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Efficient semiclassical quantum nuclear effects for shock compression studies

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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 incorporates quantum heat capacities and Bose-Einstein harmonic vibrational distributions. As a first test, we study shock-compressed methane using the ReaxFF potential. The Hugoniot curves predicted from the new approach are found comparable with existing experimental data. 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. The temperature shift associated with quantum heat capacity is determined to be the primary factor in this shift.

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