O 43: Mini-Symposium: Electrified solid-liquid interfaces II

Time: Tuesday 13:30–15:30 Location: R1

Invited Talk O 43.1 Tue 13:30 R1

Electrocatalysis beyond surface reaction energetics — •Karen Chan — Fysikvej, Building 311, Room 4, Kongens Lyngby Denmark 2200

Beyond surface reaction energetics, the structure and composition of the electric double layer exerts an influence on the activity and selectivity of electrochemical reactions. In this talk, I first discuss the impact of pH and the electrolyte on electrocatalytic activity from the perspective of adsorbate-field interactions. I then discuss the impact of mass transport on activity and selectivity. I draw examples from hydrogen evolution and CO_2 electroreduction reduction.

Invited Talk O 43.2 Tue 14:05 R1

Design and application of an ab initio electrochemical cell — Sudarsan Surendralal, Florian Deissenbeck, Stefan Wippermann, Christoph Freysoldt, Mira Todorova, and •Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Having accurate simulation techniques to explore and predict the structure and chemical reactions at the electrified electrode-water interface will be crucial to overcome major materials limitations related to energy-conversion, storage and sustainability. The last few years showed some exciting new developments that allow us a realistic description of electric fields at the interface and to (thermo)-potentiostat the electrode potential [1, 2]. These approaches are easy to implement in standard and well-established first principles codes and allow us thus to address and resolve pressing materials science questions in electrochemistry or corrosion sciences. The talk will give a brief overview over the key concepts of these new methodologies and show their application for two examples: The role of the hydrogen evolution reaction (HER) in the corrosion of Mg [1] and the role of water co-adsorption on the electrode potential and HER on Pt surfaces [3].

[1] S. Surendralal, M. Todorova, M. Finnis, J. Neugebauer, PRL 120, 246801 (2018).

[2] F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, PRL (under review), arXiv:2003.08156 .

[3] S. Surendralal, M. Todorova, J. Neugebauer, PRL (under review).

O 43.3 Tue 14:40 R1

Dielectric properties of nano-confined water: a canonical thermopotentiostat approach — •Florian Deissenbeck, Christoph Freysoldt, Mira Todorova, Jörg Neugebauer, and Stefan Wippermann — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

With the advent of robust techniques to apply electric fields in density-functional calculations, there has been continuous interest to use ab initio molecular dynamics (MD) simulations to study electrically triggered processes, such as electrochemical reactions. Here we introduce a novel approach to sample the canonical ensemble at constant temperature and applied electric potential [1]. Our thermopotentiostat approach can be straightforwardly implemented into any density-functional code. To demonstrate the power of our new approach, we compute the dielectric constant of nano-confined water without any assumptions for the dielectric volume. We show that the extremely low dielectric constant of nano-confined water is related to the existence of a dielectrically dead layer within interfacial water.

[1] F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, Phys. Rev. Lett. (submitted), arXiv:2003.08156

General discussion