Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Convergence of quasiparticle self-consistent GW calculations of transition metal monoxides[1] SUVADIP DAS, JOHN E. COULTER, EFSTRATIOS MANOUSAKIS, Florida State University — We have investigated the electronic structure of the transition metal monoxides MnO, CoO, and NiO in their undistorted rock-salt structure within a fully iterated quasiparticle self-consistent GW (QPscGW) scheme. We have studied the convergence of the QPscGW method, i.e., how the quasiparticle energy eigenvalues and wavefunctions converge as a function of the QPscGW iterations, and compared the converged outputs obtained from different starting wavefunctions. We found that the convergence is slow and that a one-shot G_0W_0 calculation does not significantly improve the initial eigenvalues and states. In some cases the "path" to convergence may go through energy band reordering which cannot be captured by the simple initial unperturbed Hamiltonian. When a fully iterated solution is reached, the converged density of states, bandgaps and magnetic moments of these oxides are found to be only weakly dependent on the choice of the starting wavefunctions and in reasonable agreement with the experiment.

[1]National High Magnetic Field Laboratory

Suvadip Das
Florida State University

Date submitted: 14 Nov 2014 Electronic form version 1.4