Structural properties and new phase transitions of silver iodide using the FP-LMTO method

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Descripción

We report first principles calculations of structural and electronic, properties of AgI compound in zinc blende (B3), CsCl (B2), rocksalt (B3), wirtzait (B4), NiAs (B8_1), PbO (B10), HCP (A3) and βSn (A5) structures employing the density functional theory (DFT) within the local density approximation (LDA) and the generalized gradient approximation (GGA). We employ the full potential linear muffin-tin orbitals (FP-LMTO) as implemented in the Lmtart code. Results are given for lattice parameters, bulk modulus and its first derivatives in the differents structures. The most important result in this work, the prediction of the possibility of two phase transitions; the firste; from cubic rocksalt (NaCl)→ hexagonal HCP (A3)(55.58 GPa) and the second; from rocksalt (NaCl)→ CsCl (B2)(68.78 GPa) for AgBr.

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Artículos relacionados

Abstract

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complicated than the alkali halides. As Kunz [8]. Many investigations different of physical properties of the binary compounds under hydrostatic pressure have been an active topic of research in condensed matter over the past few years. At high pressures semiconductors study is an exceptionally good tool in understanding their optoelectronic properties but these studies have been scarcely used in the investigation of AgI, as compared to other I-VII semiconductors. At the end of last decade Hull and Keen [15] performed X-ray diffraction (XRD) studies of AgBr, AgCl and AgI correspond to the rocksalt structure and they exhibit transitions to cesium chloride and/or other phases upon the influence of external pressure. Theorical, calculations has been realized [24] in three main structures (B2, B1 and B3) for AgCl, four structures (B1, B2, B3 and B8_1) for AgBr, and five geometries (B1, B2, B3, B8_1 and B4)