Kandidatprojekt
(2015-10-12)

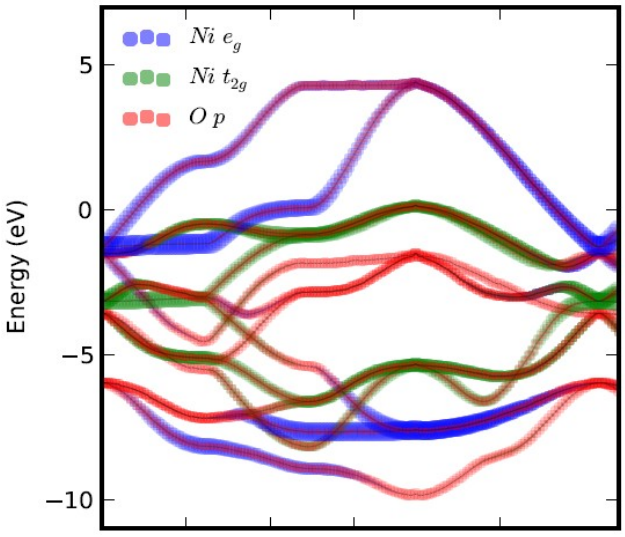
Modeling of the metal to insulator phase transition in $LaNiO_3$

In the future, multi-layer structures of transition metal oxides will possibly replace the present semiconductor based electronic devices. The reason is the observations of remarkable properties of these materials. The temperature, pressure and doping driven transitions between a vast number of phases, e.g. metallic to an insulating phase and metallic to a superconducting phase.

A major challenge is to be able to control the known inherent strong local electron coulomb interaction of these compounds which seems crucial for the properties. To perform computer simulations, the conventional computational schemes based on the Density Functional Theory (DFT) is not sufficient. You will taste the problem by applying a simple tight-binding model in order to avoid large scale calculations but still hopefully gain some insight in the physics.

Project

- Continuing working with our 2-band model for the two uppermost Ni_{3d}-O_{2p} bands (see figure next door)
- Introduce the local colomb interaction U in the spirit of the variational Gutzwiller method.
- You will do some coding and search for the metal-insulator transitions as function of U and the lattice parameter.



DFT Band structure of LNO

Background

Quantum Mechanics, Atom- and Molecular physics, elementary Solid State physics

Group size

2-3 students

Supervisor

Bo Hellsing, room 3008, third floor in Soliden, Materials and Surface Theory group, Department of Physics. E-mail: hellsing@physics.gu.se