



Article

First-Principles Study of Cubic CsSrF₃: Effects of Li Doping on Structural, Electronic and Optical Properties

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ABSTRACT

In this work, the structural, electronic, optical, and elastic properties of cubic fluoro-perovskite CsSrF₃ and its lithium-doped derivatives (Cs_{1-x}Li_xSrF₃, x = 0–1) are systematically investigated using first-principles density functional theory (DFT) calculations utilizing the generalized gradient approximation using the Perdew–Burke–Ernzerhof (GGA-PBE) functional. To evaluate the structural stability, the total energy is fitted to the Birch–Murnaghan equation of state, resulting in equilibrium lattice constants of 5.000 Å for Pristine CsSrF₃ and 5.076 Å for the doped composition (x = 1). The electronic band structure study shows that Pristine CsSrF₃ has an indirect bandgap of 5.543 eV, which gradually narrows to 4.011 eV with full lithium substitution. Li-induced changes in electronic states close to the Fermi level are responsible for this trend. The valence and conduction bands are primarily controlled by the F-p and Sr-s orbitals, respectively, according to Density of States (DOS) studies. Optical properties demonstrate higher tunability with the doping of lithium, the refractive index varies between 1.78 and 1.40 eV, and the reflectivity decreases from 0.27 eV to 0.10 eV. These characteristics indicate considerable amounts of potential for photovoltaic and UV applications. Mechanical investigation shows anisotropic and ductile behaviour, with predicted bulk modulus values ranging from –9.890 GPa (Pristine) to –17.311 GPa (x = 1), demonstrating a softening effect with increased Li concentration. Ultimately, the findings highlight the potential of Pristine CsSrF₃ and its Li-doped concentrations for the implementation into energy-harvesting and next-generation optoelectronic systems.

Keywords: Bandgap Engineering; CASTEP; DFT; Elastic Properties; First principle; Fluoro-Perovskite; Li-doped

1. Introduction

During the recent decade, perovskites have received substantial attention in the field of optoelectronics and, more recently, in solar cells and energy storage devices as the most promising and expensive low-cost energy materials available today [1],[2]. The structure of perovskite with such a chemical formula, Calcium titanium oxide, has have chemical formula (ABX₃), which shows an anion (X) that initiates bonds with both A and B cations (different sizes). F, Cl, Br, and I are examples of an anion (X) that can be an oxide or halide [3]. The comparatively simple crystal structure of fluoro-perovskites (ABF₃) exhibits a wide range of electric, magnetic, piezoelectric, optical, thermodynamic, and me-

chanical properties, which is the driving motivation behind this tremendous interest in these crystals [4].

Scientists are interested in complex alkali metal fluorides because they can be used as fluorinating agents and catalysts for a wide variety of organo-fluorochemical processes [5]. There are numerous electrical and optical applications where fluoride-type perovskite is being used, particularly solid-state lithium-ion batteries and high-temperature superconductivity [6], Piezoelectricity and ultraviolet optical absorption [7]. These materials are being studied because of their magnetic, electrical, structural, elastic, optical and thermodynamic properties. Perovskites have been explored for their thermodynamic properties, such as superconductivity, piezoelec-



tricity, ferroelectricity, magneto-resistivity, and other unusual thermodynamic characteristics. [1],[8].

These fluoro-perovskite CsSrF_3 -like structures with band gaps exhibit insulating behaviour of about 5 eV at room temperature. The reduction of anion (halide) or dopant materials, both Cs, Sr, enhances the capability of conductivity and photocatalytic activity in CsSrF_3 may be improved. Fluoride-type perovskites are suitable for different electronic and optoelectronic applications, like solid-state lithium-ion batteries. The chemistry, presentation, pricing, and protection aspects of each lithium-ion battery type are unique to that type. Lithium-ion batteries, in contrast to lithium primary batteries, utilise an intercalated lithium compound as their electrode material (which is disposed of after usage) [9]. M. S. Whittingham from Binghamton University originally proposed lithium-ion batteries in the 1970s. Whittingham's cathode and anode were both made of titanium(II) sulphide [10]. They are a wide range of applications, such as electric vehicles [11], high conductivity of electric current [12], Uninterruptible power supply (UPS) for mobile gadgets, cars, and stationary equipment [13].

