

Evaluating hydrogen storage potential of Cs_2ABH_6 : DFT-based approach

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Received 1 September 2024 ♦ Accepted 17 February 2025 ♦ Published 11 April 2025

Citation: Berri S (2025) Evaluating hydrogen storage potential of Cs_2ABH_6 : DFT-based approach. *Modern Electronic Materials* 11(1): 19–30. <https://doi.org/10.3897/j.moem.11.1.136072>

Abstract

In the current investigation, we have implemented first-principles calculations to examine the structural, elastic, electrical and optical characteristics of Cs_2ABH_6 (AB = AlGa, AlIn, AlTl, NaAl, NaGa, NaIn and TlIn). All of the calculations were performed out using first-principles density functional theory (DFT). The space group $Fm-3m$ (225) has been used. The computed values of lattice parameters are $\text{Cs}_2\text{AlGaH}_6$: 0.8739 nm, $\text{Cs}_2\text{AlInH}_6$: 0.8923 nm, $\text{Cs}_2\text{AlTlH}_6$: 0.8953 nm, $\text{Cs}_2\text{NaAlH}_6$: 0.8669 nm, $\text{Cs}_2\text{NaGaH}_6$: 0.8688 nm, $\text{Cs}_2\text{NaInH}_6$: 0.8960 nm, $\text{Cs}_2\text{TlGaH}_6$: 0.8938 nm and $\text{Cs}_2\text{TlInH}_6$: 0.9258 nm and also it is observed that the volume and density are inversely associated with each other. In addition, the computed band-gap values for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTlH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TlGaH}_6$ and $\text{Cs}_2\text{TlInH}_6$ and $\text{Cs}_2\text{YAuCl}_6$ are 1.21, 1.66, 2.58, 1.32, 1.42, 0.94 and 0.91 eV, respectively, which demonstrates the indirect semiconducting nature. Between 0 and 20 eV, optical spectra calculations are made, taking into account the real and imaginary parts of the dielectric function $\epsilon(\omega)$, reflectivity $R(\omega)$, index of refraction $n(\omega)$, coefficients of extinction $k(\omega)$ and absorption $\alpha(\omega)$. The dielectric function is wide close to the ultraviolet districts (3.10–4.13 eV). The extinction coefficient of the Cs_2ABH_6 has the ability to worn for implements like Bragg's reflectors, optical and optoelectronic equipments. The optical parameters of Cs_2ABH_6 disclose that our working constructions have an elevated dielectric constant, with a greatest absorption in the visible range holding out over $2.45 \cdot 10^5 \text{ cm}^{-1}$. All three compounds fulfil the Born stability condition. The gravimetric hydrogen storage capacities of $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTlH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TlGaH}_6$ and $\text{Cs}_2\text{TlInH}_6$ compounds are 1.64, 1.20, 1.88, 1.66, 1.48, 1.02, 1.11 and 1.20 wt.%, respectively. Cs_2ABH_6 crystals are dynamically stable.

Keywords

hydride double perovskites, density functional theory, photovoltaic, hydrogen storage

1. Introduction

In light of the escalating global energy crisis, researchers are actively exploring innovative and economically viable renewable avenues with minimal ecological impact. Within this spectrum of emerging renewable alternatives, solar energy stands out as a particularly environmentally benign and economically efficient energy paradigm. The

efficacy of solar energy conversion hinges upon the judicious selection of materials conducive to the fabrication of advanced optoelectronic apparatus. Since fossil fuels are being depleted at an alarming rate, it is crucial to find sustainable energy options that don't harm the environment. Because of its prevalent reserves, and clean as well as non-polluting benefits, solar energy is currently an integral aspect of the emerging technology. There has been

a rise in international competition to develop solar cell technology, which is capable of converting solar energy into electricity. The principal challenge at hand pertains to global warming, a phenomenon attributed to the discharge of greenhouse gases. To reduce the negative impact on the environment and meet the public's need for clean energy; we can turn to scientific research in materials science. Specifically, an exploration of semiconductor physics and its application within solar photovoltaic cells stands as a pivotal approach [1–3].

Perovskite materials have swiftly emerged as a prominent choice in the field of optoelectronics and apply to solar energy systems as well as various optoelectronic devices as a result of their advantageous features including superior absorbance, high carrier mobility, and highly luminescent. Due to their exceptional photoelectric conversion efficiency (PCE), affordable cost, and relatively simple production procedure, perovskite solar cells (PSCs) have garnered significant attention from scientists in the past few years [4–6]. Ever since the inception and fabrication of inaugural solar cells hinging upon solid-state perovskite materials $\text{CH}_3\text{NH}_3\text{PbX}_3$ ($X = \text{Cl}, \text{Br}, \text{or I}$) [7], there has been an accelerated advancement in organic-inorganic halide hybrid perovskites.

In an oxide-based crystal structure, the experimental reported high bandgap nature of perovskite materials. As a result, photovoltaic uses are not possible with these compounds [8, 9]. As a result, photovoltaic uses are not possible with these compounds. Many attempts have been undertaken in the latest decade to produce organo-inorganic hybrid composites, i.e., solids that combine an organic molecule with a lead halogen perovskite, in order to improve the efficiency of photo-electro-chemical devices [10]. However, the fundamental disadvantage of Pb-based halide perovskite is that it loses efficiency excess moisture, temperature, and other factors [11]. The other demerit is the toxicity of lead, as a result, the scientific group's attention has moved to the discovery of solids that are environmentally benign, stable at ambient temperatures, and therefore could be performed further proficiently for longer periods of time. The other demerit is the toxicity of lead.

Theoretical investigations indicate that these materials may find use in optoelectronic and thermoelectric devices [12–15]. The band gaps of $\text{Cs}_2\text{AgBiBr}_6$ and $\text{Cs}_2\text{AgBiCl}_6$ have been estimated to be 2.19 eV and 2.77 eV, respectively, by E.T. McClure et al. [16]. A thermoelectric material attaining a ZT value of 1.0 is recognized as demonstrating exceptional performance in the conversion of heat to electricity. Several double perovskites, such as ACdX_3 ($A = \text{K}, \text{Rb}, \text{Cs}$; and $X = \text{F}, \text{Cl}, \text{Br}$) [17] and $\text{Cs}_2\text{Z}(\text{Cl}/\text{Br})_6$ ($Z = \text{Os}, \text{Ir}$) [18]. Additionally, there are a series of theoretical research to investigate electronic, optical and transport aspects of numerous perovskite materials, such as $\text{M}_2\text{AgAlBr}_6$ ($M = \text{K}, \text{Rb}, \text{Cs}$) [19], CsInSbAgX_6 ($X = \text{Cl}, \text{Br}$ and I) [20], CsRbPtX_6 ($X = \text{Cl}, \text{Br}$ and I) [21], K_2AgBiX_6 ($X = \text{Cl}, \text{Br}$) [22], Cs_2KXCl_6 [23], and Rb_2YInX_6 ($X = \text{Cl}, \text{Br}, \text{I}$) [24].

