Abstract Submitted
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Dielectric screening : Effects of Core Polarization on Phonons and Quasiparticle Bands[1] AMANDEEP KAUR, ERIK YLVISAKER, University of California, Davis, DEYU LU, Brookhaven National Lab, Upton, NY, GIULIA GALLI, WARREN PICKETT, University of California, Davis — We investigate the influence of core polarization on the dielectric screening of atoms, molecules and solids with focus on non metallic systems. We compare results for dielectric band structures and for the eigenvalues of the dielectric matrix obtained by varying the number of valence electrons included in our calculations. We show that (semi)-core electronic states may substantially influence the dielectric screening, even if they lie very deep in energy compared to the outermost valence electrons. We then discuss how the changes in dielectric screening observed when including (semi)-core electrons affect computed quasi particle energies at the GW level, and phonon frequencies, e.g. the LO-TO splitting. We focus on closed shell atoms, including Be,Mg, Ca, Ar, Zn, simple diatomic molecules and simple ionic solids, e.g. LiH and NaH.

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