

## AB INITIO STUDY OF STRUCTURAL AND OPTOELECTRONIC PROPERTIES OF LEAD-FREE DOUBLE PEROVSKITES $\text{Rb}_2\text{BCuF}_6$ (B = SC, Y)

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### Abstract

This study investigates the double perovskite family  $\text{Rb}_2\text{BCuF}_6$  (B = Sc, Y) using density functional theory (DFT) within the CASTEP framework. The compounds crystallize in a cubic structure (space group Fm-3m) and were systematically evaluated for structural stability mechanical behavior electronic structure and optical response using the GGA-PBE functional. Stability criteria including Goldschmidt tolerance factor values of 0.92 for  $\text{Rb}_2\text{ScCuF}_6$  and 0.91 for  $\text{Rb}_2\text{YCuF}_6$ , along with negative formation energies confirm thermodynamic stability for both compositions. Mechanical property analysis using elastic constants and derived moduli values composition-dependent behavior where  $\text{Rb}_2\text{ScCuF}_6$  exhibits a bulk modulus of 34.26 GPa, a shear modulus of 5.33 GPa, and a Young's modulus of 15.21 GPa, whereas  $\text{Rb}_2\text{YCuF}_6$  shows a bulk modulus of 22.80 GPa, a shear modulus of 8.58 GPa, and a Young's modulus of 22.88 GPa. Electronic-structure calculations indicate that both materials are semiconductors with direct band gaps of 1.43 eV ( $\text{Rb}_2\text{ScCuF}_6$ ) and 0.91 eV ( $\text{Rb}_2\text{YCuF}_6$ ), Provide them suitable for optoelectronic applications. Optical properties, including dielectric functions, refractive indices absorption coefficients and reflectivity are characterized across the 0-40 eV energy range to assess the material's potential for optoelectronic applications. Thermoelectric properties are also evaluated. Collectively this study establishes  $\text{Rb}_2\text{BCuF}_6$  (B = Sc, Y) as promising, composition-tunable materials for photovoltaic applications and thermoelectric technologies based on theoretical predictions.

## 1. Introduction

Rapid technological development and concerns about the environment have increased the pressure on governments to find alternatives to coal oil and other fossil fuels [1, 2]. Clean energy is produced through the decomposition of organic waste, which allows for the utilization of the gases emitted to generate power using generators. Solar and thermal energy [3, 4] conversion are alternatives to pollution-causing materials, including fossil fuels. Thermoelectric and photovoltaic devices then are extremely dependable and inexpensive sources that encourage economic and technical development. Seebeck and Peltier phenomena are used for thermal energy conversion, while solar cells provide electrical energy. The purpose of the current investigation is to identify feasible alternatives to the toxic metal lead that are inexpensive, safe, stable, and convenient to utilize. Consequently, extensive studies have been planned to evaluate such materials for energy harvesting purposes [5, 6]. Highly efficient thermoelectric generators and PV cells made from perovskites ( $ABX_3$ ) are investigated in detail.  $CH_3NH_3PbI_3$  is a hybrid organic-inorganic lead perovskite that has significantly increased the efficiency of optoelectronic devices and photovoltaic cells [7-9]. Efforts made by researchers led to an enhancement in efficiency from 3.8% (2009) to 25.2% (2020) because of extensive study and great activities of experts [10], which has recently increased even more to 29.15% [11]. Strong absorbance in the visible spectrum, direct band gaps and stable electron-hole masses characterize these materials [12, 13]. Due to toxicity, environmental pollution, and health concerns, Pb-based materials are less reliable. Therefore, lead must be replaced with other alternatives due to radiation instability and environmental damage. Substituting Ge or Sn, which belong to the same family as lead, is preferable; however, this results in a 10% efficiency loss [14, 15]. As an added complication, Ge and Sn exhibit inconsistent valences (+2, +4), whose degradation limits their durability [16]. Additionally, lead may be substituted by a complicated mixture containing

monovalent and trivalent cations with the structural formula  $A_2B'B''X_6$ , where "A" denotes a big cation (such as  $Cs^+$  or  $Rb^+$ ), "B'" and "B''" designate either monovalent or trivalent cations, and "X" specifies oxygen or halogen. More recently, indium-based halide perovskites such as  $Cs_2AgInCl_6$  have been successfully synthesized and characterized. However, most of these perovskites have a band gap that is too wide (above 3 eV), meaning they absorb mainly ultraviolet light instead of visible sunlight. This limits their effectiveness for solar cell applications [17]. Furthermore, scientific research indicates that a perovskite material known as  $Cs_2AgInCl_6$  has a direct bandgap and demonstrates exceptional stability. However, when additional halides are included in the perovskite structure, its stability appears to decline. The instability of perovskite materials may be attributed to crystal defects, such as vacancies and interstitials which create localized energy levels (trap states) within the band gap. This is demonstrated by investigations of photoluminescence (PL) and charge carrier relaxation [18, 19]. Additionally, researchers found that the perovskite compounds  $Rb_2AgInCl_6$  (direct band gap  $\approx 2.6$  eV) and  $Cs_2AgInCl_6$  (direct band gap  $\approx 3.3$  eV) exhibit large direct band gaps which is very important for finding materials with excellent photovoltaic properties [20, 21]. Narrow band gap In-based perovskites  $X_2CuInCl_6$  ( $X = K, Rb, [19] Cs$ ) and  $Rb_2InSbX_6$  ( $X = Cl, Br$ ) [22] have recently been reported with optical absorption and remarkable thermoelectric characteristics.

