

First-Principles Calculations on Novel Rb-Based Halide Double Perovskites Alloys for Spintronics and Optoelectronic Applications

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Abstract

The outcomes of computational study of electronic, magnetic and optical spectra for A_2BX_6 (A = Rb; B = Tc, Pb, Pt, Sn, W, Ir, Ta, Sb, Te, Se, Mo, Mn, Ti, Zr and X = Cl, Br) materials have been proceeded utilizing Vanderbilt Ultra Soft Pseudo Potential (US-PP) process. The Rb₂PbBr₆ and Rb₂PbCl₆ are found to be a $(\Gamma - \Gamma)$ semiconductors with energy gaps of 0.275 and 1.142 eV, respectively making them promising photovoltaic materials. The metallic behavior of the materials for Rb₂BX₆ (B = Tc, W, Ir, Ta, Mn, Sb, Mo) has been confirmed showing the attendance of conducting lineaments. The dielectric function is found to be large close to the ultraviolet districts (3.10 - 4.13 eV). The extinction coefficient of the Rb₂BX₆ has the ability to be used for implements. The band structures and density of states ensure the magnetic semiconductors' nature of the Rb₂Mn (Cl, Br)₆ perovskites. The total calculated magnetic moment of Rb_2MnCl_6 and Rb_2MnB_6 is $3.00\mu_{\beta}$. Advanced spintronic technology requires room-temperature ferromagnetism. The present work confirms that, bromine and chlorine-founded double perovskites are extremely attractive for photovoltaic and optoelectronic devices.

Keywords

Halide Double Perovskites, Density Functional Theory, Spintronic, Photovoltaic Solar Cells

1. Introduction

The materials A_2BX_6 are multi-band gap materials that offer the possibility of increasing the efficiency of solar cells. In fact, solar cells based on these materials could reach theoretical efficiencies up to 63.2% [1] [2]. Moreover, interme-

diate-band materials are characterized by splitting band gaps into two or more sub-band gaps by narrow intermediate bands and have been the focus of recent studies [3] [4]. In intermediate-band materials, an electron is promoted from the valence band to the conduction band through the intermediate-band. Upon absorption of sub-band gap-energy photons, the electrons transit from valence band to conduction band and later from the intermediate-band to conduction band. By adopting a hypothesis similar to that of Shockley and Queisser [5], it was shown in 1997 [1] that balance-limiting efficiencies of 63.2% for intermediate-band solar cells and 41% for single-band gap solar cells can be achieved at a concentration of 46,050 suns at earth and sun temperatures of 300 and 6000 K, respectively. These perovskites are being utilized in third-generation solar cells and photovoltaic technology. The high absorption, low reflectivity, high optical conductivity, tunable narrow band gaps and high PCE make them promising materials for light-emitting diodes, detectors, absorbers, scintillators, energy storage devices, thermoelectric generators and solar cells [6]. The humidity, toxicity, moisture and temperature sensitivity are some of the challenges for commercialization of cubic perovskites. Therefore different variants of cubic perovskites are being reported in literature. Lead-free thallium-based cubic perovskites $TlSnX_3$ (X = Cl, Br, I) were explored by Pingak *et al* [7].

A new mesoporous carbon nano-structured material was ready and characterized by scanning electron microscopy, transmission electron microscopy, Raman spectroscopy, thermo-gravimetry, and X-ray diffractometry. The material exhibited large speed and great adsorption capacities of 827.5 and 2484.5 mg·g⁻¹ for methyl orange (MO) and malachite green (MG) dyes in 10 min. It was situated that MO and MG adsorption was limited by chemical interactions and blended diffusion. Hence, it can be finished that the adsorbent offered herein had great speed and great adsorption capacity. Thus, it can be regarded as promising in eliminating the mentioned dye pollutants [8]. Likewise, the speeded-up carbon was got ready by a green oncoming from pomegranate peel coated with zero-valent iron nanoparticles (AC-nZVI) and promoted as adsorbent for the suppression of amoxicillin from aqueous solution. The reusability of the adsorbent equally disclosed that the adsorption efficiency diminished from 83.54% to 50.79% after five consecutive duplications. Global, taking into account the fine productivity, ratification, environmental friendliness, and right regeneration, AC-nZVI can be presented as a promising absorbent for amoxicillin from aquatic environments [9]. On the other hand, in diverse laboratory conditions, Ni²⁺ was studied and isolated in tone from aquatic solutions using Jordanian natural zeolite (JNZ). The impacts of time of interaction, initial metal concentration, adsorbent dose concentration and temperature were investigated in the suppression experiments. The adsorption efficiency was examined in 153.846 mg·g⁻¹. The JNZ adsorbent's equilibrium adsorption potential was calculated and extrapolated utilizing the Langmuir and Freundlich isotherm models. The outcomes point that the experimental results were ameliorated matched utilizing Langmuir model. The adsorption conduct of JNZ for the removal of Ni²⁺ was well-depicted utilizing the pseudo-second-order kinetic model [10].

