A new generation of KS methods for molecules based on the exact local KS exchange potential.

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A new all-electron Kohn-Sham method for molecules and clusters is introduced and applied to various test molecules. The *local* Kohn-Sham exchange potential and the exchange energy are treated exactly. The new method, in contrast to present ones, is free of unphysical Coulomb self-interactions. As result, it solves some of the long standing problems of density-functional methods: the treatment of anions and the unphysical eigenvalue spectrum. Moreover it represents a new generation of Kohn-Sham methods in a systematic development of density-functional theory. The method is generally applicable, the required computational effort is comparable to that of Hartree-Fock procedures. Kohn-Sham orbitals and eigenvalues obtained with the new method are used as input in the calculation of excitation energies with time-dependent density-functional theory .