

**MATERIALS ENGINEERING
SEMINAR**

“Synthesis and Characterization of Energetic Materials”

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Purdue MSE PhD Dissertation
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ABSTRACT

Energetic materials are compounds that can store and release high amounts of energy and are broadly classified as explosives, propellants, and pyrotechnics. Energetic materials find wide application including civil, military, and medical applications. With a wide range of uses, the properties required for each compound will be different. Development of energetic materials has six goals: (1) economical synthesis; (2) environmentally friendly synthesis and use; (3) sufficient safety in production and use; (4) excellent performance; (5) high thermal stability; (6) facile synthesis. There are many materials that will satisfy any number of these goals, but fail to fulfill others, precluding widespread adoption. Trying to balance performance, environmental safety, and stability to create better materials is the challenge of the field of energetic materials seeks to address.

In the pursuit of new and high-performing energetic compounds several energetic backbones and methods of imparting stability and energetic performance were explored. The first body of work consisted of amination of 4-nitro-1,2,3-triazole and azo-coupling the resulting primary energetic materials. This yielded two new primary energetic explosives WPX-101 and WPX-102, which have impressive explosive performances; WPX-102 may find utility as a metal-free primary explosive. Utility of 1,2,3-triazole as a zwitterionic compound was also explored and resulted in the production of 3-methyl-1,2,3-triazolium-1*N*-dinitromethylide, the first fully-studied energetic material making use of the zwitterionic dinitromethyl functional group. This compound shows promising stability and prompted on-going work for a bis-dinitromethyl-1,2,3-triazole, which is expected to be higher-performing and more stable than the previous work. Other work on new explosives includes synthesis of fused ring systems with high stability towards physical stimuli while retaining performances similar to TNT. Work with fused ring systems also lead to the development of an improved synthesis of bromotetrazole. Development of a new oxidizer for use in rocket propellants that may compete with ammonium dinitramide is also presented. Finally, work with the elusive and unstable all-nitrogen pentazolone anion is presented.

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