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**An accurate high pressure scale from quantum Monte Carlo**

KENNETH ESLER, R.E. COHEN, Geophysical Laboratory, Carnegie Institution, BURKHARD MILITZER, Dept. of Astronomy, UC Berkeley, JEONGNIM KIM, University of Illinois at Urbana-Champaign, NCSA — We have developed a fundamental high-temperature and high-pressure scale based on cubic boron nitride (cBN) using a combination of Quantum Monte Carlo (QMC) for the static contribution along with density functional perturbation theory (DFPT) for the thermal pressure. The anharmonic Raman frequency was determined as a function of pressure by solving the Schrodinger equation for the vibrational well determined using QMC with the frozen phonon method. The use of cBN as a pressure scale has a number of advantages. Unlike ruby, its structure is highly constrained by symmetry and stable well beyond 100 GPa, and it has a well-separated Raman spectrum with sufficient pressure dependence to allow accurate pressure calibration. While the cBN EOS from density functional theory (DFT) gives reasonable agreement with experiment, the results from different approximate functionals disagree. Quantum Monte Carlo is a first principles simulation method which circumvents approximate functionals and is widely regarded to provide the most accurate predictions of the properties of solids available. We utilize state-of-the-art QMC methods to obtain the static EOS with the QMCPACK code. We include a novel correction based on all-electron wave functions to eliminate pseudopotential error.

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