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Optimized Nested Markov Chain Monte Carlo Sampling: Application to the Liquid Nitrogen Hugoniot Using Density Functional Theory
M. SAM SHAW, JOSHUA D. COE, Theoretical Division, Los Alamos National Laboratory, THOMAS D. SEWELL, Department of Chemistry, University of Missouri-Columbia — An optimized version of the Nested Markov Chain Monte Carlo sampling method is applied to the calculation of the Hugoniot for liquid nitrogen. The "full" system of interest is calculated using density functional theory (DFT) with a 6-31G* basis set for the configurational energies. The "reference" system is given by a model potential fit to the anisotropic pair interaction of two nitrogen molecules from DFT calculations. The EOS is sampled in the isobaric-isothermal (NPT) ensemble with a trial move constructed from many Monte Carlo steps in the reference system. The trial move is then accepted with a probability chosen to give the full system distribution. The P's and T's of the reference and full systems are chosen separately to optimize the computational time required to produce the full system EOS. The method is numerically very efficient and predicts a Hugoniot in excellent agreement with experimental data.

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