

Abstract Submitted
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Electronic Properties of Energetic Molecules Under Compression

JEFFREY KAY, Sandia National Laboratories — Understanding how the electronic structure of energetic materials change under compression is important for understanding the shock response of materials and mechanisms of shock-induced chemical reactions. In this presentation, changes in the electronic structure of prototypical energetic crystals under high degrees of compression are examined *from the molecule's point of view*, using quantum chemical calculations. The effects of compression on the electronic structure of, and interactions between, the constituent molecules are examined in particular. The insights these results provide into previous experimental observations and theoretical predictions of energetic materials under high pressure are discussed.

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