

Abstract Submitted
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Heterocyclic energetic materials: Synthesis, characterization and computational design ROMAN TSY SHEVSKY, University of Maryland, PHILIP PAGORIA, LLNL, ALEKSANDER SMIRNOV, Bakhirev Research Institute of Mechanical Engineering, Dzerzhinsk, Russia, MAIJA KUKLJA, University of Maryland — Achievement of the tailored properties (high performance, low sensitivity, etc.) in targeted new energetic materials (EM) remains a great challenge. Recently, attention of researchers has shifted from conventional nitroester-, nitramine-, and nitroaromatic-based explosives to new heterocyclic EM with oxygen- and nitrogen-rich molecular structures. They have increased densities and formation enthalpies complemented by attractive performance and high stability to external stimuli. We will demonstrate that oxadiazol-containing heterocycles offer a convenient playground to probe specific chemical functional groups as building blocks for design of EM. We discuss a joint experimental and computational approach for design, characterization, synthesis, and modeling of novel heterocyclic EM. Combinatorially, we comprehensively analyzed how overall stability and performance of each material in the family (BNFF, LLM-172, LLM-175, LLM-191, LLM-192, LLM-200) depends upon their chemical composition and details of the molecular structure (such as a substitution of a nitro group by an amino group and 1,2,5-oxadiazole fragment by 1,2,3- or 1,2,4-oxadiazol ring). We will also discuss proposed new EM with predicted superior chemical and physical properties. -/abstract- P. Pagoria, R. Tsyshevsky, A. Smirnov,

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