To study the structural, electronic and optical properties of predicted stable halide perovskites \(\text{ABX}_3\)

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Abstract

Perovskites have gained great interest in recent times. High efficiency solar materials have been developed from this family. Here in this work, structure, optical and electronic properties of recently artificial intelligence predicted stables perovskites \(\text{ABX}_3\) are studied through DFT approach. The structural analysis is done through the generalized gradient approximation. For the band structure calculations generalized gradient as well as the modified Becke-Johnson potential are used to investigate electrical and optical properties. The density of states and electronic band structure calculations reveal that the predicted stable halides Perovskites \(\text{ABX}_3\) have ultra-high to low band gaps. In the absence of experimental results, the calculated results can be valuable for further calculations. In the optical properties of the compounds dielectric function, optical reflectivity, absorption coefficient, optical conductivity, extinction coefficient, refractive index is calculated in different ranges of energy. The maximum value of static dielectric function is observed for \(\text{KNiI}_3\) and \(\text{RbIrBr}_3\) are 3.5 and 3 respectively. The highest absorption peak among the all is observed at 26 eV for \(\text{SrLiF}_3\), while refractive index of that \(\text{SrLiF}_3\) gives peak at 24 eV then refractive index decreases below the unity as energy increases up to 27.5 eV. The suitable energy bandgaps of the new compounds in the ultraviolet to infrared region certainly appeal for their use in the diverse applications.

1. Introduction

Perovskites make up a large amount of mantle of the Earth crust, hence studying their physical characteristics is essential. Perovskites are a broad class of compounds that include anything from insulators to superconductors to colossal magneto resistive compounds. They exhibit a variety of interesting features; thermoelectricity, superconductivity, spins dependent transport, colossal magnetoresistance, charge ordering, and the interaction of structural, optical characteristics and magnetic properties, are all common aspects of perovskite materials. The perovskite materials are often utilized as sensors, catalytic electrodes in fuel cells, substrates, and they also considered interesting for optoelectronic devices \([1, 2]\).

Perovskites come in a variety of shapes and sizes, such as metal-based halides perovskites (HP), which have visible and near-infrared band gaps (and thus are more suitable for use in light emitting devices and also as a photovoltaic), with a big set of transition metal fluoride perovskites in the first row, which can be used as a host material for up or down conversion emission or for lithium intercalation \([3–5]\). K\(\text{MgF}_3\) (parascandolaite) one of these fluoride perovskites \([6]\), is also one of a pure cubic HP structure discovered in nature.

Because of their superior charge-transport and optical characteristics, halide Perovskites (\(\text{ABX}_3\)) have gained a lot of interest in the scientific community as light harvesting materials, such as conformable band gaps, high external quantum efficiency, long charge carrier diffusion lengths, high chemical defect tolerance and high
absorption coefficient. Due to their high quantum yield, multicolor luminescence and simple cheap growth, the halide Perovskites become very famous [7], in short time, power conversion efficiency (PCE) of comparable photovoltaic cells improved from 3.81 percent to 23.3 percent. In addition to solar cells, the applications of HP mainly include photo detectors (PDs), light emitting diodes (LEDs), encryption devices and lasers.

The computer neural networks method have reported a list of the best stable halides perovskites (ABX₃) \{SrLiF₃, TiSrF₃, ZnScF₃, ZnLiF₃, TiBeF₃, CsBeCl₃, CaCuCl₃, CsRhCl₃, CsRuCl₃, BaAgCl₃, RbRhBr₃, RbPdBr₃, CaCuBr₃, BaAgBr₃, RbIrBr₃, CaCuI₃, KNiI₃, CsTCl₃, KIrI₃, CaAgI₃\} [8]. The newly predicted super symmetric perovskites still not being synthesized, however some of the predicted ones e.g. ZnScF₃, ZnLiF₃, TiSrF₃, TiBeF₃, RbPdCl₃, CsBeCl₃ and TiBeF₃ were already describes in former theoretical works [9]. More to further understand the characteristics of these molecules, more experimental study is required. By knowing the properties and structure of these molecules theoretically makes the experimental work more productive.

