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Theoretical N_2 Hugoniot using MondoSCF density functional quantum energies and a very efficient Monte Carlo reweighting scheme
M. SAM SHAW, C.J. TYMCZAK, Los Alamos National Laboratory — A Monte Carlo reweighting scheme is used to calculate the Hugoniot of molecular N_2 incorporating very accurate quantum energies. We first determine a reference potential fit to quantum calculations of the anisotropic pair interaction. Then the full many-body energy is evaluated for uncorrelated configurations from an NPT Monte Carlo reference simulation at pressure P_0 and temperature T_0. Each configuration is then reweighted to correspond to the distribution of the full energy at values of P and T chosen to maximize the overlap of the two distributions. Because the configurations are uncorrelated, only a few configurations are needed to give a statistically accurate EOS at P and T. The quantum energy calculations are computer intensive, but tractable due to the linear scaling of the MondoSCF density functional code. The PBE0 density functional is used with a 6-31g** basis set, shown to be convergent in the relevant energy differences. The resulting Hugoniot is in excellent agreement with Hugoniot data up to 40 GPa where N_2 remains molecular.

Milton Shaw
Los Alamos National Laboratory

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