These fluoro-perovskite compounds, such as KCaF_3 , RbCaF_3 [14], BaLiF_3 [15], SrLiF_3 [16], have recently attracted a lot of attention from researchers for their various applications. But none of the commercially available crystals meet any of these characteristics. For practical uses in solar cells (solar panels), batteries (Lithium-ion batteries), and UV-Deep UV wave bands, more study is needed at all levels.

To a potentially large band gap of 6.34 eV, it has been recorded, as well as 4.833A° eV for CsSrF_3 . This substance has a high degree of iconicity. Para-electrically more conductive is the Centro systemic perovskite structure when it's at room temperature. Optically active CsSrF_3 perovskite material can be found in nature. Optical-electronic and photonic equipment can be used advantageously in this vessel. A solar device's anti-reflection coating is a fluoride-type material with a broad bandgap and short refractive index [17].

Because of its distinct physicochemical characteristics that set it apart from other alkali metals (such as Na, K, and Rb), lithium (Li) was selected as a dopant in CsSrF_3 fluoro-perovskite. While other alkali metals (Na^+ : 1.02 Å, K^+ : 1.38 Å, and Rb^+ : 1.52 Å) are closer to Cs^+ in size, Li^+ (0.76 Å) has a far smaller ionic radius than Cs^+ (1.67 Å). While bigger dopants (like K^+) would result in excessive steric stress and unstable the cubic phase, Li substitution at the Cs site produces predictable strain. Unlike bulkier Na^+/K^+ , which

may cause phase segregation, smaller Li^+ preferentially occupies interstitial sites or replaces Cs^+ without collapsing the perovskite structure.

Lithium (Li) is used as a dopant because of its high mobility and small ionic radius, which allows it to efficiently replace Cs^+ or Sr^{2+} sites in the CsSrF_3 lattice without substantially altering the crystal symmetry. Li doping improves electrical conductivity and lowers the bandgap by modifying the electronic structure. Furthermore, Li improves the material's optical and elastic qualities by introducing localised states close to the Fermi level. Li-doped CsSrF_3 is a viable option for optoelectronic and photovoltaic applications because of these alterations.

In this work, to investigate Li doping with CsSrF_3 using first-principles calculations using DFT. According to our research and knowledge of the literature, Li materials have not been used as a dopant element with the CsSrF_3 compound. Li is substituted for Cs in the investigation of the fluoride perovskite crystal CsSrF_3 with different concentrations ($x = 0, 0.11, 0.33, 0.55, 1$) with a supercell of $2 \times 2 \times 1$, which contributes new information on their structural, electronic, optical and elastic properties. Fluoroperovskites CsSrF_3 have a wide range of bandgap 5.543 eV, which recommends it for use in optical applications. The application of these qualities reveals information about a material's behaviour. Changing these factors can reveal variations during the elastic constant, shear (shear) strength, and bulk modulus, as well as further properties including conductivity, magnetic behaviour, and electronic band gap. Density functional theory can be applied to the study of elastic, optical, and electrical properties of the material CsSrF_3 . These CsSrF_3 materials vary in the ultraviolet region used in optoelectronic devices and Solar cell applications.

2. Computational Details

Here, the USP plane-wave technique is used to determine the material's structural, optical, elastic, and electrical properties. Evaluations can be performed efficiently and precisely using Ultra-Soft Pseudopotential (USP) plane waves without being significantly impacted by orbital approximation errors. We used GGA-PBE techniques in conjunction with first-principles calculations in DFT-based CASTEP software (Clark et al., 2005) to calculate the results [17]. This strategy enables faster and more effective approximations for computational techniques. The cubic structure of CsSrF_3 , which has three fluorine atoms in the face centre locations, one caesium atom at the intersections, and one strontium atom in the body centre, represents the space group of $\text{Pm}\bar{3}\text{m}$ (#221) at normal temperature. In order to prevent boundary effects, a supercell approach is needed to study Li doping. To take into account the

