Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Vacancy-Induced Initiation of β-NTO via Bimolecular Hydrogen Transfer at High Pressure: A DFT-D Study

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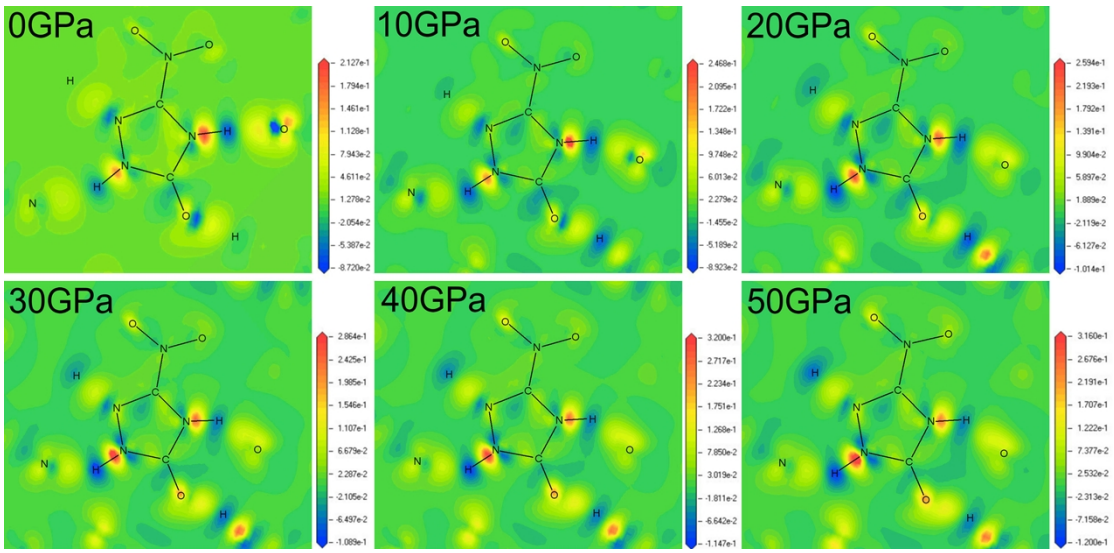

Fig. S1. Electron density difference (EDD) map displaying electron delocalization between ideal bulk and independent NTO molecules with slice cutting across the triazole ring of one molecule. The red or blue color denotes a gain or loss of electron density.

