Computational Condensed Matter 23 (2020) e00467

Contents lists available at ScienceDirect

Computational Condensed Matter

journal homepage: http://ees.elsevier.com/cocom/default.asp

Density functional study of magnetic, structural and electronic properties of quasi-one-dimensional compounds $CrSbX_3$ (X = S, Se)

Thomas Mathew [a, b], Suseel Rahul K [a, c], Vincent Mathew [a, *]

[a] Department of Physics, Central University of Kerala, India
[b] Department of Physics, St Stephen's College, Uzhavoor, Kerala, India
[c] Department of Physics, Sree Vyasa NSS College, Wadakkanchery, Kerala, India

ARTICLE INFO

Article history:
Received 9 January 2020
Received in revised form
3 March 2020
Accepted 4 March 2020

Keywords:
Density functional theory (DFT)
one-dimensional magnetism
Transition metal chalcogenides
Quasi-one-dimensional structure
Electronic structure
Magnetocrystalline anisotropy

ABSTRACT

Antimony chromium trichalcogenides $CrSbX_3$(X = Se, S) have interesting electronic and magnetic properties due to their quasi-one-dimensional structure. We investigated magnetic, structural and electronic properties of $CrSbSe_3$ and $CrSbS_3$ using density functional theory as implemented in VASP. Ground state magnetic ordering of the materials were determined using PBE functional including spin-orbit interaction and we find that $CrSbSe_3$ is ferromagnetic and $CrSbS_3$ is anti-ferromagnetic. We used exchange-correlation functionals SCAN and PBE to study structural properties. We also calculated the Magneto-crystalline Anisotropy of $CrSbSe_3$ along three different directions. We found that the axis which is parallel to the chains is the hard axis (b-axis) and the axis which is perpendicular to the chains (a-axis) is the easy axis. Electronic structure calculations confirms that $CrSbSe_3$ and $CrSbS_3$ are indirect band gap semiconductors.

1. Introduction

The compounds $MCrX_3$, a subgroup of the MTX_3 group of ternary chalcogenides (M a non-transition metal, T a transition metal, and X = S, Se), occur in different structural types. The structure and symmetry of $MCrX_3$ depend on the M cation and most structures are formed by the stacking of CrX_6 polyhedrons in different ways, leading to the formation of either one dimensional, two dimensional or three dimensional infinite networks of CrX_6. These materials are reported to have interesting electric and magnetic properties related to one dimensional, two dimensional or three dimensional magnetism [1]. A structure consisting of array of filaments, where the electron dynamics within a chain are characterized by energy scales much larger than the coupling between the chains can be considered as quasi-one-dimensional in nature [2]. The compounds $CrSbX_3$(X = S, Se) are quasi-one-dimensional magnetic semiconductors belonging to the class of ternary chalcogenides mentioned above. Single crystals of $CrSbSe_3$ was first prepared by DA Odink et al. [3] by the reaction of the elements Cr, Sb and Se in 1:1:3 M ratio. It yielded needles of $CrSbSe_3$ which were found to be air stable. $CrSbS_3$ was first synthesised by K Belov et al. [4] from the elements by solid-phase reaction. Powdered samples of $CrSbSe_3$ and $CrSbS_3$ were prepared from the elements by a two-step sintering procedure by V Volkov et al. [1]. T. Kong et al. [5] obtained millimeter long single crystals of $CrSbSe_3$ which were blade-like and malleable. It was observed that $CrSbX_3$(X = S, Se) compounds consisted predominantly of prismatic needles that were often curved and split, which suggested a strong anisotropy of the structural and physical properties [1].

Previous studies have showed that the material $CrSbSe_3$ becomes ferromagnetic below 70 K [1,3]. Recently it was verified that the ferromagnetic transition occurs at T_c = 71 K and at high temperatures $CrSbSe_3$ is paramagnetic and isotropic with a Curie-Weiss temperature of 145 K and an effective magnetic moment of 4.1 μ_B /Cr [5]. It was recently demonstrated that the thermoelectric performance of $CrSbSe_3$ can be greatly enhanced by doping with Pb [6].

There is very little information available in literature regarding the properties of $CrSbS_3$. There are contradicting claims about the magnetic properties of $CrSbS_3$. Jobic et al. prepared the compound and claimed that the compound exhibited antiferromagnetic behavior at low temperatures [7]. Based on temperature dependence of magnetic susceptibility Volkov et al. observed that $CrSbS_3$ might have a ferromagnetic transition at T_c = 104 K with an effective magnetic moment $\mu_{eff} = 3.51\mu_B$/Cr [1].

The focus of this work is to predict magnetic, structural and

* Corresponding author.
E-mail address: vincent@cukerala.ac.in (V. Mathew).

https://doi.org/10.1016/j.cocom.2020.e00467
2352-2143/