Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Pressure-driven high-spin to low-spin and orbital-selective insulator to metal transition in cubic CoO LI HUANG, XI DAI, YILIN WANG, The Institute of Physics, Chinese Academy of Sciences — We studied the magnetic and spectral properties for cubic para-magetic phases of CoO under high pressures by using *ab initio* many-body method which combining local density approximation with dynamical mean-field theory. Experimentally observed metal-insulator transition at high pressure is successfully reproduced in calculations. Our calculation predicts CoO as a Mott insulator at ambient pressure and metal at extreme high pressure. In the intermediate pressure regime, our results indicate that there is an orbital selective Mott phase with t_{2g} orbitals being metallic and e_g orbitals being insulating. In contrast with MnO and Fe_2O_3 (d^5 configuration) where metal-insulator transition is accompanied by a high-spin to low-spin transition, we found that the local moment of CoO (d^7 configuration) decreases gradually from 2.8 ($S = 3$ states) to 1.4 ($S = 1$ states) with increasing pressure, which is in agreement with experimental data.

Li Huang
The Institute of Physics, Chinese Academy of Sciences

Date submitted: 17 Oct 2011 Electronic form version 1.4