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# IAP-SEMINAR

## EINLADUNG

Termin: **Dienstag, 22.5.2012 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**

Vortragende: **Prof. Rossitza Pentcheva**  
Ludwig-Maximilians University, Munich/Germany

Thema: **Tuning Electronic Phases at Transition Metal Oxide Surfaces  
and Interfaces**

### Kurzfassung

The surfaces and interfaces of transition metal oxides give rise to a variety of intriguing electronic phenomena that are not available in the parent bulk compounds. Density functional theory calculations can provide insight into the underlying mechanisms but also enable one to identify further parameters to control these effects in view of device applications. In my talk I will address two examples: The first one deals with the surface termination and adsorption of molecules (water, hydrogen and arsenate oxoanions) at iron (hydr-)oxide surfaces such as  $\text{Fe}_3\text{O}_4(001)$  [1,2] and  $\text{FeOOH}$ . The second topic focuses on the origin of metal-to-insulator transition in polar  $\text{LaAlO}_3$  films on  $\text{SrTiO}_3(001)$  [3]. In particular, the role of a  $\text{SrTiO}_3$  capping layer [4] and metallic contacts [5] in tuning the two-dimensional electron gas at the interface will be elucidated.

Work in collaboration with N. Mulakaluri, M. Scheffler, R. Arras, K. Otte, V.G. Ruiz, and W.E. Pickett. Funding by the DFG (e.g. SFB/TR80) and a grant for computational time at the Leibniz Rechenzentrum Garching are gratefully acknowledged.

[1] N. Mulakaluri, R. Pentcheva, M. Wieland, W. Moritz and M. Scheffler, Phys. Rev. Lett. **103**, 176102 (2009)

[2] G.S. Parkinson, N. Mulakaluri, Y. Losovyj, P. Jacobson, R. Pentcheva, and U. Diebold, Phys. Rev. B **82**, 125413 (2010)

[3] R. Pentcheva and W.E. Pickett, Phys. Rev. Lett. **102**, 107602 (2009)

[4] R. Pentcheva M. Huijben, K. Otte, W.E. Pickett, J.E. Kleibeuker, J. Huijben, H. Boschker, D. Kockmann, W. Siemons, G. Koster, H.J.W. Zandvliet, G. Rijnders, D.H.A. Blank, H. Hilgenkamp, and A. Brinkman, Phys. Rev. Lett. **104**, 166804 (2010)

[5] R. Arras, V.G. Ruiz, W.E. Pickett and R. Pentcheva, Phys. Rev. B **85**, 125404 (2012)

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*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)*

