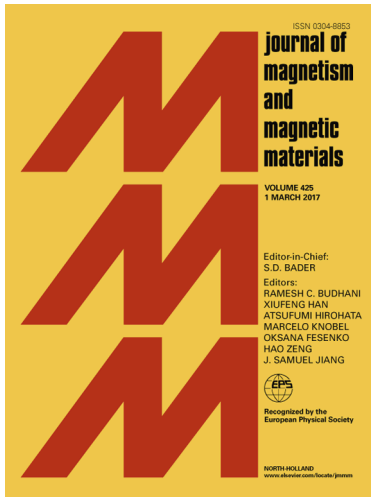

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Electronic Structure, Magnetism and Thermoelectricity in Layered Perovskites: Sr_2SnMnO_6 and Sr_2SnFeO_6

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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.

Keywords: Thermoelectric; electronic structure: electrical conductivity: ferromagnetism; half-metallicity

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