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Emergent molecular theory of initiation of detonation: the effect of molecular and crystal structure on thermal stability of high density energy materials MAIJA KUKLA, National Science Foundation, ROMAN TSYSHEVSKY, ONISE SHARIA, University of Maryland — The sensitivity to detonation initiation of high density energy materials along with their performance are two most important criteria for choosing the best material for explosive formulations, booster engines, detonators, *etc.* After numerous experimental and theoretical attempts to develop a single parameter describing sensitivity of different classes of energetic materials, one concludes that the complexity of physical and chemical explosive properties cannot be trivialized. We report here the results of our theoretical and computational studies of thermal decomposition mechanisms and kinetics of five classes of EM: pentaerythritol tetranitrate (PETN), nitramine cyclotetramethylene-tetranitramine (HMX), diamino-dinitroethene (DADNE), bis-(nitrofurazano)-furoxane (BNFF) and benchmark triamino-trinitrobenzene (TATB). Our modeling reveals how the thermal stability depends on the molecular structure of the material and how the crystal structure may additionally hinder or catalyze decomposition reactions. We will also discuss an effect of crystalline defects on sensitivity and performance of materials.

Maija Kukla
National Science Foundation

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