Abstract for an Invited Paper
for the MAR06 Meeting of
The American Physical Society

LDA+U Based Studies of Electronic, Vibrational and Spectroscopic Properties of Solids[1]

STEVEN G LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory

The LDA+U method is a physically motivated approach that attempts to incorporate the effects of important orbital-specific local Coulomb interactions in strongly correlated electron systems while retaining the simplicity of local density approximation (LDA) calculations for real materials. In this talk, we discuss several applications of this method within the ab initio pseudopotential planewave framework. For transition metal oxides, the appropriate inclusion of the effects of onsite Coulomb U significantly alters their electronic structure leading to better agreement with experiment for quantities such as the nature of the electronic state, structural parameters, magnetic moments, phonon frequencies, etc. We have also studied the effects of doping on the electronic, magnetic, and structural properties of NaxCoO2. Undoped CoO2 is a metal with a high density of states at the Fermi level within LSDA, but a charge transfer insulator within LSDA+U. It is found that, due to a strong interaction between the doped electrons and the other Co d electrons, the calculated electronic structure is sensitively depended on the doping level. Finally, we discuss the use of LDA+U results as a starting mean-field solution for calculation of the electron self energy and quasiparticle excitations within the GW approximation.

[1]This work was done in collaboration with P.-H. Zhang and M. L. Cohen and supported by the NSF under Grant No. DMR04-39768 and the U.S. DOE under Contract No. DE-AC03-76SF00098.