A self-interaction-free local hybrid functional in DFT derived from exact criteria

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The physical interpretability of the Kohn-Sham eigenvalues obtained in density-functional theory (DFT), as they are frequently used in linear response theory and for the prediction of photoemission spectra, crucially depends on the exchange-correlation (xc) functional put to task. Unfortunately, functionals that predict thermochemical properties well are known not to deliver eigenvalues of comparable quality and vice versa. With the aim of achieving a reasonable description of thermochemistry and at the same time yielding physically interpretable eigenvalues, we designed a functional of the form of a local hybrid. The ansatz was constructed to satisfy exact constraints such as the freedom of self-interaction (SI) for one-electron systems and the correct scaling behavior. The functional, which contains one free parameter, was tested on a set of simple, yet representative systems. Its predictions for binding energies and ionization potentials (IP) according to the IP-theorem are, in dependence on the free parameter, compared to experimental data.