The major goal of this study is to cover the lack of theoretical data on the optical properties of recently predicted stable halide perovskites. Since no theoretical work is reported yet on most of the perovskites and also the latest artificial intellience (AI) algorithms predict the new stable perovskites. It would be very interesting to determine the optical properties of these newly predicted halide perovskites. We selected these compounds and studied them using the density functional theory approach (DFT) [10]. The full potential linearized augmented plane wave (FP-LAPW) technique is used to calculate the parameters related to optical characteristics, with various exchange and correlation approximations. In terms of structural properties, the optimized lattice constants, ground state energies, pressure derivative of the bulk moduli and bond nature among the anions and cations have all been investigated. Density of states and band structure are used to explain the electronic properties of these materials. Electronic charge density graphs represent chemical bonding. The complex dielectric function, optical conductivity, effective number of electrons, complex refractive index, energy loss function, absorption coefficient and reflectivity participating in optical transition are used to describe optical properties. This research will contribute to the knowledge of the optical characteristics of halide perovskites and will also explain different important applications of these compounds.

2. Computational details

The Wien2k simulation [11] tool was used to investigate the properties of the predicted halides perovskite ABX₃ in this work. FP-LAPW [12] technique is used in Wien2k to calculate various compounds’ properties. The structural properties of the compounds were calculated using the generalized gradient approximation (GGA) [13, 14] For various materials, GGA calculations for band structures are mostly underestimated. Various potentials, such as the Hubbard potential [15], hybrid functional and dynamic mean field theory [16], have been used to overcome the problem of band gap, however these are computationally expensive. Tran and Blaha put Becke Johnson’s trade potential to the test [17], however band gap of materials is still underestimated. Modified Becke Johnson exchange potentials (mBJ) are the result of Tran and Blaha’s revisions to the original Becke Johnson exchange potentials. Unlike other computationally intensive methods, this potential (mBJ) accurately calculates a material’s band gap. Tran and Blaha’s modified Becke Johnson potential is as follows:

\[
v_\circ \text{mBJ}(r) = cv_\text{BR} r + (3C - 2) \frac{1}{\pi} \sqrt{\frac{3}{12}} \frac{t_0(r)}{n(r)}
\]

\(v_\circ \text{BR}\) shows the Russel potential, \(t_0\) shows the density of electron and ‘C’ is a constant, \(n_0\) indicate the energy density. The muffin tin radii (Rmt) for the elements were choosed such that no charge leakage observed from the core states. For the Brilliouin zone integrations a set of 1000 K points was used. Rmt = Kmax (cutoff) parameter was set to 7. The calculations conversion criteria were set to 0.0001 Ry energy.

3. Results and discussion

3.1. Structural properties

The predicted stabiles halides Perovskites materials ABX₃ structural properties are investigated to compare with the earlier results. The analysis of optimal lattice constants, bulk modulus, ground state volume and pressure derivative of bulk modulus is used to study the structural properties of the compounds. The total energy values of the compounds are fitted to their associated volume in Birch Murnaghan’s equation [18]. The parabolic energy versus volume curve of ABX₃ compounds are shown in figure 1. The plot shows that with the increase of unit cell volume the unit cell energy reduces, reaches to minimum value (known as ground state energy) and then again rises with the increase in volume. The calculated lattice constants of the compounds are shown in table 1 alongwith other results [8]. The calculated lattice constant from the DFT calculations agrees well with the AI predicted lattice constants. Calculated bulk moduli of the compounds show that the studied perovskites have
bulk moduli in the range 25–90 GPa. The bulk modulus derivative for the compounds has value of 5.0. The optimized volume is also presented in the table. In order to find the stability of the studied structures, the cohesive energy is important to calculate. It is just the difference of the total unit cell energy with the energy of its constituents. The negative value of the formation energy is necessary to confirms the stability of the studied structures. In the table 1, the cohesive energy is also calculated for all the compounds. It is evident from the table that all the studied new compounds have negative value of the formation energy. Hence all the compounds are stable in the perovskite structure. In the absence of experimental results, the current comparison is highly important for further research on these potential systems. The optimized lattice constants then used for the self-consistent calculations to obtain electronic and optical properties.

