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A Molecular Dynamics simulation of Hugoniot curves of HMX using ReaxFF and its application in SPH modeling of macroscale terminal effects[1] GUI-RONG LIU, GANGYU WANG, University of Cincinnati, QING PENG, SUVRANU DE, Rensselaer Polytechnic Institute — HMX is a widely used high explosive. Hugoniot curve is a valuable tool for analyzing the equations of state, and is of importance for all energetic materials including HMX. The Hugoniot curves serve as one of the key character in continuum modeling of high explosives. It can be obtained from experimental measurements, and recently also from computational studies. In this study, the Hugoniot curve of HMX is calculated using a multi-scale shock technique via Molecular Dynamics (MD) simulations, where the reactive force field ReaxFF is obtained from Quantum Mechanics calculations and tailored for HMX. It is found that our MD Hugoniot curve of HMX from the optimized ReaxFF potential agree well with experiments. The MD Hugoniot curve of HMX is also incorporated in our in-house Smoothed Particle Hydrodynamics (SPH) code for the modeling of the macro-scale explosive behaviors of HMX explosives and HMX cased in a 3D cylinder.

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Qing Peng
Rensselaer Polytechnic Institute

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