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Computational evaluation on the sensitivity of energetic materials[1] YI LIU, SERGEY ZYBIN, WILLIAM GODDARD, California Institute of Technology — An efficient computational procedure based on molecular dynamics (MD) simulation with ReaxFF reactive force field has been developed to evaluate the sensitivity of various energetic materials including TATB, RDX, PETN, HMX, and TATP. In this study, the two-dimensional slab model is first equilibrated at 300 K, followed by rapid heating up to 2000 K at a rate of 10 K/fs. The system is then allowed to evolve via MD at microcanonical ensemble, where the decomposition of energetic molecules mostly occurs. Another technique mimics the shock impact test and uses two moving wall driving by a constant force to create two impact waves running toward each other, followed by the shock reverberation and material decomposition. Our simulations show that sensitive energetic materials, in general, decompose more quickly than less sensitive ones, which agrees with experimental observations. The chemical reactions found in these simulations are analyzed to understand the mechanisms that account for diverse sensitivity of energetic materials.

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