Computational Study of Mechanical Properties of Halogenated Azobenzene Crystals

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Traditionally, molecular crystals are considered brittle and inflexible. However, numerous examples have demonstrated elastic or plastic mechanical responses, challenging this assumption. This discovery has led to growing research on flexible molecular crystals positioning them as a promising class of functional materials due to their elasticity or plasticity. Mechanical flexibility opens up many potential applications of flexible molecular crystals in numerous fields, such as pharmaceuticals, mechanical actuators and optoelectronics [1,2]. Studies have shown that azobenzene derivatives exhibit different mechanical properties, such as bending magnitude, due to a trans-cis photoisomerization [3]. This study investigates some of these derivatives, focusing on how subtle modifications in chemical structure and intermolecular interactions influence their mechanical behavior. Some of the researched structures exhibit polymorphism, which is the ability of a compound to crystallize into more than one crystal structure. Mechanical properties of known polymorphs of halogenated azobenzenes were examined in this study. The influence of chemical structure on mechanical properties was explored by varying para-substituted halogens (chlorine and bromine). Periodic DFT methods implemented in the CRYSTAL23 program were used to optimize molecular geometries and to compute properties such as interaction energies and virtual tensile tests. The synthesis of chlorine and bromine derivatives has been successful, of which chlorine's crystal structure has demonstrated elastic behavior in preliminary tests. The findings show that both molecular structure and crystal rearrangements impact interaction energies and tensile tests, which can be directly correlated to the material's mechanical properties. These results highlight the potential of computational modeling in predicting and tailoring the mechanical behavior of organic crystalline materials.

References:

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