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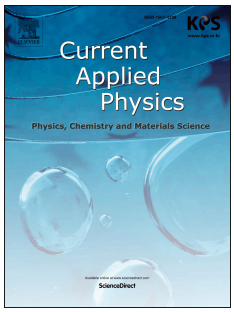

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DFT study on phase transition behavior and mechanical properties of HgSe polymorphs under high pressure

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Abstract: Total energy calculations based on density functional theory are performed for HgSe in the ambient and pressure induced phases. The electronic exchange and correlation effects are described by employing the generalized gradient approximation together with the projector augmented wave potentials. The equation of state parameters and the phase transition paths are obtained from the energy-volume landscape and enthalpy versus pressure data, correspondingly. The observed phase transition sequence of HgSe as ZB → Cinnabar → RS → $Cmcm$ and the final transition from $Cmcm$ to CsCl structure predicted by the other theoretical study are confirmed by our calculations. The pressure dependence of elastic constants of the structures considered in this study is reported. Bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and Debye temperature as isotropic mechanical properties are evaluated for HgSe polymorphs. Our calculations of energy band structure reveal the inverted band structure evoking that HgSe in ZB phase is a semimetal.

***Keywords*:** Pressure induced phases; Density functional theory; Elastic constants; Isotropic mechanical properties; Energy band gap.

1. Introduction

The mercury chalcogenides exhibit a variety of properties which differentiate them from the other members of the group of II-VI semiconducting compounds finding the application in the manufacture of various light emitting devices and sensors. They behave as neither real metals, nor semiconductors nor insulators. They possess the unusual properties of the material group called as semimetals and/or zero-gap semiconductors. Some well-known examples of the mercury chalcogenides are α-Sn and Hg based systems of β-HgS, HgSe and HgTe which

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