Abstract

Materials with versatile physical properties are the requirement of modern physical society, mainly of those who present a strong coupling between spin, lattice, and charge. This by far intact competency promises a new paradigm-shift towards environmentally friendly renewable energy resources. Therefore, the investigation of several functions into one material is highly essential. This thesis focuses on the understanding of the physical properties of thermoelectric and optoelectronic materials to suggest new, highly efficient materials for thermoelectric and photovoltaic device applications.

Research in the direction of thermoelectric materials has already highlighted perovskite oxides with potential applications. However, the sensitivity of oxides with crystal chemistry and lattice distortions can modify and engineer new materials.

In this thesis, we present the first principle study of perovskite oxide properties within the framework of density functional theory by using the Full-Potential Linearized Augmented Plane-wave method (FPLAPW). Perovskite oxides ABO_3 (A: Pr, La…. Cs, Ba, Sr… B: 3-d elements) is investigated for the structural, electronic, magnetic, optical, and thermoelectric character. To deal with strongly correlated electron systems, the most recently developed Modified Beck-Johnson potential is used in our present work. Firstly, we used optimized structural parameters to investigate physical properties. Secondly, the investigation of electronic response is made by computing band structure and density of states. Optical characteristic is also computed for each perovskite and discussed for their role in the precise direction. This thesis emphasizes on the analysis of thermoelectric characteristics in the temperature range 100-800 K.

Following the idea, we focus our calculations on the bulk properties of potential materials. The aim of working on the bulk perovskite oxides is to open a pathway for the downscaling of oxides for the integration of thermoelectric nanoparticles.

We calculate the electronic structure, which confirms the half-metallic nature of PrV/CrO_3, mixed half-metallic, and metallic nature in $LaMn/FeO_3$ and semiconducting nature is revealed in Cs doped Nb/Ta oxides. The origin and nature of ferromagnetism with Cr/V/Mn/Fe doped oxides have been shown in terms of exchange energies involved and exchange constants. Strong *p-d* hybridization generates magnetic moments at the site of

oxygen atoms, in result reduced magnetic moments at B-sites. Bond length measurements reveal Jahn-Teller distortion lifted *d*-site degeneracy in transition metal oxides by splitting it into doublets e_g and triplets' t_{2g} states. The influence of rare-earth elements (Pr, La) is also studied in electronic character.

For thermoelectric nature, electrical and thermal conductivity, See-beck coefficient, power factor, and thermal efficiency are calculated and discussed in detail. Thermodynamic stability of materials is directly related to phonon dispersion curves, and positive frequency curves confirm the studied oxides are stable in prescribed phases. The network of nano-scale orbital studies provides a powerful tool to increase the thermal efficiency of studied compounds. Hence, the evaluation of materials based on of electronic and thermoelectric study reveals suitable materials for thermoelectric applications.

The potential of studied perovskite oxides for several optical applications is also investigated. The verification of Penn's model law between bandgap E_g with the real part of dielectric constant $\varepsilon_1(0)$ confirms the accuracy of our calculated results. $CsTb/NbO_3$ are the potential candidates with the best optical response for photovoltaic devices. Absorption coefficients are also taken into accounts. However, rare-earth-based oxides are not in the best condition for device applications because of low carrier mobility. Thus, the solution can be adopted by A-site and B-site cation doping. This consideration has proven a way for future development in the study of perovskite oxides as photovoltaic materials.

Future work of perovskites as thermoelectric materials should be accepted to compute this work of thermal efficiency presented in the current thesis work.