4. Electronic properties

4.1. Band structure

Electronic nature of a material is accurately described by its energy band structure. Therefore, for the studied materials ABX₃, energy band structures (through mBJ) were calculated and presented in figure 2. The halide perovskites demonstrate a diverse energy bandgap nature. The SrLiF₃ is determined to be direct bandgap energy with a wide bandgap of 9.1 eV. All other materials have lower energy bandgaps than SrLiF₃ as depicted in table 2. Mostly the energy bandgap possessing compounds have the conduction band minima and valence band maxima lie at different symmetry points which show the materials are indirect gap nature. The lowest energy gap is calculated for CaCuBr₃ with value 0.2 eV. Remaining compounds (CaCuI₃, CsRhCl₃, CsTcI₃, KIrI₃, KNiI₃, RbIrBr₃, RbPdBr₃, RbRhBr₃) show the metallic nature due to the mixing of the valence and conduction bands. In the absence of any theoretical or experimental results, these observations can be important for the further studies on these materials.

4.2. Density of states (DOS)

Among the studied materials the SrLiF₃ has widest separation between the valence and conduction band edges. In figure, it is observed that the halide anion F contribute majorly in the valence band with minute contribution from Li-p state. In the conduction band Sr-d state forms the conduction band. So the optical transitions in SrLiF₃ are F-p to Sr-d. In TlSrF₃, the valence band consist of majority contribution of Tl-s and F-p in the energy of ~2 eV to 0 eV. Strong s-p hybridization state is seen in the valence band. While in the conduction band, majority contributions are from Tl-p in energy of 6.5 eV to 9.5 eV, while Sr-d distributed in the of 10.8 eV to 16 eV. Similarly, for ZnLiF₃ the F-p states form the valence band while lower part of it has mixed contribution from Zn-d and F-p. While Li-s,p orbitals is in the energy range of ~3 eV to 0 eV contribute minutely. While in conduction band the majority contribution is from Zn-s. In the case of TlBeF₃, Tl-d state contributes highly in
the semicore region. For the valence band near the Fermi level, F- \( p \) state possesses this region. In conduction band majority participation are from Be-\( s \) and Be-\( p \) states.

In the valence band of CsBeCl₃ the majority contribution are Cs-\( p \) and Cl-\( p \), the contribution of the Cs-\( p \) is high at \(-4.5 \) eV to \(-5.5 \) eV while contribution of Cl-\( p \) is high at \(-5.5 \) eV to 0 eV. Majority contribution are from Cs-\( d \) and Cl-\( p \) with small contribution from Be-\( s,p \) in the conduction band. Similar DOS spectra is observed for CsRuCl₃ and CsRhCl₃ with only the difference that the Ru/Rh–\( d \) states span through the valence band to the conduction band to cause the mentality of the two compounds. Also the Ru/Rh–\( d \) states contribute majorly in the valence band. In BaAgCl₃ the valence band states in the range \(-6 \) eV to 0 eV originated from Ag-\( d \) and Cl-\( p \) orbitals while the Cl-\( p \) shows the majority contribution in the range \(-6 \) eV to \(-3 \) eV while for Ag-\( d \) in the energy from \(-2.5 \) eV to 0 eV. In conduction band the majority contribution is from Ba-\( d \) in the lower part of it and Ba-\( f \) orbital in the upper part with small contributions from other states of Ag and Cl. Similar trend is seen for the BaAgBr₃ and BaCuCl₃ except that the Cu-\( d \) state contributes in the valence band and halide ion Cl.

In the figure 3, density of states of CaAgI₃ is also presented. The compound shows a narrow bandgap. In the valence band Ag-\( d \) and I-\( p \) hybridize strongly. While in the conduction band Ca-\( d \) state in the lower part with some contribution of I-\( p,d \) states in the upper region. CaCuBr₃ (figure 3) and CaCuI₃ (figure S1) shows a narrow

