

Exact-exchange-based hybrid-method investigations of small molecules

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Abstract

We have recently shown that the Kohn-Sham calculation based on the exact-exchange (EXX) energy functional leads to markedly improved eigenvalue spectra over the local-density approximation (LDA), the generalized-gradient approximation (GGA), and the Hartree-Fock (HF) approximation for molecular systems, while it gives structural properties comparable to the HF results, hence typically inferior to the LDA and GGA ones¹. In an effort to construct a density-functional scheme that generates both good structural properties and eigenvalue spectra, we study adiabatic-coupling hybrid-functional schemes that mix the EXX and the LDA or GGA. Preliminary results from the investigations of several closed-shell molecules, H₂, N₂, CO, H₂O, and CH₄, will be presented.

¹**Y.-H. Kim**, M. Städele, and R. M. Martin, Phys. Rev. A **60**, 3633 (1999)