QMC And Phonon Study of Super-Hard Cubic Boron Carbon Nitride

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ABSTRACT:
In this study, we have applied phonon and quantum Monte Carlo (QMC) calculations to c-BC2N, which is derived from c-BN by the introduction of carbon, in search of cheaper as well as harder materials that have advantages over the traditionally known hardest material, diamond. There have been theoretical density functional theory (DFT) results of the bulk modulus, which indicate that c-BC2N has a higher bulk modulus than c-BN. However, varied findings of experimental data for the properties of c-BC2N reported by various groups appear to indicate a wide range of values. We found lattice structure instability at the high pressure region of c-BC2N which has been used for theoretical estimations of bulk modulus. We also examined the widely varying predictions depending on the functionals used in previous DFT works, using QMC with a more accurate treatment of the electronic interactions. Taking the instabilities into account, the QMC energy-volume fitting is still found to support that c-BC2N has a higher bulk modulus than c-BN, but with smaller difference than the prediction of the previous theoretical works. We also find substantial reductions in the bulk modulus due to zero point vibrational effects.

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