### Table 1.

| Compounds | \( a_0(\text{Å}) \) | B(GPa) | BP | \( V_0(\text{Å}^3) \) | \( E_f(\text{Ry}) \) |
|-----------|-------------------|--------|----|----------------|----------------|
| CaAgI₃    | 5.768             | 25.387 | 5.0| 1295.975       | -0.60045      |
| CsTcI₃    | 5.653             | 30.479 | 5.0| 1219.265       | -0.86233      |
| KIrI₃     | 5.364             | 37.872 | 5.0| 1162.658       | -0.40198      |
| KNiI₃     | 5.497             | 28.541 | 5.0| 1128.541       | -0.78007      |
| BaAgBr₃   | 5.491             | 30.086 | 5.0| 1117.622       | -0.94882      |
| CsCuI₃    | 5.457             | 57.383 | 5.0| 1096.478       | -1.54425      |
| RbPdBr₃   | 5.283             | 36.583 | 5.0| 995.049        | -0.92069      |
| RbIrBr₃   | 5.238             | 44.365 | 5.0| 970.055        | -0.59132      |
| BaAgCl₃   | 5.236             | 34.422 | 5.0| 969.214        | -1.11712      |
| RbRhBr₃   | 5.219             | 40.834 | 5.0| 959.272        | -0.97639      |
| CaCuBr₃   | 5.101             | 84.551 | 5.0| 895.906        | -1.10998      |
| CsRhCl₃   | 5.004             | 47.235 | 5.0| 845.484        | -1.10074      |
| CsRuCl₃   | 4.993             | 47.494 | 5.0| 840.016        | -1.22519      |
| BaCuCl₃   | 4.958             | 40.979 | 5.0| 822.591        | -1.39408      |
| CsBeCl₃   | 4.852             | 40.979 | 5.0| 770.885        | -1.10911      |
| TlSrF₃    | 4.790             | 40.703 | 5.0| 741.523        | -1.56008      |
| ZnScF₃    | 4.218             | 82.089 | 5.0| 506.403        | -1.71715      |
| TlBeF₃    | 3.9123            | 88.919 | 5.0| 404.097        | -1.45628      |
| SrLiF₃    | 3.883             | 70.912 | 5.0| 395.239        | -1.80814      |
| ZnLiF₃    | 3.642             | 86.977 | 5.0| 326.087        | -1.25541      |

* Reference [8].
bandgap and semi-metallic nature respectively. The DOS spectra of both the compounds is similar to CaAgI$_3$, except that the I-$p$ states cross the Fermi level for CaCuI$_3$. In the valence region of CsRuCl$_3$ (figure 3), the majority part is from Cs-$p$ in the semicore region while Cl-$p$ state in the valence band. The Ru-$d$ orbitals possess the valence band and lower part of the conduction band. In the upper part of the conduction band Cs-$d$ and Cl-$d$ states.

The DOS plot of CsTcI$_3$ (figure S1) shows that it has a metallic nature. The lower band in the semicore region is occupied by Cs-$p$ while Tc-$d$ and I-$p$ states contribute highly in energy range of $-4$ eV to $-1$ eV. The conduction band is composed on Tc-$d$ state with small contribution from I-$p,d$ states. The compounds KIrI$_3$ and KNiI$_3$ shows the metallic nature due to the crossing of the valence and conduction bands through the Fermi level. Both the compounds show similar DOS character. K-$d$ states form the conduction band of the compounds. The valence band consist of mixed states of Ir/Ni–$d$ states and I-$p$ states. The DOS plots of RbIrBr$_3$, 

Figure 2. Band profiles of predicted halides Perovskites ARX$_3$. 

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RbPdBr₃ and RbRhBr₃ show similar trends. The three compounds are metallic due to the mixing of valence and conduction bands. The conduction band of the compounds is composed on Rb- \(d\) orbital. The valence band forms due to the existence of Ir/Pd/Rh – \(d\) states and Br- \(p\) state. These states cross the Fermi level to make the materials metallic nature.

5. Optical properties

The study of optical characteristics of materials is essential because it explains how compounds react to electromagnetic waves. All of the optical properties of halides Perovskites ABX₃ are computed using the FP-LAPW technique. Below is a detailed description of optical constants like the dielectric function, which includes imaginary parts and real, reflectivity, refractive index, optical conductivity and absorption coefficient.

5.1. Dielectric function

A detailed explanation of a material’s response to an incident electromagnetic disturbance is determined by the dielectric function. It consists of both real and imaginary parts, and represented by following equation.

\[ \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \]

Where \(\varepsilon_1(\omega)\) show real part and \(\varepsilon_2(\omega)\) shows the imaginary part of the complex dielectric function. The imaginary component of the dielectric is an essential quantity that explains all transitions between energy states, from conduction to valence bands.

