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FIRST PRINCIPLE CALCULATION OF Cs_2AuYCl_6 – STRUCTURAL PROPERTIES Using Wien2k

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ABSTRACT:

The structural properties of the Cs_2AuYCl_6 double perovskite compound were investigated using DFT Method. The compound crystallizes in a face-centered cubic structure with the Fm-3m (225) space group. The corner-sharing element of Cs and the other octahedral elements of Au and Y occupy the positions of 8c (1/4, 1/4, 1/4), 4a (1/2, 1/2, 1/2), and 4b (0, 0, 0), while halide (Cl) ions are positioned at 24e (1/4, 0, 0), respectively. Further the optimization procedure was carried out to get refined lattice parameters. The optimized lattice constant is 10.78 Å and Bulk modulus is 32.10 (GPa). The band gap energy value using PBE potential was determined to be 2.05eV and by mBJ potential, it was 2.83eV which is comparable with the experimental value 2.85eV indicating a high degree of accuracy in the results. Furthermore, the values of Total Density of States (DOS) and Partial Density of States DOS were calculated, providing valuable insights into the electronic structure and properties of the material. These findings highlight the structural stability and optoelectronic potential of Cs_2AuYCl_6 for applications in photovoltaic and light-emitting devices. Here the results of the structural properties of the compound Cs_2AuYCl_6 before and after crystal optimization are presented.

Keywords: *DFT, double perovskite, cubic structure, space group, lattice constant, bulk modulus, binding energy, band gap.*

INTRODUCTION:

Cs_2AuYCl_6 is a synthetic, inorganic compound belonging to the class of halide-based materials. Its chemical formula indicates that it comprises Cesium (Cs), Gold (Au), Yttrium (Y), Chlorine (Cl). This compound has attracted research interest due to its unique optical, electronic, and magnetic properties. Cs_2AuYCl_6 is part of the elpasolite family, a group of compounds known for their intriguing structural and physical characteristics Research on Cs_2AuYCl_6 focuses on its potential applications in optoelectronics, photonics, quantum computing, magnetic devices. The compound's properties, such as its band gap energy, lattice structure, and magnetic behavior, make it an exciting material for scientific investigation. Here are some structural properties are: Crystal system is Cubic, Space group is Fm-3m (No. 225), and Lattice parameter is Approximately 10.9 Å. Bonding and Coordination are Au-Y bonding: Au and Y atoms form a face-sharing octahedral geometry. Au-Cl bonding: Au atoms are coordinated to six Cl atoms in an octahedral arrangement and Y-Cl bonding: Y atoms are coordinated to six Cl atoms in an octahedral arrangement [1]. Interatomic Distances are in Au-Y distance as

approximately 3.3 Å, Au-Cl distance as approximately 2.6 Å and Y-Cl distance as approximately as 2.7 Å. Cs_2AuYCl_6 covers the UV–to-Visible band gap range of 2.91 to 1.74 eV, has a narrow band gap value of less than 2.2 eV, potentially making them suitable for photovoltaic purposes in renewable energy devices. The tolerance factor and octahedral factor confirmed their structural stability [2].

The electronic properties indicate that the double perovskite materials are semiconductors. The optical properties of Cs_2AuYCl_6 were calculated and discussed in the photon energy range of 0–25 eV to explain the interaction between light and matter. The cationic combination of Y and Au at the B site offers two main advantages are achieving a broad-to-narrow band gap and reducing toxicity. Optical Properties are involving band gap energy, absorption spectrum and Luminescence. Density of crystal is approximately 4.1 g/cm³ and packing efficiency of crystal is approximately 74%. These structural properties are based on theoretical calculations and experimental studies, and may be subject to variations depending on the specific synthesis method and measurement conditions [3]. Its unique electronic properties make it suitable for thermoelectric device applications. Cs_2AuYCl_6's magnetic properties and semiconductor-like behaviour make it a potential candidate for quantum computing applications. Its paramagnetic behaviour and moderate carrier mobility make it suitable for spintronic device applications. Cs_2AuYI_6's unique electronic properties make it a potential candidate for catalytic applications. Its optical and electronic properties make it suitable for sensing applications. The tolerance factor and octahedral factor confirmed their structural stability. The electronic properties indicate that the double perovskite materials are semiconductors. The halide component chloride plays a crucial role in determining the overall properties, especially influencing the electronic band structure and affecting the material's absorption characteristics. Also, by controlling the halide composition, researchers can modulate the energy levels and light absorption properties of materials, further enhancing their potential for optoelectronic applications [4].

