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Thermal stability and performance of oxadiazole based energetic materials[1] ROMAN TSYSHEVSKIY, University of Maryland College Park, PHIL PAGORIA, Lawrence Livermore National Laboratory, ALEKSANDR SMIRNOV, Bakhirev Scientific Research Institute of Mechanical Engineering, MAIJA KUKLJA, University of Maryland College Park, UNIVERSITY OF MARYLAND TEAM — Achievement of tailored properties of new energetic materials remains a great challenge. Among the most important and probably least understood criteria is sensitivity of energetic materials to detonation initiation. Thermal stability is a key factor that defines sensitivity. Because of the appealing properties including relatively low impact sensitivity, high decomposition temperature and low melting point, novel oxadiazole based energetic materials became attractive candidates for using as melt-castable explosives. We report results of our DFT modeling that reveals kinetically and energetically most favorable decomposition mechanisms, which govern thermal stability of the oxadiazole based materials. We show how reactivity and performance of the material depend on the chemical composition and molecular structure of the material.

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