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Nuclear Quantum Vibrational Effects in Shock Hugoniot Temperatures[1] NIR GOLDMAN, EVAN J. REED, LAURENCE E. FRIED, LLNL — We present a straightforward technique for the inclusion of nuclear quantum vibrational effects in molecular dynamics (MD) calculations of shock Hugoniot temperatures. Although *ab initio* MD simulations accurately reproduce the high pressure-density equation of state for many materials, they have been shown to under-predict experimental Hugoniot temperatures by 20-30%, partially due to the exclusion of nuclear quantum effects in standard MD simulations. Using a Grüneisen equation of state and a quasi-harmonic approximation to the vibrational energies, we derive a simple, post-processing method for calculation of quantum corrected Hugoniot temperatures. We have used this technique to determine the quantum corrected temperatures for *ab initio* MD simulations of shock compressed water, methane, and diamond. Our results indicate significantly closer agreement with all available experimental temperature data. This new technique and formalism can easily be applied to simulations of a number of different shock compressed systems, and has the potential to decrease the large uncertainties inherent in many experimental temperature measurements.

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