In contrast, only a few perovskites are known in the hydrides. Hydrides are the most prominent structures which may be applicable in the use of hydrogen storage [25]. In particular, the perovskite-type hydrides NaMgH_3 and complex transition metal hydrides such as the $R_2\text{TMH}_6$ hydrates, where $R = \text{Mg}, \text{Ca}, \text{Sr}, \text{Ba}, \text{Eu}, \text{Sm}$; $\text{TM} = \text{Fe}, \text{Ru}, \text{Os}$ are very promising and potential candidates as future hydrogen storage materials [26, 27].

O. Boudrifa et al. [28] have theoretically investigated a wide variety of ARuH_6 ($A = \text{Mg}, \text{Ca}, \text{Sr}$ and Ba) to understand their structural, electronic and optical properties. Z. Souadia et al. [29] have theoretically investigated the stability and efficiency of a series of A_2OsH_6 ($A = \text{Mg}, \text{Ca}, \text{Sr}$ and Ba). S. Bouras et al. [30] studied A_2PtH_6 ($A = \text{K}, \text{Rb}$ and Cs) and investigated its electrical and optical characteristics. Using the periodic DFT code the analysis of the inelastic neutron scattering (INS) spectrum of Rb_2PtH_6 and Rb_2PtD_6 have been deliberated by S.F. Parker et al. [31]. The elastic, electronic and optical properties for NaAeIrH_6 ($Ae = \text{Ca}, \text{Ba}$ and Sr) have been studied by S. Bouras et al. [32]. M.A. Ghebouli et al. [33] studied Li_2PtH_6 and Na_2PtH_6 with band gaps of 3.55 eV and 2.2 eV, respectively.

The double perovskites Cs_2ABH_6 have not yet been the subject of any theoretical or experimental studies. Therefore, to explore in more detail the physical properties of this materials, we investigate the electronic, lattice structural, electronic, elastic, and optical properties of Cs_2ABH_6 with the density functional theory. We prospect that our theoretical results of this paper will contribute to afford theoretical support for available experimental data and offer guidance for come experiments as well as eventual applications of Cs_2ABH_6 .

2. Computational methods

In this work, all the first-principles calculations are executed using the plane-wave pseudopotential method based on the DFT [34]. The electron-ionic core interactions are represented by employing the ultra-soft pseudopotential proposed by D. Vanderbilt [35]. The valence electrons of Na, Al, Cs, In, Ga, Tl are $2s^22p^63s^1$, $3s^23p^1$, $5s^25p^66s^1$, $4d^{10}5s^25p^1$, $3d^{10}4s^24p$ and $5d^{10}6s^26p^1$, respectively.

The exchange-correlation potential is handled by the PBEsol (Perdew–Burke–Ernzerhof for solid) [36] method in the generalized gradient approximation (GGA) [37]. Two parameters, plane-wave cutoff energy and the number of k -points for the first Brillouin zone (BZ) integration can affect the calculation accuracy. To ensure convergence, the cutoff energy is 800 eV, and Monkhorst–Pack grid k -points are $10 \times 10 \times 10$ for geometry optimizations (for electronic properties, the k -points are $30 \times 30 \times 30$). The Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm [38] is used to optimize the lattice structure and internal atomic coordinates, till the total energy converges, maximum stress, maximum displacement, the maximum

force, and are $5 \cdot 10^{-6}$ eV/atom, 0.02 GPa, $5 \cdot 10^{-5}$ nm, and 0.1 eV/nm, respectively.

The optical characteristics of the explored DPs provide insight into their behavior in the presence of light energy, highlighting their relevance to solar cell technology. Light-matter interaction, carrier transition, and recombination rate are major determinants of optical features. In this investigation, we neglect the intraband transitions of carriers in favor of their interband counterparts. The complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, absorption coefficient $\alpha(\omega)$, reflection $R(\omega)$, and refractive index $n(\omega)$, and the dispersion of light energy as calculated by the refractive index $n(\omega)$ [39, 40].

$$n(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) \right\}^{1/2} + \varepsilon_1(\omega) \right]^{1/2}; \quad (1)$$

$$k(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) \right\}^{1/2} - \varepsilon_1(\omega) \right]^{1/2}; \quad (2)$$

$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 - k^2}; \quad (3)$$

$$\alpha(\omega) = \frac{4\pi k(\omega)}{\lambda} \quad \text{or} \quad \alpha(\omega) = 2\omega k = \sqrt{2\omega} \left[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) \right]^{1/2}. \quad (4)$$

Mechanical qualities are important when designing solids for commercial production for different applications. We computed the Second-order elastic constants (C_{ij}), such as Young's modulus (Y), Poisson's ratio (ν), bulk modulus (B), shear modulus (G), brittleness, ductility, anisotropy, elastic wave propagation, Debye temperature, average velocity, longitudinal and transvers waves. Three separate elastic constants C_{11} , C_{12} , and C_{44} are used to quantify the strength of the dimensional structure in the cubic system. Where C_{11} symbolizes the resistance of materials to shear deformation, C_{12} represents shear stress, and C_{44} indicates opposition to shear deformation. These parameters were obtained from the matrix of equations and also we ought to be fulfill the born elastic solidity conditions [41], they are

derived from the estimated elastic constants by using the following Eqs (5)–(10) [42]:

$$B_V = B_R = B = \left(\frac{C_{11} + 2C_{12}}{3} \right); \quad (5)$$

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

$$G = \frac{G_V + G_R}{2}; \quad (6)$$

$$E = \frac{9GB}{3B + G}; \quad (7)$$

$$\nu = \frac{3B - 2G}{2(3B + G)}; \quad (8)$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}}; \quad (9)$$

$$C_p = C_{12} - C_{44}. \quad (10)$$

where B_V and G_V are the Voigt values, while B_R and G_R are the reuss values of B and G , respectively. The extreme values of B and G have been calculated using the scheme suggested by Hill [43]. The results are discussed and compared for their suitability in utilizing them for the hydrogen storage and other

3. Result and discussion

3.1. Structure properties

To begin our extensive examination of the many characteristics of Cs_2ABH_6 ($AB = \text{AlGa}, \text{AlIn}, \text{AlTi}, \text{NaAl}, \text{NaGa}, \text{NaIn}$ and TiIn) materials. Cs_2ABH_6 compounds have a cubic structure with the space group #225, $Fm\bar{3}m$, having the Cs, A, B, and H atoms occupying positions $8c$ (0.25, 0.25), $4a$ (0, 0, 0), $4b$ (0.5, 0, 0), and $24e$ (x , 0, 0). The calculated values of these parameters are shown in Table 1. Till now, there is no experimental evidence of Cs_2ABH_6 .

