



TECHNISCHE
UNIVERSITÄT
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INSTITUT FÜR
ANGEWANDTE PHYSIK
Institute of Applied Physics
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IAP-SEMINAR

ANNOUNCEMENT

Date: **Tuesday, 25.4.2017**
Time: **16:00 s.t.**
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**
yellow tower „B“, 5th floor, Sem.R. DB gelb 05 B (room DB05L03), 1040 Wien, Wiedner Hauptstr. 8-10

Lecturer: **Keith McKenna**
University of York, UK

Subject: **Electron trapping in nanocrystalline titanium dioxide**

Abstract: The trapping and mobility of electrons in nanocrystalline oxide materials underpins a diverse range of applications in areas such as solar energy generation, catalysis, gas sensing and nanoelectronics. However, directing probing the properties of electrons in such complex nanocrystalline systems is extremely challenging. Here, we provide insight into these important issues through first principles based modeling of the interaction of electrons with surfaces and grain boundaries in rutile TiO₂. We show that different surface orientations exhibit markedly different electron affinities: some preferring to trap electrons with others repelling electrons. The equilibrium nanocrystal morphology exposes both electron trapping and electron repelling facets and therefore is predicted to possess highly anisotropic electron trapping properties [1]. Interfaces between nanoparticles (grain boundaries) are associated with high concentrations of strong electron trapping sites which hamper electron transport between grains. However, we show how this effect is partially ameliorated at high current densities (>0.01 mA/cm²) as a result of a highly nonlinear trap filling effect [2]. We discuss how with atomistic insight into the electron trapping properties of nanocrystalline materials one can suggest ways to improve the performance of materials for applications, for example by designing optimal nanocrystal morphologies.

[1] S. Wallace and K. P. McKenna, Journal of Physical Chemistry C 119, 1913 (2015)

[2] S. Wallace and K. P. McKenna, Advanced Materials Interfaces 1, 1400078 (2014)

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

*U. Diebold, G. Parkinson e.h.
(Seminar-Chairpersons)*

*F. Aumayr e.h.
(LVA-Leiter)*