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First-principles study of the electronic structure, charge density, Fermi surface and optical properties of zintl phases compounds Sr2ZnA 2 (A=P, As and Sb)

Abstract

We present first-principles calculations of the electronic structure, Fermi surface, electronic charge density and optical properties of Sr $_2$ZnA$_2$ (A=P, As and Sb) based on density-functional theory using the local density approximation (LDA), generalized-gradient approximation (GGA) and the Engel-Vosko GGA formalism (EV-GGA). Additionally, modified Becke-Johnson (mBJ) is also used to improve the band splitting results. The calculated band structure and density of states show that Sr_2ZnA_2 compounds are metallic. The total DOS at Fermi level N(E F) is 72.92, 73.06 and 33.47 states/eV and the bare electronic specific heat coefficient (y) is 12.64, 5.805 and 12.67 mJ/mol-K2 for Sr_2ZnP_2, Sr_2ZnAs_2 and Sr $_2$ZnSb$_2$, respectively. The Fermi surface of Sr $_2$ZnA2 compounds is composed of two bands crossing along the r - A direction of Brillouin zone. There exists a strong hybridization between Zn-p/s and Sb-d, Sb-p and Sr-d and also between Sr-s and Sr-p states. The bonding features are analyzed by using the electronic charge density contour in the (101) crystallographic plane. We found that Sr forms an ionic bond with Zn, whereas Zn forms a strong covalent interaction with P/As/Sb atoms. For further insight information about the electronic structure, the optical properties are derived and analyzed.

Keywords — EVGGA, GGA, LDA, MBJ, DFT, zintl phases compound