The arrangements of atoms and structures can explain the chemical and physical properties of materials. An important property can be obtained on the rigidity, strength and toughness of the materials under study [11] [12]. Also, the optical properties of these materials are given important information on such several aspects of their physical properties [13] [14]. In fact, the physical properties are dependent on the interaction of electromagnetic radiation with matter. This is related to the radiation wavelength and frequency and to other material properties. The knowledge of these properties is an important information for the comprehension of the interaction of phonon and electron and for the statement of the nature of the material. Furthermore, this will give a useful application for determining the microelectronic properties of the materials for applications of devices [15]-[23].

Perovskites are fascinating solids that have received a great deal of attention in recent years due to the fact that they can be utilized in a diverse selection of thermoelectric devices [24]. (Cs, Br, K)-based halide double perovskites show tremendous potential for spintronic devices such as quantum computers, quantum valves and also magnetic memory devices [25]-[27]. This is due to the fact that they have been explored as low-cost magnetic things. Despite all the benefits of spintronic devices and their uses, there are still two significant obstacles to overcome: high-temperature phase instability and magnetic ion clustering. The first problem has been partially solved because recent research has made a significant contribution to tenable solutions for the Curie temperature issue. The clustering which is the second problem, is still a focus of research, though [28] [29]. Moving forward, understanding the materials' quantum nature and room-temperature magnetic properties is crucial to test the materials' appropriateness for spintronic applications [30] [31]. Recently, Retuerto *et al.* reported a new double perovskite Ca₂CrSbO₆ compound that exhibited strong ferromagnetism below Tc = 13K [32]. Bouras et al. [33] studied the electronic, optical, and elastic features of A_2PtH_6 (A = Rb, Cs and K) and revealed that both materials are direct Eg semi-conductors. Jong et al. [34] revealed the structural, and optoelectronic features of K_2SnX_6 (X = I, Cl, Br), which demonstrated both materials as semiconductors. Several other double perovskite materials are researched and published under density functional theory (DFT) study [35]-[40] for electronic, optical, elastic and thermoelectric properties in different varieties of correlation potentials. The present study reports on the structural, electronic, magnetic, and optical properties of A₂BX₆ (A = Rb; B = Tc, Pb, Pt, Sn, W, Ir, Ta, Sb, Te, Se, Mo, Mn, Ti, Zr and X = Cl, Br) materials with a cubic structure. The novelty of the work is an investigation of Ab Initio calculations on novel Rb-based halide double perovskites alloys for spintronics, optoelectronic and photovoltaic applications. The computations are performed using a computer program CASTEP (Cambridge Serial Total Energy Package). The treatment of the exchange-correlation potential has been made using the generalized gradient approximation (GGA) within the GGA approach according to Perdew-BurkeErnzerhof (PBE) function and the functional density of Heyd, Scuseria, and Ernzerhof (HSE06). More details about the calculations which could be desirable for some photovoltaic and microstructure applications have been given in Sections 2 and 3 of the present paper.

2. Computational Method

We utilized the CASTEP code within the Materials Studio Software, in employing the DFT framework. In this study, we employed the GGA with PBE schemes for calculating the exchange and correlation potentials [40]. GGA with PBE functional is a widely used approximation for evaluating electronic exchange-correlation potentials, known to perform well across a wide range of systems. The HSE06 is worn to regulate the energy band gap [41]. The Vanderbilt-type ultrasoft pseudo-potential [42] was utilized to calculate the geometrical structure and physical properties. The integration of the Brillouin zone is achieved utilizing a Monkhorst-Pack grid of a particular $11 \times 11 \times 11$ *k*-points with a cutoff of 380 eV which is worn for the plane-wave basis aggregate. To calculate optical properties, compact Monkhorst-Pack special *k*-points are employed. A $30 \times 30 \times 30$ special *k*-points mesh is requisite for A₂BX₆ compounds.

The determination of optical characteristics of perovskite materials is very useful in explaining solid-state electronic structure and hence essential for their applications such as in optoelectronics and nano-electronics. The material response to the incoming radiations is completely measured via various energy dependent parameters including, dielectric function $\varepsilon(\omega)$, optical conductivity $\sigma(\omega)$, reflectivity $R(\omega)$, index of refraction $n(\omega)$, coefficients of extinction $k(\omega)$ and absorption coefficient spectra $\alpha(\omega)$. For a medium, the $\varepsilon(\omega)$ is given by [43] [44],

