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Many-body effects on the zero-point renormalization of diamond: a frozen-phonons approach GABRIEL ANTONIUS, Université de Montréal, SAMUEL PONCÉ, Université Catholique de Louvain, MICHEL CÔTÉ, Université de Montréal, XAVIER GONZE, Université Catholique de Louvain — Electron-phonon interaction has a sizeable effect on the electronic structure of materials. Even at zero temperature, the zero-point renormalization (ZPR) can reduce the band gap of insulators by several hundreds of meV. The method of choice to compute this effect is based on the AHC theory, performing perturbative calculations with DFT wavefunctions and energies, possibly with a scissor shift. However, previous studies suggest that inclusion of many-body effects might change substantially the DFT electron-phonon coupling coefficients. We study the ZPR of the optical band gap of diamond, using a frozen-phonons method. This allows us to perform G_0W_0 and self-consistent quasi-particle GW calculations on the distorted lattice, thus including many-body effects in the electron-phonon coupling coefficients. The frozen-phonons method also allows us to study other neglected components of the AHC theory, such as the non-diagonal Debye-Waller term, and the anharmonic effects.

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