TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

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IAP-SEMINAR

EINLADUNG

Termin: **Dienstag, 29.11.2011 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: **Ao.Univ.Prof. Dr. Peter Mohn**
TU Wien, IAP and Center for Computational Materials Science

Thema: **p-Electron Magnetism in anion doped $BaTiO_{3-x}X_x$ (X=C,N,B) and CdS**

Kurzfassung

We present VASP calculations using the HSE functional for carbon, nitrogen, and boron doped $BaTiO_{3-x}X_x$ (X=C,N,B) and $CdS_{1-x}Y_x$ (Y= main group element). We calculate supercells and replace one oxygen atom by C,N, or B or a main group element for S in CdS. In the perovskite for all three substituents we find a magnetically ordered groundstate which is insulating for C and N and halfmetallic for B. The changes in the electronic structure between the undoped and the doped case are dominated by the strong crystal field effects together with the large band splitting for the impurity p-bands. Using an MO picture we give an explanation for the pronounced changes in the electronic structure between the insulating non-magnetic state and the as well insulating magnetic state for doped $BaTiO_3$. For CdS we also find in most cases magnetic order, either halfmetallic or indulating. p-element doped perovskites and CdS could provide a new class of materials for various applications ranging from spin-electronics to magneto-optics.

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

H. Störi e.h.
(LVA-Leiter)