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Mechanism of Superconductivity in Boron-Doped Diamond[1] FELICIANO GIUSTINO, JONATHAN R. YATES, IVO SOUZA, MARVIN L. COHEN, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — The recent discovery of superconductivity in boron-doped diamond above liquid helium temperature has attracted considerable interest. Theoretical investigations indicate that the superconducting pairing in this material is of the conventional phonon-mediated type. However, the nature of the phonon mechanism involved and the role of the dopants are still controversial issues. In order to elucidate such issues we performed first-principles calculations of the electron-phonon interaction in boron-doped diamond, considering a virtual crystal model and a supercell model which explicitly includes the boron atoms. For each model we calculated the Eliashberg functions with high accuracy by sampling the corresponding Brillouin zone with a million of inequivalent k-points. We found that the localized vibrational modes associated with the boron atoms provide a significant contribution to the electron-phonon coupling strength and that superconductivity in diamond is crucially linked to the breaking of the lattice periodicity induced by the doping.

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