Modified local exchange and kinetic energy functionals for atomic systems

Fuentealba,

New local functionals for the kinetic and Hartree-Fock exchange energy of atoms are proposed. They are of the following general form: T[?] =22/3CF ? ???5/3 ?f(r,? ?)dr. The function f(r,??), except for two adjustable parameters, is the same for both functionals. They are constructed to distinguish between non-uniform scaling along different coordinates. The functionals are tested and compared with other commonly used functionals for neutral atoms He to Ar. The exchange energy functional is also tested through Kohn-Sharn self-consistent calculations for atoms and ions. Total and exchange energies for hydrogen to argon atoms and for the helium and beryllium isoelectronic series are presented and compared with local density approximation (LDA) and Hartree-Fock (HF) results. The first ionization potential of the atoms of the second row of the periodic table are also calculated. In addition, for the atoms Cr, Mn and As the eigenvalues of the highest occupied orbital are also calculated and