Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Particle-Hole Corrections for Accurate DFT-based Charge Transfer Energetics TUNNA BARUAH, University of Texas at El Paso, M. PEDERSON, Naval Research Laboratory — Density functional theory (DFT) is primarily a ground state theory because it lacks a rigorous prescription for the calculation of excited states. However, a formalism due to Theophilou showed that a Hohenberg-Kohn like theorem is extendable to an ensemble of ground and excited states provided the states are mutually orthogonality. This condition is also a necessary for a variational approach to individual excited states as shown by Levy. We present a way for obtaining accurate single-electron excitation energies from the ground-state Hamiltonian and orbitals. Our approach explicitly guarantees mutual orthogonality and removes spurious interactions between the electron and hole states. The method yields excellent results for inert gas atoms, closed-shell atoms and molecules, and to charge transfer systems such as the dissociated Na-Cl molecule and a 50 nm long organic molecule containing 200 atoms. Initial applications rely entirely upon standard GGA functionals but the approach is equally amenable to any mean-field method such as Hartree-Fock or DFT with SIC.

Tunna Baruah
University of Texas at El Paso

Date submitted: 29 Nov 2005 Electronic form version 1.4