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Cluster expansion of the electron-density response function: GW+BSE with molecular environments JEEHYE LEE, T.A. ARIAS, Cornell University, Department of Physics — Molecular excitations in dielectric environments have drawn great interest because environmental manipulation provides the possibility to engineer photo-excitation processes. In exciton calculation the environments often are replaced by dielectric continuum media. These approaches have been successful for solvated molecules, but they lack molecular detail, and hence miss microscopic features. We present a new method to represent environments that allows a more accurate treatment of a wide range of systems by employing cluster expansions of environmental response functions. This initial work, at the GW+BSE level, presents results for shifts in excitation energies due to environments consisting of either individual molecules or conjugated polymers.

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