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Nuclear Quantum Effects and their Role in Shock Induced Chemical Initiation of TATB[1] BRENDEN W. HAMILTON, Purdue University, MATTHEW P. KROONBLAWD, Lawrence Livermore National Laboratory, MD MAHBUBUL ISLAM, ALEJANDRO STRACHAN, Purdue University — The approximation of classical ion dynamics in molecular dynamics (MD) leads to an overprediction of the specific heat and omits zero-point energy (ZPE). The former deficiency leads to an underprediction of temperature rise in MD shock simulations. Post-simulation corrections can accurately predict the actual rise in temperature, but do not correct for ZPE errors. We use ReaxFF and a quantum thermal bath coupled with the multiscale shock technique (MSST) to assess the separate roles of specific heat and ZPE in MD-based predictions for initiation of the explosive TATB. Compared to classical MSST simulations, the quantum bath not only increases the temperature rise that lowers the shock strength needed to induce chemical reactivity, but also leads to a decrease in the temperature threshold itself. Including ZPE lowers the apparent shock velocity threshold for reactivity by a similar amount as including a temperature-dependent specific heat. The decomposition pathways of TATB are shown to be unchanged by the quantum bath relative to predictions from purely classical simulations. Prepared by LLNL under Contract DE-AC52-07NA27344 and approved for unlimited release under document number LLNL-ABS-768122.

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