

Abstract Submitted  
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**First-principles study of cubic BC<sub>6</sub>N: Structural forms and ideal strength** YI ZHANG, Department of Physics, University of Nevada, Las Vegas, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas — We present first-principles calculations on the structural forms and ideal strength of cubic BC<sub>6</sub>N. The calculated ideal tensile and shear strength are lower or comparable to those of c-BN. Our results show that increasing carbon content does not lead to significant enhancement of the idea strength as expected by the conventional wisdom. It can be attributed to the weak C-N bonds that impose a limit on the idea strength.

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