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Spectral Representation analysis of dielectric screening in solids and molecules[1] AMANDEEP KAUR, ERIK YLVISAKER, University of California, Davis, CA, DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, NY, TUAN ANH PHAM, GIULIA GALLI, WARREN PICKETT, University of California, Davis, CA — We propose a new approach to identify and rationalize the contribution of core electron polarization to dielectric screening, based on ab initio calculations of the dielectric matrix in its eigenpotential basis. We also present calculations of phonon frequencies, dielectric constants for alkali hydrides and quasiparticle energies of several sp bonded molecules, and we discuss the quantitative effect of including core polarization. We find that inclusion of semicore (SC) electrons leads to new eigenmodes in the dielectric matrix with respect to those with valence electron only. These eigenmodes are highly localized in real space. Polarization arising from SC orbitals may contribute 4-6% to the computed dielectric constants in alkali hydrides, and to differences in QP energies of $\sim$100 meV for sp bonded molecules. Our findings illustrate efficient ways of approximating the spectral decomposition of dielectric matrices used, e.g. in many body perturbation theory and dielectric constant calculations, with substantial computational gains for large systems composed of heavy atoms.

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