# Electronic and optical properties of novel double perovskite compound $Cs_2RbInI_6$

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Novel energy materials grab the attention of researchers because of the huge demand for green energy sources. We have attempted to investigate the physical properties of such material which will be suitable for photovoltaic applications. Double perovskites of $A_2BB'X_6$ framework have been conspicuous materials by the virtue of their magnificent electronic and optical properties. We have computed the physical properties of $Cs_2RbInI_6$ double perovskite compound using the first principles method along with density functional theory (DFT). Complete computational analysis has been done within wien2k simulation code which is based on full potential linearized augmented plane wave method.

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## 1. Introduction

Solar power is acquired from the sun through photovoltaic cells. Photovoltaic cells do not negatively impact the environment in any sense and make the sun's energy usable. Currently, numbers of research communities have engaged in increasing the PCE of photovoltaic cell so that they can accomplish the global energy demand with a green energy source. Consequently, research in the field of photovoltaic cells is increasing abruptly. Investigate a suitable photo absorbing material to develop cost-effective and efficient photovoltaic cells is still a great challenge. Overall efficiency of cells mainly depends on absorption of photo absorbing material and their fabrication method. However, there are several kinds of solar cells that have been investigated till now such as thin film solar cell [1], dye sensitized solar cell [2-3], organic solar cell [4], hybrid solar cell, heterojunction solar cell [5-7], tandem solar cell [8] etc; Research has already on their epitome still we are far from enough beneficiary results. Kunzmann *et al* [9] have designed the low temperature dye sensitized solar cell and achieve the photo conversion efficiency of 8.75% in 2018. The power conversion efficiency of 14.7% has been achieved with single junction organic solar cell [10]. Lee *et al* [11] have discussed the applicability and reliability of amorphous silicon, copper indium gallium selenide and cadmium telluride based thin film solar cells. There are a number of materials that have been investigated as good photo absorbers till now such as silicon, perovskites etc.

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Commercially 90% of the market is taken over by wafer based silicon solar cells [12]. According to Andreani *et al* [12], crystalline silicon based solar cells can reveal the limiting efficiency upto ~ 29% but we are much optimistic about it and believe that the better is yet to come. However, silicon is a good photo absorbing material due to their convenient band gap but their high-cost fabrication method is undeniable obstruction [13]. To achieve better power conversion efficiency one should need the work on fabrication methods. Eperon *et al* [14] have fabricated the organo-metal halide perovskite based solar cell and attained the highest surface coverage with the help of morphological control. With the help of such an easier and cheaper processing method they achieved an efficiency of 11.4%.

In the era of silicon based thin film solar cells, perovskites emerged as promising semiconducting material for high efficient solar cells [15]. Any material based on the formula $ABX_3$, is called perovskites where A, B are cations and X is an anion. The first discovered perovskite was calcium titanate $CaTiO_3$. Due to availability of multiple substitutions for A, B and X, one can obtain a huge number of compounds with this structure [16]. Their fabulous intrinsic properties such as defect tolerance, high emission color purity, high photoluminescence quantum efficiency and broad tunability of bandgap made them applicable for several devices [17]. These compounds manifest variety of applications in the field of photovoltaic, light-emitting diodes, lasers, light signal detectors, biomedical sensing, video imaging, environmental monitoring and photo-detectors due to their wide range properties [18-21]. Herein, our all concern is about photovoltaic cells. In 2009, Kozima *et al*. [22] has been designed the very first Organo-metal halide based perovskite solar cell; they have achieved the efficiency of 3.13% and 3.81% with $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ respectively. Eperon *et al.* [23] have designed the Organo-metal halide perovskites based tandem solar cell and achieved the efficiency of 20.3%. Green *et al*. [24] reported that the power conversion efficiency of thin film perovskite solar cell increased up to 25% by 2020. Silicon based single junction solar cell reveals the PCE up to 26% till now which is comparable to the perovskite based thin film solar cell [24]. NREL has been achieved the PCE of 31.3% with perovskite based tandem cell. On the basis of Shockley-Queisser limit, one can achieve the PCE up to 31.4% with lead halide perovskite [25]. Among the whole class of perovskites, the most beneficiary results have been achieved with lead halide perovskites [26-28]. Bhatt *et al.* [29] demonstrated that organic-inorganic lead halide perovskites having excellent electronic and optical properties such as ferroelectric properties, domain walls, lattice point defects, dynamic disorder, controlled doping ability and proper band alignments. Zhou *et al.* [30] have discussed that the lead halide perovskites are not only good light absorber but also potential candidate for charge transport layer due to their high charge mobility, long carrier diffusion length, high extinction coefficient and long carrier lifetime. Brivio *et al.* [31] have done the first principle calculation for hybrid perovskites. They have studied the structural and electronic properties of $MAPbI_3$ with VASP computational code. On the basis of performance, organometallic perovskite based solar cells are much better than organic solar cell or dye-sensitized solar cell [32]. Sun *et al.* [33] proposed an efficient way to analyze the thermodynamic stability of halide perovskites and reported that the cubic perovskites are thermodynamically stable compounds. Tenuta *et al.* [34] have revealed that the chemical stability of inorganic halide perovskites is much better than hybrid halide perovskites.

