Abstract Submitted
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Ab Initio Reactive Monte Carlo JEFFERY LEIDING, JOSHUA COE, Los Alamos National Laboratory — Equations of state of HE product mixtures under extreme conditions are of obvious interest to the shock physics community. There is also considerable overlap in thermodynamic and chemical space of HE product mixtures and planetary interiors. Chemical equilibrium EOSs provided by thermochemical models are underconstrained due to lack of experimental data, particularly on chemical composition. First-principles data fill this much needed gap. The standard first-principles simulation technique for bulk materials is ab initio molecular dynamics (AIMD). While AIMD is often reliable, I will show that chemical reactions, which are critical to the EOSs of HE product mixtures, can be rare events in AIMD. This causes AIMD to exhibit hysteresis along thermodynamic paths. To solve this problem, we have developed the first ab initio reactive Monte Carlo algorithm (AIRxMC), which samples chemical reactions directly. Standard MC sampling is too inefficient for use with ab initio calculations. I will discuss the techniques used to make the algorithm practical, and compare the results of AIRxMC to those of AIMD for warm dense ammonia, using DFT.

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