Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Self-consistent linear density response within the LDA+U method: Application to transition-metal oxides(*) A. G. EGUILUZ(1), O. D. RESTREPO(1), (University of Tennessee and CMSD, ORNL (2)), J. KUNES, W. E. PICKETT (3), (University of California, Davis) — We formulate a scheme to calculate self-consistently the dynamical linear density-response function based on correlated LDA+U theory. The orbital dependent V_U term in the Kohn- Sham potential, leads to an additional self-consistent condition in the density fluctuations. The end result is a density response function which includes electron-hole interactions (that is, it goes beyond the random-phase approximation). We assess the performance of our scheme by calculating the electron-hole excitation spectrum of prototype transition metal oxides for arbitrary momentum transfers. (*) DOE-CMSN PCSCS collaboration. (1) Supported by NSF ITR-DMR 0219332. (2) Managed by UT-Battelle for the U.S. DOE under contract DE- AC05-00OR22725. (3) Supported by DOE Grant DE-FG03-01ER45876

oscar restrepo
University of Tennesse and ORNL

Date submitted: 30 Nov 2005 Electronic form version 1.4