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Electron-Phonon Renormalization of Electronic Band Structures of C Allotropes and BN Polymorphs[1] ROXANNE M. TUTCHTON, CHRISTOPHER MARCHBANKS, ZHIGANG WU, The Colorado School of Mines
— The effect of lattice vibration on electronic band structures has been mostly neglected in first-principles calculations because the electron-phonon (e-ph) renormalization of quasi-particle energies is often small (< 100 meV). However, in certain materials, such as diamond, the electron-phonon coupling reduces the band gap by nearly 0.5 eV, which is comparable to the many-body corrections of the electronic band structures calculated using the density functional theory (DFT). In this work, we compared two implementations of the Allen-Heine-Cardona theory in the EPW code and the ABINIT package respectively. Our computations of Si and diamond demonstrate that the ABINIT implementation converges much faster. Using this method, the e-ph renormalizations of electronic structures of three C allotropes (diamond, graphite, graphene) and four BN polymorphs (zincblend, wurtzite, monolayer, and layered-hexagonal) were calculated. Our results suggest that (1) all of the zero-point renormalizations of band gaps in these materials, except for graphene, are larger than 100 meV, and (2) there are large variations in e-ph renormalization of band gaps due to differences in crystal structure.

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