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Research articles

Electronic structure, magnetism and thermoelectricity in layered perovskites: Sr_2SnMnO_6 and Sr_2SnFeO_6

Shakeel Ahmad Khandy, Dinesh C. Gupta *

Condensed Matter Theory Group, School of Studies in Physics, Jiwaji University, Gwalior 474 011 (MP), India

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ABSTRACT

Layered structures especially perovskites have titanic potential for novel device applications and thanks to the multifunctional properties displayed in these materials. We forecast and justify the robust spin-polarized ferromagnetism in half-metallic Sr_2SnFeO_6 and semiconducting Sr_2SnMnO_6 perovskite oxides. Different approximation methods have been argued to put forward their physical properties. The intriguingly intricate electronic band structures favor the application of these materials in spintronics. The transport parameters like Seebeck coefficient, electrical and thermal conductivity, have been put together to establish their thermoelectric response. Finally, the layered oxides are found to switch their application as thermoelectric materials and hence, these concepts design the principles of the technologically desired thermoelectric and spin based devices.

1. Introduction

Recurrent use of available energy resources (coal and petroleum) has generated energy crisis throughout the world. While utilizing a particular energy source, the corresponding device utilizes a small amount of it in doing the work while the maximum part is wasted as heat. Material scientists are therefore in a quest to somehow manage the excessive usage as well as to increase the efficiency of these devices. Thermoelectric devices with a working principle of Seebeck effect convert the waste heat into useful electrical energy and thereby reduce the wastage of energy, hence proving to be reasonably economical as well as a source of green energy. Thus, the solid state thermoelectric materials are being investigated to replace the commercial devices. The absence of moving parts in solid state devices strengthens their reliability. Although, the low efficiency of these devices limits their usage still, they have found many applications in refrigerators, temperature sensors, power generators for space stations or satellites, etc [1–4].

The compelling advances in layered structures including double perovskites, or simply perovskites which cloud in them a titanic sum of functional properties such as half-metallicity, ferromagnetism and high thermopower have fueled their exploration [5–7]. The applicability of organic-inorganic hybrid perovskites in solar thermoelectric generators by conversion of incident sunlight into electricity has further envisaged the importance of this family [8,9]. The toxicity, costly, environmentally hazardous and instability at high temperatures constraint the use of other thermoelectric materials (e.g., Heusler alloys [10,11], lead chalcogenides [12], skutterudites [13], Clathrates [14], etc.) and to subdue these concerns, metal oxides particularly perovskites stretch a new expectation for the researchers [15,16]. Cubic Ba_2MnMoO_6 was synthesized and reported to have long-range antiferromagnetic ordering below Neel temperature, $T_N = 10.8$ K [17]. Wide band gap semiconductors, $LiAA'O_6$ (A = Nb, Ta and A′ = W, Mo) were observed to have application in optoelectronics when investigated by modified Becke-Johnson potential [18]. Spin-glass behavior below 80 K and 2:1 trigonal cation ordering was observed in $Sr_3Fe_2TeO_9$ [19]. Sahnoun et al. studied the structural, electronic and thermodynamic properties of indirect band gap materials Ba_2MWO_6 (M = Mg, Ni, Zn) and the variation of band gaps by different methods [20]. Ferromagnetic perovskites Sr_2SnMnO_6 and Sr_2SnFeO_6 are reported to be semiconductor and semimetal, respectively in Fm-3m space group [21]. However, to the best of our knowledge no detailed studies are reported in the literature regarding electronic, elastic and transport properties of these double perovskites. In this paper, the variation of energy gap and therefore, the electronic structure with respect to different approximations have been envisaged in detail. Also, the contribution towards thermoelectricity by various energy states around Fermi level in the band structures, the relative position of the upper

* Corresponding author.
E-mail addresses: shakeelkhandy11@gmail.com (S.A. Khandy), sosfizix@gmail.com (D.C. Gupta).

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