Abstract Submitted
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First-principles approach to reactivity in the presence of shock-wave CHRISTOPHER MUNDY, LLNL, I.-F. WILL KUO, LLNL, ALESSANDRO CURIONI, IBM, EVAN REED, LLNL, LARRY FRIED, LLNL — Gaining insight into the mechanisms leading to detonation in energetic materials within a planar shock geometry had been thought to be computationally prohibitive. The use of the Multiscale Shock Method (MSSM) of Reed et. al has opened the possibilities to study the chemistry of complex molecular systems undergoing uniaxial shock compression using Kohn-Sham density functional theory (KS-DFT). Here, we present results of nitromethane under various levels of shock loading and reveal the chemical mechanisms underlying the detonation process. We will also discuss an alternative non-Hamiltonian formulation of the MSSM. The aforementioned formulation is present in both CPMD and CP2K software packages. We also will compare and contrast different formulations of KS-DFT (both plane- wave and hybrid schemes) and discuss future of scaling the MSSM method to tera- scale platforms such as Blue Gene/L.

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