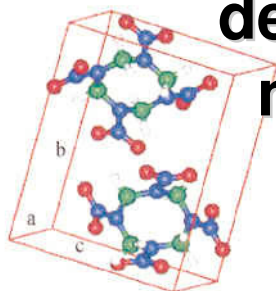


# Defect-induced decomposition in energetic materials: *ab initio* study



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**Abstract:** Most energetic materials are molecular solids having complex crystal structures composed of polyatomic organic molecules. Being exposed to some external stimuli they are capable of undergoing fast chemical decomposition with large energy release. Macroscopic properties of energetic substances are fairly well understood, especially in gas or liquid phases. Microscopic processes and behavior of the explosive solids are poorly known due to complexity of their structures and rapidity of the detonation initiation process.

In this presentation, a brief review of results recently obtained from *ab initio* modeling of defects in a series of energetic materials will be presented. The significant role of defects in changing properties of solids and controlling sensitivity to initiation of chemistry under extreme conditions will be discussed.

**Friday September 15, 2006  
2:30 pm Robeson Hall Room 210**

