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Ab initio study of Structural, Electronic, Optical, Magnetic, and Thermoelectric properties of Ba 2 HoXO 6 (X = Rh, Os, Ru) for spintronics application

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Research Article

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Ab initio study of Structural, Electronic, Optical, Magnetic, and Thermoelectric properties of Ba_2HoXO_6 (X = Rh, Os, Ru) for spintronics application

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Abstract

In this article, we explore the Ba_2HoXO_6 (X=Rh, Ru, and Os) double perovskite for its physical properties i.e. structural, electronical, optical, magnetic, and thermoelectric properties of theoretically investigated cubic compounds under PBE-GGA approximation by quantum-based density functional theory (DFT) within WIEN2K software. The structural, electronical, optical, magnetic, and thermoelectric properties of studied materials have been investigated for the energy renewable devices. Electronic properties of studied materials are explained by describing the band gap and density of states under study PBE-GGA approximation and the results abundantly evident that the studied material have indirect band gap and half metallic semiconductor. For optical behavior of studied materials, we analyzed complex dielectric functions, optical conductivity $\sigma(\omega)$, Absorbance $\alpha(\omega)$, Reflectivity $R(\omega)$, and Loss parameter $L(\omega)$. Also, we analyze the thermal behavior of studied materials by calculating charge carrier concentration (n), electrical conductivity σ/τ, Seebeck coefficient (S), thermal conductivity K/τ, specific heat capacity C_v, magnetic susceptibility χ, and power factor theoretically which predict the materials are eco-friendly and could be used in energy renewable devices. These properties are calculated by Boltz-Trap code under Wien2K code. All these properties are studied though first-Principle calculation and leads to new renewable devices.

Keywords First Principle, Spintronics, electronics, double perovskite, WIEN2K software

1 Introduction

Moore's Law's influence that there's a growing demand for IT which wanes and traditional electronics reach their limits and its solution that minimize power consumption while maximizing speed [1-5]. To address the challenges, emerging technologies such as quantum information, molecular electronics, spintronics, and nano-electronics are being explored and developed. These innovations aim to push the boundaries of conventional electronics and pave the way for more efficient and powerful IT solutions [6-8]. Exploiting the spin properties of electrons for use in

technological devices is the goal to create new types of devices and overcome the obstacles that traditional electronics face [9, 10].

Quantum spintronics is a subfield that explores the quantum properties of electron spins that has the potential to reveal the ultra-secure communication and quantum computing, taking advantage of its physical properties and superposition principle [11, 12]. One of the significant advantages of development of new materials which exhibit unique electronic and spin properties that brig a revolutionary change in the field of IT. For this purpose, the materials such as topological insulators, two-dimensional materials like graphene, and double perovskite materials have great potential. The use of spintronics increasing day by day which facilitate the transmission of spin information, which may further enhance data transfer speeds and reduce energy consumption in integrated circuits. The study of exploiting the spin properties of electrons for use in advance technological devices is possible now, because of the effective theoretical quantum-based approaches. By including additional flavors as ab-initio calculations has expended in scope [13-15].

The investigation of innovative materials with improved properties is the main focus of material scientists. Advancements in theoretical design and algorithmic quantum theory now leads the researchers to perform well-organized and accurate calculations for both experimental as well as quantum-based mechanical data. These materials are supposed to create devices which are more efficient in spintronic devices, including low-power transistors and memory storage elements. The use of spintronics with the integration of existing semiconductor technologies is beneficial but the researchers trying to explore about development of hybrid devices that combine the advantages of both spintronics and conventional electronics [16, 17].

To achieve materials with required properties, the double perovskite materials which have a lot of required features or qualities i.e. band gap property which attract the attention to use these materials for spintronics. Theoretically and experimentally perovskites are beneficial because of numerous economic and technical features and it's a lot of applications. Double perovskites have a wide range of characteristics, combinations and structure. Double perovskite is a subgroup of perovskite compounds that have changed their crystal structure [18]. The general formula for a double perovskite is $A_2BB'O_6$ since the A-site and B-site cations are swapped out for two distinct types of cations and X is referred to as oxygen or halogen. Hundreds of compounds have this type of structure. Double perovskite materials as semiconductors, magneto-optics materials, magneto dielectrics, multi ferroic materials thermoelectric materials and spintronics materials are very useful. They have also other interesting magnetic properties like spin singlet ground states, simple anti-ferromagnetism, ferromagnetism, and spin glasses. Numerous double perovskites have been studied for this purpose [19, 20].

