Journal of Magnetism and Magnetic Materials, vol.358–359, 2014, pages 16–22

# Density of states, optical and thermoelectric properties of perovskite vanadium fluorides $Na_3VF_6$

**Abstract**

The electronic structure, charge density and Fermi surface of $Na_3VF_6$ compound have been examined with the support of density functional theory (DFT). 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 to solve Kohn–Sham equations. The calculation show that $Na_3VF_6$ compound has metallic nature and the Fermi energy ($E_F$) is assessed by overlapping of V-d state. The calculated density of states at the $E_F$ are about 18.655, 51.932 and 13.235 states/eV, and the bare linear low-temperature electronic specific heat coefficient ($\gamma$) is found to be 3.236 mJ/mol-$K^2$, 9.008 mJ/mol-$K^2$ and 2.295 mJ/mol-$K^2$ for LDA, GGA and EVGGA, respectively. The Fermi surface is composed of two sheets. The chemical bonding of $Na_3VF_6$ compound is analyzed through the electronic charge density in the (1 1 0) crystallographic plane. The optical constants and thermal properties were also calculated and discussed.

Keywords; Electronic structure, Electronic charge density, Fermi surface, Optical properties, Thermal properties