

Abstract Submitted
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The atomic and electronic structure of defects in 1,1-diamino-2,2-dinitroethylene MAIJA KUKLJA¹, National Science Foundation, SERGEY RASHKEEV², Vanderbilt University, FRANK ZERILLI³, Naval Surface Warfare Center, Indian Head — The atomic and electronic structure of defects in the molecular crystal 1,1-diamino-2,2-dinitroethylene (FOX-7) is studied by means of both first-principles Hartree-Fock and density-functional theory methods. The defect-related local electronic states in the band gap and their contribution to the optical and transport properties of FOX-7 are modeled. The decomposition energy of the material in the solid phase in the presence of defects is accurately calculated using the nudged elastic band approach and compared with results obtained from other methods. The possible correlation between the lowering of the decomposition barrier and the electronic properties of the material has been investigated.

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