Local representation of the electronic dielectric response function: Theory and applications

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The microscopic electronic dielectric response function is a central physical quantity that captures the many-electron correlation effects in the ground state total energy and electronic excitations. Key quantities include molecular polarizabilities in different chemical environments, the correlation energy under the random phase approximation, and the screened Coulomb interaction under the GW/BSE framework. Although it is non-local by definition, a local representation of the dielectric response function in real space can provide insightful understanding of its chemical nature and improve the computational efficiency of first principles excited state methods. Recently we proposed a local representation of the electronic dielectric response function [1], based on a spatial partition of the dielectric response into contributions from each occupied Wannier function using a generalized density functional perturbation theory. We show that the locality of the bare response function is determined by the locality of three quantities: Wannier functions of the occupied manifold, the density matrix, and the Hamiltonian matrix. In systems with a gap, the bare dielectric response is exponentially localized, which supports the physical picture of the dielectric response function as a collection of interacting local response that can be captured by a tight-binding model. Several applications of the local response theory will be discussed including response density partition, bond polarizability, dielectric band structure interpolation, and molecular polarizability in condensed phase.

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[1] X. Ge and D. Lu, Phys. Rev. B 92, 241107(R), 2015.