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Autocatalytic Decomposition Mechanisms in Energetic Molecular Crystals MAIJA KUKLJA, University of Maryland, SERGEY RASHKEEV, Idaho National Laboratory — Atomic scale mechanisms of the initiation of chemical processes in energetic molecular crystals, which lead to the decomposition and ultimately to an explosive chain reaction, are still far from being understood. In this work, we investigate the onset of the initiation processes in two high explosive crystals - diamino-dinitroethylene (DADNE) and triamino- trinitrobenzene (TATB). We found that an autocatalytic decomposition mechanism is likely to take place in DADNE crystal that consists of corrugated, dashboard-shaped molecular layers. The presence of a dissociated NO2 group in the interstitial space between two layers induces a significant shear-strain between these layers, which, in turn, facilitates the further dissociation of NO2 groups from surrounding molecules through lowering the C-NO2 decomposition barrier. Unlike this, in TATB (that consists of flat, graphite-like molecular layers), an interstitial NO2 group positioned between two layers tends to produce a tensile stress (rather than a shear-strain), which leads to local molecular disorder in these layers without any significant modification of the C-NO2 decomposition barrier. The observed differences between the two materials are discussed in terms of their structural, electronic, and chemical properties.

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