Poster Presentation

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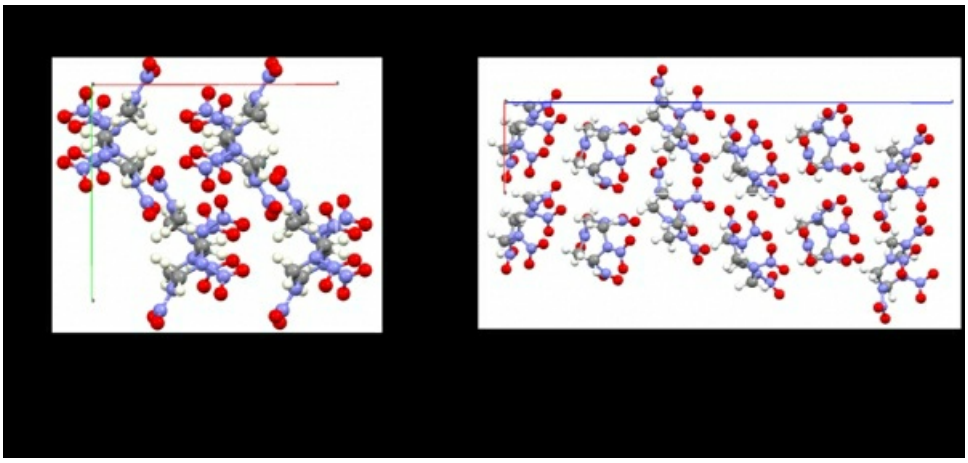
The big-bang theory: predicting energetic materials properties

Adam Alexander Leon Michalchuk[1], Sarah Piggott[1], Ivana Lapsanska[1], Colin Pulham[1], Carole Morrison[1]
[1]*University Of Edinburgh, Edinburgh, United Kingdom*
E-mail: adam.michalchuk@ed.ac.uk

Energetic materials (EM) are used in a variety of industrial and commercial applications. From defence applications to public use in automobile airbags, EMs are encountered daily by both trained and untrained individuals. Ensuring these materials are safe for use is therefore of paramount importance. To date, many fundamental questions surrounding these materials remain poorly understood, perhaps most importantly: how easily can an EM be triggered? To answer these questions, laborious testing is required, on a case-by-case basis. The development of novel EMs is therefore very hazardous, with no a priori knowledge as to the safety of new materials, or known materials under new conditions. In the present contribution we discuss a new approach to the prediction of impact sensitivity of EMs from first principles. This model is based on a fundamental understanding of the energy transfer processes that occur within crystalline materials.[1] The energy transfer processes underpinning this model are found to be highly dependent on the packing of molecules within a crystal lattice and thus captures the unique impact sensitivities of different polymorphic forms of the same energetic molecule Figure 1. Based on this approach, we successfully predict the relative impact sensitivities of a wide variety of known materials, and predict these values for currently untested EMs. This work therefore allows a fundamental rationalisation of the structure-property relationships in EMs.

In this contribution we will present the developed theory, and subsequently discuss its implications for the rational design of novel energetic materials based on structural characteristics. How sensitive is an EM? How safe will an EM be to handle? How will novel conditions affect safe handling of EMs? Can new EMs be rationally designed?

[1] D. Dlott and M.D. Fayer (1988) J. Chem. Phys 88 949



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