Table 1. Lattice constants a (nm), bulk modulus B (GPa), formation energy E_f (eV/atom), binding energy E_{coh} (eV/atom) and total energy E_{tot} (eV) of Cs_2ABH_6 compounds

Compounds	a (nm)	B (GPa)	E_{tot} (eV)	E_f (eV/atom)	E_{coh} (eV/atom)
$\text{Cs}_2\text{AlGaH}_6$	0.8739	29.439	-3304.2735	-0.253	-1.636
$\text{Cs}_2\text{AlInH}_6$	0.8923	29.516	-2812.3701	-0.199	-1.765
$\text{Cs}_2\text{AlTiH}_6$	0.8953	30.164	-2629.5522	-0.186	-1.478
$\text{Cs}_2\text{NaAlH}_6$	0.8669	36.965	-2557.3596	-0.242	-2.375
$\text{Cs}_2\text{NaGaH}_6$	0.8688	34.229	-4552.6783	-0.212	-1.352
$\text{Cs}_2\text{NaInH}_6$	0.8960	28.642	-4060.3597	-0.128	-1.762
$\text{Cs}_2\text{TiGaH}_6$	0.8938	32.907	-4625.0939	-0.162	-1.965
$\text{Cs}_2\text{TiInH}_6$	0.9258	19.515	-4132.7384	-0.084	-1.783

Faber and co-workers identified one hundred twenty-eight novel structures through the development of a machine learning (ML, complementary to experts' intuitions) model that trained to reproduce the formation energies of two million combinations of elements presenting the ABC_2D_6 formula. The one hundred twenty-eight new structures are added later to the Materials Project database [44]. Since no theoretical or experimental data is available on these alloys, so our findings will serve as guidelines for future theoretical and experimental analysis. Further, the thermodynamic stability is also checked using convex hull calculations performed with Open Quantum Materials Database (OQMD) [45]. The Cs_2ABH_6 ($A = \text{Al, Na, Tl, In}$ and $B = \text{Ga, In, Tl, Al, Ga}$) compound decomposes into ternary (CsAlH_4 , Cs_3AlH_6 , CsGaH_4), binary ($\text{Cs}_8\text{Ga}_{11}$, CsIn_3 , CsTl_3 , NaH , CsH), with a convex hull value of 0.087, 0.087, 0.049, 0.023, 0.070, 0.008 and 0.077 eV/atom for $\text{Cs}_2\text{AlGaH}_6$, $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$ and $\text{Cs}_2\text{TlInH}_6$, respectively, which is less than 0.1 eV/atom [46]. Hence Cs_2ABH_6 ($AB = \text{AlGa, AlIn, AlTi, NaAl, NaGa, NaIn}$ and TlIn) phase is thermodynamically stable.

In order to further verify the stability of the studied compounds, the formation energy E_f and binding energy E_{coh} of the system were calculated by Eqs (12) and (13) [47]:

$$E_f = E_{\text{Cs}_2\text{ABH}_6} - 2xE_{\text{Cs}} - E_A - E_B - 6xE_{\text{H}}; \quad (12)$$

$$E_{\text{coh}} = E_{\text{Cs}_2\text{ABH}_6}^{\text{bulk}} - 2xE_{\text{Cs}}^{\text{bulk}} - E_A^{\text{bulk}} - E_B^{\text{bulk}} - 6xE_{\text{H}}^{\text{bulk}}. \quad (13)$$

3.2. Elastic properties

Elastic constants C_{ij} , volume modulus B and shear modulus G are the key parameters of elastic properties of materials. Understanding the elastic properties of materials is helpful to their industrial application. The elastic constant C_{ij} reflects the response of a material to external stress and can derive important mechanical information such as the mechanical stability, load-bearing capacity and bonding characteristics of the compound. For cubic crystals, the Born–Huang stability criteria $C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$ should be met [48]. The basic parameters of the elastic properties of Cs_2ABH_6 ($AB = \text{AlGa, AlIn, AlTi, NaAl, NaGa, NaIn}$ and TlIn) are listed in Table 2, and they all satisfy the mechanical stability. The bulk modulus (B) is a parameter that characterizes the resistance to breakage of materials. The fracture resistance is higher in $\text{Cs}_2\text{TlInH}_6$ than in Cs_2ABH_6 ($AB = \text{AlGa, AlIn, AlTi, NaAl, NaGa}$ and NaIn). The deformation that changes volume without changing shape is called compression, and the deformation that changes shape without changing volume is called shear. B and G are used to measure the ability of the crystal to resist deformation. The larger the B and G , the stronger the de-

formation resistance. The mechanical strength of compounds is depicted by Young's modulus. A higher Young's modulus value indicates that the fracturing tendency of the material is more sophisticated [49]. Calculated values of all these allied parameters are presented in the Table 2 and compared with isostructural double perovskites [15, 50, 51].

In materials science and solid mechanics, the Poisson's ratio ν is being defined as the deformation of a certain material in directions perpendicular to the specific direction of loading. It is the transversal elongation divided by the compression for small values of these changes. Principally, ν is a measure of a rock's strength which is another critical rock property that is related to closure stress. It is dimensionless that is in the range between 0.1 and 0.5. In fact, low ν such as 0.10–0.25, indicates that the rocks are easier to fracture, whereas high ν such as 0.35–0.50 means that the rocks are harder to fracture. Meaning ν varies from layer to layer. The lowest ν 's are taken from the best formations to hydraulically fracture. It is of big importance for both theoretical and numerical analysis of rock engineering. However, it was rarely studied as compared to state modulus and strength. As a matter of fact, the rock materials are different from the metallic ones. In the process of uniaxial tension or compression, the pure elastic deformation stage is usually very short or nonexistent. Accordingly, the ν increases with the externally applied stress. Hence, as an elastic constant it is worthy of a second thought. According to I.N. Frantsevich et al. rule [52], the critical value which predicts ductility/brittleness of the material is 0.26. For brittle materials, Poisson's ratio is < 0.26 . Otherwise the material behaves in a ductile manner. Here the calculated Poisson's values are greater than (0.26) revealing that all these compounds are ductile in nature. In addition to the Poisson's ratio, we also calculated the Pugh's ratio (B/G) and Cauchy's pressure, $C_p = C_{12} - C_{44}$ and presented in the Table 2. From the Table 2, we observed that $B/G < 1.75$ and the C_p value is negative, which collectively indicate a brittle nature of the Cs_2ABH_6 ($AB = \text{AlGa, AlIn, AlTi, NaAl, NaGa, NaIn}$ and TlGa) compounds. Utilizing the following relation of the melting temperature T_m (K), as proposed by M.E. Fine et al. [53], we have calculated the same for our studied compounds Cs_2ABH_6 ($AB = \text{AlGa, AlIn, AlTi, NaAl, NaGa, NaIn}$ and TlGa) and listed in the Table 2.

