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High pressure-induced phase transitions in AgI semiconducting compound up to 1 Mbar

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Abstract

In this work, we have resorted to a recent version of the full potential linear muffin-tin orbitals (FP-LMTO) method based on the density functional theory (DFT), within both the local density approximation (LDA) and the generalized gradient approximation (GGA) for the calculation of the equilibrium structural parameters, and phase transition under high pressure of AgI semiconducting compound. Results are given for lattice parameters, bulk modulus and its first pressure derivative in different structures. In general, the use of the GGA approach in this work appears more appropriate than the LDA, and it is most correctly predicts the majority of the ground state properties for AgI material. The energy differences of NiAs ($B8_1$)/NaCl (B1) phases are around 1.76 and 1.15 meV, using the LDA and the GGA, respectively. Importantly, the phase transitions for this material from sixfolds coordinated NaCl-type structure (B1) to the eightfold coordinated CsCl-type structure (B2), and then to the hexagonal close packed HCP-type structure (A3) are possible under high pressure. Our calculations show that AgI semiconducting compound transforms firstly from B1 to B2 at pressure of around 55.58 GPa, and then from B2 to A3 at pressure of around 95.03 GPa, respectively.

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Keywords

AgI
Structural properties
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