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Ab-initio Prediction of Impact Sensitivity PETER HASKINS, MALCOLM COOK, ANDREW WOOD, HELEN FLOWER, QinetiQ — An important goal of the energetic materials community has been to develop a first-principles technique for the prediction of sensitivity. There have been a number of attempts by previous researchers to develop a simple criterion that might achieve this, but they have only been partially successful. Here we review previous attempts and propose some alternative approaches. These are based, variously, on ab-initio quantum chemistry determinations of activation barriers, crystal packing predictions of the lattice energy, and estimates of the reaction energy. Using these basic parameters we have attempted to obtain correlations with experimental drop weight impact data for a wide range of explosives. We compare and contrast the methods and draw conclusions with regard to the most important factors. Finally, we use the best correlations to make predictions for novel, as yet un-synthesised, poly-nitrogen materials.

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