$$T_m = [553 + (5.91 \times C_{11})] \text{ K}. \quad (14)$$

The calculations suggested that the melting temperature of the Cs_2ABH_6 is differing from 701.02 to 810.31 K and such high melting temperature would project the Cs_2ABH_6 as suitable material for thermal barrier applications.

The generation of microcracks in the use of materials is closely related to elastic anisotropy, and the generation of microcracks will affect the service life of materials [54]. Therefore, we have calculated the elastic anisotropy

Table 2. Calculated C_{ij} (GPa), A , G (GPa), B (GPa), Y (GPa), ν , C_p , B/G Ratio, melting temperature T_m (K) for Cs_2ABH_6 material

Compounds	C_{11}	C_{12}	C_{44}	$C_p = C_{12} - C_{44}$	G	B	Y	ν	A	B/G	T_m (K)
$\text{Cs}_2\text{AlGaH}_6$	35.40	6.61	12.77	-6.16	13.42	16.21	33.32	0.16	0.02	1.21	750.89
$\text{Cs}_2\text{AlInH}_6$	35.73	6.95	12.77	-5.83	13.42	16.54	33.47	0.16	0.02	1.23	752.73
$\text{Cs}_2\text{AlTiH}_6$	44.38	9.70	19.26	-9.56	18.49	21.26	40.90	0.18	0.01	1.15	801.08
$\text{Cs}_2\text{NaAlH}_6$	39.98	15.85	28.64	-12.79	22.01	23.89	30.99	0.28	0.95	1.09	776.49
$\text{Cs}_2\text{NaGaH}_6$	26.48	7.45	20.82	-13.37	16.30	13.79	23.22	0.22	0.77	0.85	701.02
$\text{Cs}_2\text{NaInH}_6$	32.38	14.42	22.79	-8.37	17.27	20.41	23.50	0.31	1.12	1.18	734.00
$\text{Cs}_2\text{TiGaH}_6$	44.29	11.75	20.39	-8.64	18.74	22.60	39.36	0.21	0.06	1.21	800.58
$\text{Cs}_2\text{TlInH}_6$	46.03	14.47	13.20	1.28	14.23	23.99	39.11	0.24	0.04	1.68	810.31
$\text{Cs}_2\text{BiAuF}_6$ [15]	27.25	19.92	4.09	–	13	25.11	35.12	0.29	0.052	2.69	–
$\text{Cs}_2\text{AgIrF}_6$ [15]	49.855	21.199	15.51	–	15.04	30.75	37.20	0.29	0.007	2.00	–
$\text{Cs}_2\text{CuBiF}_6$ [15]	26.81	21.26	16.82	–	11.32	37.44	5.40	0.67	0.120	3.30	–
$\text{Cs}_2\text{GaAuF}_6$ [15]	-15.26	56.84	9.42	–	-8.77	32.81	-170.65	1.37	-7.30	–	–
$\text{Cs}_2\text{InAsF}_6$ [15]	31.31	10.98	11.18	–	10.77	19.76	25.60	0.28	0.010	1.83	–
$\text{Cs}_2\text{InAgF}_6$ [15]	56.77	35.88	22.40	–	17.61	42.84	28.97	0.39	0.033	2.43	–
$\text{Cs}_2\text{InSbF}_6$ [15]	48.98	16.27	14.42	–	15.19	27.17	40.87	0.25	0.018	1.78	–
$\text{Cs}_2\text{InBiF}_6$ [50]	98	35	57	–		49.2	103.2	0.15	1.80	1.09	–
K_2AgRhF_6 [51]	100.18	24.94	10.96	–	21.62	49.23	56.70	0.31	2.27	1.96	–
K_2NaPdF_6 [51]	90.25	21.34	17.98	–	20.78	48.39	18.88	0.36	3.51	1.27	–

of Cs_2ABH_6 ($AB = \text{AlGa}, \text{AlIn}, \text{AlTi}, \text{NaAl}, \text{NaGa}, \text{NaIn}$ and TlIn), which is usually expressed by the anisotropy index the standard Eq. (9). If $A = 0$ or 1, then the material is isotropic. Otherwise, it is anisotropic [55, 56]. The greater the deviation of A from 0 or 1, the easier it is to produce cracks. From Table 2, it can be seen that Cs_2ABH_6 ($AB = \text{AlGa}, \text{AlIn}, \text{AlTi}, \text{NaAl}, \text{NaGa}, \text{NaIn}$ and TlIn) are anisotropic materials, but Cs_2ABH_6 ($AB = \text{AlGa}, \text{AlIn}, \text{AlTi}, \text{NaAl}, \text{NaGa}, \text{TiGa}$ and TlIn) deviate from 0 or 1 to a very small extent, resulting in good mechanical durability. Cs_2ABH_6 ($AB = \text{NaGa}$ and NaIn) deviates from 0 or 1 to a large extent, so microcracks are more likely to occur.

3.3. Electronic structure

Band structure is an important parameter in the application of semiconductors in photovoltaic and optoelectronic devices, which affects the whole process of carrier generation, separation and recombination [57]. Band gap value, direct or indirect band gap and dispersion of electronic state reflect the most important information of electronic properties, which usually determine the physical properties of the materials under study. Therefore, the electronic band structures of the double antiperovskites Cs_2ABH_6 have been calculated and analyzed. Energy band structures calculated by using GGA approach for compounds Cs_2ABH_6 ($AB = \text{AlGa}, \text{AlIn}, \text{AlTi}, \text{NaAl}, \text{NaGa}, \text{NaIn}$ and TiGa) are shown in Fig. 1. Calculated values of energy band gaps are 1.213, 1.666, 2.576, 1.318, 1.417, 0.939 and 0.912 eV for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$,

$\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TlInH}_6$ respectively. Fermi level in these energy band structures is taken at 0 eV. The VBM was found at the highest symmetry point (W point), and both bands indicate the indirect band gap for the both perovskites, whereas the CBM was situated at the maximal symmetry point (point L for $\text{Cs}_2(\text{NaAl}, \text{NaGa}, \text{NaIn})\text{H}_6$ and Γ for $\text{Cs}_2(\text{AlIn}, \text{AlTi}, \text{and TiGa})\text{H}_6$.

