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Predicting Elastic Properties of β-HMX from First-principles Calculations[1] QING PENG, - RAHUL, Rensselaer Polytechnic Institute, GUANGYU WANG, GUI-RONG LIU, University of Cincinnati, STEFAN GRIMME, Universitt Mnster, SUVRANU DE, Rensselaer Polytechnic Institute — We investigate the performance of the van der Waals (vdW) functions in predicting the elastic constants of the β-polymorph of cyclotetramethylene tetranitramine (HMX) energetic molecular crystal using density functional theory (DFT) calculations. We confirm that the accuracy of the elastic constants is significantly improved using the vdW corrections with environment dependent C_6 together with PBE and revised PBE exchange-correlation functionals. The elastic constants obtained using PBE-D3(0) calculations yield the most accurate mechanical response of β-HMX, with compared to the experimental stress-strain data. The PBEsol without vdW corrections can also predict the elastic constants well. Our results suggest that PBE-D3 calculations are reliable in predicting the elastic constants of this material.

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