O.37 Influence of spin-orbit coupling interaction on the electron-phonon renormalized electronic energy levels in polar materials

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Electron-phonon (e-p) interaction calculations from first-principles are well documented in the literature. The predominance of non-adiabatic effects in the zero-point renormalization (ZPR) of the band gap for polar materials has been recently assessed in the light of the Fröhlich interaction [1].

Yet, even for benchmark materials, spin-orbit coupling (SOC) is frequently neglected to reduce the numerical cost of calculations. SOC manifests itself in the electronic structure through the split-off energy and by lifting band degeneracies away from time-reversal invariant momenta (TRIM). This modification of the energy levels will affect both e-p coupling energies and ZPR. Materials lacking inversion symmetry also exhibit an in-plane shift of the band extrema away from the TRIM, known as Rashba splitting. This could lead to resonant couplings at finite phonon wavevectors, which will strengthen the e-p coupling energies.

We explicitly compute e-p coupling energies and ZPR for binary semiconductors, using density-functional perturbation theory (DFPT), with and without SOC. We analyze our results in the light of a generalized three-dimensional Fröhlich Hamiltonian including SOC.

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[1] Miglio, A., Brousseau-Couture, V., Godbout, E. et al. Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. *npj Comput Mater* **6**, 167 (2020).