Compounds with indirect band gaps are relatively less optically active semiconductors as compared to materials with direct band gaps due to the reason that CBM and VBM exist at different points in the Brillouin zone. In addition to photons and electrons, phonons are also the part of optical transitions when compounds with indirect energy band gap are used. Materials having direct band gap are ideal materials to be used in optoelectronic devices. In this work, two double perovskites, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TlInH}_6$ have the band gap values of 0.94 and 0.91 eV, similar to that of silicon (1.14 eV), but in the direct nature, making them ideal candidates as good solar absorbers.

Calculations reveal that since $\text{Cs}_2\text{NaAlH}_6$ possesses indirect band-gap of 2.58 eV and lower absorption coefficient in the UV region, it is not a suitable material in single-layered solar cell. On the other hand, due to indirect band-gap slightly larger than 2.0 eV, the $\text{Cs}_2\text{NaAlH}_6$ would be suitable for the development of highly efficient tandem solar cells, where photovoltaic efficiency of a conventional solar cell is enhanced without much affecting the manufacturing cost by using $\text{Cs}_2\text{NaAlH}_6$ as a tandem with a conventional solar cell absorber.

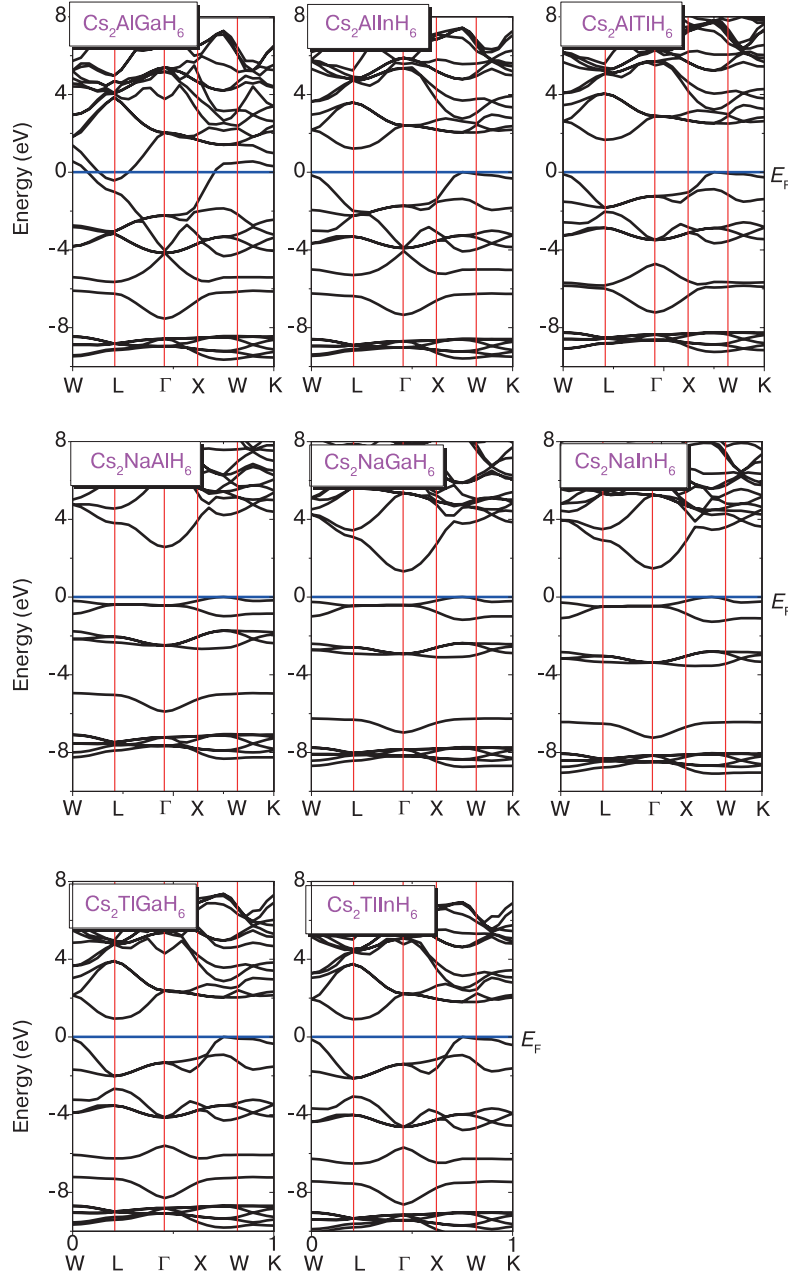


Figure 1. The calculated electronic band structure

3.4. Optical properties

Nature of interactions between material and electromagnetic radiations is utmost important to understand its optical characteristics, which in turn play a crucial role for optoelectronics and photo-voltaic applications. Material's interaction with the incident radiation of desirable frequency may produce two types of transitions, which are intra-band and interband transitions. As the intra-band transitions are typical characteristic of metals, we focused our study on inter-band transitions for our semi-conducting specimen Cs_2ABH_6 . Optical characteristics of any material are primarily controlled by the complex dielectric function $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, where ω is the frequency of the incident radiation. Moreover, the real part $\epsilon_1(\omega)$ provides insights regarding dispersion of incident

radiation, whereas the imaginary part $\epsilon_2(\omega)$ reveals the extent up to which the studied material can absorb the incident radiation [58].