The predicted ABX₃ compounds dielectric function real parts are shown in the figure 4. The BaAgBr₃ the static dielectric function is gotten as \(\varepsilon(0) = 3.5\). It begins to increase from its zero frequency limit and reaches its peak of 7.5 at 5 eV. After reaching another peak at 17.5 eV for the energy 18 eV to 20 eV, it begins to decline farther beneath zero in the negative scale. This material exhibits metallic behavior when the real dielectric function \(\varepsilon(\omega)\) is negative, otherwise it is dielectric. Similarly, the static dielectric function \(\varepsilon(0)\) is obtained for BaAgCl₃, BaCuCl₃, CsCuI₃, CsRhCl₃, CsRuCl₃, CsBeCl₃, PdRhBr₃, SrLiF₃, TlBeF₃ are 3, 3.5, 5, 4.5, 6, 8, 4, 3.2, 8, 1.8, 2.8 respectively. The highest static dielectric function \(\varepsilon(0)\) is obtained for KNiI₃, KIrI₃ and CsTcI₃ are 13, 14 and 16 respectively. This indicates slightly higher polarizability. For some compound like BaAgCl₃, BaAgBr₃, BaCuCl₃, CsCuI₃, CsBeCl₃, SrLiI₃, TlBeF₃, ZnScF₃, TlSrF₃ the peak value of real dielectric function \(\varepsilon(\omega)\) are observed in ultraviolet (UV) region, and for CaAgI₃ the peak value is observed in visible region. While RbIrBr₃, KIrI₃, KNiI₃, the peaks observed in infrared region.

The imaginary part of dielectric function for ABX₃ has been computed in figure 5. The threshold values of dielectric functions are occurring at 0.2 eV, 0.5 eV, 0.6 eV for CaCuBr₃, CsCuCl₃, and CaAgI₃ respectively while for BaCuCl₃, BaAgBr₃, BaAgCl₃, CsBeCl₃ the threshold value occurring 2 eV, 2.1 eV, 2.4 eV, 2.7 eV respectively while high threshold value are observed for compound TlBeF₃, ZnLiF₃, TlSrF₃ and SrLiF₃ are 4.9 eV, 5.4 eV 6.4 eV.

| Compounds  | Band gap (E₉) eV | Other works | Bandgap nature |
|------------|----------------|-------------|----------------|
| SrLiF₃     | 9.1            |             | Indirect       |
| TlSrF₃     | 6.4            |             | Direct         |
| ZnLiF₃     | 5.4            |             | Indirect       |
| TlBeF₃     | 4.9            |             | Indirect       |
| CaBeCl₃    | 3.5            |             | Indirect       |
| BaAgCl₃    | 2.4            |             | Indirect       |
| BaAgBr₃    | 2.1            |             | Indirect       |
| BaCuCl₃    | 2              |             | Indirect       |
| CaAgI₃     | 0.6            |             | Indirect       |
| CaRuCl₃    | 0.5            |             | Indirect       |
| CaCuBr₃    | 0.2            |             | Indirect       |
| ZnScF₃     | 0              |             | Metal          |
| CaCuI₃     | 0              |             | Metal          |
| CaRhCl₃    | 0              |             | Metal          |
| CaTcI₃     | 0              |             | Metal          |
| KIrI₃      | 0              |             | Metal          |
| KNiI₃      | 0              |             | Metal          |
| RbIrBr₃    | 0              |             | Metal          |
| RbPdBr₃    | 0              |             | Metal          |
| RbRhBr₃    | 0              |             | Metal          |

Table 2. Band gap value of Predicted Stables halides Perovskites ABX₃.

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eV and 9.1 eV respectively. The absorption peaks of BaAgCl₃, BaCuCl₃, CaCuBr₃, CsRuCl₃, and CsBeCl₃ are found in the energy range of 5 eV-20 eV. While absorption maxima for ZnLiF₃ and TlSrF₃ are found in the energy range of 6 eV to 12 eV. These absorption peaks are caused by the interband transition area. The Complex dielectric function contains all of the required data for determining additional optical parameters like as

Figure 3. TDOS and PDOS for predicted ABX₃ Perovskites.
refractive index, reflectivity, transmission coefficient, extinction coefficient, adsorption coefficient, transmissivity among others.