In contrast to other materials of same family Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 have not been investigated using DFT. Therefore, we tried to analyze the physical characteristics of these materials in the current work. So, this work is about to investigate the physical properties (structural, electronic, optical, magnetic and thermoelectric) of Double perovskite Ba_2HoXO_6 (X=Rh, Ru, Os) cubic compounds by using PBE-GGA approximation under the Quantum based Density Functional Theory (DFT) within Wien2K code which has proven the most effective.

Basically, this research has four parts,

2 Computational Method

In simulation of many-body atomistic systems density functional theory (DFT) has played a key role for past few decades. To explore the properties and characteristics like electrical, mechanical, optical, transport, and magnetic features of the cubic structure crystals Ba_2HoXO_6 (X=Rh, Ru, Os) the Wien2k cod is employed which is based on DFT, is used in this article. The full-potential linearized augmented plane wave (FP-LAPW) approach is used by the Wien2k code, which uses quantum-based properties. For solving the Kohn-shame equation (FP-LAPW) is one of the most precise schemes [21-23]. For the structural analysis, we utilized the next version of general gradient approximation (GGA) along with PBE which combined called PBE-GGA approximation. The optimization of electronic structures is optimized by PBE approximation which minimize the inter atomic forces and stabilize the structure. Electronic calculations as well as optical characteristics are also be verified using PBE_{sol} and Trans and Blaha modified Becke Johnson potential (TB-mBJ). These approximations have best edge in combined and is suitable for simulation results which are nearly equal to experimental results. The electronic band gap property is suppressed by PBE because it analyses the ground state properties more correctly [24]. The TB-mBJ have been used in this work to increase the accuracy of band gap in replacement of PBE approximation. Mostly for magnetic studies, we choose the Hubbard approximation and modified Becke-Johnson (mBJ). Hubbard U and mBJ has been used for every interaction of diagonal matrix of density. we use the self-interaction correction method (SIC) in our calculations for introducing the U term into computation although there are various methods. By using the following values for the beginning parameters in the reciprocal lattice, the angular momentum $l = 0$, Gaussian parameter G_{max}, the combination of the wave vector as well as muffin-radius $K_{max} \times R_{MT} = 10$, and so on. The k-mesh has been chosen to be official size 12x12x12 by 1000, which is the k-point at which the system's energy output stabilizes [25, 26]. For the precision of calculated results this is the convergence criteria's upper limit. Charge convergence is assumed to be 0.01 mRy. To be calculate the transport properties using optimized electronic structures Classical Boltzmann transport theory in addition with Boltz trap code is being utilized using TB-mBJ [27, 28].

3 Results and Discussion

3.1 Structural Properties

To understand the materials characteristics, firstly we have to learn the internal structure an composition of materials the arrangements of the composition, in this purpose structures gives information of the materials. Here, crystal structures are used to find out the ground state of the materials. The studied materials Ba_2HoXO_6 (X=Rh, Ru, Os) have space group Fm3m-225 with cubic crystals as in fig 1, in (a) Ru and Os are at edge centered position shown in gray balls in these materials [29]. Where Ho at the corner of the cube and Ru at the center of the face of each

side and Ba at the body centered and O at the middle of the edge with the red ball. While Rh element at the corner of the crystal cube shown as purple balls in their cubic structure and Ho at the edge center of the crystal while O at the middle of edge with red color balls [30]. Ba also present at the body center position with blue balls shown in figure (c) They have same lattice parameter in cubic structure. Theoretically values of lattice parameter a=b=c and α=β=γ=90° which is calculated through simulation calculations. The lattice parameter for Ba_2HoRhO_6 =16Å, the lattice parameter for Ba_2HoOsO_6 which is equal to 17Å and for Ba_2HoRuO_6 =17Å. The compounds Ba_2HoOsO_6 and Ba_2HoRuO_6 has same lattice parameter while Ba_2HoRhO_6 has larger lattice parameter both of them due to it allied in different group of atoms in periodic table [31]. We can see that Ba_2HoOsO_6 =Ba_2HoRuO_6.

