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Combined density functional and Hartree Fock calculations of the total electronic energy of atoms KENNETH WALSH, HENRI JANSEN, OSU — The total electronic energy of an atom has been calculated using unrestricted Hartree Fock methods. In a first step, we perform density functional calculations and obtain the ground state energies and wave functions for spherically symmetric potentials. These wave functions are then used as basis functions for solving the unrestricted Hartree Fock equations. Spherical symmetry is broken by expanding the basis set into spherical harmonic states and by complete angular consideration in the coulomb potential. The wave functions generated by the density functional calculations provide nearly converged basis sets. Breaking the spherical symmetry allows splitting degeneracies in the electronic contribution to the total energy. The resulting Hartree Fock energies are compared with experiment.

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