O 83: Overview Talk: Bernd Meyer

Time: Thursday 9:30–10:15 Location: TRE Phy

Invited Talk O 83.1 Thu 9:30 TRE Phy

Molecular adsorption on oxide surfaces: Insights from first-principles calculations — •Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

In the past decade, much progress was made in characterizing and understanding chemical processes occurring at oxide surfaces. Compared to metals, oxides show a much wider variety of phenomena upon adsorption and reaction of molecules. The more versatile behavior of oxide surfaces can be attributed to more pronounced changes in the electronic structure, a reduced screening and the more important role of surface defects. In this talk I will review recent theoretical studies in this field, starting with examples of how the adsorption of small molecules can lead to phenomena such as surface metalization and how new types of substrate-mediated adsorbate–adsorbate interactions can result in the formation of unexpected complex adsorbate structures. I will then turn to the functionalization of oxide surfaces by larger organic molecules and the characterization of hybrid organic–inorganic interfaces, which play an important role in molecular electronics and dye-sensitized solar cells. Finally, first ab initio molecular dynamics simulations on chemical processes at the oxide/liquid interface will be discussed.