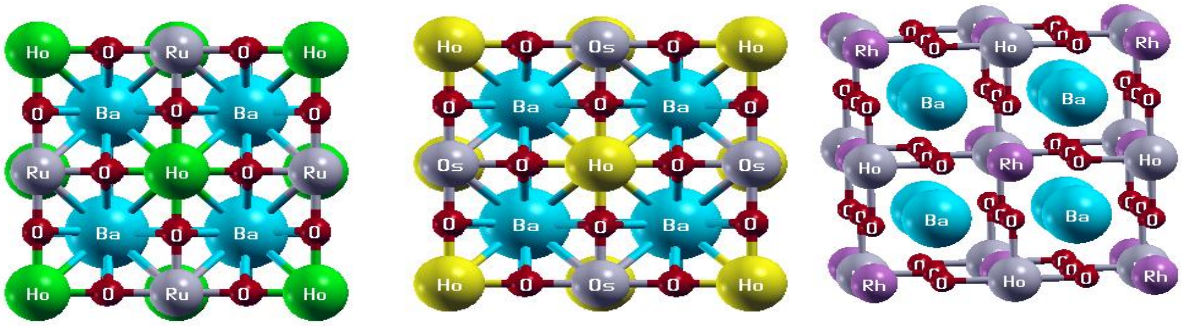


Figure 1 Cubic structures of Ba_2HoXO_6 (X=Rh, Ru, Os) oxide with space group Fm3m-225

3.2 Electronic Properties

Electronic properties of studied materials can be explained by describing the band structure and density of states.

3.2.1 Band Structures

The band structure of a material provides necessary information related to energy band gap whether it is direct or indirect. It also tells us either the material is semiconductor, insulator or metal. The band structure of studied material Ba_2HoRuO_6 can be described by using PBE- GGA approximation. The energy band gap structures of Ba_2HoRuO_6 are shown figure 2(a) with energy range -4eV to 4eV. At 0eV the Fermi level occurs. Below the 0eV valance band occur and above the 0eV conduction band occur. The electronics band gap structure for spin up shows that the material is semi-conductor material show at the right-side graph while the spin down channel shows the metallic character shows at left hand side graph. The band gap values of our studied compound shows that these compounds have cubic structure. It is half metallic semiconductor material. The spin up channel shows the semiconductor nature which is indirect band gap with 1.3eV so this spins up and spin down channels shows both unsymmetric. The band structure of studied material Ba_2HoOsO_6 can be described by using PBE-GGA approximation [32, 33]. The energy band gap structures of Ba_2HoOsO_6 are shown figure (b) with energy range -4eV to 4eV. At 0eV the Fermi level occurs. Below the 0eV valance band occur and above the 0eV conduction band occur. The electronics band gap structure for spin up shows that the material is semi-conductor material show at the right side of the graph while the spin down channel shows the metallic character shows at left hand side graph. The band gap values of our studied compound shows that these compounds have cubic structure. It is half metallic semiconductor material. The spin up channel shows the semiconductor nature which is indirect band gap with 2eV so this spins

up and spin down channels shows both unsymmetric. Similarly, Ba_2HoRhO_6 compound also shows half metallic properties as shown in figure (c) which is also indirect band gap semiconductor for spin up channel which is approximately equal to 1.1 eV [34].