In recent progressive erudition regarding energy research, having the number of double perovskite frameworks like $A_2BB'X_6$, $A_2B_2X_6$ and $A_2BX_6$ have been of great concern. Some double perovskite compounds of these frameworks have been behaving as conductors, some as insulators and few of them as semi-conductors. For the purpose of optoelectronic applications, we have interested in semi-conducting materials. Herein, we have computed the structural, electronic and optical properties of the $Cs_2RbInI_6$ with the first principles method.

## 2. Computational method

For the simulation of physical properties like crystal structure, electronic and optical properties of solids, DFT has been used in immense. Wien2k code is basically based on DFT along with full potential linearized augmented plane wave method (FPLAPW) which considered the all

electrons (core electron + valance electron) for further analysis [35]. In this method, iterations operated for Kohn-sham equations until self-consistency has reached which gives us the electron density for all occupied states. For exchange and correlational functional, we have various approximations like Perdew-Burke-Ernzerhof (PBE), Wu-Cohen (WC), local density approximation (LDA), TB-mBJ and Koller-mBJ. According to Wu *et al.*[36] have been most convenient approximation for volume optimization which manifests the lattice constant.

## 3. Results and discussion

### 3.1. Structural Properties

$Cs_2RbInI_6$ possesses the $Fm\bar{3}m$ space group with corner sharing octahedral geometry and $Cs^{+1}$ having the position in cuboctahedral void [37]. In the case of $Cs_2RbInI_6$, anions of $I^-$ form the octahedral along this $Rb^{+1}$ and $In^{+3}$ having the alternate position in octahedral voids. We have been considered the Wyckoff positions [38] for $Cs_2RbInI_6$ are: Cs: 8c (0.25,0.25,0.25), Rb : 4α (0,0,0), In: 4b (0.5,0.5,0.5) and I: 24e (y,0,0). As structural properties, we have computed the ground state energy, lattice constant and bulk modulus of $Cs_2RbInI_6$. We have done the volume optimization accompanying the least square curve fitting of ground state energy versus volume by WC approximation which is represent in figure 1. With the help of volume optimization, the computed lattice constant for $Cs_2RbInI_6$ is 12.3609Å. Ground state energy and bulk modulus of $Cs_2RbInI_6$ is -134327.043Ry and 14.6905GPa.