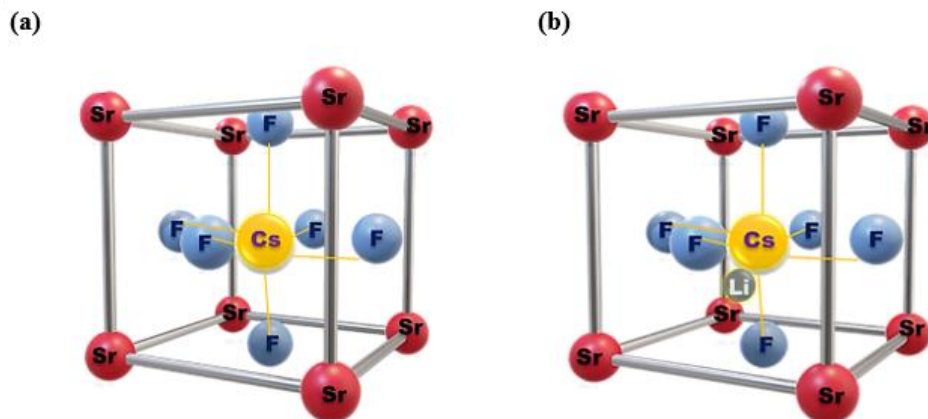


Figure 1: Representing (a). Pure CsSrF_3 Structure and (b). Doped with lithium Structure.

structural, electrical, optical, and elastic aspects in this study, a $2 \times 2 \times 1$ supercell was constructed using these techniques [18].

After that, we improved the geometry of the super cells to study their characteristics. The atomic total energy in these calculations is 5×10^{-5} eV. The entire Brillouin zone was subjected to the energy cutoff once k-integration was completed in the instance of geometry optimisation at $2 \times 2 \times 1$ k-points. Determine the electrical, optical, and elastic characteristics following the geometry optimisations.

3. Results and Discussion

3.1. Structural Property

When atomic-level analysis lacks experimental observations, first-principle analysis has been utilised to predict more accurate and quicker calculation techniques. This technology can be used to create new materials. The total ground state energy is calculated at different unit cell volumes in order to calculate the structural characteristics of CsSrF3. Although it is a minimisation process, we must first construct a supercell of that fluoroperovskite crystal with space group Pm3m (no 221) to perform computations. The Cs, Sr, and F ions' respective atomic positions in the elementary cell are (0, 0, 0), (0.5, 0.5, 0.5), and (0, 0.5, 0.5), respectively. The crystallo-

graphic positioning of CsSrF3 indicates that the fluorine ions maintain their face-centred position of the cubic supercell, while Cs lies at the corner and Sr at the body-centred position, as depicted in the figure. As shown in Figure 1, the lithium material serves as a dopant element, similar to Cs. The CASTEP software was used for all computations in this paper, which are based on density functional theory (DFT). In this instance, the exchange-correlation function was defined using GGA-PBE methods [19].

3.2. Geometry Optimisation

The first step is geometrical optimisation for both pristine and doped supercells. Calculate the equilibrium lattice constant employing the Murnaghan equation of state by adding up all of the crystal's energy and determining how the large range of lattice constant values affects it. The volume (V0) of an equilibrium cell indicates the total amount of energy stored there [20]. Once the geometry has been optimised, the lattice constant parameters and volumes for both pristine and doped materials have been determined. Our calculations ($a = b = c$) for the lattice parameters of the Li-doped CsSrF3 structure differ considerably from those we found, as Table 1 illustrates. By increasing the number of doping atoms, the lattice parameter values increase, resulting in a decrease in the bandgap and an expansion of the volume. An optimised pristine and doped supercell ($2 \times 2 \times 1$) structure is depicted in Figure