The above discussion has motivated us to explore further the structural, elastic, electro-optic, and thermoelectric behavior of  $Rb_2BCuF_6$  (where  $B = Sc, Y$ ). In  $Rb_2BCuF_6$ , the B-site is occupied by scandium (Sc) or yttrium (Y), the B'-site by copper (Cu), and the halogen site by fluorine (F). This combination provides a novel pathway toward stable, non-toxic, and efficient perovskite materials. Compared to indium-based and lead-based counterparts,  $Rb_2BCuF_6$  compounds are expected to exhibit distinct electronic structures arising from the covalent interaction between copper and fluorine ligands, potentially leading to favorable band gaps and charge transport properties. The

outcomes of the research will be extremely beneficial for the evolution of new materials with improved features for photovoltaic and thermoelectric applications. By investigating the aforementioned properties of double perovskites experimental researchers can design materials that are more efficient and effective for use in these important applications[23, 24].

We present a first-principles investigation of the double perovskite family  $\text{Rb}_2\text{BCuF}_6$  ( $\text{B} = \text{Sc}, \text{Y}$ ) using density functional theory (DFT) within the CASTEP framework. These compounds crystallize in a cubic structure with space group  $\text{Fm-3m}$  (No. 225). Rubidium occupies the A-sites while Sc, Y, Cu, and copper alternate at the B-sites within a network of corner-sharing  $[\text{BF}_6]$  and  $[\text{CuF}_6]$  octahedra. We systematically evaluate the structural stability mechanical behavior electronic structure optical response[25, 26] and thermoelectric properties of both compositions using the generalized gradient approximation with the Perdew-Burke-Ernzerhof functional (GGA-PBE) [27, 28].

## 2. Results and Discussion

### 2.1 Structure Analysis

$\text{Rb}_2\text{BCuF}_6$  ( $\text{B} = \text{Sc}, \text{Y}$ ) crystallizes in a cubic double perovskite structure with the space group  $\text{Fm-3m}$  (No. 225). In this arrangement (Fig. 1),  $\text{Rb}^+$  cations occupy the 8c Wyckoff sites, while  $\text{B}^{3+}$  ( $\text{Sc}^{3+}$  or  $\text{Y}^{3+}$ ) and  $\text{Cu}^{2+}$  cations alternately occupy the 4a and 4b octahedral sites in a rock-salt type ordering pattern. The F anions are located at the 24e Wyckoff positions, forming corner-sharing  $[\text{BF}_6]^{9-}$  and  $[\text{CuF}_6]^{4-}$  octahedral. The calculated tolerance factors ( $\tau \approx 0.92$  for Sc, 0.91 for Y) and octahedral factors ( $\mu = 0.56\text{-}0.73$ ) fall within the stability ranges ( $0.8 < \tau < 1.0$ ,  $0.41 < \mu < 0.90$ ), confirming the cubic symmetry. The B-F bond lengths are  $\sim 2.02 \text{ \AA}$  (Sc-F) and  $\sim 2.23 \text{ \AA}$  (Y-F), while Cu-F is  $\sim 1.95 \text{ \AA}$ . Substituting  $\text{Sc}^{3+}$  with the larger  $\text{Y}^{3+}$  expands the lattice parameter from  $\sim 8.66 \text{ \AA}$  to  $\sim 8.95 \text{ \AA}$  and the unit cell volume from  $\sim 535 \text{ \AA}^3$  to  $\sim 576 \text{ \AA}^3$ , offering composition-dependent tunability.

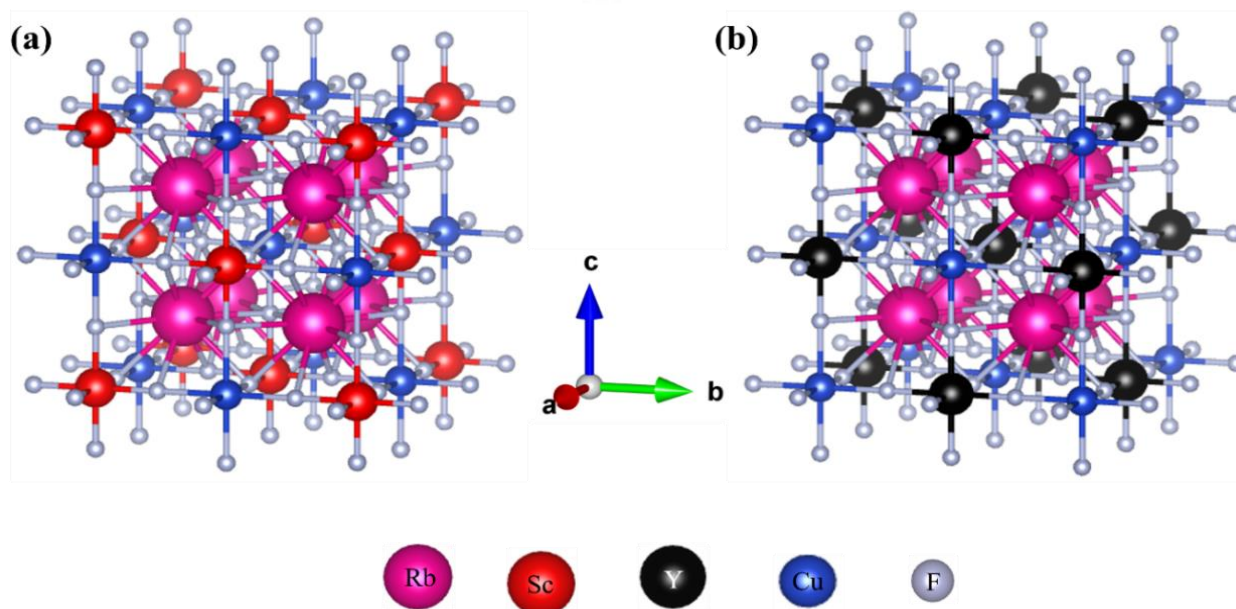


Fig. 1: Computed crystal structure of (a)  $\text{Rb}_2\text{ScCuF}_6$ , (b)  $\text{Rb}_2\text{YCuF}_6$

