On behalf of the

Science College CMS

Vienna Computational Materials Laboratory

and Center for Computational Materials Science

we cordially invite you to the following seminar

Dr. Hena Das

S. N. Bose National Centre for Basic Sciences, Kolkata, India

First Principles Study of Complex Oxides

The study of complex oxide materials has been a great source of stimulation for quantum condensed matter physics. Many fundamental concepts such as ferromagnetism, antiferromagnetism, colossal magnetoresistance, ferroelectricity, dielectricity, superconductivity etc have been motivated by and are realized in these systems. Oxide materials offer rich physics due to the interplay of spin, orbital and lattice degrees of freedom, often driven by the strong electronelectron correlation. Because of the correlated nature of the electrons these systems have been traditionally described using model Hamiltonians. Model Hamiltonian-based calculations have the obvious limitation that the parameters of the model Hamiltonian are vastly unknown, and therefore fails to capture the material specific complexity of the oxide materials. On the other hand, the first principles density functional based calculations, which take into account all the structural and chemical aspects correctly, fail to predict the properties of such materials due to the presence of strongly electron electron interaction. In recent years there has been a significant effort to combine the two above mentioned method in terms of building up a first principles derived model Hamiltonian, followed by the solution of the model Hamiltonian by means of many body techniques. Since often the electronic structure of these oxide materials involve only few active degrees of freedom, a crucial step in the model Hamiltonian building involves filtering out the informations provided by a full first principles calculation to arrive to a feworbital, low energy description starting from a full first principles calculation. This has been achieved in recent years in terms of Nth order mun tin orbital (NMTO) based downfolding calculation. In the present study we have investigated properties of few chosen transition metal oxides following the above mentioned approach.

Date: Monday, Oct 25, 2010 16:00

Location: Seminar room 138C (TU Freihaus 9. Stock, gelb)
A-1040 Wien, Wiedner Hauptstaße 8-10