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

Deyu Lu
Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, 11973

The microscopic electronic dielectric response function is a fundamental physical quantity that captures the many-electron correlation effect. Although it is non-local by definition, a local representation in real space can provide insightful understanding of its chemical nature and to improve the computational efficiency of first principles excited state methods. In a recent work [Phys. Rev. B 92, 241107(R), 2015], we have developed a local representation of the electronic dielectric response function, 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 "bond polarizability", dielectric band structure interpolation, and molecular polarizability in condensed phase.

This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.