SFB 608

Einladung zum Kolloquium

Ort: Universität zu Köln
II. Physikalisches Institut
Seminarraum 201

Zeit: 28.05.2008, 14:30 Uhr

Sprecher: **J. Kunes,**
Theoretical Physics III
University of Augsburg

Thema: Crystal-Field Driven Mott Transition in MnO under High Pressure

MnO is a classical example of strongly correlated (Mott) insulator. Recent high pressure experiments found high-spin to low-spin transition accompanied by insulator-metal transition and isostructural volume collapse around 100 GPa. I will present a numerical electronic structure study which combines the first-principles bandstructure of MnO with dynamical mean-field theory (LDA+DMFT), and discuss the relationship and origin of the observed transitions. Part of the talk will be devoted to the role of metal-ligand hybridization in transition metal oxides in general.

Gez. A. Rosch