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First principles studies of PETN molecular crystal under uniaxial compression JIJUN ZHAO, J.M. WINEY, Y.M. GUPTA, Institute for Shock Physics, Washington State University, Pullman, WA 99164, WARREN PERGER, Department of Physics and Department of Electrical Engineering, Michigan Tech University, Houghton, MI 49931 — First principles calculations are important tools to understand changes of atomic structures and physical properties of energetic molecular crystals under compression. Using the plane-wave pseudopotential technique (CASTEP program), we have performed first principles calculations to determine the structural and vibrational properties of pentaerythritol tetranitrate (PETN) crystals under uniaxial compression to about 5 GPa along the [001], [100], and [110] orientations. Our results under uniaxial elastic strains are discussed and compared with those from hydrostatic compression. For a given compression, the geometry of various chemical groups in the PETN molecule show different changes in terms of their bond length and bond angle. The deformation of PETN crystal under compression is also found to be sensitive to the loading conditions. The shift of vibrational frequencies of PETN crystal due to uniaxial compression along different orientations is discussed.

Jijun Zhao
Institute for Shock Physics, Washington State University
Pullman, WA 99164

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