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Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional SIVAN REFAELY-ABRAMSON, Weizmann Institute of Science, Israel, SAHAR SHARIFZADEH, Lawrence Berkeley National Laboratory, USA, NIRANJAN GOVIND, Pacific Northwest National Laboratory, USA, JOCHEN AUTSCHBACH, University at Buffalo, State University of New York, USA, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, USA, ROI BAER, Institute of Chemistry, Hebrew University, Israel, LEEOR KRONIK, Weizmann Institute of Science, Israel — We present a method for obtaining outer-valence quasiparticle excitation energies from a density-functional-theory-based calculation, with an accuracy that is comparable to that of many-body perturbation theory within the GW approximation. The approach uses a range-separated hybrid density functional, with an asymptotically exact and short-range fractional Fock exchange. The functional contains two parameters, the range separation and the short-range Fock fraction. Both are determined nonempirically, per system, on the basis of the satisfaction of exact physical constraints for the ionization potential and many-electron self-interaction, respectively. The accuracy of the method is demonstrated on four important benchmark organic molecules: perylene, pentacene, 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA), and 1,4,5,8-naphthalene-tetracarboxylic dianhydride (NTCDA). We envision that for finite systems the approach could provide an inexpensive alternative to GW, opening the door to the study of presently out of reach large-scale systems (Phys. Rev. Lett., in press).

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