The plots of $\epsilon_1(\omega)$, $\epsilon_2(\omega)$, $n(\omega)$, $k(\omega)$, $R(\omega)$ and $a(\omega)$ are depicted in Figs 2–5, where the largest peak of $\epsilon_1(\omega)$ is observed at 2.43, 2.67, 2.50, 3.54, 3.27, 2.33 and 2.09 eV for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$, respectively. Since the energy and frequency of electromagnetic waves are intimately related, the movement of the peak of highest intensity towards lower energy causes the $\epsilon_1(\omega)$ value to increase from 1.19 to 4.22 [59]. We see that the static dielectric constants obtained for the materials (Table 3). When $\epsilon_1(0)$ is inversely linked to a material's band gap from which it becomes clear that our computed results are quite in line with that of Penn's rule [60, 61], when

Table 3. Optical parameters for Cs_2ABH_6 material

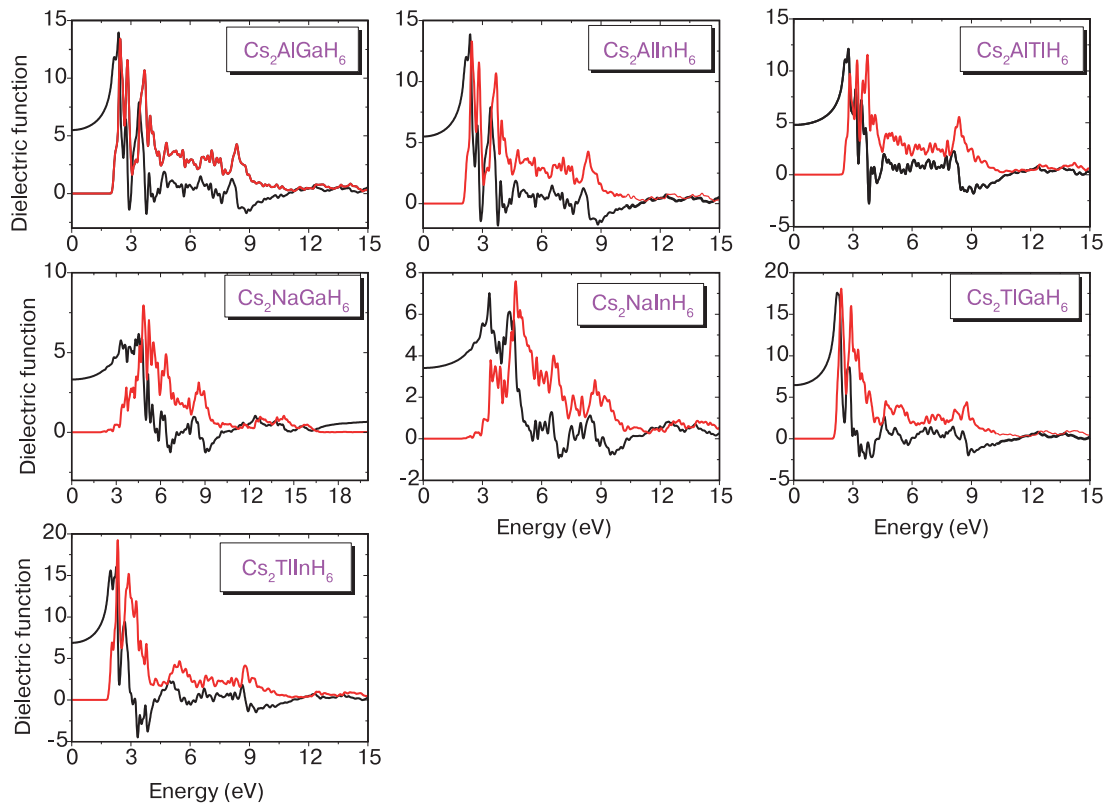
Compounds	E_g (eV)	$E_{g\text{ optic}}$	$E(0)$	$n(0)$	$R(0)$
$\text{Cs}_2\text{AlGaH}_6$	—	—	—	—	—
$\text{Cs}_2\text{AlInH}_6$	1.21	1.90	5.49	2.34	0.16
$\text{Cs}_2\text{AlTiH}_6$	1.66	2.44	4.77	2.18	0.13
$\text{Cs}_2\text{NaAlH}_6$	2.58	1.91	5.50	2.35	0.16
$\text{Cs}_2\text{NaGaH}_6$	1.32	2.29	3.30	1.82	0.08
$\text{Cs}_2\text{NaInH}_6$	1.42	1.95	3.40	1.84	0.08
$\text{Cs}_2\text{TiGaH}_6$	0.94	2.00	6.45	2.54	0.18
$\text{Cs}_2\text{TiInH}_6$	0.91	1.68	6.87	2.62	0.20

the compound's band gap narrows, its spectral peaks rise. Fig. 2 shows the change in $\epsilon_1(\omega)$ with incident energy. The variation of $\epsilon_2(\omega)$ with photon energy (0–15 eV) is seen in Fig. 2. An absorptive transition among the different bands is indicated by the existence of several peaks in the energy region which is primarily due to transition of electrons. The opacity of a compound when light photons strike its surface is measured by the refractive index $n(\omega)$. For materials that are completely transparent, $n(\omega)$ must be equal to 1 [62]. The most efficient optical materials have refractive indices of 2 to 3. The trend of $n(0)$ is noticed to be replica of the $\epsilon_1(\omega)$. At zero frequency it is known as static refractive index $n(0)$ that is determined as $n(0)^2 = \epsilon_1(0)$. The initial summits of $n(\omega)$ for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$ are 2.34, 2.18, 2.35, 1.82, 1.84, 2.54 and 2.62, respectively. After reaching its peak (see

Fig. 3), or a resonance frequency it then starts to decelerate. Fig. 3 illustrates the extinction coefficient spectra $k(\omega)$ versus photon energy. For $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$, the amounts of $k(\omega)$ started of from 0 eV (see Fig. 3) and reached the first peak of 2.47, 3.00, 2.55, 5.01, 5.55, 2.56 and 2.32 eV, identifying. The greatest accounts of $k(\omega)$ are 3.92, 3.67, 3.77, 6.47, 6.64, 3.56 and 3.34 eV for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$, respectively. A greater quantity of light absorption is associated with each peak in the extinction coefficient spectrum.

Figure 4 depicts another crucial element for optoelectronic applications, reflectivity $R(\omega)$, which is used to evaluate the light that is reflected from the surface[63, 64]. For zero frequency reflectivity, the computed values for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$ are 0.16, 0.13, 0.16, 0.08, 0.08, 0.18 and 0.20, respectively (see Fig. 4). Furthermore, the highest values of $R(\omega)$ are 0.50, 0.61, 0.49, 0.48, 0.43, 0.45 and 0.55 for $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$ at 9.11, 10.55, 8.89, 9.58, 10.18, 10.42 and 3.95 eV, respectively. The $\epsilon_1(0)$, $n(0)$, $E_{g\text{ optic}}$ and $R(0)$ is represented in Table 3.

