

Abstract Submitted
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Shear strain induced structural and electronic modifications of the energetic molecular crystal 1,1-diamino-2,2-dinitroethylene¹ SERGEY RASHKEEV, Idaho National Laboratory, MAIJA KUKLJA, National Science Foundation — First-principles calculations of the structural and electronic properties of the deformed energetic molecular crystal 1,1-diamino-2,2-dinitroethylene (FOX-7) under shear-strain loading are presented. The reaction of the crystal to applied shear-strain loading is found to be highly anisotropic. When the external loading is removed, the relaxation of the system is mainly defined by stretching, bending, and rotations of the NO₂ groups of neighboring molecules. In general, the deformed molecular crystal never relaxes to its initial, ideal crystalline FOX-7 structure. Instead, different planes remain shifted relatively to each other on vectors, which are typically incommensurated with any translational vector of the ideal crystal. We also found that no metallization occurs under shear-strain loading. We suggest that the considered mechanisms of the shear-strain relaxation of the structural and electronic degrees of freedom are typical for layered anisotropic molecular crystals, and that they should significantly affect their chemical reactivity, conductivity, optical properties, and initiation of detonation in energetic materials.

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