TECHNISCHE UNIVERSITÄT WIEN

INSTITUT FÜR ANGEWANDTE PHYSIK
Institute of Applied Physics
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IAP-SEMINAR

ANNOUNCEMENT

Date: **Tuesday, 14.6.2016**
Time: **16:00 p.m.**
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**
yellow tower „B“, 5th floor, Sem.R. DB gelb 05 B (room number DB05L03), 1040 Wien, Wiedner Hauptstraße 8-10

Lecturer: **Harald Oberhofer**
Theoretical Chemistry, TU Munich, Germany

Subject: **Modelling surface photo-electrochemistry: beyond the computational hydrogen electrode**

Abstract: The role, computer-modelling plays today in understanding and optimising catalysts for photo-electrochemical reactions, is undisputed. Yet, state of the art simulation approaches tend to rely on a number of assumptions and simplifications, which – according to newest results – may not be fully justified. For example, simulation of the all-important electro-catalytic water oxidation reaction is mainly based on idealised surfaces and the computational hydrogen electrode (CHE) approach, which evaluates the thermodynamic feasibility of a catalyst looking at pathway where each hydrogen abstraction is coupled to the removal of one electron (PCET). This in turn is used to justify neglecting solvation effects as only overall neutral reaction intermediates need to be considered. Yet, especially on semi-conducting catalysts the assumption of PCET is not necessarily fulfilled. The great success of the CHE approach is in part due to its low computational cost allowing a computational screening of suitable catalyst materials. Any other scheme going beyond PCET and ideal surfaces should therefore match this advantage, ideally avoiding costly molecular dynamics sampling of solvent degrees of freedom. Yet, recent developments in thermodynamic modelling as well as embedding techniques, both liquid and solid-state, especially considering the interface between catalyst and solvent, point the way towards photo-electrochemistry modelling beyond the computational hydrogen electrode.

All interested colleagues are welcome to this seminar lecture
(45 minutes presentation followed by discussion).

U. Diebold e.h.
(Seminar-Chairperson)

H. Störi e.h.
(LVA-Leiter)