The $\alpha(\omega)$ is a crucial parameter for the reason that it establishes how far light of some energy can proceed via the substance prior being used [65]. $\alpha(\omega)$ equally accounted for the photon-induced processing of electrons from replete to unfilled states [66]. The $\alpha(\omega)$ for the two substances is produced at 0 eV (see Fig. 5). For $\text{Cs}_2\text{AlInH}_6$,

**Figure 2.** Computed real part of the dielectric functions for Cs_2ABH_6 material

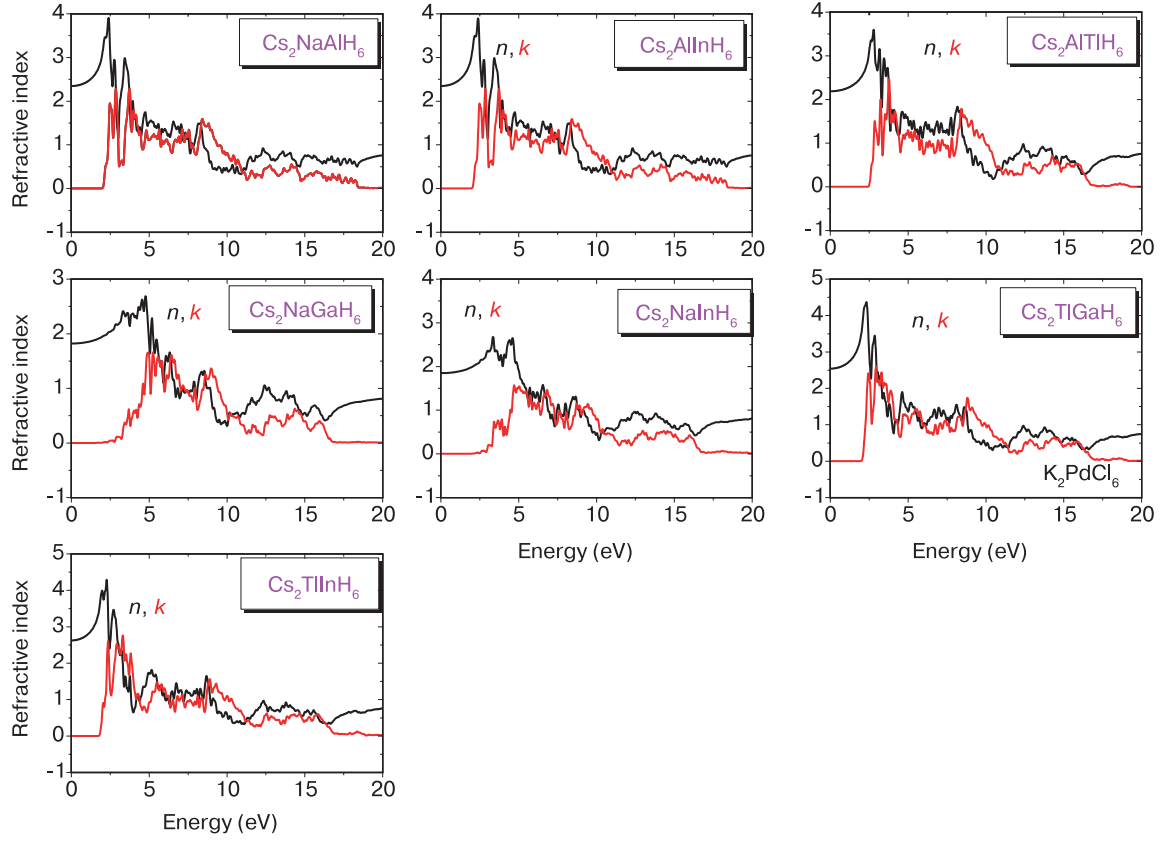


Figure 3. The calculated refractive index $n(\omega)$ and extinction coefficient $k(\omega)$ for Cs_2ABH_6 material

