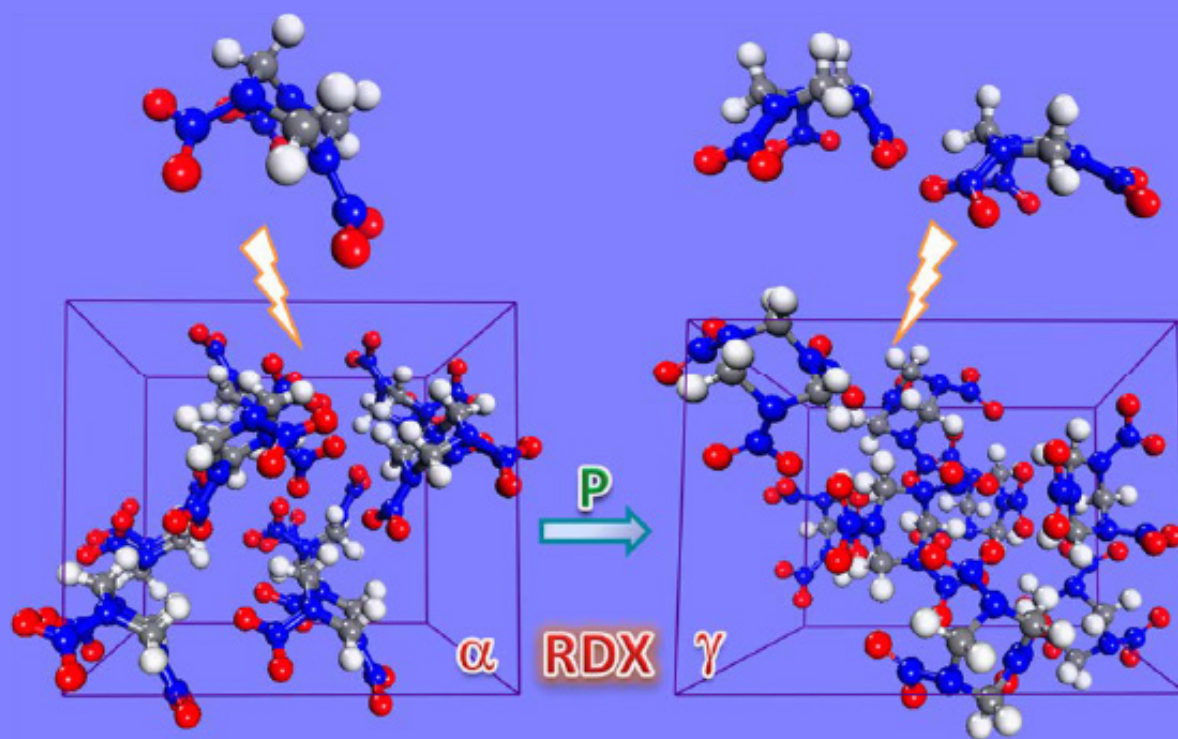# COMPUTATIONAL MODELING OF
HIGH ENERGY MATERIALS

NETL
NATIONAL ENERGY TECHNOLOGY LABORATORY

OVERVIEW

Understanding intermolecular interactions among different materials and integrating them into design strategies is paramount to developing novel structured materials or enhancing the performance of existing ones.

Predictions of the crystal density and detonation velocity are essential metrics in computer-assisted methods for the development of new formulations of energetic materials. Such properties are directly dependent on the structure and type of interactions present in energetic materials, which, in turn, can undergo significant modifications under the high-temperature and high-pressure conditions characteristic of detonation processes.

In the case of composite materials containing both energetic materials and polymeric binders, understanding how these interact is particularly important in several areas, for example to develop new polymer-based sensors for explosives detection, to increase the collection efficiency of the explosive residues adsorbed on surfaces for enhanced detection sensitivity, or to formulate new polymer-based explosives or munitions.

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RESEARCH

NETL accomplishments for this research includes:

- Used first-principles calculations to investigate the compression, the low-pressure phase transition, and the shock Hugoniot properties of energetic material RDX (hexahydro-1,3,5-trinitro-1,3,5-s-triazine) in the pressure range of 0–9 GPa using Born-Oppenheimer molecular dynamics (BOMD) simulations.

- Studied the interactions of crystalline and amorphous polyethylene (PE) with RDX surface using force-distance spectroscopy and molecular dynamics (MD) simulations.

- Used density functional theory (DFT) to calculate the crystallographic lattice parameters for a set of 26 ionic high nitrogen content compounds. The main objective of this study was to screen different DFT functionals which incorporate long-range dispersion interactions and to identify those functionals that are capable of predicting the unit cell volumes within a target error of less than 3%, a value which is a required threshold for accurate predictions of energetic materials formulations.
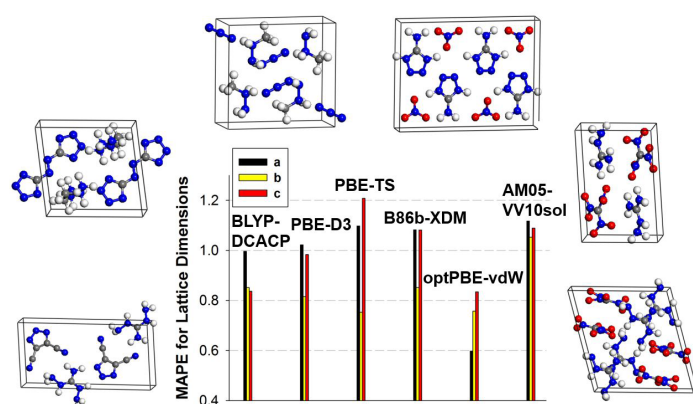

Figure 1. The mean absolute percent error of the predicted lattice dimensions by some of the best performing DFT functionals. The errors bars are below 1 %, similar to the values obtained by experimental methods.
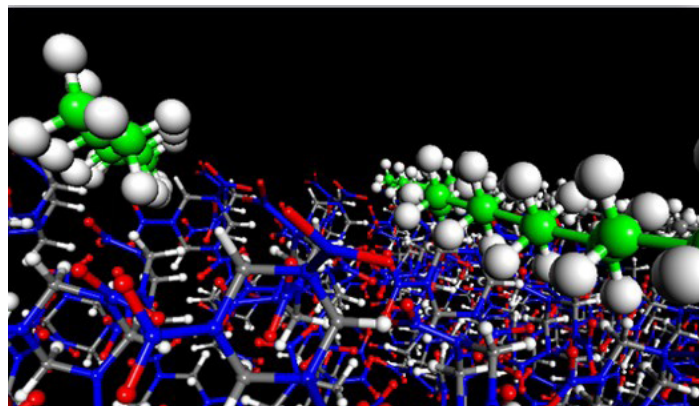

Figure 2. Snapshot of a PE chain interacting with RDX surface.

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