5.2. Complex refractive index
The real part $n(\omega)$ of the complex refractive index is known as ordinary refractive index, whereas the imaginary part $k(\omega)$ of complex refractive index is termed as extinction coefficient. For predicted stables halides Perovskites ABX$_3$, its imaginary and real parts of the complex refractive index are presented in figure 6. The value of static function $n(0)$ at zero frequency (static refractive index) for KNiI$_3$ are 3.5 for RBlrBr$_3$ are 3 for RbRhBr$_3$ and CsRhCl$_3$ are 2.9 for CsBeCl$_3$ are 2.8 for CaCuI$_3$ are 2.5 for CaAgI$_3$ are 2.3 for RbPdBr$_3$ and CaCuBr$_3$ are 2.1 for CsRuCl$_3$ are 2 for BaAgBr$_3$ and BaCuCl$_3$ are 1.9 for BaAgCl$_3$ are 1.7 for TlSrF$_3$ are 1.5 while for ZnLiF$_3$ are 1.25.

From the figure 6 it is observed that all compounds refractive index values rise from static frequency limit and...
achieve a number of peaks in different energy ranges. The highest peaks are observed for BaCuCl₃ and CsBeCl₃ at 7.5 eV, for TlSrF₃ at 7.2 eV, for BaAgCl₃ at 6.5 eV, for BaAgBr₃ at 5 eV, for CsRuCl₃ and BaAgBr₃ at 5 eV for KNiI₃ at 4.8 eV, for CaCuBr₃ at 5 eV, for CaCuI₃ at 2.75 eV, for CaAgI₃ at 2.5 eV while for RbIrBr₃ and RbPdBr₃ at 2 eV. While ZnLiF₃ has refractive index is constant up to the energy range of 25 eV, then decrease. The SrLiF₃ possesses maximum peak at 24 eV, then refractive index decreased below unity as energy increase up to 27.5 eV. It is clear that all maximum peaks are observed in visible and ultraviolet region. In figure 7, it can be seen that some compounds like BaAgBr₃, BaAgCl₃, CaCuBr₃, CaCuI₃, CsRuCl₃, CsBeCl₃, ZnLiF₃ has significant value in the UV region. While compounds like KIrI₃, KNiI₃, RbIrBr₃, RbPdBr₃, and ZnScF₃ have prominent peaks both in visible and ultraviolet region.

5.3. Absorption coefficient

The absorption coefficient α (ω) is a compound’s linear attenuation coefficient when it reacts with light [19]. The dielectric function is crucial in determining a compound’s absorption coefficient. The absorption coefficients predicted halide perovskites ABX₃ are given in figure 8. At various high symmetry points, the peaks are associated to the inter band transition on the electronic band spectrum. In the energy range of 0 to 30 eV, all
compounds show various peaks, but the highest absorption peaks observed among all is at 26 eV of value $5.0 \times 10^6$ cm$^{-1}$ for SrLiF$_3$ and the second highest peaks are observed for CaCuBr$_3$ ($4.7 \times 10^6$ cm$^{-1}$), CaAgI$_3$ ($4.1 \times 10^6$ cm$^{-1}$), and CaCuI$_3$ ($3.95 \times 10^6$ cm$^{-1}$) at 28 eV, while for BaAgCl$_3$ ($3.9 \times 10^6$ cm$^{-1}$) and BaCuCl$_3$ ($3.40 \times 10^6$ cm$^{-1}$) are observed at 18 eV. The maximum absorption peaks for the BaAgBr$_3$, CsBeCl$_3$, TlBeF$_3$, CsRuCl$_3$, RbRhBr$_3$, RbPdBr$_3$, TlSrF$_3$, ZnLiF$_3$, ZnSrF$_3$, RbIrBr$_3$, CsRuCl$_3$, CsTcI$_3$, KIrI$_3$, KNiI$_3$ are $3.30 \times 10^6$ cm$^{-1}$, $2.62 \times 10^6$ cm$^{-1}$, $1.45 \times 10^6$ cm$^{-1}$, $2.92 \times 10^6$ cm$^{-1}$, $2.20 \times 10^6$ cm$^{-1}$, $2.05 \times 10^6$ cm$^{-1}$, $2.88 \times 10^6$ cm$^{-1}$, $1.20 \times 10^6$ cm$^{-1}$, $1.10 \times 10^6$ cm$^{-1}$, $2.40 \times 10^6$ cm$^{-1}$, $2.40 \times 10^6$ cm$^{-1}$, $2.70 \times 10^6$ cm$^{-1}$, $1.99 \times 10^6$ cm$^{-1}$, $1.50 \times 10^6$ cm$^{-1}$, $1.66 \times 10^6$ cm$^{-1}$, $1.50 \times 10^6$ cm$^{-1}$, $1.99 \times 10^6$ cm$^{-1}$ respectively. The broad absorption energy range of these compounds promises uses in the optoelectronic as well as optical instruments operating energy range 0.5–30 eV [19].

