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Electron-phonon renormalization of the electronic structure of diamond FELICIANO GIUSTINO, Department of Materials, University of Oxford, STEVEN G. LOUIE, MARVIN L. COHEN, University of California at Berkeley and Lawrence Berkeley National Laboratory — The calculation of band structures from first-principles has reached a high level of accuracy. Calculations combining density-functional theory with many-body perturbation theory often are in good agreement with measurements by photoemission, tunneling, and other spectroscopic probes. While significant efforts have been devoted to improving the description of electron-electron interactions in these calculations, the effect of lattice vibrations has largely been overlooked so far. In this work we study from first principles the electron-phonon renormalization of the band gap of diamond. The calculated temperature dependence of the gap and the broadening of the absorption edge are in excellent agreement with spectroscopic ellipsometry data. Interestingly we find a gap renormalization due to zero-point vibrations as large as 0.6 eV. We discuss the implications of our findings for the electronic structure of other carbon-based bulk materials and nanostructures.

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