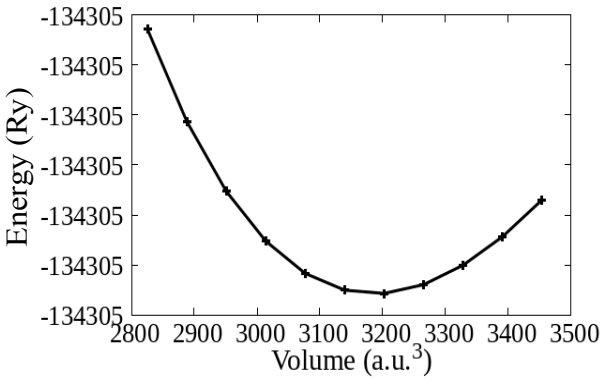


*Fig. 1. Volume optimization of $Cs_2RbInI_6$ with WC approximation.*

### 3.2. Electronic Properties

We have estimate the energy band gap within the PBE, TB-mBJ and Koller-mBJ exchange energy functional. $Cs_2RbInI_6$ exhibit the band gap of 0.726eV, 1.515eV and 1.529eV with PBE, TB-mBJ and Koller-mbj respectively. According to Koller *et al.* [39] have predicted the band gap with better accuracy whereas PBE and TB-mBJ exchange potentials underestimate the band gap of perovskite materials. Therefore we have evaluated all electronic and optical properties of $Cs_2RbInI_6$ within Koller-mBJ potential. As electronic properties, we have estimated the total density of states, projectile density of states and dispersion curve for $Cs_2RbInI_6$ as shown in figure1. Fermi energy level set at 0eV. In the figure 2(A) energy from -4eV to 0eV represent the valance band and energy from 0eV to 6eV represent the conduction band. In the upper valance band there is immense contribution of p orbital of $I^-$ and $Rb^+$ for total density of states. Total density of states of lower conduction band is form of s orbital of $In^{+3}$.

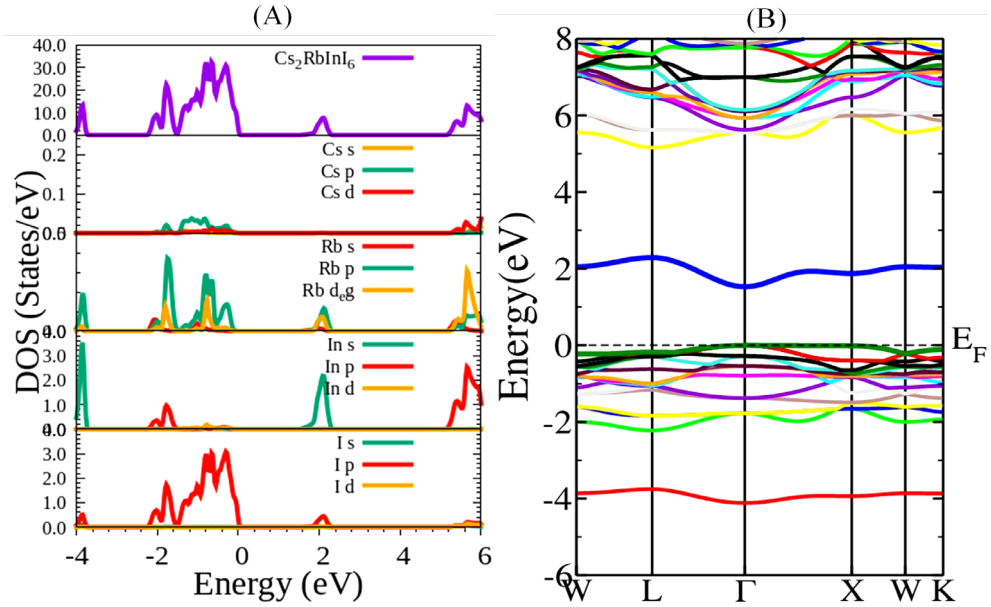


*Fig. 2. (A) Total density of states for $Cs_2RbInI_6$ with projectile density of states corresponding to orbitals associated with conduction band minima and valence band maxima, (B) Dispersion curve for $Cs_2RbInI_6$ where $E_F$ is Fermi energy level.*

Dispersion curve for $Cs_2RbInI_6$ manifest the valance band and conduction band separated by fermi energy level which is set at 0eV. $Cs_2RbInI_6$ possesses the direct band gap of 1.529 eV in Γ-direction. According to Shockley-Queisser limit the band gap of 1.529 eV is convenient band gap for photovoltaic applications.

### 3.3. Optical Properties

We have computed the optical properties like absorption coefficient α(ω), reflectivity R(ω) and optical conductivity σ(ω) for $Cs_2RbInI_6$ as shown in figure 3.