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \tag{1}$$

The refractive index $n(\omega)$, extinction coefficient $k(\omega)$, reflectivity $R(\omega)$, and absorption coefficient spectra $\alpha(\omega)$ have been computed using the following formula [45]-[48]:

$$n(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) \right\}^{1/2} + \varepsilon_1(\omega) \right]^{1/2}$$
(2)

$$k(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)^2 \right\}^{1/2} - \varepsilon_1(\omega) \right]^{1/2}$$
(3)

$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 - k^2}$$
(4)

$$\alpha(\omega) = \frac{4\pi k(\omega)}{\lambda} \quad \text{or} \quad \alpha(\omega) = 2\omega k = \sqrt{2}\omega \left[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)\right]^{1/2} \tag{5}$$

3. Results and Discussion

The cubic A_2BX_6 perovskites crystallize in space group number 225 Fm $\overline{3}$ m [49]. A and B location cations possesses Wyckoff's locations 8e (1/4, 1/4, 1/4)

and 4b (0, 0, 0), respectively, whereas the location of anion occupies 24a (u, 0, 0) site. u is slightly separate (changing about 0.24) for dissimilar structures. The lattice constant a (Å), total energy, bulk modulus (B) and the formation energy for the materials A_2BX_6 (A = Rb; B = Tc, Pb, Pt, Sn, W, Ir, Ta, Sb, Te, Se, Mo, Mn, Ti, Zr and X = Cl, Br) computed using the GGA-PBE approximation are shown in **Table 1**. Also exhibited for comparison are the lattice constants given by experiments [50]-[53]. We remark that our calculated results regarding the lattice constant are in very good agreement with those of experiments when using the GGA-PBE approximation. This table holds as well the inputs which are disposable in the written works for assimilation [50]-[64]. The results concerning a (Å) are found to be within 2% slighter than those of experiment. This exhibits the substantially of introducing calculations in extra computations of other physical properties of interest. **Table 1** clearly indicates that cubic A_2BX_6 perovskites have negative formation energy, implying their chemical stability. As a result, the materials can be synthesized experimentally at normal conditions.

Table 1. Lattice constants *a* (Å), bulk modulus *B* (GPa), Formation energy (eV/atom), energy band-gap *Eg* (eV) and the total energy E_{T} (eV) of A₂BX₆ compounds.

Compounds	References	<i>a</i> (Å)	B(GPa)	Etot (eV)	Formation energy (eV/atom)	<i>Eg</i> (eV)	Туре
Rb_2TcCl_6	Present work	10.208	19.815	-5986.587	-2.26	-	-
Rb_2TcBr_6	Present work	10.823	20.238	-5624.761	-1.35	-	-
Rb ₂ PbCl ₆	Present work	10.586	23.032	-5436.940	-4.20	1.142	direct
Rb ₂ PbBr ₆	Present work	11.214	18.408	-5180.960	-3.32	0.275	direct
Rb ₂ PtCl ₆	Present work	10.263	15.078	-4495.036	-2.28	1.916	Indirect
Rb_2PtBr_6	Present work	10.833	19.289	-4239.236	-1.18	1.230	Indirect
Rb ₂ SnCl ₆	Present work	10.484	24.810	-3874.482	-2.08	2.380	direct
Rb_2SnBr_6	Present work	11.117	24.132	-3618.082	-2.65	1.193	direct
Rb_2WCl_6	Present work	10.244	24.757	-5711.917	-4.62	-	-
Rb_2WBr_6	Present work	10.657	25.575	-5832.267	-3.55	-	-
Rb_2IrCl_6	Present work	10.239	22.764	-4335.360	-2.64	-	-
Rb_2IrBr_6	Present work	10.759	24.237	-4672.258	-4.18	-	-
Rb_2TaCl_6	Present work	10.412	16.708	-3916.900	-4.64	-	-
Rb_2TaBr_6	Present work	10.753	18.157	-3620.145	-3.32	-	-
Rb_2MnCl_6	Present work	10.082	21.374	-4430.466	-4.72	-	direct
	EXP. [50]	9.838	-	-	-	-	-
Rb ₂ MnBr ₆	Present work	10.567	26.157	-4862.127	-3.30	-	direct
Rb ₂ SbCl ₆	Present work	10.753	18.246	-3928.819	-3.32	-	-
Rb ₂ SbBr ₆	Present work	11.145	19.135	-3842.245	-4.22	-	-

