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Investigation of the transport, structural and mechanical properties of half-metallic $REMnO_3$ (RE = Ce and Pr) ferromagnets

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Systematic investigation of the ground state structure, which includes elastic and transport properties, of perovskite oxides $REMnO_3$ (RE = Ce and Pr) has been carried out by first principles calculations. We present the analytical as well as DFT calculated equilibrium lattice constants which show good agreement with experimental data. Three independent elastic constants are emphasised to yield the corresponding mechanical properties, including the elastic moduli (*B*, *G* and *Y*), Poisson's ratio (ν), anisotropy factor (*A*) and Pugh ratio *B*/*G*, for these compounds. These calculations predict the brittle $PrMnO_3$ as a less hard material than the ductile $CeMnO_3$ oxide. Post DFT treatment involving Boltzmann's theory is conveniently employed to investigate the thermoelectric properties of these compounds. The analysis of the thermal transport properties specifies the dimensionless figure of merit of 0.24 and 0.19 at room temperature for $PrMnO_3$ and $CeMnO_3$, respectively. Their half-metallic nature with efficient thermoelectric parameters, including electrical conductivity, Seebeck coefficient and thermal conductivity, suggest the likelihood of these materials to have a potential application in the design of shape memory devices and imminent thermoelectric materials.

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Introduction

Ferromagnets, which have efficient thermoelectric (TE) performance and half-metallicity, have proven to be a thrust area for researchers and industrial technologists to feed the demands of smart and spintronic materials, and highly competent thermoelectric materials for future devices. Thermoelectric materials, because of their multiple applications, from the reuse of waste heat to Peltier cooling in order to conserve or to reduce fuel consumption in automobiles, are in high demand. The characterization of a material as an efficient thermoelectric is represented by a dimensionless constant, $zT = S^2\sigma T/\kappa$, called the thermoelectric figure of merit. Where, S is the Seebeck coefficient, σ is electrical conductivity, T is temperature, and κ is the thermal conductivity, which is comprised of the electron, ε, and lattice, λ contributions of the material. Larger values of zT indicate a more pronounced thermoelectric performance in a material and hence higher efficiency in converting waste heat into useful electricity.[1,2] The enhancement of zT can be achieved by the combination of different strategic parameters. The prime idea to achieve this involves the minimization of the lattice contribution towards thermal conductivity.[3] The second way of improvement is to maximize the product $S^2\sigma$, which is defined as the power factor, by varying the carrier concentration with different doping levels.[4,5] Lastly, the band engineering of materials with strongly correlated electrons in order to induce peaks in the DOS is an alternative approach.

From the above perception, perovskite oxides are very attractive materials which display diverse structural phase-transition sequences, metal–insulator transitions, ferroelectricity, superconductivity, piezoelectricity, and half-metallic ferromagnetism (HMF) or thermoelectric properties, thus labeling them as ultimate candidates for multi-functional devices.[6,7] In transition metal ABO_3 perovskites, the flexibility of the structure exposes the possible ways to tailor the electronic, magnetic and orbital states, which in turn alter the bond lengths, angles and distances, and thus guide various parameters such as electronic band gap and transport properties. Owing to strong coulomb repulsion (correlations), the energy and occupancy of the t_{2g} (triplet) and e_g (doublet) states are strongly affected in transition metal perovskites. This has a strong influence on their physical properties, for example magnetic order and/or orbital order can emerge from the interplay of the correlation phenomenon with charge, spin and orbital degrees of freedom.[8–10]

Na_xCoO_2 cobaltates, which have large thermopower and the highest recorded zT value of up to 1.0 at 800 K for oxides, have promoted the study of the TE properties of oxide materials.[6,11] Recently, tuning of the DOS in double perovskites, including Sr_2NbIrO_6, $LaSrTiIrO_6$, Sr_2TaIrO_6 and Sr_2NbRhO_6, was revealed to yield efficient thermoelectric materials when optimally doped.[1] Also, the n-type doped $SrTiO_3$ oxide shows large power

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