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Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the band structure GABRIEL ANTONIUS, University of Montreal, SAMUEL PONCÉ, Université Catholique de Louvain, ÉTIENNE LANTAGNE-HURTUBISE, GABRIEL AUCLAIR, MICHEL CÔTÉ, University of Montreal, XAVIER GONZE, Université Catholique de Louvain — The electron-phonon coupling in solids renormalizes the band structure, reducing the band gap by several tenths of an eV in light-atoms semiconductors. Using the Allen-Heine-Cardona theory (AHC), we compute the zero-point renormalization (ZPR) as well as the quasiparticle lifetimes of the full band structure in diamond, BN, LiF and MgO. We show how dynamical effects can be included in the AHC theory, and still allow for the use of a Sternheimer equation to avoid the summation over unoccupied bands. The convergence properties of the electron-phonon coupling self-energy with respect to the Brillouin zone sampling prove to be strongly affected by dynamical effects. We complement our study with a frozen-phonon approach, which reproduces the static AHC theory, but also allows to probe the phonon wavefunctions at finite displacements and include anharmonic effects in the self-energy. We show that these high-order components tend to reduce the strongest electron-phonon coupling elements, which affects significantly the band gap ZPR.

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