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Multi-level approach for design and synthesis of energetic materials with tailored properties[1] PHILIP PAGORIA, Lawrence Livermore National Laboratory, ROMAN TSYSHEVSKIY, University of Maryland College Park, GUZEL GARIFZIANOVA, Kazan National Research Technological University, ALEKSANDR SMIRNOV, Bakhirev Scientific Research Institute of Mechanical Engineering, MAIJA KUKLJA, University of Maryland College Park — A typical approach to design novel high energy density materials usually involves sophisticated synthesis procedures combined with extensive sensitivity characterization tests. Such empirical explorations are time and effort consuming and often very expensive while the successful outcomes are never guaranteed. Thus, many new energetic materials were attained only to be rejected due to their dangerously high sensitivity. Therefore, an efficient approach that could potentially replace rather expensive trial and error method has yet to be established. Here we discuss a multi-level protocol developed for searching for novel energetic materials with tailored properties. Our approach combines state-of-the-art first principles modeling and semi-empirical big data analysis with advanced synthetic procedures and experimental characterization. We demonstrate how this protocol has been used to design fused and linear heterocyclic materials.

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