Abstract

The increasing energy demand has compelled numerous researchers to explore and foster the development of renewable energy sources as a substitute for conventional resources. Kinetic, hydropower, wind, and solar energy have emerged as significant renewable sources. Nonetheless, these systems produce heat as a result of energy conversion. Worldwide, almost 70% of energy derived from fossil fuels generates waste heat that elevates environmental temperatures. The efficient use of thermal energy is essential for a genuinely sustainable and renewable energy system.

Thermoelectric generators (TEG) may harness waste heat energy to turn it into electrical energy. They provide several attributes like minimal processing costs, optimal efficiency, stability, and sufficient lifespan. The mechanical architecture of the TEG features no moving components, resulting in reduced maintenance costs and enabling its application in remote locations.

This study focuses on exploring the synthesis, stability, and thermoelectric characteristics of various metal oxides featuring adaptive structures. The primary benefits of metal oxides include their remarkably low costs, minimal or absent toxicity, high availability, and enduring stability. In contrast, their growth as thermoelectric materials has been hindered by a low figure of merit ($ZT = S^2\sigma T/\kappa$), which is ascribed to the high thermal conductivity and limited mobility of charge carriers.

Nonetheless, the study of thermoelectric oxides remains a relatively nascent area, indicating significant potential for advancement. In this scenario, metal oxide featuring adaptive structures has the potential to address many of the limitations associated with conventional metal oxides. The interplay of intrinsic defects and expansive unit cells, coupled with the potential to independently adjust electronic transport properties from thermal characteristics, places them as highly promising options for thermoelectric applications at elevated temperatures.

In the First Experiment, divanadate oxides XV_2O_6 (X = Mg, Ca, and Ba) were investigated for waste heat recovery applications utilizing DFT and experimental methods to investigate their thermoelectric, electrical, photoluminescence, and

structural characteristics. The synthesis was carried out using the solid-state reaction technique, and the XRD results confirmed that the synthesized oxides had a monoclinic structure. EDS mapping verified that Mg, Ca, Ba, V, and O were present with the right compositions, and SEM images showed that well-shaped particles were formed. 3.20 eV, 2.14 eV, and 1.76 eV were determined to be the band gap values for MgV_2O_6, CaV_2O_6, and BaV_2O_6, respectively. Calculations were conducted for the total and partial density of states to investigate the impact of atomic orbitals on the formation of bands. The transport properties were investigated using the BoltzTraP algorithm in Wien2k. The optical properties of the synthesized oxides were studied with the help of photoluminescence (PL) analysis. We have found that all divanadate oxides XV_2O_6 (X = Mg, Ca, Ba) have productive values for the Seebeck coefficient (S), electrical conductivity (σ), power factor (PF), and figure of merit (ZT). The semi-metallic nature, low synthesis cost, and thermoelectric data of the oxides under investigation demonstrate their exceptional potential for waste heat recovery applications and their high efficiency in energy harvesting devices, particularly in thermoelectric generators.

The second experiment examined the thermoelectric, electronic, and structural properties of Nb-based metal oxides XNb_2O_6 (X = Mg, Ca, and Ba) for energy harvesting applications using experimental methods and DFT. The orthorhombic structure of the synthesized oxides was confirmed via XRD analysis. SEM revealed the creation of well-defined particles, whereas EDS confirmed the presence of Mg, Ca, Ba, Nb, and O in suitable compositions. The polycrystalline nature of the $BaNb_2O_6$ sample was confirmed by TEM. In the metal oxides $MgNb_2O_6$, $CaNb_2O_6$, and $BaNb_2O_6$, the band gaps were 2.19 eV, 2.13 eV, and 0.90 eV, respectively. The total and partial density of states were computed to investigate the impact of atomic orbitals on the formation of bands. BoltzTraP algorithm was implemented in the Wien2k code to investigate the novel transport characteristics. The fruitful values of the figure of merit (ZT) indicate that the materials under investigation are potentially suitable for thermoelectric applications.

The third experiment investigates the influence of Ti-doping on the thermoelectric properties of Ba_2ZrCoO_6 (BZC), a double perovskite compound synthesized for energy harvesting applications. The solid-state reaction approach was used to synthesize ceramic samples of $Ba_2Zr_{1-x}Ti_xCoO_6$ (TBZC), where x ranged from 0.05 to 0.15. The XRD analysis of these double perovskites has verified the presence of a cubic crystal structure, specifically with the space group $Pm\bar{3}m$. SEM shows the existence of uniform TBZC crystals. By using TEM and electron diffraction examinations, it is confirmed that polycrystalline $Ba_2Zr_{0.95}Ti_{0.05}CoO_6$ crystals are present in a cubic-ordered phase. Furthermore, energy-dispersive X-ray spectroscopy (EDX) mapping reveals the uniform distribution of all elements inside the synthesized materials, as well as the convergence of the elements Ba, Zr, Ti, Co, and O. Using UV–vis spectroscopy, the band gap values for $Ba_2Zr_{1-x}Ti_xCoO_6$ (x=0.0, 0.05, 0.10, and 0.15), were found to vary from 3.18 eV to 3.58 eV. The shift from a semiconductor to a metal state of these oxides was influenced by temperature, as evidenced by the change in electrical conductivity and power factor at approximately 700 K. The p-type behavior of the TBZC ceramic samples was indicated by a positive Seebeck coefficient. For the $Ba_2Zr_{0.95}Ti_{0.05}CoO_6$ sample, the power factor rose with temperature and reached a value of 93.8 $\mu W/mK^2$ at 750 K. The findings of this study suggest that the titanium-doped Ba_2ZrCoO_6 double perovskites have significant promise as thermoelectric materials for thermoelectric devices.