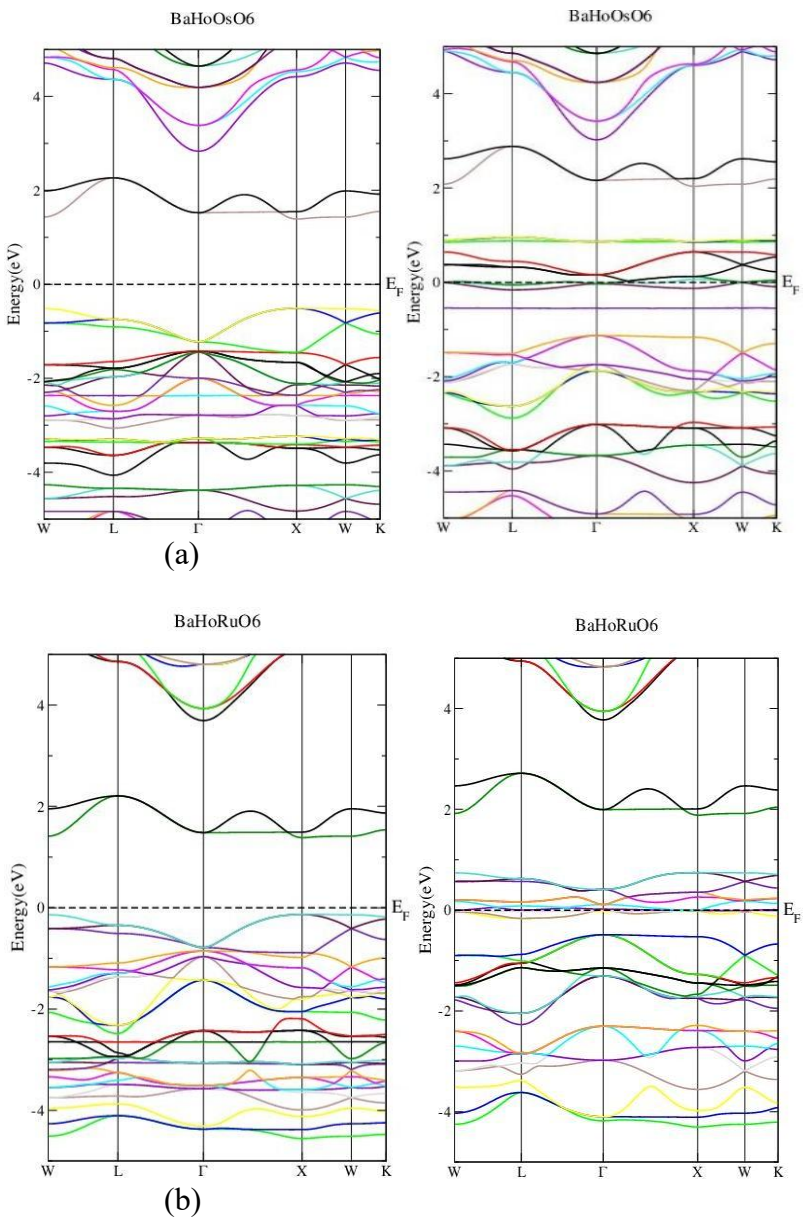
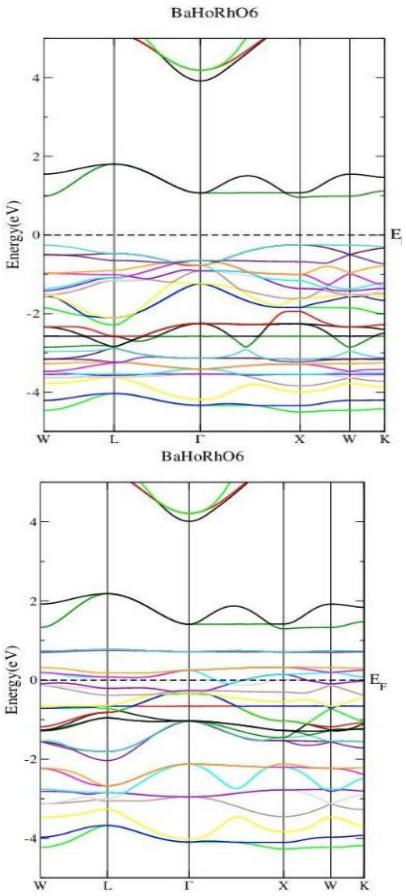


Figure 2 a) Both spin up and spin down channels show the un-symmetric, spin down show metallic and spin up shows the semiconductor nature of Ba_2HoRuO_6. **b)** Both spin up and spin down channels show the un-symmetric, spin down show metallic and spin up shows the semiconductor nature for Ba_2HoOsO_6. **c)** Spin up and spin down channels show the un-symmetric, spin down show metallic and spin-up channel shows the pure metallic nature of Ba_2HoRhO_6.



(c)

3.2.2 Density of States

3.3 Optical Properties

Optical properties cover about the materials that which material is effective for the manufacturing for which kind of applications. When light falls on the materials it performs some phenomena's that determines the types of materials and use of materials. The properties of the double perovskite Ba_2HoXO_6 (X=Ru, Rh, Os) materials depend on the light and explained with optical conductivity σ (ω), Absorbance α(ω), Reflectivity R(ω) and Loss parameter L(ω) [35-37]. The optical conductivity talks about the material's conductivity behavior when light falls on the material. At the value of 0 eV the conductivity is 0.5×10^3, 1×10^3 and 1.5×10^3 for Ba_2HoOsO_6, Ba_2HoRhO_6 and Ba_2HoRuO_6 respectively. But the value of optical conductivity does not increase continuously but there are ups and downs in the curve and at 6.1 eV these materials have maximum values 5.8×10^3, 5×10^3 and 4.8×10^3 for Ba_2HoOsO_6, Ba_2HoRhO_6, and Ba_2HoRuO_6 respectively and then decreases gradually with increase in energy as shown in fig 3(a). But in case of absorption coefficient α, the Ba_2HoOsO_6, Ba_2HoRhO_6, and Ba_2HoRuO_6 have an increasing trend with an increase in energy as shown in fig 3 (b). In case of reflectivity (R) its value is high at 0 eV and then suddenly drops and then become consistency in fluctuations in reflectivity with increase in energy of photons as shown in fig 3 (c) and after reaching 13.4 eV energy the reflectivity coefficient increases exponentially

for these materials Ba_2HoOsO_6, Ba_2HoRhO_6, and Ba_2HoRuO_6 [38]. For the case of the Loss parameter there is no identical pattern as shown in fig 3(d). The Loss parameter is zero at zero eV. The graphs of these materials are in an increasing trend with an increase in energy but in fluctuations.