Table 1: The derived structural parameters for  $\text{Rb}_2\text{BCuF}_6$  ( $\text{B} = \text{Sc}, \text{Y}$ )

| Sample                            | $\text{Rb}_2\text{ScCuF}_6$ | $\text{Rb}_2\text{YCuF}_6$ |
|-----------------------------------|-----------------------------|----------------------------|
| Lattice Constant ( $\text{\AA}$ ) | 8.66                        | 8.95                       |

|                  |         |         |
|------------------|---------|---------|
| Formation Energy | -3.2 eV | -2.1 eV |
| Tolerance Factor | 0.92    | 0.91    |

## 2.2 Electronic properties of $\text{Rb}_2\text{BCuF}_6$ (B = Sc, Y)

Light absorption is a significant characteristic of solar cell absorbers, as photons in the infrared part of the solar spectrum must be efficiently absorbed with appropriate band gaps. Band structures are calculated using the CASTEP potential to assess the impact of anion substitution on the electronic band gap [29, 30]. The obtained band structures for  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$  are presented in Fig.

2(a & b). According to band-structure analysis there is an indirect band gap because the lowest conduction band and the highest valence band are not aligned. The obtained band gap is 1.43 eV and 0.91 eV for  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$ , respectively. The band gap decreases with increasing ionic radii and is consistent with reported literature.

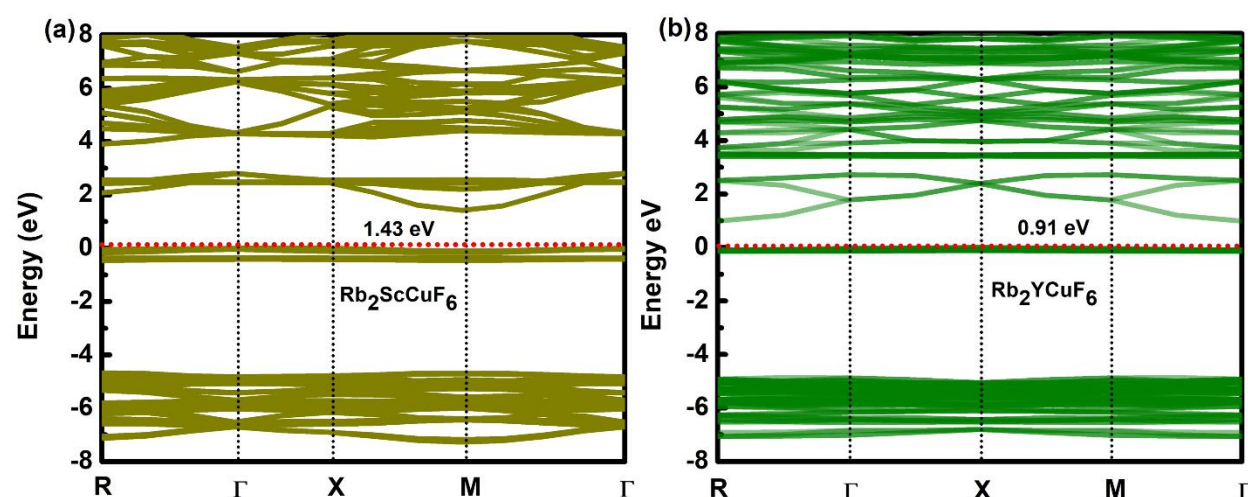


Fig. 2: Electronic band structures of (a)  $\text{Rb}_2\text{ScCuF}_6$  (b)  $\text{Rb}_2\text{YCuF}_6$

We examine the total density of states (TDOS) and partial density of states (PDOS) to gain deeper insight into the electronic properties [31]. The TDOS and PDOS of  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$  are shown in Fig. 3 (a & b) respectively. Fig. 3 confirms no band overlap at the Fermi level, indicating the semiconducting nature of both materials and supporting the band-structure result. Fig. 3 (a) shows that, in the valence band near the Fermi level, Cu makes a large contribution, whereas in the conduction band, Y contributes more. A similar trend is observed for  $\text{Rb}_2\text{YCuF}_6$  as well. The Sc and F have contributions to both the valence and conduction bands near the Fermi level, but their contributions are smaller than those of Cu and Y. Rb makes no contribution to the near-Fermi level [32].

The TDOS of  $\text{Rb}_2\text{ScCuF}_6$  exhibits a well-defined band gap in Fig. 3(c) at the Fermi level, confirming its semiconducting nature. The valence band is dominated by F-p states with pronounced sharp peaks, indicating strong localization of electronic states. The conduction band arises primarily from Sc-d and Cu-d hybridized states. The separation between the valence band maximum (VB) and the conduction band minimum (CB) is relatively wide, suggesting a broad band gap similar to that of chloride-based compounds, but with slightly increased ionic character due to fluorine's high electronegativity.

In  $\text{Rb}_2\text{YCuF}_6$ , the TDOS shows the sharpest band gap in Fig. 3(d) among the studied fluorides in this series, with a significant energy separation around the Fermi level. The valence band is almost exclusively composed of F-p states, displaying

highly localized, narrow peaks. The conduction band is derived from Y-d and Cu-d states. Compared to  $\text{Rb}_2\text{ScCuF}_6$ , the larger ionic radius of  $\text{Y}^{3+}$  introduces minor lattice expansion yet the

band gap remains wide due to the strong ionic potential of  $\text{F}^-$ . The number of electronic states near the Fermi level is lower reinforcing its insulating-like semiconducting behavior.

