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Enhanced Static Approximations for Efficient Calculation of Electronic Excitation Energies[1] WEI KANG, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Laboratory — The GW method for the calculation of excited-state energies has been proven accurate for many physical systems. However, the unfavorable scaling with the size of the system has severely limited its applications. In particular, quantitative prediction of frontier electronic energy levels, crucial in the design of complex and nanostructured materials, has not been feasible. While the static COHSEX approximation significantly simplifies the calculations, the quantitative results are substantially less accurate. Analysis shows that much of the error in the COHSEX approximation traces to the overestimation of short wavelength contributions to the Coulomb-hole term of the self-energy. We have implemented modified static methods that compensate for most of this error. Results will be shown for a series of material applications.

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