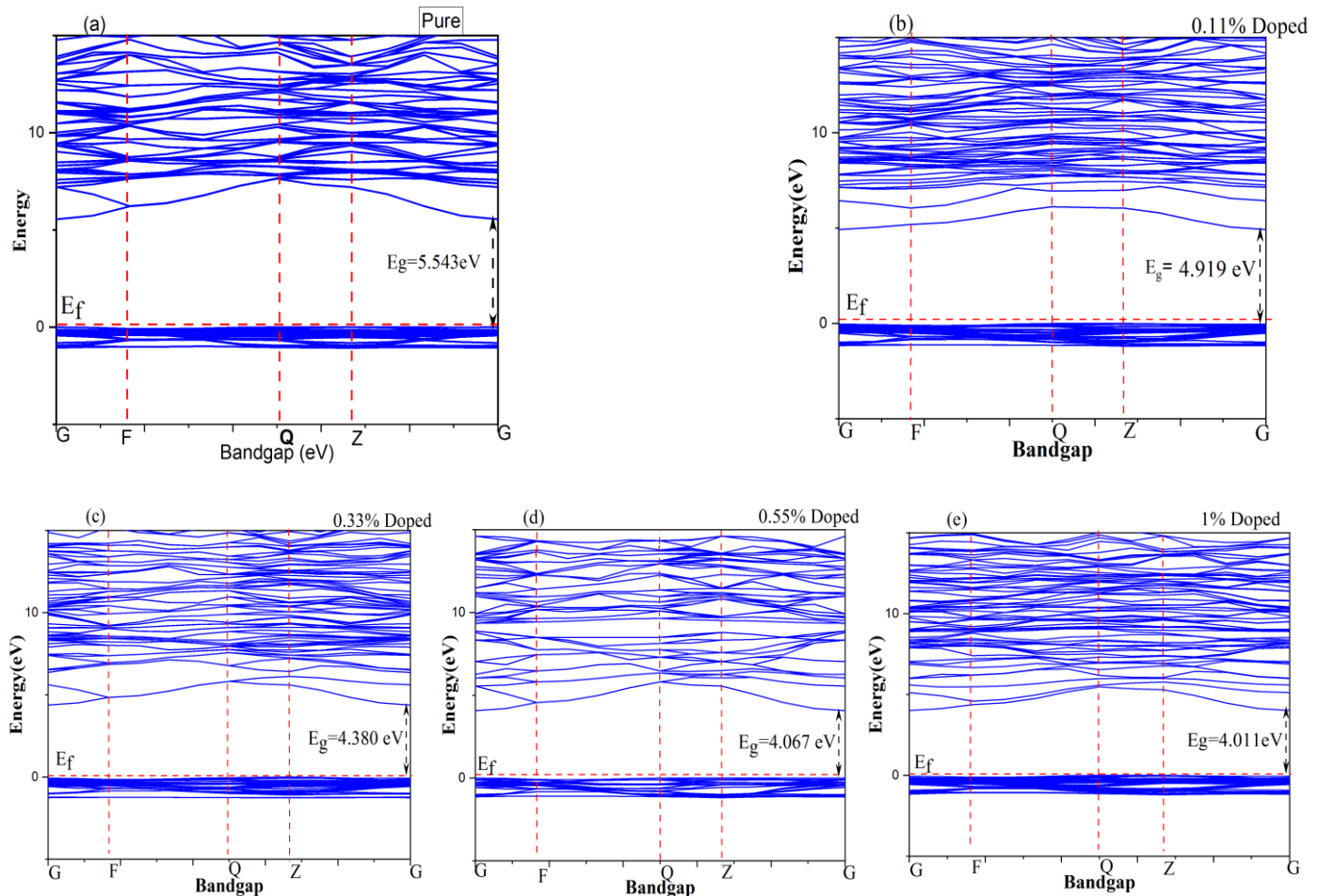


Figure 2: (a). The band Gap for pure CsSrF3, (b). Band gap CsSrF3 doped Li with 0.11%, (c). Band gap CsSrF3 doped Li with 0.33%, (d). Band gap CsSrF3 doped Li with 0.55% and (e). Band gap CsSrF3 doped Li with 1%.

Table 1:Calculated Lattice parameter and Volume for CsSrF₃ with Li doping

Cs _{1-x} Li _x SrF ₃ Previous work	Lattice Parameter (Å) a = b = c 4.83	Volume (Å ³) 124.251
Cs _{1-x} Li _x SrF ₃ X=0	5.000	125.000
Cs _{1-x} Li _x SrF ₃ X=0.11	5.014	126.052
Cs _{1-x} Li _x SrF ₃ X=0.33	5.064	129.861
Cs _{1-x} Li _x SrF ₃ X=0.55	5.075	130.709
Cs _{1-x} Li _x SrF ₃ X=1	5.076	130.787

