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Multistage reaction pathways in detonating high explosives[1] YING LI, Argonne National Laboratory, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California, CACS COLLABORATION, ALCF TEAM — Atomistic mechanisms underlying the reaction time and intermediate reaction products of detonating high explosives far from equilibrium have been elusive. This is because detonation is one of the hardest multiscale physics problems, in which diverse length and time scales play important roles. Here, large spatiotemporal-scale reactive molecular dynamics simulations validated by quantum molecular dynamics simulations reveal a two-stage reaction mechanism during the detonation of cyclotrimethylenetrinitramine crystal. Rapid production of N_2 and H_2O within 10 ps is followed by delayed production of CO molecules beyond ns. We found that further decomposition towards the final products is inhibited by the formation of large metastable carbon- and oxygen-rich clusters with fractal geometry. In addition, we found distinct uni-molecular and intermolecular reaction pathways, respectively, for the rapid N_2 and H_2O productions.

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