Intelligent Design of Energetic Materials

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Abstract:

Energetic materials present a unique opportunity for the Army to incorporate green chemistry principles and “Materials by Design”, or computational prescreening, into the design process to improve the Army’s environmental footprint. As the Army is responsible for the entire life cycle of the materials from synthesis through demilitarization, potential benefits of “greener” energetic materials that maintain performance standards are far-reaching. With this in mind, the US Army Research Laboratory and collaborators have utilized significant advances in the development of computational methods to predict properties related to performance, sensitivity, and environmental impact of a new material. Here we present a framework for integration and validation of emerging methods and models for energetic materials design. This presentation will discuss research into predictive toxicological modeling, progressive standards for conducting environmental health assessments, high-level efforts to foster a fundamental green chemistry ethic, and projects to seek alternative energetic materials.