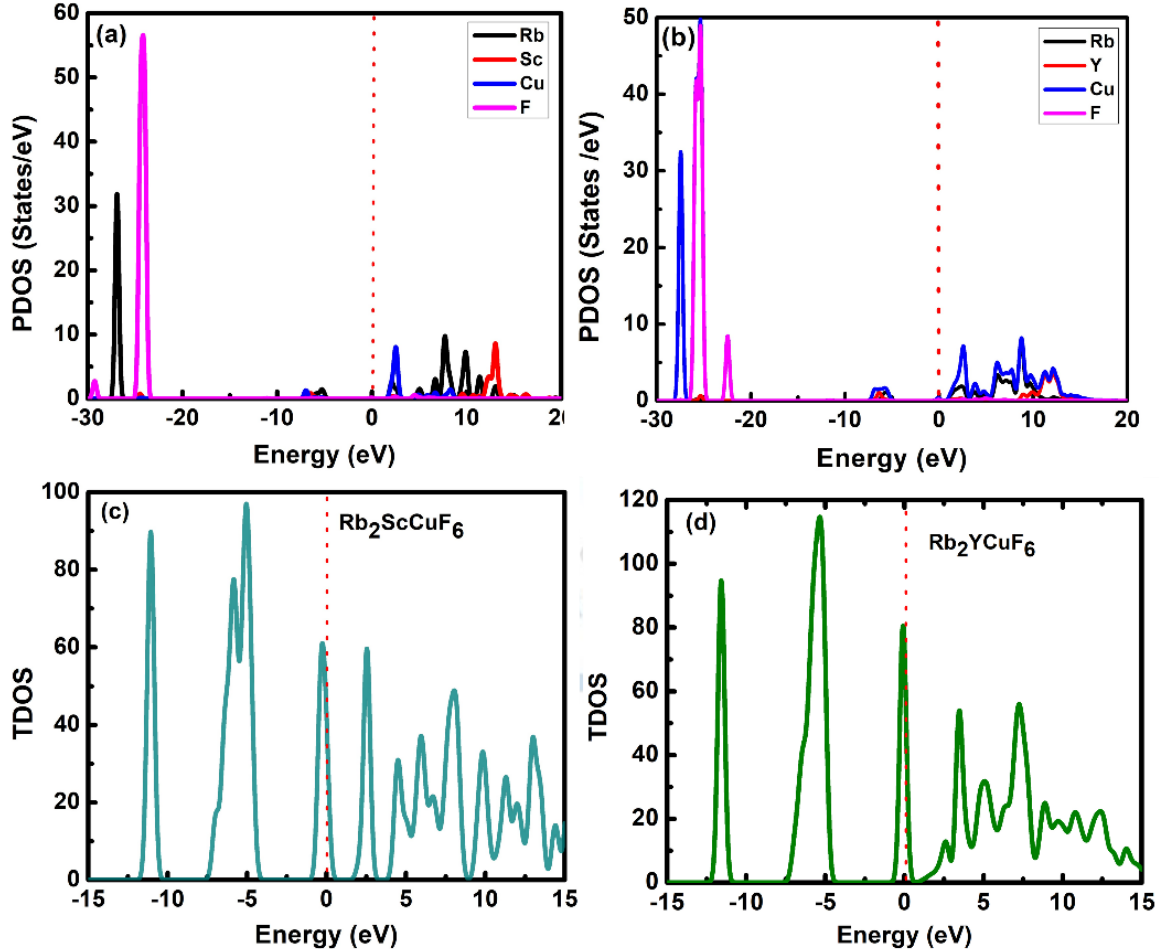


Fig. 3: The obtained PDOS (a)  $\text{Rb}_2\text{ScCuF}_6$  (b)  $\text{Rb}_2\text{YCuF}_6$ , TDOS (c)  $\text{Rb}_2\text{ScCuF}_6$  (d)  $\text{Rb}_2\text{YCuF}_6$

### 2.3 Mechanical properties of $\text{Rb}_2\text{BCuF}_6$ (B = Sc, Y)

Elastic properties are fundamental in evaluating a material's mechanical strength. Understanding the mechanical behavior of an alloy is particularly important, and it is primarily determined by the elastic constants of  $\text{Rb}_2\text{BCuF}_6$  (B = Sc, Y), with a focus on three key elastic constants:  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$ . A material must meet the Born stability criteria and have a non-negative elastic constant to be considered mechanically stable [33]. For the

cubic phase, these criteria are:  $C_{11} > 0$ ,  $C_{44} > 0$ ,  $C_{11} - C_{12} > 0$ ,  $C_{11} + 2C_{12} > 0$ ,  $C_{12} < B < C_{11}$ . Further parameters, i.e., bulk modulus (B), Young's modulus (Y), and shear modulus (G), can be derived from the elastic constants using the mathematical relationship below [34, 35]. These parameters, summarized in Table 2, provide insight into the mechanical characteristics of  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$ .

