

MM 1: Tutorial: Electro Chemistry 4 Condensed Matter Physicists

Organized by Erich Runge and Jörg Neugebauer on behalf of the Semiconductor Physics Division (HL) and the Metal and Material Physics Division (MM), respectively.

Time: Sunday 16:00–18:25

Location: H 1058

Invited Talk MM 1.1 Sun 16:00 H 1058

Challenges in the theoretical description of structures and processes at electrochemical interfaces — ●AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — Helmholtz Institut Ulm, 89069 Ulm, Germany

In spite of its technological relevance in the energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces is still rather limited. The theoretical description of these interfaces is hampered by three challenges [1]. i) In electrochemistry, structures and 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 interfaces includes a proper description of the liquid which requires to determine free energies instead of just total energies. This means that computationally expensive statistical averages have to be performed. iii) Electronic structure methods based on density functional theory (DFT) combine numerical efficiency with a satisfactory accuracy which makes them appropriate for electrochemical systems. However, there are severe shortcomings of the DFT description of liquids, in particular water, using current functionals.

In this tutorial talk, I will give an overview over concepts and theoretical methods for the realistic description of electrochemical interfaces. Examples of insights gained from theoretical studies will be presented but open challenges will be identified as well.

[1] N.G. Hörmann *et al.*, *J. Power Sources* **275**, 531 (2015).

Short break

Invited Talk MM 1.2 Sun 16:50 H 1058

Raman under water - Of photons, phonons and the fun of tuning the Fermi level — ●KATRIN F. DOMKE — MPI for Polymer

Research, Ackermannweg 10, D-55128 Mainz

t.b.a.

Short break

Invited Talk MM 1.3 Sun 17:40 H 1058

Scanning probe microscopies for electrochemical problems — ●GUNTHER WITTSTOCK — Carl v. Ossietzky University of Oldenburg, School of Mathematics and Science, Department of Chemistry, D-26111 Oldenburg

Electrified solid-liquid interfaces are characterized by a vertical and horizontal inhomogeneity in structure. Even well prepared single crystal electrodes show, adatoms, steps kinks and other defects. The investigation of such structures by STM has dramatically enhanced our understanding of such interfacial structures. However, the experiments were mostly performed in the absence of a Faradaic reaction (i.e. electrolysis). With a few exceptions, electrodes are designed for controlling Faradaic reactions. High current densities are requested for efficient energy conversion devices; very low current densities are a requirement for materials that shall resist corrosion under harsh environments. Such materials (polycrystalline, multiphase or composites) show a large variation of local current densities that are neither accessible by I-V-curves nor by STM. Scanning electrochemical microscopy (SECM) provides this information. It uses the electrolysis current of a dissolved redox-active compound at a probe microelectrode to generate the signal. The electrolysis at the probe is coupled to local reaction at the sample by diffusion of reactants in the probe-sample gap. Different working modes and examples will be explained with the aim to differentiate between fundamental barriers and current instrumental limitations that might be overcome by the impact of well trained physicist.