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# Electronic band structure and specific features of $Sm_2NiMnO_6$ compound: DFT calculation


## Abstract

The band structure, density of states, electronic charge density, Fermi surface and optical properties of $Sm_2NiMnO_6$ compound have been investigated with the support of density functional theory (DFT). The atomic positions of $Sm_2NiMnO_6$ compound were optimized by minimizing the forces acting on the atoms, using the full potential linear augmented plane wave method. We employed the local density approximation (LDA), generalized gradient approximation (GGA) and Engel-Vosko GGA (EVGGA) to treat the exchange correlation potential by solving Kohn-Sham equations. The calculation shows that the compound is metallic with strong hybridization near the Fermi energy level (EF). The calculated density of states at the EF is about 21.60, 2452 and 2621 states'eV, and the bare linear low-temperature electronic specific heat coefficient (y) is found to be 3.74, 4.25 and 4.54 mJ/mol $K^2$ for EVGGA, GGA and LDA, respectively. The Fermi surface is composed of two sheets. The bonding features of the compounds are analyzed using the electronic charge density in the (011) crystallographic plane. The dispersion of the optical constants was calculated and discussed.


**Keywords —** Electronic charge density, electronic structure, fermi surface and optical, properties, DFT