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Quantum Mechanical Corrections to Simulated Shock Hugoniot Temperatures[1] NIR GOLDMAN, EVAN REED, LAURENCE E. FRIED, Lawrence Livermore National Lab — We present a straightforward method for the inclusion of quantum nuclear vibrational effects in molecular dynamics calculations of shock Hugoniot temperatures. 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 the quantum corrected Hugoniot temperatures. We have used our novel technique on *ab initio* simulations of both shock compressed water and methane. Our results indicate significantly closer agreement with all available experimental temperature data for these two systems. Our formalism and technique can be easily applied to a number of different shock compressed molecular liquids or solids, and has the potential to decrease the large uncertainties inherent in many experimental Hugoniot temperature measurements of these systems.

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