

O 25: Overview Talk: Axel Groß

Time: Tuesday 9:30–10:15

Location: TRE Phy

Invited Talk

O 25.1 Tue 9:30 TRE Phy

Electrochemistry: A new frontier for a theoretical surface scientist — ●AXEL GROSS — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm/Germany

Despite its relevance in energy conversion and storage, our knowledge about microscopic structures and processes at electrochemical electrode-electrolyte interfaces is still rather limited. The theoretical description of these interfaces from first principles is hampered by at least two factors that are typically not present in surface science. i) In electrochemistry, properties of the electrode-electrolyte interfaces are governed by the electrode potential which adds considerable complexity to the theoretical treatment since charged surfaces have to be considered. ii) The theoretical treatment of processes at solid-liquid inter-

faces necessitates a proper description of the liquid which in principle requires to perform computationally expensive statistical averages.

I will in particular focus on how, despite these obstacles, the electrochemical environment can be appropriately and efficiently taken into account in theoretical studies. For example, the presence of the electrolyte can be treated in a grand-canonical approach as a reservoir. Thus the equilibrium coverage of metal electrodes with ions present in the solution was derived [1]. In an implicit solvent model, the aqueous electrolyte is treated as a dielectric continuum. Using this approach, we demonstrate the importance of the presence of the electrochemical environment in the methanol electro-oxidation on Pt(111) [2].

[1] F. Gossenberger *et al.*, *Electrochim. Acta* **216**, 152 (2016).

[2] S. Sakong and A. Groß, *ACS Catal.* **6**, 5575 (2016).