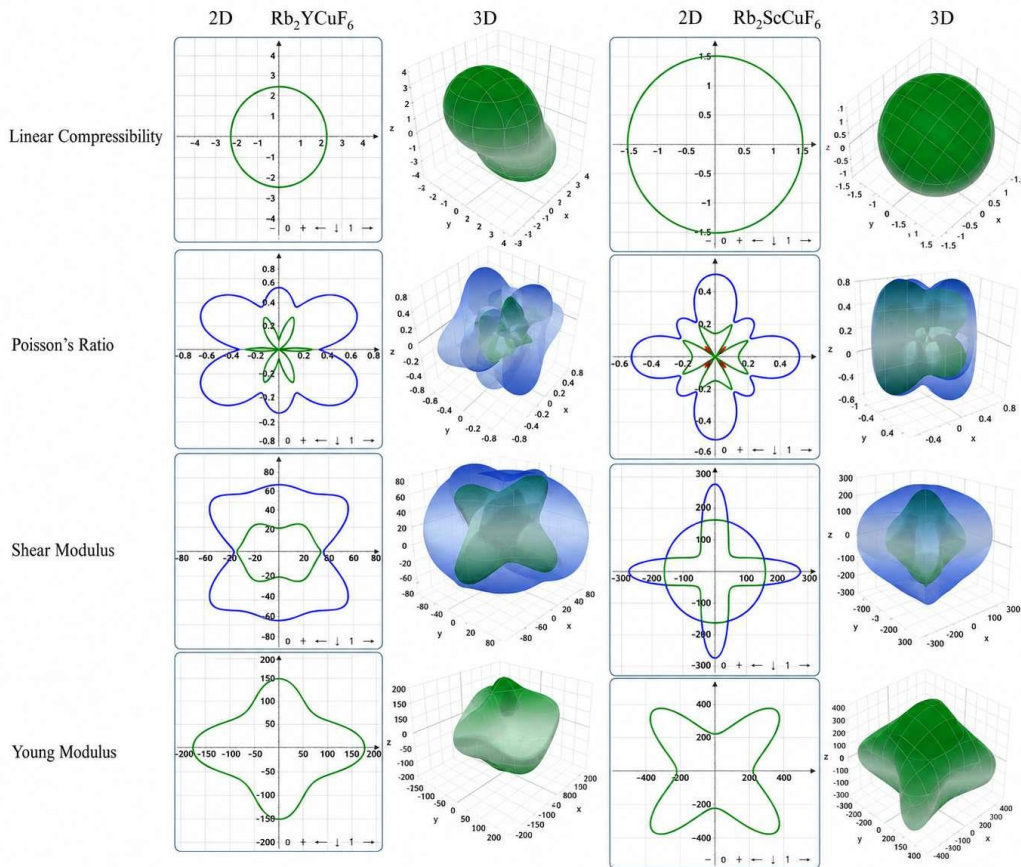


Fig. 4: Directional dependence of elastic properties for Rb<sub>2</sub>YCuFe (left) and Rb<sub>2</sub>ScCuFe (right). (a) Young's modulus, (b) linear compressibility, (c) Shear modulus, and (d) Poisson's ratio are presented in two-dimensional (2D) polar plots and three-dimensional (3D) surfaces. The 2D plots illustrate anisotropy in different crystallographic directions, while the 3D surfaces provide a spatial visualization of mechanical behavior. The nearly spherical shapes in Rb<sub>2</sub>YCuF<sub>6</sub> indicate isotropic characteristics, whereas the distorted shapes in Rb<sub>2</sub>ScCuF<sub>6</sub> demonstrate pronounced anisotropy

$$\frac{(C_{11}+2C_{12})}{3} \dots \dots \dots (1)$$

$$G = \frac{(G_V+G_R)}{2} \dots \dots \dots (2)$$

$$G_V = \frac{(C_{11}-C_{12}+3C_{44})}{5} \dots \dots \dots (3)$$

$$G_R = \frac{5(C_{11}-C_{12})C_{44}}{3(C_{11}-C_{12})+4C_{44}} \dots \dots \dots (4)$$

$$Y = \frac{9BG}{3B+2G} \dots \dots \dots (5)$$

$$\nu = \frac{3B-2G}{2(3B+G)} \dots \dots \dots (6)$$

Resistance to structural deformation of a material is measured by its elastic modulus. Rb<sub>2</sub>BCuX<sub>6</sub> (X =Sc, Y) shows a greater resistance to volumetric deformation than shape deformation, as shown by a larger bulk modulus (B) in comparison to the

shear modulus (G). The material stiffness is further confirmed by higher shear modulus (G) and Young's modulus (Y) values. The other important parameters, Poisson's ratio (ν), Pugh's

ratio (B/ G), and anisotropy ratio (A), can be written as:

Table 2: The computed elastic parameters of (1) Rb<sub>2</sub>ScCuF<sub>6</sub> and (2) Rb<sub>2</sub>YCuF<sub>6</sub>.

| Samples                            | C <sub>11</sub> (GPa) | C <sub>12</sub> (GPa) | C <sub>44</sub> (GPa) | B (GPa) | A    | G    | E     | N    | B/G  |
|------------------------------------|-----------------------|-----------------------|-----------------------|---------|------|------|-------|------|------|
| Rb <sub>2</sub> ScCuF <sub>6</sub> | 11.27                 | 45.76                 | 20.38                 | 34.26   | 0.45 | 5.33 | 15.21 | 0.42 | 5.65 |
| Rb <sub>2</sub> YCuF <sub>6</sub>  | 4.74                  | 31.10                 | 21.40                 | 22.80   | 0.68 | 8.58 | 22.88 | 0.33 | 4.33 |

$$CP = (C_{11} - C_{12}) /$$

2 .....  
(8)

Ductility is assessed through Poisson's ratio (ν), Pugh's ratio (B/G), and A material is considered ductile if the following criteria are met: Poisson's ratio more than 0, and Pugh's ratio more than 1 [36]. The anisotropy ratio (A) quantifies the degree of anisotropy in a lattice. If A is unity the crystal is isotropic. In contrast for the compounds Rb<sub>2</sub>ScCuF<sub>6</sub> and Rb<sub>2</sub>YCuF<sub>6</sub>, the anisotropy ratio deviates from 1 indicating that these materials exhibit anisotropic behavior.