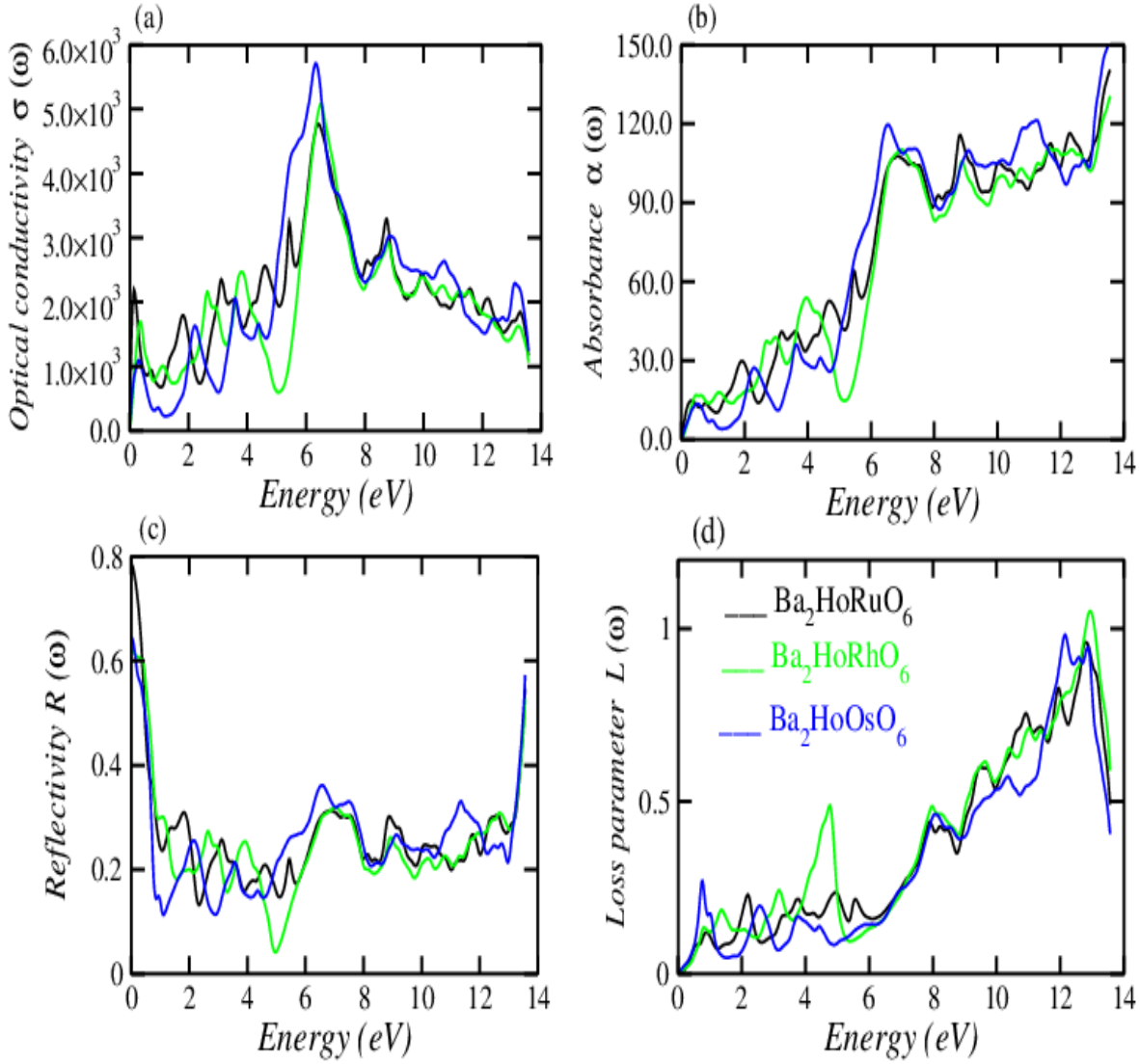


Figure 3 a) Optical conductivity σ (ω) **b)** absorbance α (ω) **c)** reflectivity R(ω) and **d)** Loss Parameter L(ω) of Ba_2HoOsO_6, Ba_2HoRhO_6, and Ba_2HoRuO_6 materials

