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**Mesoscale challenge of extending atomistic scale chemistry of initiation reactions to deflagration-to-detonation transition<sup>1</sup>**  
SANTANU CHAUDHURI, University of Illinois at Urbana-Champaign

Predictive simulations connecting chemistry that follow the shock or thermal initiation of energetic materials to subsequent deflagration or detonation events is currently outside the realm of possibilities. Molecular dynamics and first-principles based dynamics have made progress in understanding reactions in picosecond to nanosecond time scale. However, connecting the events that leads to deflagration will require simulations using much larger length and time scale to connect the full reaction network. This constitutes a mesoscale challenge in energetic materials research. Recent advances in addressing this mesoscale chemistry challenge in other domains will be discussed. Development in coarse-grain simulations and accelerating reactive MD simulations faces the challenge of simplifying the chemistry by making assumptions on the mechanism with consequences on the outcome. For example, results from thermal ignition of different phases of RDX shows a complex reaction and deterministic behavior for critical temperature before ignition. First-principles calculations for validation of key pathways observed will be discussed. The kinetics observed is dependent on the hot spot temperature, system size and thermal conductivity. Smaller hot spots in simulations needed higher temperature for ignition of the solid. For cases where ignition is observed, the incubation period is dominated by intermolecular and intramolecular hydrogen transfer reactions. The gradual temperature and pressure increase in the incubation period is accompanied by accumulation of heavier polyradicals. The polyradicals with triazine rings from the RDX molecules intact undergo ring-opening reactions which fuel a series of rapid exothermic chemical reactions. Our ongoing work on connecting mesoscale and continuum scale will be discussed.

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