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Mechanical Stability of Beryllium chalcogenides: BeX (X= S, Se, and Te)

Beryllium chalcogenides (BeX) are semiconductor materials which belong to the family of II-IV semi-conductors. They manifest in four-fold coordinated zinc-blende structure at 0GPa and 0K DFT conditions which is unique in the chalcogen family. These compounds have many useful technological applications yet some properties are yet to be explored due to their toxicity and thus the ab initio methods are recommended. All calculations in this work were done based on Density Functional Theory (DFT) framework and a plane wave basis set as implemented in the quantum ESPRESSO computer code. The projector Augmented Wave pseudopotentials were used to describe core valence electron interactions with the GGAs and LDA chosen as the exchange correlations. A comparison with previous DFT work and experimental work was also done. The calculated values of the lattice parameters agreed with the experimental ones and only varied by 0.1\%. The bulk modulus obtained from pz was found to high due to its known effect of overbinding the lattice parameter. The other mechanical moduli agreed with the existing experimental and theoretical data and there was clear indication that all beryllium chalcogenides are brittle except BeTe that was ductile. The rich mechanical properties of these chalcogenides informs the suitability of these compounds for optical use.

Keywords

chalcogenides; elastic properties; Density Functional Theory

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