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Explosive initiation of pentaerythritol tetranitrate (PETN) by laser irradiation ROMAN TSYSHEVSKIY, ONISE SHARIA, MAIJA KUKLJA, Materials Science and Engineering Department, University of Maryland, College Park, MD — Understanding of explosive decomposition of energetic materials triggered by laser irradiation is of great importance for design of new economical formulations with high performance and tunable sensitivity. Earlier, laser irradiation was only considered as a source of heat. Nowadays, it is realized that optical excitation may set off initiation of rapid chemical reactions and govern further decomposition in energetic materials. However, mechanisms of this phenomenon are yet to be established. We present quantum-chemical calculations of the electronic structure of molecular and crystalline PETN to explore the effect of common impurities on its optical properties. We found that charged or excited PETN molecules exhibit significantly different electronic, optical, and chemical behavior. For example, new decomposition pathways that were not available in the ground state become favorable in the charged state of PETN. Three calculated lowest excitation energies of ionized PETN require 0.6, 0.7 and 1.13 eV, which is considerably lower than those for equilibrium PETN. The activation energy of the rate limiting decomposition stage is within 9-12 kcal/mole, while it is 35 kcal/mole in the ground state. We discuss possible ways that originate charge transfer in PETN and presented results in the context of recent experimental data.

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