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**Energetic materials under thermal shock: Molecular dynamics simulation with reactive force field**[1] YI LIU, SERGEY ZYBIN, ADRI VAN DUIN, WILLIAM GODDARD, California Institute of Technology — The physical and chemical response of energetic materials under thermal shock loading has been investigated for RDX, PETN and HMX by molecular dynamics method with ReaxFF reactive force field parameterized from first-principles calculations. We study the propagation of a thermal front and following reactive wave from the hot spot created by fast heating of a local region and keeping it at high constant temperature. The hot spot serves as heat source to heat up adjacent materials where no temperature constraint is imposed, and trigger the chemical decomposition of energetic molecules. The mechanism and evolution of chemical reactions induced by thermal shock is discussed along with the propagation of heat, mass, pressure, and reaction waves.

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