

FULL PAPER

Investigation of structural, magneto-electronic, and thermoelectric response of ductile SnAlO₃ from high-throughput DFT calculations

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Successfully optimized calculations for the stability of SnAlO₃ perovskite in its paramagnetic phase and various structural parameters have been figured out in this study. Structural stability and ductile character is reflected from the calculated elastic constants and mechanical properties. Moreover, the melting temperature of the present material has also been calculated. We have discussed in detail, the ground state electronic band structure and paramagnetic character. In addition, the Boltzmann's transport theory has been employed to obtain the Seebeck, electrical and thermal conductivity coefficients so as to manifest the thermoelectric response of the material. Remarkably, the observed high electrical conductivity in inclusion of metallicity and paramagnetic nature is a characteristic of perovskite type electrode materials. The above discussed material properties suggest the possible application of this compound as an efficient electrode material.

KEYWORDS

electrode materials, electronic structure, mechanical properties, perovskite, Seebeck coefficient

1 | INTRODUCTION

The search for novel materials and the tunability of the properties of multifunctional materials have achieved much more interest from the researchers worldwide particularly the perovskite oxides. These oxides certainly allow the tailoring of their electronic structure; transport and charge distributions, spin coupling phenomena, and the energetic parameters (e.g., lattice constants, phonon spectra, thermodynamics of phase transitions, etc.). Such enhanced features are easily achieved by various reliable theoretical methods.^[1,2] The improved structural, magnetic, and other related properties has become a very important theme meant for modern scientific and technological applications. Nevertheless, theory has helped to resolve various experimental doubts and to predict new experiments/phenomena in a number of well-documented circumstances.^[3,4]

Perovskite compounds like PrMO₃ (M = Al, Ga, and In) have been recently investigated for their electronic optical and thermoelectric properties.^[5] SnTaO₃, a simple metal with cubic *Pm-3m* structure is predicted to be a potential electrode material.^[6] Metallic paramagnets like SrMoO₃ and BaMoO₃ which are being used as electrode materials have simple cubic structure.^[6,7] More recently, cubic PbTaO₃ with simi-

lar properties was also reported to be useful for electrode material synthesis.^[8] The high value of electrical resistivity ($2 \times 10^{-4} \Omega\text{cm}$) and metallic nature of SrRuO₃ has been studied for its electrode properties.^[9] Also, the LaInO₃ oxide a useful candidate for solid oxygen fuel cells (SOFCs)^[10,11] and oxygen sensors,^[12] has achieved much more interest from the researchers worldwide. From the above discussed stimulating advances in physical or chemical properties of perovskite oxides, forecasting new materials with tunable multifunctional properties has proven to be a hot subject among the material scientists and researchers globally.

Apart from this, predicting the most stable structure for a particular solid state inorganic compound or any other chemical composition is an unending challenge for chemists and material scientists. The ability to successfully predict the structure of a previously unknown composition has considerably progressed with the advent of modern simulation methods.^[13-15] More interestingly, the candidness of tolerance factor to predict the stability of a perovskite structure has been widely recognized.^[16-18] The recent interest in perovskites for their application in electrode materials has steered our intention to use the tolerance factor as a way to explain and predict structure of the present material. Since, no structural prediction or any kind of theoretical