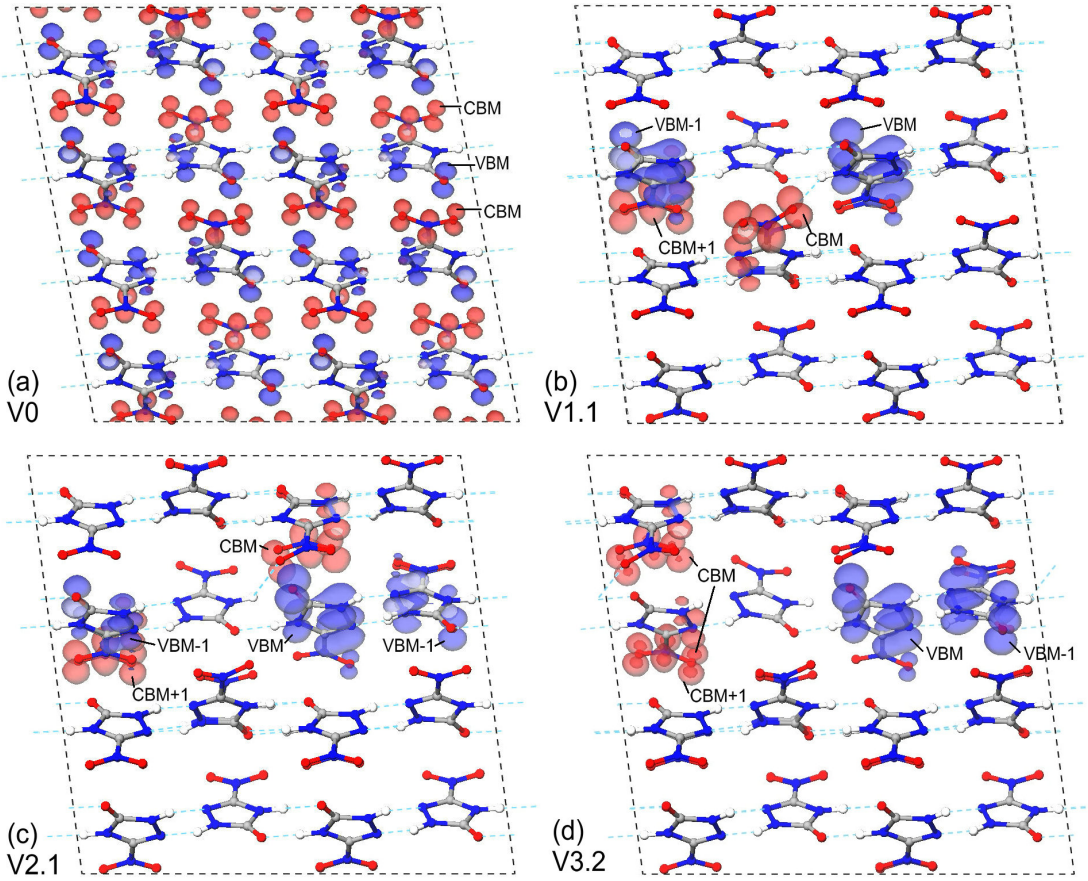

Fig. S2. Distributions of frontier orbitals of the ideal bulk crystal and vacancy systems at 0 GPa. The blue orbitals stand for the top of the valence bands and the red ones for the bottom of the conduction bands. The isovalue is defined by 0.005 in (a) and 0.04 in (b)-(d). The hydrogen bond paths are denoted by the dotted lines.

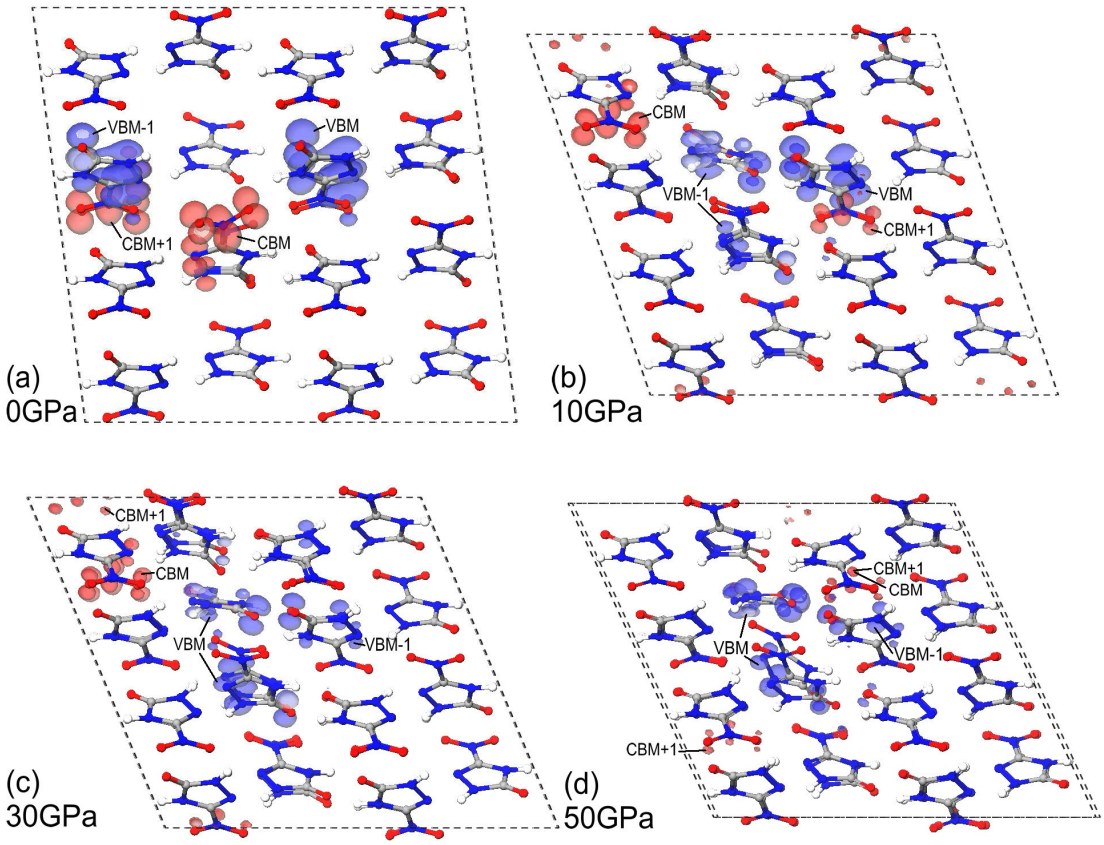

Fig. S3. VBM-1, VBM, CBM, and CBM+1 of the monovacancy V1.1 at 0 GPa, 10 GPa, 30 GPa, and 50 GPa. The isovalue is defined by 0.04.