Journal of Magnetism and Magnetic Materials 458 (2018) 176–182

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Research articles

Electronic structure, magnetism and thermoelectric properties of double perovskite Sr_2HoNbO_6

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ARTICLE INFO

Article history:
Received 31 October 2017
Received in revised form 29 January 2018
Accepted 10 March 2018
Available online 12 March 2018

Keywords:
Double perovskites
Seebeck coefficient
Band structure
Electrical conductivity
Figure of merit

ABSTRACT

First principles calculations on structural, electronic, magnetic and thermoelectric properties of newly synthesized perovskite Sr_2HoNbO_6 are carried out at the behest of much reliable density functional theory (DFT). The equilibrium lattice parameters at the cost of structural optimizations are observed to agree with the available experimental data. Three different methods for exchange correlations are utilized to investigate the electronic structure of this oxide. Spin polarized band structure calculations predict the semiconducting nature of this compound along with a large energy gap of 3.6 eV. Ferromagnetic interactions among the constituent atomic spin moments determine the total magnetic moment $\mu = 4.0$ μB for this material with a maximum contribution from $\mu_{Ho} = 3.95$ μB. In addition, the temperature dependent thermoelectric properties based on the electronic results of Sr_2HoNbO_6 in temperature range from 50 to 1000 K are investigated. The total negative Seebeck coefficient signifies the p-type conduction or holes as charge carriers along the selected temperature range. The outcome of this study specifies the maximum value of dimensionless figure of merit $zT \approx 0.97$ at room temperature.

1. Introduction

The heavy resource loaded regions have limited the global fuel supply due to overexploitation, inefficient and low standard technology in addition to political instability directly consequences the cost, as well as the extinction of these resources. Present-day energy situation provisions the transformation of energy bases from fossil fuels to renewable sources e.g. thermoelectrics (TE), biomass, solar cells, photovoltaics, piezoelectrics, etc. [1–4]. Presently, the TE materials have become an interesting theme for material scientists because they promote the environment friendly and efficient tactics to conserve the energy available in the form of waste heat. Undoubtly, these materials can be visualised as *green energy* reservoirs and control measures to overcome the worldwide energy crisis. The process by which a material is capable to refurbish the waste heat (via incompetency in servicing the released energy and partial combustion of fuels) into electric power is known as the thermoelectric phenomenon. It is generally specified by a dimensionless constant $zT = (S^2\sigma T/\kappa)$ called figure of merit, where S is Seebeck coefficient, σ electrical conductivity, κ thermal conductivity and T temperature. Here, κ is a combination of electrical (κ_ε) and phonon (κ_λ) contributions of thermal conductivity of a lattice. Among the four quantities involved in zT relation, one is mainly interrelated to the lattice (κ_λ) and three of them (S, σ and κ_ε) are mainly linked to the electronic structure of the material. To reduce lattice thermal conductivity, there are three possible strategies. The first is to create rattling structures or point defects or by alloying so that the phonons scatter within the unit cell. The second approach is to separate the electron-crystal from the phonon-glass by using complex crystal structures without disrupting the crystallinity of the electron-transport region. A third tactic is to use the multiphase nano-composites to scatter phonons at interfaces [5]. Maximum value of zT means the enhanced efficiency of a TE material [6]. To optimize the various thermoelectric parameters for enhanced thermoelectric response, fruitful tailoring strategies have been developed from the exhaustive knowledge of electron and phonon transport. Engineering of band structure leads to the increased power factor $S^2\sigma$, and hosting the additional phonon scattering without the alteration of power factor makes the k_λ to reduce [7–8]. At the same time, the material exhibits maximum Seebeck coefficient with minimum resistivity and thermal conductivity. However, in conventional semiconductors, these quantities are itself the functions of carrier concentration and their independent control is little possible; therefore, such materials are rarely found.

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https://doi.org/10.1016/j.jmmm.2018.03.017
0304-8853/