Abstract Submitted
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Energetic Material Simulations Framework WILLIAM MATTSON, BETSY RICE, US Army Research Laboratory — We have created a computational framework for the easy implementation of the modeling needs of the advanced energetic materials (AEM) community, with rapid turnaround. The framework constructs simulations described in eXtensible Markup Language (XML) from a set of components in shared object libraries. The complete set of standard molecular simulation components can be combined in any fashion creating typical simulations and providing unanticipated functionality. The framework includes multi-million atom molecular dynamics in a several thermodynamic ensembles, including the recently developed uniaxial Hugoniostat method. This constrains the system to states that correspond to points on the shock Hugoniot curve. It also includes ab initio crystal prediction capability. This procedure predicts the crystal structure and density of a solid using only the molecular structure of a single molecule. This predictive capability is considered crucial to the design and development process of AEM, since one of the fundamental properties required for the initial screening of a candidate energetic material is its crystalline density.

William Mattson
US Army Research Laboratory

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