## 2.4 Optical properties of Rb<sub>2</sub>BCuF<sub>6</sub> (B = Sc, Y)

A material's electrical properties and its interaction with incident light are revealed by its optical characteristics. Photon energies between 0 and 40 eV are used to study the optical constants, which are crucial for the photoelectric and device applications of these DP materials. These constants include the dielectric function, refractive index, absorption coefficient, energy loss function, and reflectivity [37]. The relationship between photon energy and the real and imaginary components of the complex dielectric function is illustrated by the Equation following.

$$\begin{aligned} \epsilon_1(\omega) &= \epsilon_1(\omega) + \\ i\epsilon_2(\omega) &..... (8) \\ \epsilon_1(\omega) &= 1 + \\ \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' &..... (9) \end{aligned}$$

## 2.5 Dielectric constants

The real part of the dielectric function,  $\epsilon_1(\omega)\epsilon_1(\omega)$ , for Rb<sub>2</sub>ScCuF<sub>6</sub> and Rb<sub>2</sub>YCuF<sub>6</sub>. Both compounds exhibit low static dielectric constants (~2.5–2.6), characteristic of wide-band-gap ionic fluorides.

The  $\epsilon_1(\omega)\epsilon_1(\omega)$  spectra show a moderate peak near 4 eV, corresponding to inter-band transitions from F-p<sub>p</sub> to cation-dd states, with Rb<sub>2</sub>ScCuF<sub>6</sub> displaying a higher peak (3.8) than Rb<sub>2</sub>YCuF<sub>6</sub> (3.0). A zero-crossing is observed near 19-20 eV, indicating the screened plasma frequency, followed by a negative region up to ~30 eV. The negative  $\epsilon_1\epsilon_1$  values (minimum -0.5 for Rb<sub>2</sub>ScCuF<sub>6</sub>) suggest collective plasmon excitations. Above 30 eV, both compounds return to near-zero positive values. These results indicate that both materials are promising for transparent dielectric or UV optoelectronic applications.  $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$

## 2.6 Conductivity

The Fig. 5(b) illustrates the optical conductivity  $\sigma(\omega)$  of Rb<sub>2</sub>BCuF<sub>6</sub> as a function of photon energy. Rb<sub>2</sub>BCuF<sub>6</sub> shows strong optical responses, with real conductivity peaking at 2.3 at ~8.9 eV for Rb<sub>2</sub>ScCuF<sub>6</sub> and 2.1 at ~7.5 eV for Rb<sub>2</sub>YCuF<sub>6</sub>, indicating efficient photon absorption. All compounds exhibit actuations, with conductivity declining beyond 20 eV, suggesting diminishing optical transitions at higher energies.

## 2.7 Absorption coefficient of Rb<sub>2</sub>BCuF<sub>6</sub> (B = Sc, Y)

The absorption coefficient is a key indicator of a material's light-absorbing ability, directly influencing the efficiency of solar energy conversion in corresponding solar cells. Fig. 5(d) illustrates the calculated absorption coefficient for the Rb<sub>2</sub>ScCuF<sub>6</sub> and Rb<sub>2</sub>YCuF<sub>6</sub> double perovskites. The absorption coefficient can be expressed as [38].

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c} [\sqrt{\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2} - \epsilon_1(\omega)]^{\frac{1}{2}} ..... (5-14)$$

Fig. 5(d) depicts the obtained curve for the absorption coefficient. The absorption coefficient curve corresponds to the imaginary part of the dielectric function. The peak occurs beyond 2 eV, indicating the semiconducting nature of both materials and consistent with their electronic properties. When it comes to absorption, both materials perform well between 3 and 9 eV. The maximum values for absorption coefficients are 1008867 at 8 eV for  $\text{Rb}_2\text{ScCuF}_6$  and 837174 at 5 eV for  $\text{Rb}_2\text{YCuF}_6$ . The obtained maximum value is much higher than the reported value for the double perovskite  $\text{K}_2\text{AgSbBr}_6$ .

## 2.8 Refractive Index of $\text{Rb}_2\text{BCuF}_6$ (B = Sc, Y)

The refractive index characterizes how light propagates through a material. This property varies across materials and plays a key role in many photonic and optical applications. The complex refractive index is related to the complex dielectric function as follows:

$$n(\omega) = n(\omega) + i\kappa(\omega) = \sqrt{\varepsilon(\omega)} = \sqrt{\varepsilon_1(\omega) + i\varepsilon_2(\omega)} \dots\dots\dots (5-15)$$

The real part  $n(\omega)$  represents the ordinary refractive index, which determines the speed of light within the material, while the imaginary part  $\kappa(\omega)$  represents the extinction coefficient [39].

Fig. 5(c) shows the obtained refractive index curve [40]. It is determined that the static refractive index  $n(0)$  is 1.6 for  $\text{Rb}_2\text{ScCuF}_6$  and 1.5 for  $\text{Rb}_2\text{YCuF}_6$ , respectively. The maximum values of the refractive index have been determined to be 6.7 eV for  $\text{Rb}_2\text{ScCuF}_6$  and 6.4 eV for  $\text{Rb}_2\text{YCuF}_6$ , respectively. A refractive index greater than unity indicates that the speed of light decreases within the material.

