



TECHNISCHE
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IAP-SEMINAR

EINLADUNG

Termin: **Dienstag, 13.12.2011 um 16:00 Uhr**

Ort: **Technische Universität Wien,
Institut für Angewandte Physik,
Seminarraum 134A, Turm B (gelbe Leitfarbe), 5. OG
1040 Wien, Wiedner Hauptstraße 8-10**

Vortragender: **Peter Agoston**
TU Darmstadt/D

Thema: **Thermodynamics and electronic structure of In_2O_3 and ITO
surfaces: Insights from first-principles calculations**

Kurzfassung

Indium oxide is the most widely used transparent conducting oxide (TCO) especially when doped with tin (ITO). Despite its technological importance the surface properties of In_2O_3 are not well understood and many open questions arise from experimental studies.

This presentation provides an overview on the thermodynamics and electronic structure of In_2O_3 and ITO surfaces. The results are based on first-principles total energy calculations. It is shown that the surface chemistry and electronic structure of low index In_2O_3 surfaces differs qualitatively for different surface orientations. On the basis of the properties of the (111) and (001) surfaces this finding is illustrated and discussed. The thermodynamic stability of these two surfaces is assessed as a function of the oxygen and water content in the surrounding atmosphere. In addition, the effect of doping and dopant segregation is discussed in terms of surface stability. The results obtained for In_2O_3 surfaces are compared not only among each other but also with the surface properties of SnO_2 as well as with other group III post-transition metal oxides in the C-type rare earth modification. In addition, the relation of the surface reconstructions to the bulk point defect equilibria is pointed out.

*Alle interessierten Kolleginnen und Kollegen sind zu diesem Seminar
(45 min mit anschließender gemeinsamer Diskussion) herzlich eingeladen.*

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

*H. Störi e.h.
(LVA-Leiter)*