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Continued							
Rb ₂ TeCl ₆	Present work	10.300	19.320	-3999.619	-3.98	2.729	Indirect
	EXP. [51]	10.233	-	-	-	-	-
Rb ₂ TeBr ₆	Present work	11.287	23.452	-3744.000	-2.25	2.032	Indirect
	EXP. [52]	10.713	-	-	-	-	-
Rb ₂ SeCl ₆	Present work	10.445	22.294	-40356.786	-4.10	2.581	Indirect
	EXP. [53]	9.978	-	-	-	-	-
Rb ₂ SeBr ₆	Present work	10.961	27.189	-3780.168	-3.28	1.760	Indirect
Rb ₂ MoCl ₆	Present work	10.258	14.893	-5715.100	-4.27	-	-
Rb ₂ MoBr ₆	Present work	10.745	13.874	-5246.632	-3.11	-	-
Rb ₂ TiCl ₆	Present work	10.296	17.535	-5385.347	-2.29	2.193	Indirect
Rb ₂ TiBr ₆	Present work	10.849	16.553	-5128.338	-3.99	1.545	Indirect
Rb ₂ ZrCl ₆	Present work	10.558	19.565	-5064.433	-3.97	3.617	direct
Rb_2ZrBr_6	Present work	11.107	16.351	-4807.675	-4.31	2.776	direct
Rb_2SnI_6	EXP. [54]	11.620	-	-	-	-	-
	Others [55]	11.630	19.55	-	-	1.19	-
K ₂ PdCl ₆	Others [56]	10.000	28.7	-	-	2.00	-
K ₂ PdBr ₆	Present work	10.750	20.9	-	-2.67	1.30	-
Cs ₂ SeCl ₆	EXP. [57]	10.26	-	-	-	2.790	-
	Others [64]	10.567	29.589	-3816.773	-	-	-
Cs ₂ SnCl ₆	EXP. [58]	10.3552	-		-	-	-
	Others [64]	10.646	33.175	-3655.474	-	-	-
Cs_2TaCl_6	EXP. [58]	10.271	-		-	-	-
	Others [64]	10.490	30.855	-3697.998	-	-	-
Cs_2TiCl_6	EXP. [54]	10.445	-	-	-	-	-
	Others [64]	10.619	31.503	-3781.054	-	2.284	direct
Cs ₂ WCl ₆	EXP. [54]	10.219	-	-	-	-	-
	Others [64]	10.473	29.832	-5166.458	-	-	-
Cs_2ZrCl_6	EXP. [59]	10.245	-	-	-	-	-
	Others [64]	10.441	32.128	-5492.849	-	3.731	direct
K ₂ MoCl ₆	EXP. [60]	10.428	-	-	-	-	-
	Others [64]	9.816	-	-4670.072	-	-	-
K ₂ OsCl ₆	EXP. [61]	9.850	-	-	-	-	-
	Others [64]	9.994	-	-	-	-	-

Continued							
K ₂ PdCl ₆	EXP. [62]	9.729	32.809	-7325.458	-	-	-
	Others [64]	9.916	-	-	-	1.131	Indirect
K ₂ PtCl ₆	EXP. [63]	9.7097	-	-	-	-	-
	Others [64]	9.988	33.809	-4814.825	-	1.96	Indirect
K ₂ ReCl ₆	Others [64]	9.990	36.388	-4734.604	-	-	-
K ₂ RuCl ₆	Others [64]	9.965	31.215	-6475.831	-	-	-
K_2SnCl_6	Others [64]	9.956	36.304	-6618.537	-	-	direct
K ₂ TaCl ₆	Others [64]	10.166	30.575	-4113.999	-	-	-
K_2TcCl_6	Others [64]	10.127	27.269	-4156.545	-	-	-
K ₂ TiCl ₆	Others [64]	9.980	32.946	-6226.061	-	-	-

To gain insights for the electronic structure of entitled materials, we have calculated the band structure and density of the states of these materials using GGA and HSE06 methods. The energy band represents quasi-continuous permissible energy levels separated by the forbidden zone. In order to characterize the electron and transport properties of solids, the Fermi level (E_F) position is taken to be critical. Figure 1 shows the GGA-PBE band configurations of entitled materials. Along W-L-Γ-X-W-K symmetry direction, the band structure has been estimated employing different XC potentials such as HSE06 and GGA-PBE. It is evident from Figure 1. The studied Rb_2BX_6 (B = Pb, Pt, Sn, Te, Se, Ti, Zr) compounds show semiconductor behavior notably in PBE-GGA and HSE06 potentials. For the A_2B (Cl, Br)₆ (A = Rb; B = Tc, W, Ir, Ta, Mn, Sb and Mo), the energy bands are overlapping with the Fermi level indicating the presence of metallic character in these materials. The Rb₂PbBr₆ and Rb₂PbCl₆ compounds are direct semiconductors ($\Gamma \rightarrow \Gamma$) with energy gaps of 0.275 and 1.142 eV, respectively. This makes these materials promising photovoltaic ones. Direct band gap materials are more efficient for optoelectronic applications when compared to indirect band gap ones. This is because of phonon involvement, which makes indirect band gap semiconductors bad emitters of light [65] [66]. The total densities of Rb_2BX_6 (B = Pb, Pt, Sn, Te, Se, Ti, Zr) materials are shown in Figure 2. According to the DOS plots, the examined compounds are semiconductors by nature. Our theoretical projections agree with previous research [67]. Most double perovskites were predicted to display an indirect gap from calculations, unless some new experimental strategies were developed for changing them into direct gaps. Unfortunately, these compounds usually show large indirect band gaps (over 2.0 eV), which cannot achieve effective optical absorption and limit the performance. For example, the synthesized Rb_2BCl_6 (B = Sn, Te, Se, Ti, Zr) and Rb_2BBr_6 (B = Te, Zr) compounds, which have an oversized, indirect band gap of more than 2.0 eV, giving low conversion efficiencies merely up to ~1% [68].



