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First-Principles Dielectric Spectra of Silicon: THz through UV[1]

H.M. LAWLER, S. DALOSTO, University of Washington, Z.H. LEVINE, E.L. SHIRLEY, NIST, J.J. REHR, University of Washington — We present an implementation of the GW-Bethe-Salpeter-equation approach to first-principles calculations of dielectric response based in part on input from the plane-wave, pseudopotential code ABINIT. This work, together with lattice dynamical calculations, aims to develop versatile codes capable of calculating dielectric spectra in insulators for the full spectral range from THz to the UV. Below the bandgap, lattice vibrations absorb light in the THz range. These spectra are generally composed of sharp infrared-active features (absent by symmetry in silicon); weak, temperature dependent continuum effects from IR-active-multiphonon state hybridization; and contributions to the macroscopic polarization directly from multiphonon states. Above the bandgap, density-functional band structures are taken as a starting point for the inclusion of many-body interactions within the GW-BSE approximation. Emphasis will be on treating the excitionic effects and non-zero-momentum application of the modern theory of polarization with ABINIT.

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