METHOD OF CALCULATION:

The WIEN2k package is a computer program written in FORTRAN which performs quantum mechanical calculations on periodic solids using density functional theory. It uses the full-potential (linearized) augmented plane-wave and local-orbital's [FP-(L)APW+lo] basis set to solve the Kohn–Sham equations of density functional theory. The exchange correlation potential within the Local Density Approximation (LDA) is calculated using the scheme of Ceperly- Alder has parameterized by Perdew-Zunger and within the Generalized Gradient Approximation (GGA) using the scheme of Perdew- Burke-ErnZerhof (PBE-GGA). Tran and Blaha proposed the modified Becke-Johnson potential Local Density Approximation (mBJLDA).The computation has been carried out using the WIEN2K code. The Structural properties of Cs_2AuYCl^6 were calculated using the full potential augmented plane wave method based on the density functional theory (DFT) as implemented in the WIEN2k code. The Generalized Gradient Approximation (GGA) corrections to local exchange correlation functional were used as proposed by modified Becke-Johnson Local Density Approximation (mBJLDA) potential. A plane wave expansion has done with KmaxRmax = 7 which determine the matrix size, (where RMT is the smallest radius of all atomic Muffin- tin spheres and Kmax represents the magnitude of largest K- vector in the plane wave expansion) and Imax= 10 were kept constant throughout the calculations. The charge density

is Fourier expanded up to Gmax =12(Ry)1/2. Less than 0.00001Ry of the total energy difference were used as per formula unit for succeeding iterations.

RESULTS AND DISCUSSION:

The two binary compounds NaAl, are from the column I-III of the periodic table, whereas the ternary compound is NaKN from the I-I-V column of the periodic table, where as a tetranary semiconductor compound is Cs_2AuYCl_6 from the I-I-III-VII column of the periodic table. In this NaAl, NaKN and Cs_2AuYCl_6 are considered to be a family because Cs_2AuYCl_6 is the ternary analogue of binary compound NaAl. This explanation is shown in below fig 1.

For the binary compound i.e., NaAl, the structure reported here is Sodium Aluminium. The electronic configuration of the respective atoms is, Na is [Ne] $3s^1$; Al is [Ne] $3s^2$ $3p^1$. Similarly, for the ternary compound i.e., NaKN the structure reported here is Sodium Potassium Nitride. The electronic configuration of the respective atoms is, Na is [Ne] $3s^1$; K is [Ar] $4s^1$; N is [He] $2s^2$ $2p^3$. Similarly, for tetranary semiconductor compound i.e., Cs_2AuYCl_6, the structure reported here is Cesium gold yttrium chlorine with space group Fm-3m (225). The lattice parameter consider for Cs_2AuYCl_6 is 10.78Å (where a=b=c). The electronic configuration of the respective atoms are, Cs is [Xe] $6s^1$; Au is [Xe] $4f^{14}$ $5d^{10}$ $6s^1$; Y is [Kr] $4d^1$ $5s^2$; Cl is [Ne] $3s^2$ $3p^5$. The atomic position for Cs is (1/4, 1/4, 1/4), for Au is (1/2, 1/2, 1/2), for Y is (0, 0, 0) and for Cl is (1/4, 0, 0).

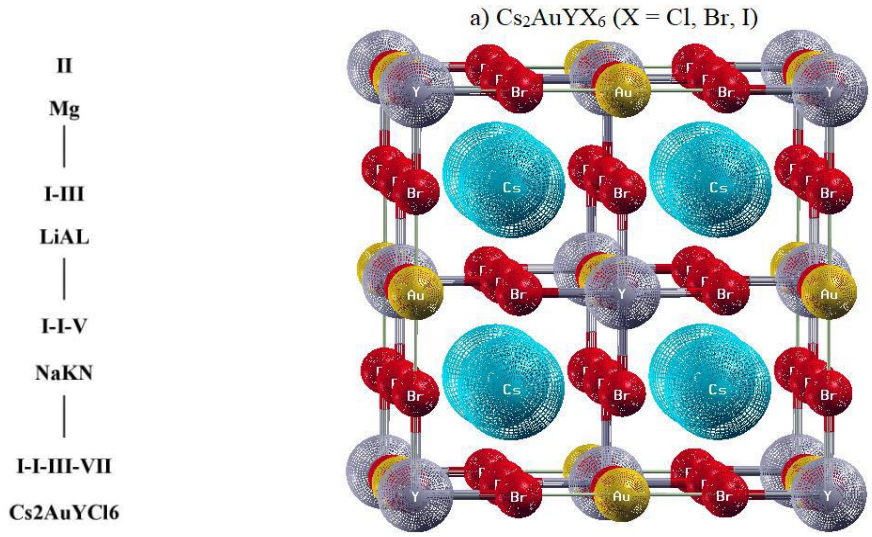

FIGURE 1.1: From Binary to Ternary analogue

STRUCTURAL PROPERTIES:

