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DFT calculation of the electronic structure and optical properties of two strontium germanium nitrides: α-Sr_2GeN_2 and β-Sr_2GeN_2

Abstract

The existence of α-Sr_2GeN_2 and β-Sr_2GeN_2 were reported recently with their structural properties. In this paper, electronic and optical properties have been investigated using density functional theory. The Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBE) is used for the exchange and correlation potential to calculate the optimized parameters of the structures. Our results confirm the previous observation of the atomic positions and lattice parameters for both crystals. The values of the unit cell volume of α- and β-Sr_2GeN_2 are in good agreement with the experimental values. The local density approximation (LDA), (GGA), the Engel-Vosko GGA approximation (EV-GGA) and the modified Becke-Johnson method (mBJ) were used to calculate the electronic and optical properties. Our results show that α-Sr_2GeN_2 has a small band gap of about 0.0 eV (LDA), 0.050 eV (GGA), 0.210 eV (EVGGA) and 0.268 eV (mBJ) while β-Sr_2GeN_2 has energy band gap of about 0.10 eV (EVGGA) and 0.15 eV (mBJ). Additionally, optical dielectric constants were calculated for both ternary compounds. We believe that the current study can provide more information to understand the properties of these ternary nitrides.

Keywords

α-Sr_2GeN_2; β-Sr_2GeN_2; Ab initio calculations; Inorganic materials; Optical constants; Ternary nitride