## 2.9 Reflectivity of $\text{Rb}_2\text{BCuF}_6$ (B = Sc, Y)

Optical reflectivity is essential for understanding electronic transitions between the valence and conduction bands in crystalline materials. When electromagnetic radiation interacts with a material the reflectivity spectrum directly reveals the frequency-dependent complex dielectric function from which the absorption coefficient refractive

index and optical conductivity can be derived. The peaks and features in reflectivity spectra correspond to specific interband transitions at critical points within the Brillouin zone. These provide detailed information about the electronic band structure energy gaps joint density of states and optical anisotropy of the material. Consequently optical reflectivity serves as a powerful non-destructive probe for characterizing the optoelectronic properties and electronic behavior of perovskite materials [41].

Reflectivity measurement provides critical insight into the amount of light entering a surface and interacting with semiconductors, and is closely related to the material's absorption characteristics. Specifically, lower reflectivity values generally correspond to increased absorption of visible or ultraviolet light. Analyzing the relationship between reflectivity and absorption is essential for elucidating the optical properties and possible uses of semiconductor materials [42]. The reflectivity can be expressed as;

$$R(\omega) = \frac{(1-n)^2 + \kappa^2}{(1+n)^2 + \kappa^2} \dots\dots\dots (5-16)$$

Fig. 5(e) demonstrates the reflectivity characteristics of  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$ . At zero frequency, the initial values of reflectivity are 0.05 at ~2.1 eV for  $\text{Rb}_2\text{ScCuF}_6$  and 0.04 at ~2.9 eV for  $\text{Rb}_2\text{YCuF}_6$ , respectively. Up to 7 eV, they have very low values below 0.3, indicating significant absorption across this frequency range.

## 2.10 Energy loss function of $\text{Rb}_2\text{BCuF}_6$ (B = Sc, Y)

The electronic energy loss function (EELF) is an essential metric for distinguishing the optical characteristics of low and high energy regions. This function is essential for studying phenomena including energy dissipation, momentum transfer, and inelastic scattering. It provides important information on how a material reacts to incident radiation and defines its behavior across different energy ranges [43]. The EELF connects macroscopic optical constants and microscopic electronic excitations by characterizing the likelihood that a moving charged particle will lose

a given amount of energy per unit path length represented by the symbols  $R(0)$  are 2.9 and 3.0, respectively.

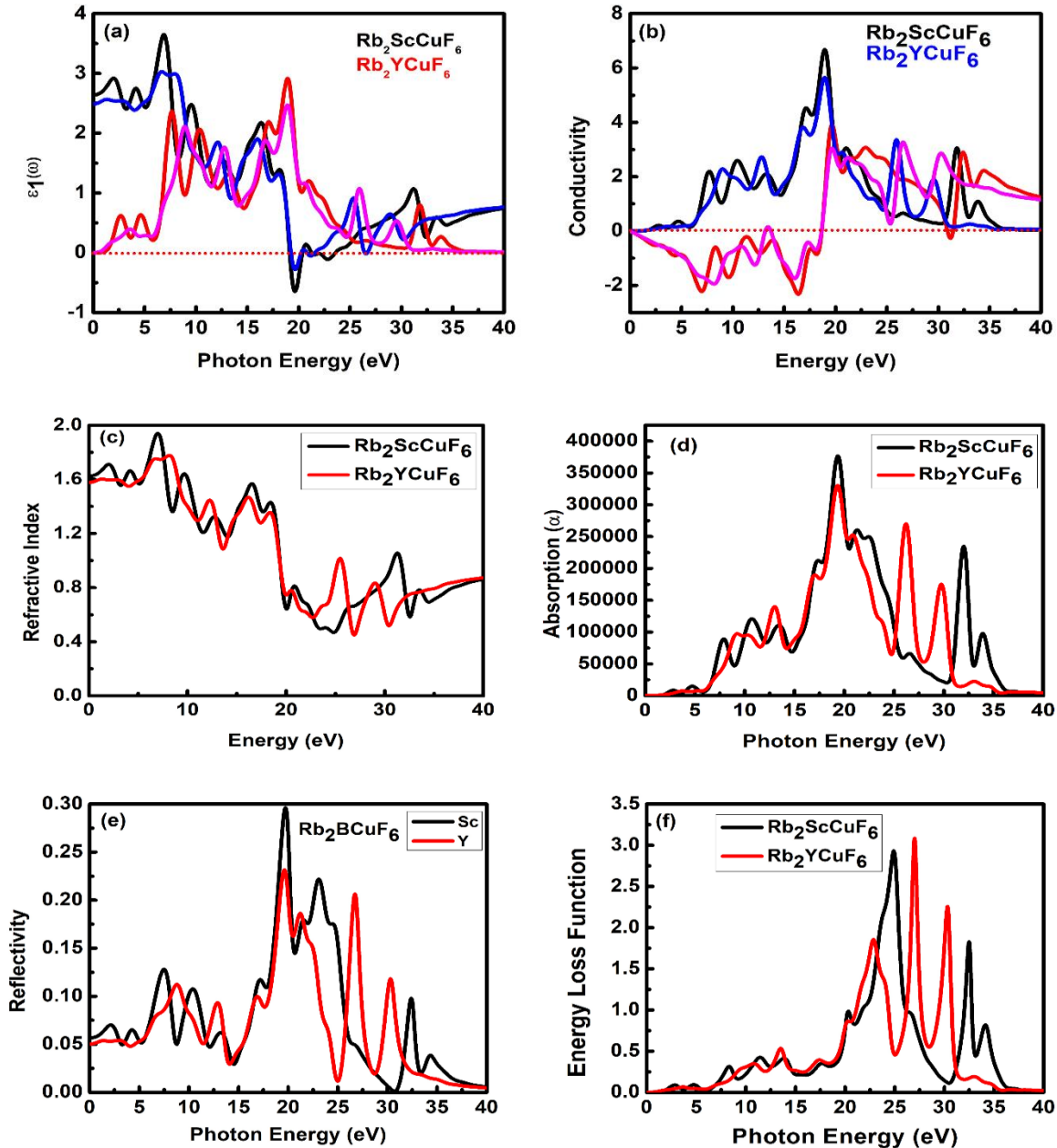


Fig. 5: Optical aspects (a) real component of dielectric function (b) Conductivity (c) refractive index Absorption (d) Reflectivity (e) Energy Loss Function (f)

