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The challenge of predicting physical properties of energetic molecular crystals by first principles calculations[1] LOREDANA VALENZANO, WILLIAM SLOUGH, WARREN PERGER, Michigan Tech Univ — The challenge to accurately predict the physical properties of energetic materials is accepted by presenting an ab-initio study on the mechanical and vibrational features of PETN and TATB. While first principles approaches describe properties of materials occurring at 0K, experimental results are mainly provided at 300K. This difference leads to discrepancies in the desired agreement of calculated and measured properties. Also, the congenital limitation of DFT in dealing with long-range dispersion interactions, makes the challenge even more intriguing. Our results are obtained through a full 3D approach that takes into account the van der Waals interaction between the molecules assembled in the solid using the B3LYP-D* functional. Results are compared with experiments showing exceptional agreement and validating the importance of including volume expansion effects in the description of molecular crystals at temperatures above 0K. To the authors' knowledge, the results presented for the elastic constants of TATB are the first ab-initio data for this energetic material. Also, the possibility of using MOFs as a precursor to the detection of explosives is reported.

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