Key properties of energetic materials (explosives and propellants) include reliable performance under a range of environmental conditions, long-term stability, environmental impact, processability, and sensitivity to accidental initiation through stimuli such as impact, shock, friction, and electrostatic discharge. Many of these properties are dependent on the crystal structure of the energetic material and how the molecules interact with each other within the crystal lattice. This talk will provide an introduction to energetic materials and highlight how intermolecular interactions can be modified by both pressure and temperature, as well as the technique of co-crystallisation whereby the energetic material is crystallised with one or more molecular components in order to modify the properties of the components. Results will be presented to illustrate how crystal-engineering techniques can be used to modify intermolecular interactions (e.g. hydrogen bonding, π-π stacking) such that properties such as density, solubility, and impact sensitivity of these materials can be tailored. In particular, experimentally measured impact sensitivities can be correlated with structural features in these materials. At the same time, the presentation will demonstrate how computational studies are able to shed light on how these structural features affect how the energy of shock and impact is distributed within intermolecular and intramolecular bonds.