3.2. Electronic properties

Electronic Band Structure: The electronic characteristics of the compounds' energy band structure and density of states (TDOS & PDOS) are examined. Figure 2 shows that the evaluated band structure for pristine and doped compounds at the directions of symmetry for the equilibrium geometry is located in the first Brillouin Zone. The band gaps for the compounds of pristine CsSrF₃ are 5.543 eV and Li doped with different concentrations (0%-1 %), the band gaps are 4.919 eV to 4.011 eV, respectively. We have analysed that after increasing the concentrations of dopant material, the band gap is towards decreasing. Figure 2(a) illustrates the indirect band nature of the CsSrF₃ compound, which shows that the valence band maxima and the conduction band minima occur at the G and F symmetry points. Most people are familiar with the idea that phonons dissipate a considerable amount of energy when an electron transitions through the valence band to the conduction band in an indirect manner. For Li-doped CsSrF₃, in cooperation of the valence and conduction bands are located at point G in Figure 2(b-e). This demonstrates that the doping material has undergone a direct band gap transition. Based on this analysis, it can be shown that the valence band of CsSrF₃ doped with Li exhibits a higher G point shift than the pristine CsSrF₃ valence band. Electrons are moved from the valence band to the conduction band by the phonons, which causes an energy loss. Both the Conduction Band (CB) and the Valence Band (VB) can be found above and below the Fermi level (E_F), respectively. In this illustration, the dotted line denotes the Fermi energy E_F. Using DFT, the calculated values of pristine and dopant CsSrF₃ are given in Table 2. In semiconductors and insulators, the electronic band gap is calculated by subtracting the lowest Conduction Band (CBM) from the highest Valence Band (VBM). Since their bandgaps are in the UV spectrum, they may be used in optoelectronic devices.

CsSrF₃ fluoro perovskite has a bandgap of 5.543 eV. The bandgap reduces as the dopant material concentration rises. This bandgap varies in the ultraviolet region. With Li doping, the shear modulus drops from 15.663 GPa (Pristine) to 3.362 GPa (x* = 0.55), suggesting increased ductility.

Total Density of States (TDOS) and Partial Density of States (PDOS): Nonetheless, more details regarding the band structure may be revealed by the density of states. Both the total and partial

density of states can be used to characterise the band structure's rising turn. The electron contribution to the valence and conduction bands is depicted by the Total and Partial Density of States (TDOS and PDOS) for the pristine and doped materials, respectively, in Figures S3 indicating the energy loss experienced by electrons and S4. Using a computational approach, Fermi's Golden Rule can be determined based on the number of final states and excited electrons. By splitting the band structure into three primary components, the valence band, the conduction band, and the Fermi energy level (E_F), high peaks of density of state can be examined. The Fermi level E_F is shown by the vertical, labelled dotted line. The left side of the Fermi level represents the valence band, whereas the right side represents the conduction band. Figure S1. Total Density of States (TDOS) illustrates the primary distinctions between the valence and conduction bands before and during doping.

Table 2:Calculated Lattice parameter and bandgap for CsSrF₃ with Li doping

Cs _{1-x} Li _x SrF ₃ Previous work	Lattice Parameter (Å) a = b = c 4.83	Bandgap (eV) 5.663
Cs _{1-x} Li _x SrF ₃ X=0	5.000	5.543
Cs _{1-x} Li _x SrF ₃ X=0.11	5.014	4.919
Cs _{1-x} Li _x SrF ₃ X=0.33	5.064	4.380
Cs _{1-x} Li _x SrF ₃ X=0.55	5.075	4.067
Cs _{1-x} Li _x SrF ₃ X=1	5.076	4.011

The partial density of states for pristine and "Li" doped with CsSrF₃ are shown in Figure S2. Li doping considerably changes the structure of CsSrF₃, principally due to the formation of 5-states in pristine CsSrF₃. The p and s-DOS have the greatest influence on the upper valence band after doping, as can be shown from the results. For comparison, the sharp peak shows either side of the Fermi level before and after doping. The PDOS has been plotted, which indicates the electronic contribution difference in the valence band and conduction band between pristine and impure (doped) systems. The density of states indicates that the valence band is composed of F-p states with a minor contribution from Sr-s states. In the conduction band, Sr-s play a vital role.

