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Possibility of superconductivity in high pressure phases of BC_3[1]
JONATHAN E. MOUSSA, MARVIN L. COHEN, UC Berkeley & LBNL — Using an ab-initio pseudopotential-local-density-approximation, we study the possibility of a high-pressure transition of graphitic planar sp^2 bonded BC_3 into an sp^3 bonded covalent network. Energy barriers are examined for the predicted transition to the sp^3 phase and for the observed onset of phase separation in BC_3 under high pressure, high temperature conditions [V. L. Solozhenko *et al.*, Appl. Phys. Lett. **85**, 1508 (2004)]. The sp^3 phase of BC_3 is predicted to be metallic and superconducting and is similar to 25% boron-doped diamond without boron clusters. Calculations of phonon frequencies and electron-phonon coupling allow for an estimate of the superconducting transition temperature.

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