5.4. Optical conductivity

To explore the spectrum of optical conductivity for the studied materials the optical conductivity $\sigma(\omega)$ is an importance parameter to it, as shown in figure 9. The electronic conductions related to the incidence of
Electromagnetic radiations are represented by this spectrum. Figure shows those compounds’ highest peaks $\sigma(\omega)$ arises in the visible to ultraviolet range, (1.7 eV to 30 eV). The maximum optical conductivity is observed for SrLiF$_3$ at 24 eV while the second maximum peaks are observed for BaAgBr$_3$, BaAgCl$_3$ and BaCuCl$_3$ at 18 eV.

5.5. Reflectivity
The complex refractive index can be used to calculate the optical reflectivity of any material [19]. In figure 10, the optical reflectivity versus the photon energy ranging from infrared to deep ultraviolet region is depicted. For all the compounds, the reflectivity starts with non-zero value in the low frequency region. For the compounds which have energy bandgap it starts from certain value and then stays almost same and then sharply increases in the region where the interband transition rates become high. For the semimetal materials (low electron density

**Figure 7.** Imaginary part complex reactive index for predicted halides perovskites.
at the Fermi level), it started from nonzero values and sharply increased to peak value and then decreases with again different peaks rises in the higher energy region. For metallic system (high electron density at the Fermi level) show asymptotic behaviour. The zero frequency reflectivity of the studied compounds is very high and then sharply decreases in the visible region due to interband transitions. Among all these compounds highest reflectivity is observed for BaAgCl$_3$, BaAgCl$_3$ at 18 eV and for BaCuCl$_3$ at 22.5 eV. CaCuI$_3$ shows relatively higher reflectivity compared to other compounds therefore can be used as Bragg reflector.

6. Conclusions

The structure, electrical structure, and optical responses of the simple cubic perovskites ABX$_3$ were calculated for the first time using DFT. From Structure calculation it is evaluated that all predicted halides perovskites ABX$_3$ are stable. The band gaps of the new compounds show that the studied materials possess a wide range of electronic properties: SrLiF$_3$, TlSrF$_3$, ZnLiF$_3$, TlBeF$_3$ have ultra-wide energy bandgaps of 9.1 eV, 6.4 eV, 5.4 eV, 4.9 eV, while the band gaps of compound like BaAgCl$_3$, BaAgBr$_3$, BaAgCl$_3$ and CsBeCl$_3$ are 2 eV, 2.1 eV, 2.4 eV,
and 2.7 eV respectively. There is no band gap found in some compounds like KIrI₃, KNiI₃, CaCuI₃, RbPdBr₃, RblIrBr₃, and RbRhBr₃. Optical measures such as complex dielectric function, reflectivity, and absorption coefficient, and conductivity, extinction coefficient have been used to investigate the optical response of these compounds. The highest static dielectric function ε₁(0) is obtained for KNiI₃, KIrI₃ and CsTcI₃ are 13, 14 and 16 respectively. Among all these compounds highest reflectivity is observed for BaAgCl₃, BaAgBr₃ at 18 eV and for BaCuCl₃ at 22.5 eV. The new compounds with very wide energy gap (SrLiF₃, TlSrF₃, ZnLiF₃, TiBeF₃, CsBeCl₃) can be utilized for solar blind applications e.g. optical lenses, UV absorbers, high frequency light detectors etc. The compounds with energy bandgaps in the visible region (BaAgCl₃, BaAgBr₃, BaCuCl₃) can be used for visible light emitting and detecting devices, solar cells etc. The narrow gap materials having values less than 1 eV (CaAgI₃, CsRuCl₃, CaCuBr₃) can be used for thermoelectric generators, they can also be used as infrared light detectors and emitters. The metallic compounds (ZnScF₃, CaCuI₃, CsRhCl₃, CsTcI₃, KIrI₃, KNiI₃, RblIrBr₃, RbPdBr₃, and RbRhBr₃) can find applications as electricity and thermal conductors for various purposes.

Figure 9. Optical conductivity for predicted halides Perovskites ABX₃.
Figure 10. Evaluated reflectivity for predicted halides perovskites ABX₃.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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