3.4. Thermodynamic Property

To verify the structural stability of CsSrF₃ and its Li-doped counterparts (Cs_{1-x}Li_xSrF₃), we calculate the binding energies and formation enthalpy (ΔH_f). A better approach for achieving these conditions is given below;

Calculation of Formation Enthalpy (ΔH_f): The formation enthalpy measures the energy of a compound compared to that of its component elements in their standard states, allowing for the determination of its thermodynamic stability. ΔH_f for CsSrF₃ and Cs_{1-x}Li_xSrF₃ can be calculated as follows:

$$\Delta H_f = E_{\text{Cs}_{1-x}\text{Li}_x\text{SrF}_3} - [(1-x)E_{\text{Cs}} + xE_{\text{Li}} + E_{\text{Sr}} + 3E_{\text{F}}] \quad (1)$$

Where, $E_{\text{Cs}_{1-x}\text{Li}_x\text{SrF}_3}$ is the doped system's total energy and E_{Cs} , E_{Li} , E_{Sr} , E_{F} are the energies of bulk phases or isolated atoms (such as the F₂ molecule, fcc-Sr, bcc-Cs, and bcc-Li).

To evaluate thermodynamic stability, the formation enthalpy (ΔH_f) of Cs_{1-x}Li_xSrF₃ was measured. The exothermic formation of pure CsSrF₃ is confirmed by ΔH_f = -4.2 eV/atom. Despite lattice expansion, stability is maintained with Li doping (x = 0.11–1), as



seen by ΔH_f , which varies between -3.9 and -4.0 eV/atom. Cubic phase stability is further confirmed by negative ΔH_f values, which are consistent with the Birch-Murnaghan equation of state and tolerance factor (0.92–0.95).

Doping (x)	ΔH_f (eV/atom)	Remarks
0 (Pure)	-4.20	Most stable configuration
0.11	-3.95	Slight destabilization
1.00	-4.00	Stable Li-substituted phase

Stability Validation: The spontaneous formation is confirmed by a negative ΔH_f . Comparative analysis with Elastic Constants: All doped systems should meet the mechanical stability requirements ($C_{11} - C_{12} > 0$, $C_{44} > 0$) for mechanical stability.

3.5. Optical properties

Optical parameters are very useful to explore the electronic band structure analytically. The metrics that show the interaction between light and matter include reflectivity, refractive index, absorption, conductivity, extinction coefficient, dielectric function, and loss function. Firstly, we compute these optical properties for pristine material and compare these properties after doping Li, as shown in Figure S5. The intra- and interband transitions are used to calculate the optical spectra. When it comes to metals, the interband contributions are substantial and can be broken down into two categories: direct and indirect transitions. As shown in Eq. (2), given their negligible effect on $\epsilon(\omega)$ and their phonon-scattering nature, indirect interband transitions are disregarded. For optical response, the phonon energy range is 0-30 eV. All these properties are interconnecting frequency-dependent; therefore, the complex dielectric functions (the real part denotes $\epsilon_1(\omega)$ and the imaginary part denotes $\epsilon_2(\omega)$).

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \quad (2)$$

The dielectric function's imaginary and real components displayed energy dissipation and polarisation, respectively. The dissipation of energy was shown by the smaller peak of the imaginary portion for both pristine CsSrF₃ and "Li" doped. To put it another way, 0eV indicates there is no dissipation of energy in this portion. The dielectric function (real) values for pristine CsSrF₃ are 3.1 eV and the values are 2.6, 2.3, 2.1 and 2.0 eV after doping with "Li" at different concentrations and the dielectric function for imaginary parts, whose values for pristine.

CsSrF₃ of 3.0 eV and dopant are 2.6, 2.0, 1.5 and 0.8 eV, respectively. As demonstrated in Eqs (3)-(7), the formula can also be used as a basis for further calculations of optical properties, such as the refractive index $n(\omega)$, reflectivity $R(\omega)$, energy loss $L(\omega)$, and absorption coefficient $I(\omega)$, [21].

