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# IAP-SEMINAR

## ANNOUNCEMENT

- Date: **Tuesday, 16.6.2015**  
Time: **16:00 p.m.**  
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**  
yellow tower „B“, 5<sup>th</sup> floor, Seminarraum 134A (room number DB05L03)  
1040 Wien, Wiedner Hauptstraße 8-10
- Lecturer: **Prof. Dr. Bernd Meyer**  
Friedrich-Alexander-Universität Erlangen-Nürnberg/Germany
- Subject: **Proton distribution and transfer dynamics at the solid/liquid interface**
- Abstract: Car-Parrinello Molecular Dynamics (CPMD) simulations have been pivotal in advancing our understanding of proton transport in hydrogen-bonded bulk liquids on the molecular scale. Two examples will be discussed which demonstrate that the bulk proton dynamics can change significantly in spatially confined liquids and at solid/liquid interfaces. The first example will be water in contact with hydroxylated oxide surfaces. We find that the energetic hierarchy of preferred protonation sites and the proton distribution on the surface depend on the environment and change from the vacuum to thin water films and the full solid/liquid interface. The surfaces readily deprotonate in the CPMD simulations due to their inherent acidity and the protons are redistributed by surface assisted and water-mediated transfer events. In the second example we studied the proton diffusion in sulfuric acid confined between the graphene layers in graphite intercalation compounds. Here we will show that the confinement and the oxidation state of the graphene sheets have a profound impact on the dynamics of proton transfer events in the sulfuric acid liquid.

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*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)*