Figure 1. Calculated electronic band structures for Rb₂PbCl₆, Cs₂PbBr₆, Rb₂PtCl₆, Rb₂PtBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TeCl₆ and Rb₂TeBr₆ materials.



Figure 2. Total density of states (TDOS) for Rb₂PbCl₆, Cs₂PbBr₆, Cs₂PtCl₆, Rb₂PtCl₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TeCl₆ and Rb₂TeBr₆ materials.

The correct knowledge of materials properties is vital to utilize them in spintronic devices. Thus, we have carried out comprehensive theoretical study on structural, electronic, and magnetic properties of Rb₂MnX₆. These properties are calculated by employing DFT based on WIEN2k software to recognize their prospective for spintronic properties [69] [70].

Discussions of the energy band gap and DOSs are of great interest to those who study electronic properties. The Rb_2MnX_6 exhibits a fascinating electronic characteristic that helps to explain ferromagnetism. To accurately explore physical properties, the evaluation of a proper energy band gap is crucial. For this purpose, the correct energy band gap of the materials under study has been predicted using GGA + *U* potential. With the help of this method, the calculated band structure is depicted in **Figure 3**. Between the conduction and valence bands, the Fermi level was set to be 0 eV. At specific locations in both spin channels, the maxima/minima of valence/conduction bands collide. As a result, it makes sense that both Rb_2MnX_6 double perovskites have direct band gaps. The band structure demonstrates that both (up, down)-spin channels are semiconductors.



Figure 3. Electronic band structure and total density of states (TDOS) of Rb₂MnCl₃ and Rb₂MnBr₃ materials.

We have studied the magnetic properties of Rb₂MnX₆ compound by using the graphs of TDOS, PDOS and band structure. We have calculated the magnetic moment of Mn, Rb and (Cl, Br) separately by using GGA and GGA + U potential. The value of magnetic moment shows the magnetic characteristics of Rb₂MnX₆. The interstitial magnetic moment of Rb₂MnX₆ has also been calculated. Table 2 compiles the total magnetic moment μ_{tot} and interstitial magnetic moment of Rb₂MnX₆. It represents also individual magnetic moment of each atom (Mn, Rb, C, Br) obtained with GGA and GGA + U potentials, respectively. The calculated total magnetic moment of Rb₂MnCl₆ and Rb₂MnBr₆ compounds is $3.00\mu_{\beta}$ and $3.00\mu_{\beta}$, respectively. It can be seen that the Rb₂Mn (Cl, Br)₆ have strong magnetic moment μ_{β} and show ferromagnetic characteristics [71]. The magnetic moment value of Mn atom is higher as compared to other atoms like Rb, Cl and Br. Furthermore, the absolute magnetic moment μ_{β} is largely consisting of Mn atom with a small addition of Rb, Cl and Br atoms and interstitial sites. The negative value of magnetic moment of antimony (Cl, Br) atoms revealed diamagnetic behavior at all sites in the unit cell. This shows anti-parallel increment to the entire ferromagnetic direction [72]. In consequences, X atom definitely affects the ferromagnetic behavior of Rb₂MnX₆ compound. Moreover, the calculated interstitial site, Mn atom along with the entire magnetic moment values of Rb₂MnX₆ compound upload ferromagnetic nature, while X site opposing to it [73]. Using GGA and GGA + U potentials, the existence of opposite sign between the magnetic moment of interstitial site, Mn, X and Rb atoms along with the total magnetic moment of Rb₂MnX₆ compound shows that the valence band electrons associated in anti-parallel behavior [74] to the total magnetic moment of the compound. Rb₂MnX₆ are magnetic semiconductors. Furthermore, the relationship between the Curie temperature Tc and the total magnetic moments m_{tot} is [75]:

$$Tc = 23 + 181m_{tot}$$
 (6)

Maria dia mandri di	Rb ₂ N	InCl ₆	Rb ₂ MnBr ₆		
Magnetic moment μ_{β}	GGA	GGA + U	GGA	GGA + U	
$\mu_{ m Mn}$	3.12374	3.13373	3.33211	3.33617	
$\mu_{\rm X}$	-0.03123	-0.03219	-0.06074	-0.06157	
$\mu_{ m Rb}$	0.00195	0.00189	0.00155	0.00175	
$\mu_{ m tot}$ (Interstitial)	0.06120	0.0645	0.03189	0.03624	
$\mu_{ m tot}$	$3.00148 \mu_{\beta}$	$3.00887 \mu_{\beta}$	3.00265 <i>μ</i> β	$3.00649 \mu_{\beta}$	
<i>Tc</i> (K)	566	-	566	-	

Table 2. Magnetic properties and Curie temperature Tc of Rb₂MnX₆ compound with GGA and GGA + U, respectively.

