Density Functional Theory Method for Nondynamic/Strong Correlation

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Nondynamic and strong correlation imposes the major challenge to the current density functional theory (DFT), and counts for the majority of the failures of DFT in a variety of areas such as catalysis, organic open-shell molecules and materials. The problem is often characterized as multireference in nature. In this talk, we will present a density functional model based on single-determinant Kohn-Sham density functional theory [1]. It combines Becke'13 method with a new model for kinetic correlation via adiabatic connection based on physical arguments and some exact conditions for both the weak and strong correlations. The result is a single-term functional for correlation of all strength, and is named as KP16/B13 (Kong-Proynov'16/Becke'13). KP16/B13 is the first model of its kind implemented with self-consistent field. The preliminary results show that the model, with only three empirical parameters, recovers the majority of left-right nondynamic/strong correlation upon bond dissociation and performs well for near equilibrium properties such as heats of formation, singlet−triplet energy splittings of diradicals. It also describes well a linear chain of H atoms with many strongly correlated electrons. The new development offers the hope for efficient computation of systems with multireference in nature.

[1] J. Kong and E. Proynov, "Density Functional Model for Nondynamic and Strong Correlation", *J. Chem. Theor. Comp*., **2016**, *12*, 133.