3.4 Thermoelectric Properties

The most energy saving material is essential for environmental friendliness and energy production. So, we need to search those materials which have small band gap because small band gap semiconductor has a greater number of charge carriers than broad band gap semiconductor. The studied material shows those properties which are important for thermodynamic material. The thermodynamic properties can be explained with the help of charge carrier concentration (n), electrical conductivity σ/τ, Seebeck coefficient (S), thermal conductivity (K/τ), specific heat capacity (C_v), magnetic susceptibility (χ) and power factor (PF) [39-41]. The carrier concentration is an important parameter to calculate the thermoelectric properties of the studied material. The relation between charge carrier concentration and temperature as shown fig 4 (a). The charge concentration increases with increases the temperature of compound Ba_2HoOsO_6 linearly and for the compound Ba_2HoRhO_6 is also linear but slower than Ba_2HoOsO_6 as shown in fig 4 (a) while compound Ba_2HoRuO_6 charge concentration decreases up to 300K and after it increasing with temperature it increases linearly. The size of atom is large so the electron is loosely bond so when we increase temperature the number of charges increases [34, 38, 42].

The electrical conductivity (σ/τ) of studied compound as shown in fig 4 (b). it can be calculated by $\sigma=\mu ne$. At the static values the electric conductivity is maximum for Ba_2HoOsO_6 and Ba_2HoRhO_6 at low temperature and when we increase temperature it decreases and after reaching 400K both of them become linear but in case of Ba_2HoRuO_6 the electric conductivity increases with increase in temperature and become linearly increasing which is low at low temperature and after reaching the temperature 800K the; electric conductivity become constant, no change in conductivity with increase in temperature [43-45].

The Seebeck coefficient of studied material as shown fig 4 (c). Seebeck gives information about potential difference due to temperature across the material. The static value of Seebeck coefficient is 0 for Ba_2HoRhO_6 and Ba_2HoRuO_6 where Ba_2HoRhO_6 increases up to 200K and after it become linear while for Ba_2HoRuO_6 decreases 70K and reaches its minimum value but further increase temperature, it increases its Seebeck values and for Ba_2HoOsO_6 the Seebeck value decreases up to 170K reaches its minimum values but further increase in temperature the Seebeck value increases.

Thermal conductivity (K/τ) of studied material are computed by Wiedemann-Franz Law [46]. It can be calculated by this. The thermal conductivity of studied double perovskite material as shown in fig 5 (a) [32]. The thermal conductivity is increasing for these materials for Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 by increasing temperature. Because at high temperature, electrical conductivity is increased and at very low temperature, the thermal conductivity becomes low as electrical conductivity. The specific heat capacity of a materials Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 gives information about absorption of heat. The C_V of studied compound as shown fig 5 (b). The static value of heat capacity for Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 is 1.2. At higher temperature, the heat capacity of Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 increase linearly.

When magnetic field applied on a material, the magnetic susceptibility describes the behavior of the material [47, 48]. The relation between magnetic susceptibility and temperature as shown in fig 5 (c). The static value of magnetic susceptibility for Ba_2HoRhO_6, Ba_2HoRuO_6, and Ba_2HoOsO_6, are 6.2×10^{-9}, 4×10^{-9}, 6.5×10^{-9} respectively. For these materials Ba_2HoRhO_6, Ba_2HoOsO_6 the magnetic susceptibility decreases up to 400K and after becomes linear while for Ba_2HoRuO_6 its magnetic susceptibility increases and after 600K it's become constant with increase in temperature. The power factor for materials Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 is shown in fig 5 (d). The static values for Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 are 4×10^{10}, 5×10^{10}, 5.2×10^{10} respectively. The values of power factor decrease for Ba_2HoRuO_6, Ba_2HoOsO_6 decreases up to 250K and increases with increases in temperature but in case of Ba_2HoRhO_6 it decreases up

to 100K and then increases with increases in temperature but after 300K it becomes constant [36, 49].