Advanced spintronic technology requires room temperature ferromagnetism, which is ensured by *Tc* values represented in **Table 2**. This value is essential for applications involving devices based on spintronic technology.

Lately, alike crystal structures have been specified utilizing precise electronic computations, however, this zone is in its infancy relative to the upcoming quantity of experimental and theoretical investigation on optical properties. The utilization of optical measurements to survey a physical framework is not a starting from traditional physics since it is presumably real that more physics has been learned utilizing photons on probes than by any other means [76]. When assessing the optical properties of a material, the fact that the transitions take place as a result of light coming into contact with the substance is an essential aspect. Electronic transitions can be broken down into two primary categories: intra-band and inter-band transitions. As a result, transitions between bands are more common than transitions within bands. We present the optical properties of the calculated materials of interest. These properties are allied to a complex dielectric constant that is important to comprehend the response between the crystal system and the electromagnetic waves. It is overmuch hard to experimentally perform a specimen of a single-crystal structure. Thus, the ab initio is a right approximation to analyze optical properties, including dielectric constant, reflectivity, and absorption coefficient. The dielectric constant is the capacity of the framework to accommodate and store electrons [77]. The complex dielectric constant $(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ contains two components: the real component $\varepsilon_1(\omega)$ that measures dispersion and the imaginary component $\varepsilon_2(\omega)$ which measures light absorption. $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are used to calculate the other major optical properties, such as reflectivity $R(\omega)$, absorption $\alpha(\omega)$, and refractive index *n*(*ω*) [78] [79].

The plots of $\varepsilon_1(\omega)$, $\varepsilon_2(\omega)$, $n(\omega)$, $k(\omega)$, and $a(\omega)$ are depicted in Figures 4-7, where the largest peak of $\varepsilon_1(\omega)$ is observed at 6.16, 6.33, 6.88, 3.44, 6.01, 2.99, 6.69, 6.61, 6.12, 4.28, 5.64, 4.29, 6.12, 6.35 eV for Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb2PtBr6, Rb2SnCl6, Rb2SnBr6, Rb2TeCl6, Rb2TeBr6, Rb2SeCl6, Rb2SeBr6, Rb2TiCl6, Rb_2TiBr_6 , Rb_2ZrCl_6 , Rb_2ZrBr_6 , respectively. Since the energy and frequency of electromagnetic waves are intimately related, the movement of the peak of highest intensity towards lower energy causes the $\varepsilon_1(\omega)$ value to increase from 5.30 to 6.41 [80]. The static dielectric constants obtained for the materials under consideration are shown in **Table 3**. Note that when $\varepsilon_1(0)$ is inversely linked to a material's band gap, it becomes clear that our computed results are quite in line with those of Penn's rule [81] [82]. When the compound's energy band gap narrows, its spectral peaks rise. Figure 4 shows the change in $\varepsilon_1(\omega)$ with incident energy. The variation of $\varepsilon_2(\omega)$ with photon energy (0 - 10 eV) is shown in Figure 4. An absorptive transition among the different bands is indicated by the existence of several peaks in the energy region which is primarily due to transition of electrons. These results suggest that variation in the studied group of these materials strongly influences their optical properties; hence, they can be used to manipulate these properties.



Figure 4. Computed real Re (Epsilon) and imaginary Im (Epsilon) parts of the dielectric functions for Rb₂PbCl₆, Cs₂PbBr₆, Cs₂PtCl₆, Rb₂PtBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TeCl₆ and Rb₂TeBr₆ materials.



Figure 5. Calculated refractive index $n(\omega)$ and extinction coefficient $k(\omega)$ for Rb₂PbCl₆, Cs₂PbBr₆, Cs₂PtCl₆, Rb₂PtCl₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TeCl₆ and Rb₂TeBr₆ materials.



Figure 6. Calculated reflectivity $R(\omega)$ for Rb₂PbCl₆, Cs₂PbBr₆, Cs₂PtCl₆, Rb₂PtCl₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TeCl₆ and Rb₂TeBr₆ materials.



Figure 7. Optical absorption coefficient $a(\omega)$ of Rb₂PbCl₆, Cs₂PbBr₆, Cs₂PtCl₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂SeBr₆, Rb₂TeCl₆ and Rb₂TeBr₆ materials versus photon energy.