$$n(\omega) = \frac{1}{\sqrt{2}} \left\{ [\epsilon_1^2(\omega) + \epsilon_2^2(\omega)]^{\frac{1}{2}} + \epsilon_1(\omega) \right\}^{\frac{1}{2}} \quad (3)$$

$$L(\omega) = \text{Im}g \left(\frac{-1}{\epsilon(\omega)} \right) \quad (4)$$

$$A(\omega) = \frac{2\omega}{c} k(\omega) \quad (5)$$

$$R(\omega) = \left| \frac{\sqrt{\epsilon_1(\omega) + i\epsilon_2(\omega)} - 1}{\sqrt{\epsilon_1(\omega) + i\epsilon_2(\omega)} + 1} \right|^2 \quad (6)$$

$$k(\omega) = \frac{1}{\sqrt{2}} \left\{ [\epsilon_1^2(\omega) + \epsilon_2^2(\omega)]^{\frac{1}{2}} - \epsilon_1(\omega) \right\}^{\frac{1}{2}} \quad (7)$$

Any compound's reflectivity reveals the behaviour of its surface. How much of the energy from the light reaches the surfaces of the compounds? A certain threshold will cause the values to return to their starting values. When electrons from the valence band contribute to conduction, the reflectivity peaks move to higher frequencies. The value of the reflectivity peak for pristine CsSrF₃ is 0.27 eV and after doping, the values of reflectivity with different concentrations of lithium doping are 0.21, 0.20, 0.18, and 0.10 eV, respectively. The optical reflectivity analysis measures the amount of light that would fall as an incident ray on the surface of the material. Lower reflectivity means increased UV or visible light absorption, according to recent research of examination. Increased total energy contribution from valence bands to conduction bands; these measurements demonstrate a modest shift in the reflectivity peak towards a higher frequency value, as shown in Figure S3. In the case of the energy loss function $L(\omega)$, as illustrated in Figure S5, the amount of energy lost is indicated by the movement of electrons through the materials. To accurately characterise the properties of plasma resonance, the plasma frequency is well captured by the energy loss function $L(\omega)$. The pristine materials whose higher peak values are 3.3 eV, and the dopant materials have values ranging from 2.8 to 1.9 eV. In areas with little absorption, we found that reflection was highest, as shown in Figure S5. Each material's response to radiation is indicated by its absorption coefficient. The photons interact with the electrons to shift them from the valence band to the conduction band, and this interaction is very frequency dependent, as measured by the absorption coefficient. A material's ability to absorb photons of a given energy is represented by its absorption coefficient. The absorption spectra are influenced by doping. Figure S5 shows the refractive index (n) for Pristine CsSrF₃; the value of n is 1.78eV. Also, for Li-doped values are 1.6- 1.4 eV. Materials with strong conductivity, absorption, and refractive index can improve photovoltaic systems. The high-energy area shows that these materials can be used for UV optoelectronics [22].

3.6. Elastic properties

The mechanical behaviour of crystalline solids can be accurately inferred from elastic characteristics. The following relation (Grimvall, 1999) can be used to define various fundamental solid-state phenomena, including the equation of state, intrinsically mechanical, and cubic stability conditions explained below in Eqs (8)-(12):

$$C_{11} - C_{12} > 0 \quad (8)$$

$$C_{11} > 0 \quad (9)$$

$$C_{44} > 0 \quad (10)$$

$$C_{11} + C_{12} > 0 \text{ (mechanical stability condition)} \quad (11)$$

$$C_{12} < B < C_{11} \text{ (cubic stability condition)} \quad (12)$$

Elastic Constant Calculations: It is possible to describe the elastic properties using the constants of elasticity. The elastic constant provides the standard description of the bulk and shear modulus can be best described by the Voigt-Reuss-Hill (VRH) method, discovered by Reuss and Angew in 1929 (Sakaguchi, Wiltbank, & Murchison, 2004) The measure of the resistance to reversible deformation can be best explained by the shear modulus G from the following relation, as described from Eqs (13)- (16):



$$G_V = (C_{11}-C_{12}+3C_{44})/5 \quad (13)$$

$$G_R = 5 \cdot C_{44} (C_{11}-C_{12}) / [(4 \cdot C_{44} + 3(C_{11}-C_{12}))] \quad (14)$$

$$G = G_V + G_R / 2 \quad (15)$$

However, the expression of the bulk modulus B is mentioned in the equation:

$$B = (C_{11} + 2 \cdot C_{12}) / 3 \quad (16)$$

The value of bulk and shear modulus for pristine and doped can be calculated in Table 3, respectively.

