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An effect of charged and excited states on the decomposition of FOX-7 ANNA KIMMEL, Department of Physics, University of Nevada Las Vegas, USA, PETER SUSHKO, ALEXANDER SHLUGER, Department of Physics and Astronomy, University College London, London, UK, MAIJA KUKLJA, Division of Materials Research, National Science Foundation, USA — Various decomposition mechanisms in 1,1-diamino-2,2-dinitroethylene (FOX-7) in both gas and solid phases have been investigated by means of density functional theory calculations using an embedded cluster model. We found that the molecular excitations and charge trapping have a dramatic effect on the decomposition process by facilitating some mechanisms of dissociation and precluding the others; the excited states not only reduce the energetic reaction barriers but also change the type of the dominating chemistry from endothermic to exothermic. We found that the decomposition of FOX-7 in the gas phase is defined by two competing low- energy mechanisms, the C-NO_2 scission and C-NO_2 to CONO isomerisation. Decomposition in solid state of FOX-7 is much more complex and is controlled by cooperative behavior, which involves the excitation processes and structural inhomogeneities in crystalline lattice.

Maija Kuklja
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