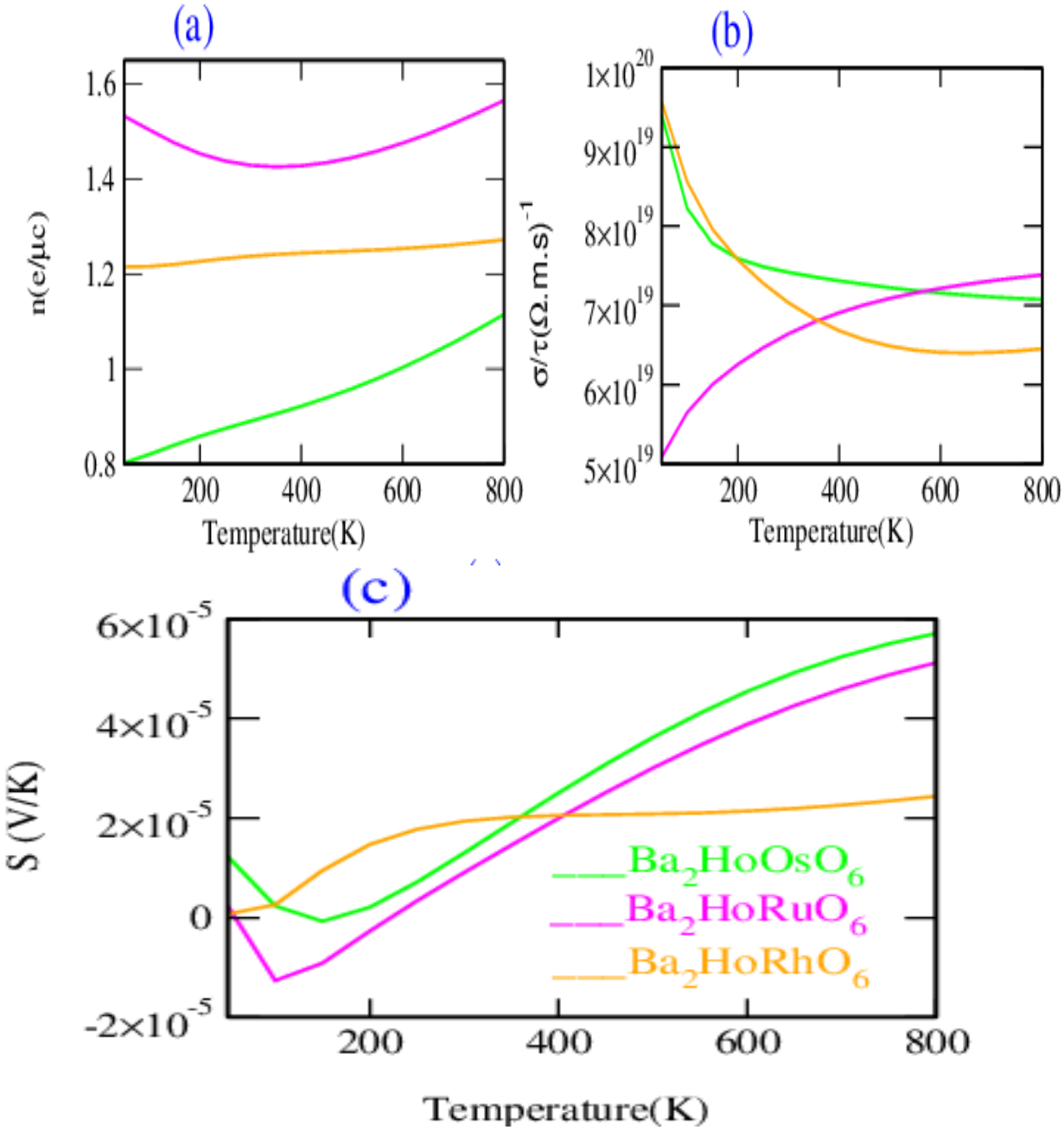


Figure 4 a) Charge carrier concentration (n) **b)** electrical conductivity σ/τ **c)** Seebeck Coefficient (S) of Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 materials