The ELF can be written as: The ELF is typically expressed as the imaginary part of the negative reciprocal of the dielectric function:  $ELF = -\text{Im}$

$(-1/\epsilon(q, \omega))$ , where  $\epsilon(q, \omega)$  depends on both momentum transfer  $q$  and energy loss  $\hbar\omega$ . This formulation enables the investigation of bulk

Plasmon's, interband transitions, and collective electronic excitations [44]. Consequently, the EELF is indispensable for applications ranging from electron energy-loss spectroscopy to modeling radiation effects in materials.

$$L(\omega) = \frac{\epsilon_2(\omega)}{(\epsilon_1(\omega))^2 + (\epsilon_2(\omega))^2} \quad \dots\dots\dots (5-17)$$

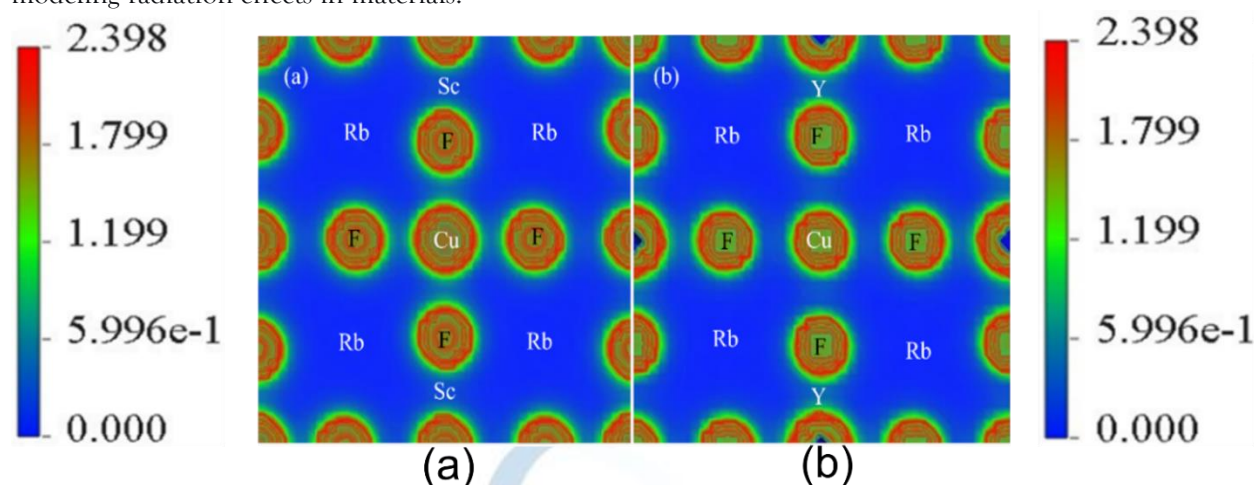


Fig. 6: The electronic charge density (ELF) determined along the a)  $\text{Rb}_2\text{ScCuF}_6$ , b)  $\text{Rb}_2\text{YCuF}_6$

Demonstrate the ELF characteristics of  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$ , Fig. 6. From the graph, it can be observed that both materials exhibit very low energy loss up to 8 eV. The two peaks at 16 and 14 eV are observed for  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$ , respectively.

### 3. Conclusion

In this work the lead-free double perovskites  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$  were systematically investigated using first-principles DFT. Negative formation energies confirm the thermodynamic stability of both compounds in the cubic phase supporting their experimental synthesizability. Mechanical analysis reveals that both materials are elastically stable anisotropic and ductile indicating good processability and fracture resistance for device fabrication. Electronic structure calculations show indirect band gaps of 1.43 eV ( $\text{Rb}_2\text{ScCuF}_6$ ) and 0.91 eV ( $\text{Rb}_2\text{YCuF}_6$ ), making them suitable for visible-light optoelectronic applications. Effective mass analysis indicates superior charge carrier mobility in  $\text{Rb}_2\text{ScCuF}_6$  compared to  $\text{Rb}_2\text{YCuF}_6$ .

Optically both compounds exhibit strong absorption in the 3-9 eV range covering ultraviolet to visible regions with static dielectric constants of 2.48 and 2.64, highlighting their potential for solar energy harvesting.

Regarding thermoelectric performance both materials display a high isotropic Seebeck coefficient (up to  $1.55 \times 10^3$  V/K) and moderately low lattice thermal conductivity (2.26 W/mK for  $\text{Rb}_2\text{ScCuF}_6$  and 2.18 W/mK for  $\text{Rb}_2\text{YCuF}_6$  at 300 K). A notably high-power factor of  $48 \times 10^{10}$  W/K<sup>2</sup>ms is achieved for  $\text{Rb}_2\text{YCuF}_6$ , with strong thermoelectric efficiency maintained at room temperature under both p-type and n-type doping. Collectively, these findings establish lead-free  $\text{Rb}_2\text{ScCuF}_6$  and  $\text{Rb}_2\text{YCuF}_6$  as promising multifunctional materials for optoelectronic and thermoelectric applications. This theoretical study provides valuable guidance for experimental synthesis and further optimization of environmentally friendly fluoride-based double perovskites.

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