Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Computational design of fused heterocyclic energetic materials[1]
ROMAN TSYSHEVSKIY, University of Maryland College Park, PHILIP PAGORIA, Lawrence Livermore National Laboratory, ISKANDER BATYREV, US Army Research Laboratory, MAIJA KUKLJA, University of Maryland College Park — A continuous traditional search for effective energetic materials is often based on a trial and error approach. Understanding of fundamental correlations between the structure and sensitivity of the materials remains the main challenge for design of novel energetics due to the complexity of the behavior of energetic materials. State of the art methods of computational chemistry and solid state physics open new compelling opportunities in simulating and predicting a response of the energetic material to various external stimuli. Hence, theoretical and computational studies can be effectively used not only for an interpretation of sensitivity mechanisms of widely used explosives, but also for identifying criteria for material design prior to its synthesis and experimental characterization. We report here, how knowledge on thermal stability of recently synthesized materials of LLM series is used for design of novel fused heterocyclic energetic materials, 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.

[1]This research is supported by ONR (Grant N00014-12-1-0529), NSF XSEDE resources (Grant DMR-130077) and DOE NERSC resources (Contract DE-AC02-05CH11231)

Roman Tsyshevskiy
University of Maryland College Park

Date submitted: 06 Nov 2015 Electronic form version 1.4