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Zero-point motion effect on the bandgap of diamond: validation of codes[1] SAMUEL PONCÉ, Univ Catholique de Louvain, GABRIEL ANTONIUS, Univ Montreal, PAUL BOULANGER, Institut Néel, ELENA CANNUCCIA, Institut Laue Langevin, ANDREA MARINI, Consiglio Nazionale delle Ricerche, MICHEL CÔTÉ, Univ Montreal, XAVIER GONZE, Univ Catholique de Louvain — Verification and validation of codes, as well as new theoretical methods, are of utmost importance if one wants to provide reliable results. In this work we present a rigorous and careful study of all the quantities that enters into the calculation of the zero point motion renormalization of the direct band gap of diamond due to electron-phonon coupling. This study has been done within the Allen-Heine-Cardona (AHC) formalism as implemented into Abinit and Yambo on top of Quantum Espresso. We aim at quantifying the agreement between the codes for the different quantities of interest. This study shows that one can get less than $10^{-5} Ha/at$ differences on the total energy, 0.07 cm^{-1} on the phonon frequencies, 0.5% on the electron-phonon matrix elements and less than 4 meV on the zero-point motion renormalization. At the LDA level, the converged direct bandgap renormalization in diamond due to electron-phonon coupling in the AHC formalism is -409 meV (reduction of the band gap) [1].

[1] S. Poncé *et al.*, arXiv:1309.0729 [cond-mat.mtrl-sci] and submitted for publication in Comput. Mat. Science (2013).

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