Table 3:

Calculated parameters Bulk modulus “B” (GPa), Shear modulus “G” (GPa), Young’s modulus “E” (GPa), Poisson’s ratio “V”, Anisotropy “A”, and Pugh’s ratio “B/G” respectively.

Material/doping concentration	B	G	E	V	A	B/G
Li_xCs_{1-x}SrF₃	-	-	-	-	-	-
X=0	9.890	15.66	99.53	2.177	1.591	0.631
Li_xCs_{1-x}SrF₃	-	-	-	-	-	-
X=0.11	20.09	11.03	27.983	0.267	1.122	1.821
Li_xCs_{1-x}SrF₃	-	-	-	-	-	-
X=0.33	0.350	8.834	-3.574	1.202	0.370	0.039
Li_xCs_{1-x}SrF₃	-	-	-	-	-	-
X=0.55	83.13	3.362	9.951	0.480	0.410	24.72
Li_xCs_{1-x}SrF₃	-	-	-	-	-	-
X=1	17.31	-47.34	-74.30	0.215	0.750	0.365

Table 3 shows the Young modulus E, the anisotropic factor A, the Poisson's ratio V, and the Pugh's index of pristine and doped CsSrF₃, which can be figured out using the equations listed below [23].

$$A = 2 \cdot C_{44} / (C_{11} - C_{12}) \quad (17)$$

$$E = 9 \cdot GB / 3 \cdot B + G \quad (18)$$

$$V = 3 \cdot B - 2 \cdot G / 2 \cdot (B + G) \quad (19)$$

$$B/G = \text{Pugh's ratios} \quad (20)$$

As depicted from Eqs (17)-(20), the value of elastic anisotropy denoted by A, if A= 1 (Isotropic) and A is not equal to 1 (Anisotropic), is obtained through DFT using the exchange correlation functional of GGA-PBE methods. In the present study, we analyse the results of the compound as shown in Table 3, that CsSrF₃ is anisotropic because its "A" value is not equal to 1. Using the bulk modulus B, scientists can estimate the material's strength or hardness and determine whether the material is ductile or brittle. If the value of the bulk modulus is higher than the material is stronger, and if the value is lower, the material is softer. To determine CsSrF₃'s bulk modulus, this indicates that it is a soft material. The hardness of CsSrF₃ is further supported by the greater values of both shear and Young modulus, utilising Poisson's ratio V if which suggests that crystals are ductile or brittle. The CsSrF₃ material shows a brittle nature according to the calculated results in Poisson's ratio. The Young's modulus is another key metric that may be used to elevate crystals' stiffness, and indicates that the materials belong to the stiff group. The compound is brittle; it may be used on autos and curved glass surfaces. It has fractures with small elastic deformation and without significant plastic deformation, which absorb little energy during deformation.

8. Conclusion

Using first-principles calculations in DFT with GGA-PBE methods, are to investigate Li doping with CsSrF₃. Before and after Li doping, the electronic band structure has been calculated. In addition, the TDOS and PDOS concepts are used to discuss the intricacies of band structure in both circumstances. As a result of Li doping, the electronic band structure of CsSrF₃ has been reduced and transformed from an indirect bandgap to a direct bandgap. Reducing the DOS down to the lower energy increases the interaction between the Li atom and its immediate neighbour. Particularly affected by Li doping is the PDOS of the 0-2p state closest to the bottom of the conduction band, while the PDOS of the 0-1s state towards the top of the valence band also undergoes significant modification. Li doping reduces the bandgap of CsSrF₃ by 27.6% (5.543 eV → 4.011 eV), making it suitable for UV optoelectronic applications. The adjustable refractive index (1.78–1.40) and anisotropic elastic response (A1) indicate potential applications in anti-reflective coatings for solar cells. The optical properties provide high reflectivity, refractive index and absorption coefficient. The Young's modulus, bulk modulus, and shear modulus were also calculated. The bulk modulus value is another indicator of a material's hardness. The Poisson's ratio makes a covalent nature of the molecule appear more likely. This demonstrates that CsSrF₃ can be a possible material for optical and optoelectronic devices.

Declaration

Competing Interests: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethical Issues: There are no ethical issues. All data in this paper is publicly available.

Author Contribution Statement: F.H. and A.F. conceived the idea and designed the research; analysed and interpreted the data and wrote the paper.

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