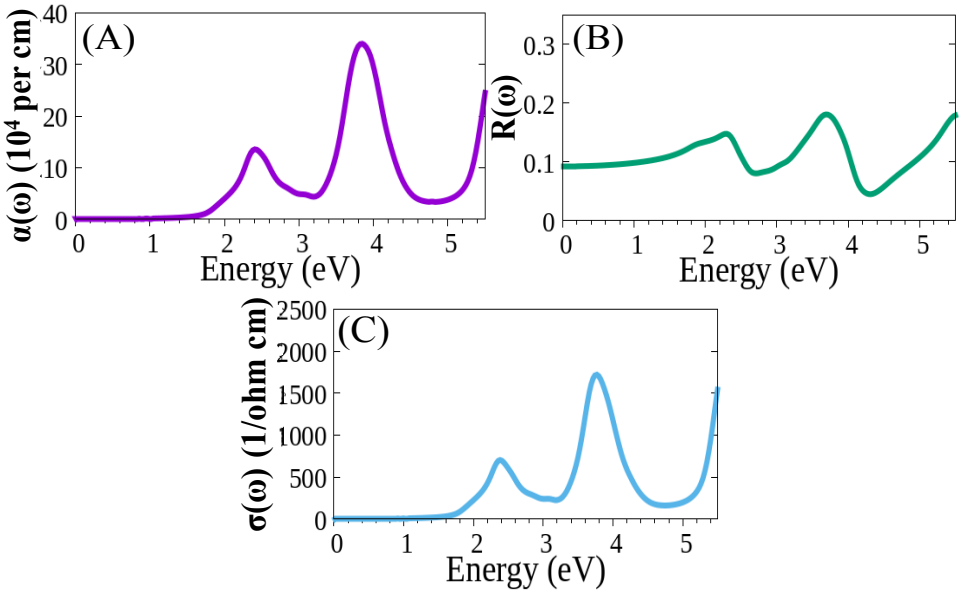


*Fig. 3. Dependency of (A) absorption coefficient α(ω), (B) reflectivity R(ω) and (C) optical conductivity σ(ω) on energy for $Cs_2RbInI_6$.*

$Cs_2RbInI_6$ exhibit the high absorption, low reflectivity and high optical conductivity. Absorption coefficient of the compound is depending on number of transitions occurs from valance band to conduction band which is based on Fermi-Golden rule accompanying by momentum matrix element. Real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ dielectric constant is evaluated by the Kramers-Kronig relations as manifest in fig.4. Static dielectric constant for the $Cs_2RbInI_6$ is 3.506. High dielectric constant leads to the low carrier recombination rate along with high power conversion efficiency. We have also enumerated the refractive index $\eta(\omega)$ and extinction coefficient $\kappa(\omega)$ for our compound which can be seen in figure 4(C)and 4(D).

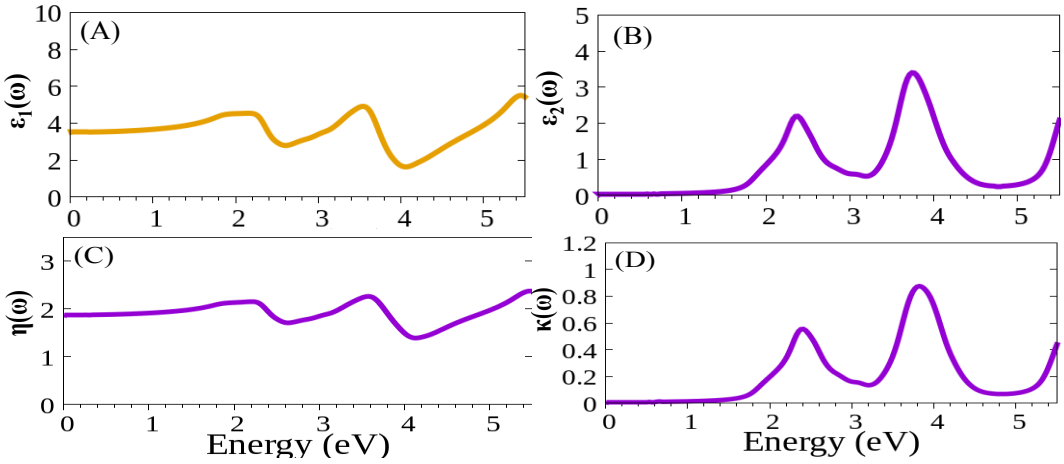


*Fig. 4. Real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ dielectric constant, refractive index $\eta(\omega)$ and extinction coefficient $\kappa(\omega)$ are plotted with energy which is enumerated from Kramers-Kronig relation.*

## 4. Conclusions

In the order to research of novel energy materials, our concern is to investigate the low band gap semiconducting materials. $Cs_2RbInI_6$ has the direct band gap of 1.529 eV which is a significant band gap for getting weighable power conversion efficiency according to Shockley-Queisser limit. $Cs_2RbInI_6$ demonstrates as the high absorption and high dielectric constant materials which are preferable for various optoelectronic applications.

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