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Total energy performance of non-Koopmans functionals ANDREA FERRETTI, DMSE, Massachusetts Institute of Technology, ISMAILA DABO, YANLI LI, University Paris Est, MATTEO COCOCCIONI, CEMS, University of Minnesota, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — We have recently introduced a non-Koopmans correction to local and semilocal exchange-correlation functionals, able to identify orbital energies with opposite removal energies in the frozen orbital approximation. This approach directly improves on some of the key failures of common exchange-correlation functionals, often related to self-interaction (e.g. the dissociation energies of simple molecules or the polarizability of linear chains), and provides a link between the Hartree-Fock and the density-functional theory approaches to the electronic-structure problem. We evaluate here the performance of this corrected functional to total energy properties; these include geometries, dissociation energies, and linear and non linear polarizabilities of linear molecules and chains. Our results indicate that the method is very effective in correcting for the self-interaction problem of local and semi-local functionals, with large improvements, among others, for the predictions of polarizabilities and hyperpolarizabilities.

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