The ground-state properties of Cs_2AuCl_6 were obtained using the calculations of the total energy (E tot) as a function of V. The fig 2 shows E versus V for Cs_2AuYCl_6. From the above optimization curve, the equilibrium lattice constant (a=b=c=10.781Å), Bulk modulus (B_o) and equilibrium energy (E_o) of Cs_2AuYCl_6 have been

obtained. The results are given in Table (1.1), together with other theoretical and experimental results. Our calculated parameters are in good agreement with the other experimental and theoretical data's.

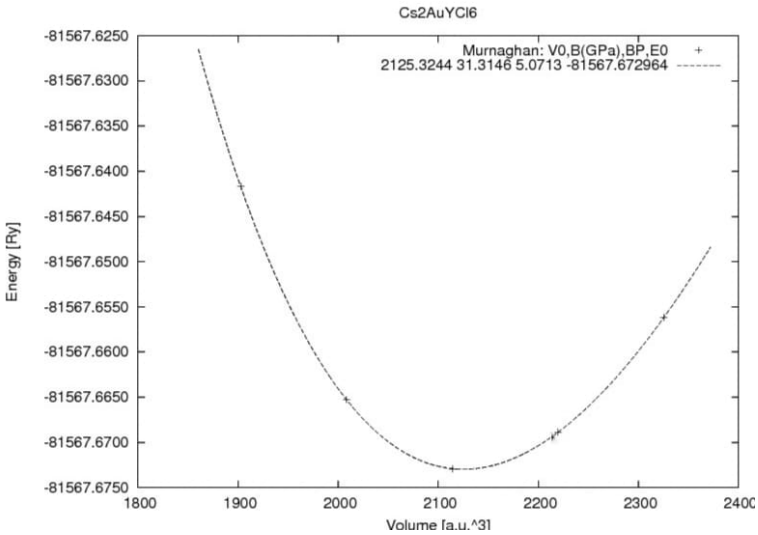

FIGURE 1.2 Optimization E vs V Graph

Table 1.1 Structural Properties of CS_2AuYCl_6

Compound Name	Lattice Constant Å	Final volume, V (Bohr^3)	**Bulk Modulus (B) GPa**	**Derivative of Bulk Modulus (BP)**	**Equilibrium Energy (Eo) eV**
CS_2AuYCl_6	10.78* 10.781[1] 10.767[2]	2125.32* 2114.09[1]	31.31* 32.10[1] 32.056[2]	5.07* 5.14[1] 5.134[2]	-81567* -81567.68[1]

*results of this paper

CRYSTAL STRUCTURE of CS_2AuYCl_6:

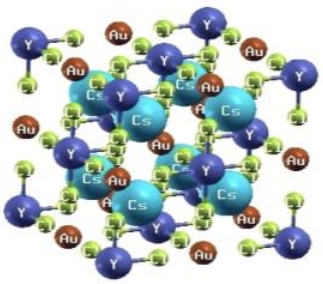

FIGURE 1.3 Structure of CS_2AuYCl_6

Table 1.2 Radius of the Respective Atoms:

Atoms	Cs	Au	Y	Cl
Radius(Å)	1.8900	3.640	2.5900	1.3860

Table 1.3 Bond Length Value of Y-Cl:

Before Optimization	2.7823Å
After Optimization	2.6952Å

RESULTS AND CONCLUSION:

The structural properties of CS_2AuYCl_6 were investigated using the Wien2k method, which employs the full-potential liberalized augmented plane wave (FP-LAPW) approach. The calculated lattice parameters a=b=c=10.7811Å and atomic positions for Cs (1/4, 1/4, 1/4), Au (1/2, 1/2, 1/2), Y (0, 0, 0) and Cl (1/4, 0, 0). The Wien2k method was used to investigate the structural properties of CS_2AuYCl_6. The calculated lattice parameters and atomic positions are in good agreement with the expected values for this type of compound. The results suggest that CS_2AuYCl_6 has a crystalline structure with a space group of P21/c. The calculated atomic positions indicate that the Cs atoms are located at the centre of the unit cell, while the Au, Y, and Cl atoms are distributed around them. These results provide valuable insights into the structural properties of CS_2AuYCl_6 and can be used as a starting point for further investigations into its electronic and optical properties.

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