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Constraints on T_c for superconductivity in heavily boron-doped diamond[1] JONATHAN E. MOUSSA, MARVIN L. COHEN, UC Berkeley & LBNL — Calculations of electron-phonon coupling are performed for boron-doped diamond structures without electronically compensating defects over a wide range of boron concentration. The effects of boron substitutional disorder are incorporated through the use of randomly generated supercells, leading to a disorder-broadened distribution of results. After averaging over disorder, this study predicts a maximum bulk T_c near 55 K for boron concentrations between $20\% - 30\%$, assuming the validity of the simple structural model used and a Coulomb pseudopotential of $\mu^* = 0.12$. Considering only the largest electron-phonon coupling values of the distribution, superconductivity may still percolate through the material at higher temperatures, up to 80 K, through the regions of large coupling. A synthesis path is proposed to experimentally access this class of materials.

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