Master of Science project
in computational material physics
(2013-12-05)

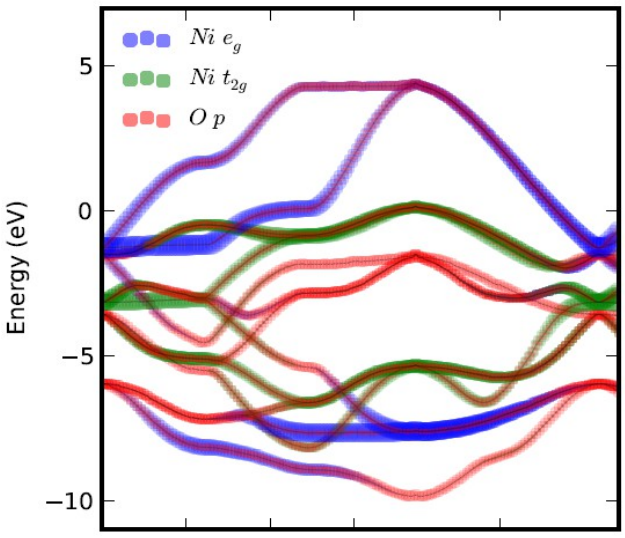
Two-band Hubbard model for $LaNiO_3$

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. We are presently working on merging the variational Gutzwiller method with the GPAW-DFT code in order to take into account the local correlations.

Project

- Construct a 2-band tight-binding model model for the two uppermost Ni3d-O2p bands
- Map the phase diagram applying a Hubbard Hamiltonian, including local electron correlation *U*. Applying our Gutzwiller computer code you will search for the metal-insulator transitions as function of *U* and the lattice parameter *a*.



DFT Band structure of LNO

Background

you have an interest in computational material science related to many-body phenomena in condensed matter physics. You have taken the courses in Quantum physics, Solid state physics and Statistical physic and have some experience in computational physics

Contact

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