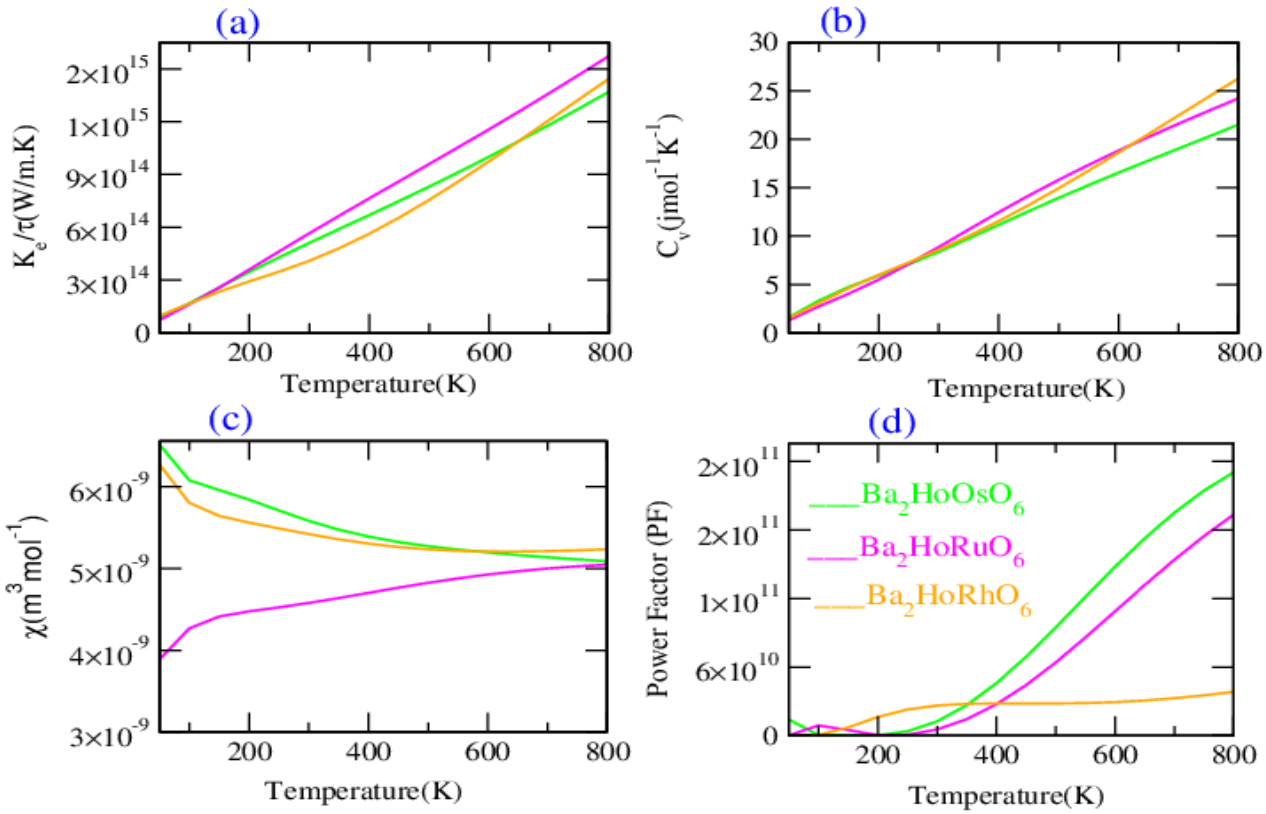


Figure 5 a) Thermal conductivity (K/τ) **b)** Specific heat capacity C_V **c)** Magnetic Susceptibility (χ) **d)** Power Factor (PF) of Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 materials

3.5 Magnetic Properties

The individual contribution of atoms in total magnetic moment and interstitial magnetic moments and total magnetic moment as shown table 1, which shows that the magnetic moment of have more contribution in magnetic moments than other atoms [50, 51]. The value of magnetic moment X= Rh, Ru, and Os are 3.91586, 3.84831 and 3.83362 respectively. The Ba, Ho and O also have a significant role in total magnetic moment of host compound. The total magnetic moment of Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 are 6.00039, 6.21634 and 6.64084 respectively [52, 53].

Table 1 Total, partial magnetic moment and interstitial magnetic moment (μ_B) of Ba_2HoRhO_6, Ba_2HoRuO_6, Ba_2HoOsO_6 crystals

Crystals	Total μ_B	Ba (μ_B)	Ho (μ_B)	X (μ_B)	O (μ_B)	Interstitial (μ_B)
Ba_2HoRhO_6	6.00039	0.00125	3.91586	0.77102	0.18536	0.19885
Ba_2HoRuO_6	6.21634	-0.00028	3.84831	1.19796	0.16835	0.16055
Ba_2HoOsO_6	6.64084	-0.00005	3.83362	1.57024	0.13352	0.43600

4 Conclusion

In this study we observe the electronic, optical, magnetic, and structure characteristics of double perovskites by using the density functional theory through the wien2k software. The materials which are studied namely Ba2HoXO6 (X=Rh, Ru, Os) show face-centered cubic crystal structure with space group Fm3m-225 with a lattice constant or unit lengths a=b=c are 16 Å, 17 Å, 18Å respectively. The materials are cubic structured and half metallic semiconductor with direct band gap which is suitable for spintronics devices. The magnetic properties of double perovskites materials have importance in spintronics as they offer high spin polarization, strong spin orbit coupling with tunable magnetic behavior which is important for designing spintronics functionality. Complex dielectric functions optical conductivity σ(ω), Absorbance α(ω), Reflectivity R(ω) and Loss parameter L(ω) have been analyzed to explain the optical behavior of the materials. This research opens possibilities for further experimental investigations and the potential application of these materials in various device technologies and Spintronics holds significant potential in the realms of science and technology on a global scale.

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