Compounds	<i>ɛ</i> (0)	<i>n</i> (0)	<i>R</i> (0)
Rb ₂ PbCl ₆	2.78	1.66	0.83
Rb_2PbBr_6	3.70	1.92	0.84
Rb ₂ PtCl ₆	2.88	1.69	0.78
Rb_2PtBr_6	2.41	1.55	0.79
Rb_2SnCl_6	2.65	1.63	0.81
Rb_2SnBr_6	2.54	1.59	0.86
Rb ₂ TeCl ₆	3.13	1.77	0.82
Rb_2TeBr_6	2.68	1.63	0.79
Rb ₂ SeCl ₆	3.16	1.77	0.85
Rb ₂ SeBr ₆	2.19	1.48	0.87
Rb ₂ TiCl ₆	2.70	1.64	0.71
Rb_2TiBr_6	3.27	1.80	0.84
Rb_2ZrCl_6	2.28	1.51	0.86
Rb_2ZrBr_6	2.69	1.64	0.83

Table 3. Optical parameters for A₂BX₆ materials.

The opacity of a compound when light photons strike its surface is measured by the refractive index $n(\omega)$. For materials that are completely transparent, $n(\omega)$ must be equal to 1 [83]. The most efficient optical materials have refractive indices of 2 to 3. The trend of n(0) is noticed to be replica of the $\varepsilon_1(\omega)$. At zero frequency it is known as static refractive index n(0) is determined as $n(0)^2 = \varepsilon_1(0)$. The initial summits of $n(\omega)$ for Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb₂PtBr₆, Rb₂SnCl₆, Rb₂SnBr₆, Rb₂TeCl₆, Rb₂TeBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TiCl₆, Rb2TiBr6, Rb2ZrCl6, Rb2ZrBr6, are 1.66, 1.92, 1.69, 1.55, 1.63, 1.59, 1.77, 1.63, 1.77, 1.48, 1.64, 1.80, 1.51 and 1.64, respectively. After reaching its peak (see Figure 4), or a resonance frequency, it then starts to decelerate. The curve behavior for the n(x) significantly changed for all of the engaged species. It is clear from Figure 4(b) that the n(x) curves shift to other energy areas for the various doped configurations. Similarly, a change in the n(x) is seen below the energy band-gap accounts for doped models. The important change seen in n(x) accounts supplies an occasion to handle the optical properties by doping with various concentrations. Additionally, the change is more pronounced in the base energy area in contrast to the great energy area.

Figure 5 illustrates the extinction coefficient spectra $k(\omega)$ versus photon energy. For Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb₂PtBr₆, Rb₂SnCl₆, Rb₂SnBr₆, Rb₂TeCl₆, Rb₂TeBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TiCl₆, Rb₂TiBr₆, Rb₂ZrCl₆ and Rb₂ZrBr₆, the amounts of $k(\omega)$ started from 0 eV (See **Figure 5**) and reached the first peak of 0.71, 1.37, 1.41, 1.46, 1.97, 2.53, 1.66, 1.95, 1.38, 1.45, 1.62, 1.74, 1.63 and 1.55 eV. The greatest accounts of $k(\omega)$ are 2.98, 3.16, 3.69, 3.45, 3.93, 3.78, 4.07, 3.54, 3.15, 3.25, 3.57, 3.45, 3.82 and 3.23 eV for Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb₂PtBr₆, Rb₂SnCl₆, Rb₂SnBr₆, Rb₂TeCl₆, Rb₂TeBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TiCl₆, Rb₂TiBr₆, Rb₂ZrCl₆ and Rb₂ZrBr₆, respectively. A great quantity of light absorption is associated with each peak in the extinction coefficient spectrum.

Figure 6 depicts another crucial element for optoelectronic applications, reflectivity $R(\omega)$, which is used to evaluate the light that is reflected from the surface [84] [85]. For zero frequency reflectivity, the computed values for Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb₂PtBr₆, Rb₂SnCl₆, Rb₂SnBr₆, Rb₂TeCl₆, Rb₂TeBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TiCl₆, Rb₂TiBr₆, Rb₂ZrCl₆ and Rb₂ZrBr₆ are 0.10, 0.11, 0.10, 0.07, 0.08, 0.09, 0.08, 0.12, 0.10, 0.11, 0.10, 0.09, 0.08 and 0.11, respectively (see **Figure 6**). Furthermore, the high values of $R(\omega)$ are 0.83, 0.84, 0.78, 0.79, 0.81, 0.86, 0.82, 0.79, 0.85, 0.87, 0.71, 0.84, 0.86 and 0.83 for Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb₂TiBr₆, Rb₂ZrCl₆ and Rb₂ZrBr₆ at 5.01, 11.39, 11.04, 9.81, 5.81, 5.01, 6.13, 5.26, 7.15, 6.24, 11.24, 8.13, 7.26 and 8.15, respectively. The $\varepsilon_1(0)$, n(0) and R(0) are represented in **Table 3**. In the visible region, the doped systems have a lower reflectivity coefficient, indicating that the systems all have "clear-type" properties. This is conducive to fundamental insights into a tunable band gap semiconductor with enormous potential in device fields.

