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Enhanced sensitivity of explosives in the Condensed Phase: 2,4,6-trinitrotoluene as a model YEHUDA ZEIRI, NRCN and Ben-Gurion University, Beer-Sheva, Israel, DAVID FURMAN, FAINA DUBNIKOVA, NAOMI ROM, BARAK HIRSHBERG, Hebrew University, Jerusalem, Israel, SERGEY V. ZYBIN, WILLIAM A, GODDARD III, Caltech, Ca. USA, RONNIE KOSLOFF, Hebrew University, Jerusalem, Israel — This study is based on the results of Molecular Dynamics (MD) employing a reactive force field (ReaxFF) and electronic structure (DFT) calculations of 2,4,6-trinitrotoluene (TNT) decomposition and high temperatures and pressures. The sensitivity to decomposition shows a marked increase for the condense phase as compared with single molecule. The simulations suggest that bimolecular processes dominate the initial stages of decomposition. The DFT calculations used to explore the role of bimolecular pathways. These pathways are responsible to the $\sim$23 kcal/mol reduction in the barrier height that lead to the enhanced sensitivity. These pathways involve (1) an H atom transfer between two neighboring TNT molecules in from the aromatic ring of one to one of the nitro groups of the other. The loss of the H atom promotes breaking the adjacent C-NO_2, and (2) the H atom transfer to the NO_2 leads subsequently to the formation of HONO and NO products. The thermal decomposition process was followed using the MD simulations for 400 ps to reach the final stable decomposition products. In addition to stable gas products, we obtained carbon clusters formed by the agglomeration of aromatic rings. The TNT decomposition mechanism is compared to that of other explosives.

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