Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Vibrational properties of correlated systems from ab-initio calculations MATTEO COCOCCIONI, BURAK HIMMETOGLU, Department of Chemical Engineering and Materials Science, University of Minnesota, ANDREA FLORIS, Department of Physics, King's College London — In this talk I will present a recent extension of Density Functional Perturbation Theory to the DFT+U energy functional that allows to compute the vibrational properties of materials from their correlated ground state. The new computational tool, named DFPT+U, is used to investigate the phonon spectrum of MnO and NiO. The more accurate account of electronic correlation through the Hubbard-corrected functional results in a significant improvement in the agreement between the computed phonon frequencies and available experiments. In particular, we obtain a significant reduction in the splitting between the center-zone optical modes (due to the antiferromagnetic order) that confirms the importance of electronic localization in the description of magnetic couplings between metal ions. The order of the split optical modes is also shown to correlate with the occupation of the d states of the transition metal atoms opening for the possibility to use measurements of the vibrational frequencies to investigate certain aspects of the electronic structure of these compounds. In the last part of the talk I will also present the application of DFPT+U to Cu compounds and will discuss the possibility to use it to compute the electron-phonon coupling of high T_c superconductors.

Matteo Cococcioni
Department of Chemical Engineering and Materials Science,
University of Minnesota

Date submitted: 26 Oct 2011 Electronic form version 1.4