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First-principles study of BC_2N[1] EUNJA KIM, TAO PANG, Department of Physics and Astronomy, UNLV, NV 89154, USA, WATARU UTSUMI, Synchrotron Radiation Research Center, Japan Atomic Energy Research Institute, Japan, VLADIMIR SOLOZHENKO, LPMTM-CNRS, Universite Paris-Nord, France, YUSHENG ZHAO, LANL, Los Alamos, New Mexico, 87545, USA — First-principles calculations are performed and analyzed to identify different cubic phases of BC_2N synthesized experimentally. With a proper choice of the supercell, cutoff energy, and sampling k points, the cubic phases are found to be stable theoretically. The bulk modulus from elastic stiffness constants for each of the phases is in excellent agreement with available experimental data. All the phases are defect free and do not possess any B–B or N–N bond. Two high-density phases with nearly degenerate energies are interpreted to represent two experimental systems of different x-ray patterns. The high-density phases are characterized by the existence of C–C bonds whereas the low-density phase is characterized by the absence of C–C bonds. From the calculated equation of state and the available experimental data, we show for the first time that the unique feature of each of the cubic BC_2N phases is a direct result of the corresponding local electronic structure and chemical bonding in the system.

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