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**Prediction of boron carbon nitrogen phase diagram** SANXI YAO, Carnegie Mellon Univ, HANTAO ZHANG, Univ of Science and Technology of China, MICHAEL WIDOM, Carnegie Mellon Univ — We studied the phase diagram of boron, carbon and nitrogen, including the boron-carbon and boron-nitrogen binaries and the boron-carbon-nitrogen ternary. Based on the idea of electron counting and using a technique of mixing similar primitive cells, we constructed many "electron precise" structures. First principles calculation is performed on these structures, with either zero or high pressures. For the BN binary, our calculation confirms that a rhombohedral phase can be stabilized at high pressure, consistent with some experimental results. For the BCN ternary, a new ground state structure is discovered and an Ising-like phase transition is suggested. Moreover, we modeled BCN ternary phase diagram and show continuous solubility from boron carbide to the boron subnitride phase.

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