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Theoretical study of defects in c-BC_2N ONYEKWELU OKEKE, Harvard University — Periodic supercells with 64 atoms using a zincblende stoichiometry for c-BC_2N are generated for various native point defects and random distribution of boron and carbon atoms in B-C-N compound. The atomic structures of these systems were relaxed by first-principles density functional theory. The elastic properties including the bulk modulus, shear modulus, and Young's modulus of the bulk c-BC_2N crystals and the defective systems were examined and compared

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