

Abstract Submitted
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Modeling the material strength and equations of state of beta-HMX from both first-principles calculations and molecular dynamics simulations¹ QING PENG, Rensselaer Polytechnic Institute, GUANGYU WANG, G.R. LIU, University of Cincinnati, SUVRANU DE, Rensselaer Polytechnic Institute — We investigate the elastic constants and equations of state (EOS) of the β -polymorph of cyclotetramethylene tetranitramine (HMX) energetic molecular crystal using density functional theory (DFT) calculations. The combination of vdW-DF2 van der Waals functionals and PBE exchange-correlation functionals gives optimized results. The DFT results are used to optimize the Reactive Force Field (ReaxFF). The material strength and EOS of beta-HMX at finite temperatures are then predicted from ReaxFF molecular dynamics simulations. Our results suggest that the optimized ReaxFF predicts the mechanics and EOS of beta-HMX well.

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