



INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Dr. Claude Ederer
Department of Materials Theory
ETH Zurich, Switzerland

Monday, February 18, 4:30 pm, ICAMS Seminar room 0.08
Universitätsstr. 90a, 44789 Bochum

Combining electronic structure calculations with model approaches for the study of functional complex oxides

Complex transition metal oxides exhibit a wealth of properties that are highly interesting for applications in information and energy technologies (magnetism, ferroelectricity, thermoelectric and/or ferrocatalytic effects, metal-insulator transitions). These properties generally arise from a complex interplay between different degrees of freedom with similar energy scales (e.g. spin, orbital, charge, lattice). Therefore, the construction of effective electronic Hamiltonians describing the "essential" degrees of freedom in complex transition metal oxides is very desirable in order to obtain a clear picture of the physical mechanisms leading to the diverse phase diagrams and order phenomena.

Furthermore, since the standard approximations to density functional theory (DFT) often fail to correctly describe the electronic properties of such "correlated" materials, the construction of realistic tight-binding-like Hamiltonians can be used as starting point for a more sophisticated treatment of electron-electron interaction using numerical many-body techniques such as e.g. dynamical mean-field theory (DMFT).

In this talk I will discuss the use of (maximally localized) Wannier functions for the construction of effective low-energy Hamiltonians of complex transition metal oxides. In particular I will focus on two specific examples: i) the construction of effective two-band models for the prototypical material LaMnO_3 , and ii) the interesting case of the p-electron magnet and Mott insulator rubidium superoxide, RbO_2 .