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Searching for new energetic materials: Computational design of novel nitro-substituted heterocyclic explosives ROMAN TSYSHESVKY, University of Maryland, PHILIP PAGORIA, Lawrence Livermore National Laboratory, MAIJA KUKLJA, National Science Foundation — The continuous search for safe and powerful energetic materials is an exciting research challenge that attracts experts in material science, chemistry, physics, and engineering. Elucidation of meaningful correlations between sensitivity and structures of explosives is a fundamental problem, which ought to be resolved to ensure successful design of new materials and improvements of existing energetics. In this report, quantum-chemical DFT study of thermal decomposition of a series of recently synthesized oxadiazole-based explosives, BNFF (3,4-bis(4-Nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-N-oxide), BNFF-1 (3,4-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole) and ANFF-1 (3-(4-amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole) is presented. We also show how the knowledge of discovered correlations between structures and thermal stability of these compounds is used to design several novel candidate heterocyclic energetic molecules, including DNBTT (2,7-dinitro-4H,9H-bis([1,2,4]triazolo)[1,5-b:1',5'-e][1,2,4,5]tetrazine), compound with high thermal stability, which is on par or better than that of TATB.

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