The absorption coefficient spectra $\alpha(\omega)$ is a crucial parameter for the reason that it establishes how far light of some energy can proceed via the substance prior being used [10]. $a(\omega)$ equally accounted for the photon-induced processing of electrons from replete to unfilled states [47]. The $\alpha(\omega)$ for the two substances is produced at 0 eV (See Figure 7). For Rb₂PbCl₆, Rb₂PbBr6, Rb₂PtCl₆, Rb₂PtBr₆, Rb₂SnCl₆, Rb₂SnBr₆, Rb₂TeCl₆, Rb₂TeBr₆, Rb₂SeCl₆, Rb₂SeBr₆, Rb₂TiCl₆, Rb₂TiBr₆, Rb_2ZrCl_6 and Rb_2ZrBr_6 , the $\alpha(\omega)$ acquires maximum merits of 20.94×10^4 , 21.91 $\times 10^4$, 25.42 $\times 10^4$, 24.54 $\times 10^4$, 22.39 $\times 10^4$, 22.16 $\times 10^4$, 19.41 $\times 10^4$, 19.17 $\times 10^4$, 20.14×10^4 , 21.63×10^4 , 20.14×10^4 , 22.30×10^4 and 21.25×10^4 at 110.24, 9.28, 10.25, 9.77, 10.25, 8.97, 9.93, 8.83, 9.82, 10.12, 10.14, 9.58, 9.43 and 9.17 eV, respectively. The peaks around 10 eV are called the vacuum ultraviolet region. It is clear that the replacement of Rb₂PbCl₆ by Rb₂PtCl₆ and Cs₂PbBr₆ by Cs₂PtCl₆ augments $a(\omega)$ at around 10 eV and significantly shifts the peaks to low energy. As stated by the provided optical representatives of Rb₂PbCl₆, Rb₂PbBr6, Rb2PtCl6, Rb2PtBr6, Rb2SnCl6, Rb2SnBr6, Rb2TeCl6, Rb2TeBr6, Rb2SeCl6, Rb2SeBr6, Rb₂TiCl₆, Rb₂TiBr₆, Rb₂ZrCl₆ and Rb₂ZrBr₆ compounds, the energy band-gap lies in the visible region. Both materials reveal a great absorption, that makes them potential applicants for energy harvesting systems.

4. Conclusion

Halides perovskites are promising materials for generating green energy that could fulfill worldwide desires for addressing energy scarcity crises. In this study, we have utilized the Ultra-Soft Pseudo-Potentials (PP-PW) approach of DFT to systematically analyze the A_2BX_6 (A = Rb; B = Tc, Pb, Pt, Sn, W, Ir, Ta, Mn, Sb,

Te, Se, Mo, Ti, Zr and X = Cl, Br) materials. The structural stabilities of the scrutinized materials have been ascertained from structural optimization. The results concerning the lattice constant are found to be within 2% slighter than those of experiment. The cubic A₂BX₆ perovskites have negative formation energy, implying their chemical stability. Thus, the materials can be synthesized experimentally at normal conditions. The electronic band structure and density of states are determined using GGA and HSE06 approximations. The electronic properties reveal that the studied Rb₂BX₆ (B = Pb, Pt, Sn, Te, Se, Ti, Zr) materials possess energy band gaps which vary from 1.131 to 3.731 eV. The Rb₂PbBr₆ and Rb₂PbCl₆ materials are found to be direct semiconductors (Γ - Γ) with energy gaps of 0.275 and 1.142 eV, respectively. This makes them promising photovoltaic materials. A metallic nature has been seen for Rb₂BX₆ (B = Tc, W, Ir, Ta, Mn, Sb, Mo) compounds showing the attendance of conductivity lineaments. The Band structure demonstrates that both (up, down)-spin channels are semiconducting materials. The Rb₂Mn (Cl, Br)₆ has strong magnetic moment μ_{β} and shows ferromagnetic characteristics. The negative value of magnetic moment of antimony (Cl, Br) atoms revealed diamagnetic behavior at all sites in the unit cell. This indicates an anti-parallel increment to the entire ferromagnetic direction. Calculations have also been made for optical characteristics with the values of the dielectric function, absorption coefficient, reflectivity, and refractive indices. A great quantity of light absorption is associated with each peak in the extinction coefficient spectrum. According to our findings, all investigated materials are able to emit light in the visible as well as in the ultraviolet energy ranges, making them suitable for use in optical applications. The obtained results will act as a theoretical road map for upcoming experimental and commercial A2BX6 applications.

Conflicts of Interest

The authors declare no competing interests.

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