Core Polarization Effects from Dielectric Eigenpotentials

A. Kaur,[1] E. R. Ylvisaker,[1] D. Lu,[2] T. A. Pham,[3]
G. Galli,[1,3] and W. E. Pickett[1]

[1] *Department of Physics, University of California, Davis, CA 95616, USA.*
[2] *Center for Functional Nanomaterials, BNL, Upton, NY 11973, USA.*
[3] *Department of Chemistry, University of California, Davis, CA 95616, USA.*

The dielectric function eigenpotential representation is used to investigate various consequences when core polarization is included with the valence electron polarization. The semicore leads to additional dielectric screening which becomes evident in the extra bands in the dielectric band structure in solids and in additional eigenpotential in molecules and atoms. We illustrate how (semi)core contributions influence dielectric screening for phonons and the dielectric constant in ionic crystals, and for quasiparticle energies at the G_0W_0 level. We conclude that in a variety of applications it is crucial to include (semi)core electrons to describe adequately dielectric screening and its consequences, for both static and dynamical behavior.

Contact: ackaur@ucdavis.edu