Abstract Submitted
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Initiation of PETN decomposition under shock compression: Reactive molecular dynamics simulation[1] PENG XU, California Institute of Technology, SERGEY ZYBIN, AIDAN THOMPSON, Sandia National Lab, JOANNE BUDZIEN, Sandia Nationa Lab, WILLIAM GODDARD III, California Institute of Technology — The initial physical and chemical response of energetic materials under mechanical shock has been investigated for PETN by molecular dynamics method with ReaxFF reactive force field parameterized from first-principles calculations. We study the propagation of a shock wave and shock-induced chemical reactions created by moving piston mimicked by a potential wall. We simulate both the continuous and impulsive piston loading to investigate its influence on the initiation and decomposition reactions in energetic materials as well as the orientational dependence using large-scale parallel ReaxFF-MD simulations. The mechanism and evolution of chemical reactions induced by mechanical shock and pure shear is discussed along with the propagation of heat, mass, pressure, and reaction waves.

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