DFT energy corrections to multiconfigurational wavefunctions

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Traditionally, strong correlations in molecules are dealt with multiconfigurational wavefunction theories (WFT), while density functional theory (DFT) approximations efficiently recover instantaneous electron-electron interactions, i.e., dynamic correlation. A variety of methodologies aim to take advantage of the distinct strengths of these two nearly antagonistic theories [1]. One of these strategies lies on merging WFT with DFT through the range separation of the Coulomb operator [2], in which DFT functionals evaluate the short-distance region, while long-range inter-electronic interactions are quantified by WFT (WFT-*sr*DFT). A less explored alternative combines the two theories by splitting the orbital space, with orbitals with large occupancies included in the WFT model and those with small occupation evaluated with a density functional [3] (WFT-*so*DFT). During my presentation, I will discuss the performance of both approaches in the characterization of close and open-shell systems. I will rationalize the role of spin polarization effects in the *sr*DFT exchange energy and how to deal with them [4,5]. I will also show preliminary results within the WFT-*so*DFT scheme.

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