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Internally Consistent Local Approximation to Density Functional theory ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON M. NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — We propose a new non-local functional for the implementation of density functional theory (DFT) within a local approximation. This functional is obtained through the replacement of the conventional form $T_s + \frac{1}{2}\int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2 \frac{n(\mathbf{r}_1)n(\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|}$ to represent the kinetic and Coulomb energy of a non-interacting system with the expression $T_s + \frac{1}{2}\int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2 \frac{n_s(\mathbf{r}_1,\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|}$ where $n_s(\mathbf{r}_1,\mathbf{r}_2)$ is the two-particle density formed from the non-interacting wave function, and $n(\mathbf{r})$ is the single-particle density. Based on this new functional we develop a local approximation and show that it is self-interaction free and also leads to energies that form an upper bound to the exact ground-state energy. We provide a brief comparison with the conventional Kohn-Sham local density approximation and some of the schemes introduced to correct for the presence of self-interaction in the conventional formalism, and comment on our immediate plans for future development.

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