O 49: Invited talk (Timo Jacob)

Time: Wednesday 15:45–16:30 Location: HE 101

Batteries, fuel cells, photocells and many other applications are powered by fundamental electrochemistry. Compared to surface science under UHV conditions, electrochemical systems combine a whole variety of additional effects. These range from the presence of an electrolyte and a multi-component environment to reaction conditions such as finite temperature, pressure, and electrode potential. Due to this complexity our knowledge of the ongoing processes is mostly limited to the macroscopic regime. However, nowadays theoretical methods are able to provide deeper insight into structures and processes at the

atomic level, which together with experiments could lead to a better understanding.

We compare the concepts of surface science and electrochemistry, addressing their similarities and differences. Using the oxygen reduction (ORR) on Pt as a model reaction, theoretical studies of the exact mechanism will be described, where, starting with the gas-phase system, effects from the reactive surrounding as well as environmental parameters are successively included. We find that the pure, perfect surface models, typically used to study this reaction, are insufficient. Nanofaceting of Ir(210) provides another example of a phenomenon showing how analogies can be made between surface science and electrochemistry. Here pyramidal-like nanostructures that were first observed under UHV conditions were later produced electrochemically.