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Pressure-induced phase transitions in energetic materials

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Explosives and propellants, known generically as energetic materials, are widely used in applications that include mining, munitions, and automotive safety. Key properties of these materials include: reliable performance under a range of environmental conditions; long-term stability; environmental impact; processability; sensitivity to accidental initiation through stimuli such as impact, shock, friction, and electrostatic discharge. Many of these properties are affected by the crystal structure of the energetic material. Explosives experience elevated pressures and temperatures under detonation conditions – such conditions often induce phase transitions in the energetic material. Hence detailed studies of pressure-induced structural changes in these materials are essential in order to understand and model fully their behaviour. This presentation will describe some recent high-pressure studies (using a combination of X-ray and neutron diffraction techniques) on 2,4-dinitroanisole (DNAN), an insensitive explosive that is replacing TNT in some applications [1,2]. DNAN shows rich pressure-induced polymorphism, with at least four high-pressure forms having been identified to date. One of the structures provides insight into as to why DNAN is particularly insensitive to initiation by shock. The presentation will also describe the interplay between experiment and theory, which will be illustrated by experimental and computational high-pressure studies of 1,1-diamino-2,2-dinitroethene (DADNE or FOX-7). A very subtle phase transition has been identified at a pressure of ~2.0 GPa and the implications of this will be discussed in relation to the observed structural changes and properties of this material.

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