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Quantum Monte Carlo determination of the equation of state of cubic boron nitride K.P. ESLER, B. MILITZER, R.E. COHEN, Carnegie Institution of Washington — The pressure inside a diamond anvil cell is usually determined by measuring the pressure-dependent frequency shift of a small ruby sample or by x-ray diffraction on a small chip of a pressure standard. However, there are no primary pressure standards for the megabar range. Recently, cubic boron nitride (cBN) has been suggested as an accurate pressure gauge.[1] Unlike ruby, its structure is highly constrained by symmetry and stable beyond 100 GPa, and it has a well-separated Raman spectrum with sufficient pressure dependence to allow accurate pressure calibration. Its use as a pressure standard requires reliable equation of state (EOS) data. A density functional theory (DFT) calculation of the cBN EOS based on the generalized gradient approximation agrees well with experiment up to 100 GPa, but a calculation that does not depend on an approximate exchange-correlation functional would be desirable. Quantum Monte Carlo (QMC) is a correlated, first-principles simulation method with fewer uncontrolled approximations than DFT methods. We present the results of applying state-of-the-art QMC methods to the bulk cBN solid in order to determine the EOS.

[1] A.F. Goncharov et al., Phys. Rev. B **72**, 100104R (2005).

Kenneth Esler
Carnegie Institution of Washington

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