

Local dielectric response theory: A pathway for electronic excitation embedding

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Understanding environmental effects on electronic excitations is of fundamental importance to predict excited state properties of materials in either solvents or matrices, e.g. a solute molecule solvated by solvent molecules, that can be treated at the mean-field level of theory. A main challenge to this problem arises from the intrinsic non-local nature of the electronic susceptibility, which hinders a real space partition of the dielectric response function. As a result, how to rigorously define and calculate the effective response function of the system of interest embedded in different chemical environments remains an open question. Recently we developed an *ab initio* local dielectric response theory [Phys. Rev. B 92, 241107(R), 2015] that partitions microscopic susceptibilities in real space based on a Wannier representation. Exemplary studies were carried out for the molecular polarizability of water, which we show behaves substantially differently in condensed phases from that in the vacuum due to the interaction with the environment caused by the crystal field and the charge transfer.

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-SC0012704. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.