, but our understanding of the role the electrolyte plays in shaping these structures is limited. It is furthermore essential to understand how a surface evolves under the influence of changing environmental conditions, such as an applied bias voltage, and unravel the elementary steps of the ensuing reactions.

Ab initio modelling using density functional theory (DFT) has proven immensely successful in providing atomistic insight into various questions of materials science, but its application to electrochemical problems is challenging, due to the presence of the solvent or to constraints imposed by the periodic boundary conditions common to many DFT codes. Utilising concepts from semiconductor physics has enabled us to overcome some of these obstacles, as will be discussed using the examples of surface stabilisation of polar ZnO(0001) surfaces in aqueous environment and the anomalous hydrogen evolution on anodically polarised Mg(0001) surfaces. We show that solvation effects are highly selective and favour the stabilisation of semiconducting surfaces experiencing a high electrostatic penalty in vacuum. Furthermore, the ability to perform DFT calculations under applied bias enabled us to identify the reaction responsible for the anomalous hydrogen evolution on anodically polarised Mg(0001)/H<sub>2</sub>O interfaces, which has puzzled the corrosion community for more than a 100 years.

[1] M. Todorova and J. Neugebauer, Faraday Discuss. 180, 97 (2015)

[2] S. Yoo, M. Todorova and J. Neugebauer, Phys. Rev. Lett. 120, 066101 (2018)

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion)

Friedrich Aumayr  
(LVA-Leiter)

Markus Valtiner  
(Seminar Chair)