Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

The Role of Quantum Nuclear Effects in Shock-Induced Chemistry and Colored Thermostats for Their Efficient Description EVAN REED, TINGTING QI, QIAN YANG, Department of Materials Science and Engineering, Stanford University — A fast methodology is described for atomistic simulations of shock-compressed materials that incorporates quantum nuclear effects in a self-consistent fashion. We introduce a modification of the multiscale shock technique (MSST) that couples to a quantum thermal bath described by a colored noise Langevin thermostat. The new approach, which we call QB-MSST, is of comparable computational cost to MSST and self-consistently, semi-classically incorporates quantum heat capacities and Bose-Einstein harmonic vibrational distributions. We study shock-compressed methane using the ReaxFF potential. We find that the self-consistent nature of the method results in the onset of chemistry at 40% lower pressure on the shock Hugoniot than observed with classical molecular dynamics. We employ new statistical and data mining methods to reveal the nature of the chemistry.

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Date submitted: 06 Jun 2013 Electronic form version 1.4