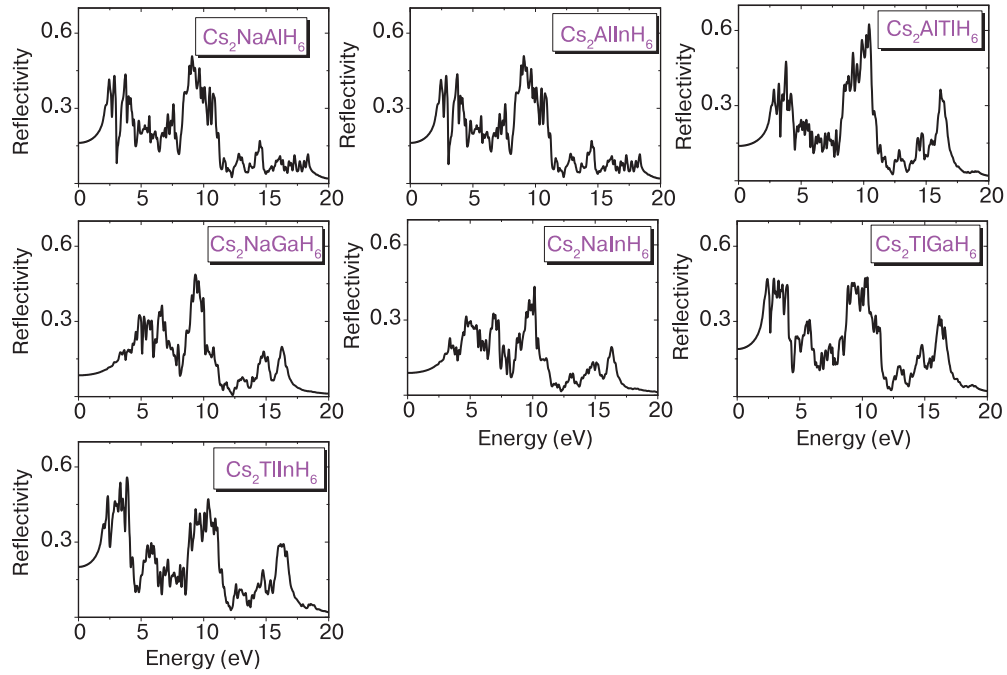


Figure 4. The calculated reflectivity $R(\omega)$ for Cs_2ABH_6 material

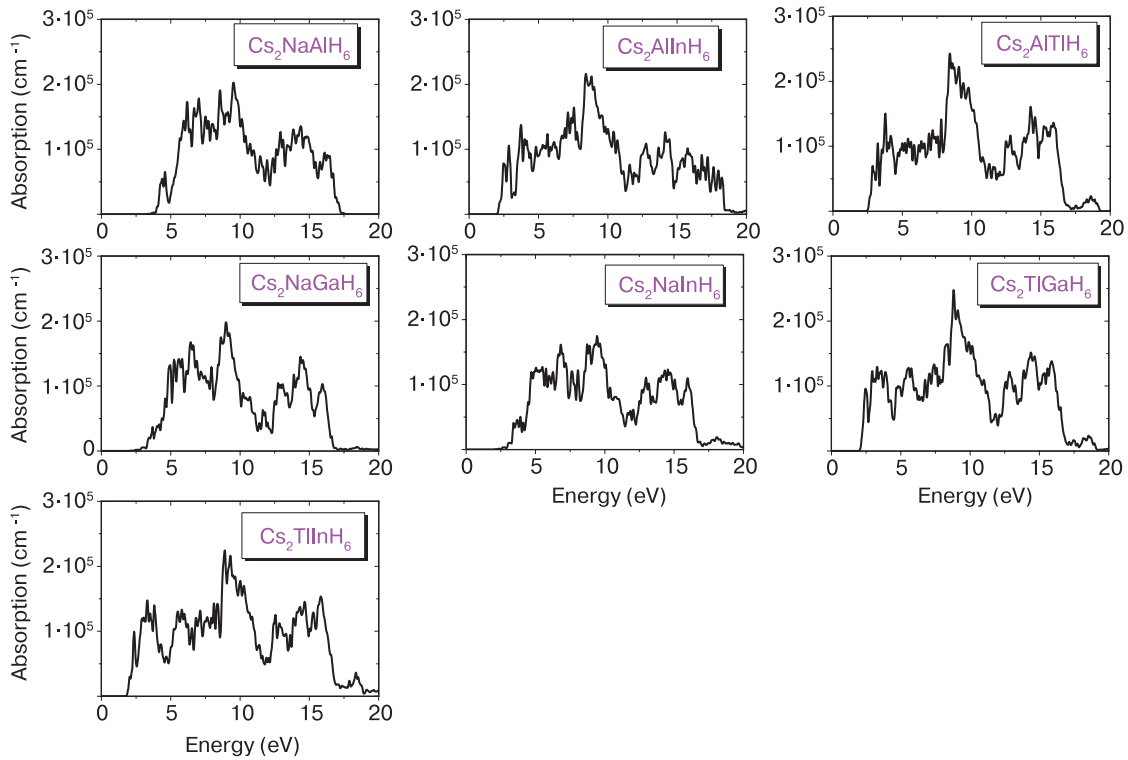


Figure 5. Optical absorption coefficient $\alpha(\omega)$ curves of the Cs_2ABH_6 versus photon energy

$\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$, the $\alpha(\omega)$ acquires maximum merits of $2.01 \cdot 10^5$, $2.38 \cdot 10^5$, $1.99 \cdot 10^5$, $1.71 \cdot 10^5$, $2.45 \cdot 10^5$, $1.99 \cdot 10^5$ and $2.21 \cdot 10^5 \text{ cm}^{-1}$ at 8.28, 8.36, 9.47, 9.82, 9.02, 9.50, 8.81 and 9.02 eV, respectively. As stated by the provided optical representatives of $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$ compounds, the energy band-gap lies in the visible region. Both materials reveal a great absorption, that makes them potential applicants for energy harvesting systems.

3.5. Hydrogen storage properties

Gravimetric hydrogen density is an important parameter to search for hydrogen storage material before studying atomic structure prediction and mechanical stability. The gravimetric hydrogen density for Cs_2ABH_6 compounds is estimated using the following equation [67].

$$C_{\text{wt.\%}} = \frac{nM_{\text{H}}}{nM_{\text{H}} + M_{\text{com}}} \cdot 100\%. \quad (15)$$

where n represents the ratio of hydrogen to material atoms, and M_{H} and M_{com} represent the molar masses of hydrogen and the compound, respectively. The gravimetric hydrogen density for the compounds $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$ was calculated to be 1.64, 1.20, 1.88, 1.66, 1.48, 1.02, 1.11 and 1.20 wt.%, respectively. In this regard, sluggish kinetics and thermodynamic reactions of adsorption and desorption are major disadvantages of elemental hydride [68]. Metal alloy/

complex hydrides of $A_xB_yH_z$ form such as Mg_2NiH_4 , $\text{FeTiH}_{1.95}$, $\text{LaNi}_5\text{H}_{6.7}$, $\text{ZrMn}_2\text{H}_{3.6}$, are reported to have gravimetric weight percentages of 7.6, 3.6, 1.89, 1.37, 1.75, 2.10 wt.%, respectively [68].

4. Conclusions

This work investigated into the structural, electrical, elastic, and optical properties of Cs_2ABH_6 , where $AB = \text{AlGa}$, AlIn , AlTi , NaAl , NaGa , NaIn or TiIn . Calculations of calculated formation enthalpy and cohesive energy show its thermodynamic stability. The calculated lattice constant of the Cs_2ABH_6 double perovskite is in close proximity with the same reported in the Materials Project Database. Our calculated C_{11} , C_{12} and C_{44} follow the trend $C_{11} > C_{44} > C_{12}$. The Cs_2ABH_6 crystal obeys Born's stability criteria and hence it is mechanically stable.

Elastic anisotropy of this crystal is confirmed from the computed shear moduli G as well as the anisotropy factor A . The brittleness of this crystal is confirmed from the computed Poisson's ratio (σ), Pugh's ratio (B/G) and Cauchy's pressure CP . Computed Poisson's ratio (σ), close to 0.25, suggests substantial dominance of ionic bonding over the covalent in the chemical bonding of the cubic Cs_2ABH_6 . The examination of band structures suggested that $\text{Cs}_2\text{AlInH}_6$, $\text{Cs}_2\text{AlTiH}_6$, $\text{Cs}_2\text{NaAlH}_6$, $\text{Cs}_2\text{NaGaH}_6$, $\text{Cs}_2\text{NaInH}_6$, $\text{Cs}_2\text{TiGaH}_6$ and $\text{Cs}_2\text{TiInH}_6$ exhibited indirect band gaps with respective values of 1.21, 1.66, 2.58, 1.32, 1.42, 0.94, and 0.91 eV. In the present study, optical features of the Cs_2ABH_6 have been computed in terms of real part $\epsilon_1(\omega)$ and imaginary part $\epsilon_2(\omega)$ of dielectric

function, refractive index $n(\omega)$, extinction co-efficient $k(\omega)$, normal incidence reflectivity $R(\omega)$ and optical absorption coefficient $\alpha(\omega)$.

These materials have substantial optical features, including absorption and reflection in the visible spectrum, making them suitable for solar cell applications. The analysis of optical characteristics reveals that both materials with low reflectivity have significant absorption

capability throughout the ultraviolet-visible spectrum. In terms of real and imaginary part of the dielectric function as well as some other auxiliary parameters, we have investigated the optical properties of the $\text{Cs}_2\text{NaAlH}_6$. Since the computed indirect band-gap of the $\text{Cs}_2\text{NaAlH}_6$ is larger than 2.0 eV, it would be suitable for fabricating low-cost tandem solar cells.

References

- Moskvin S., Makhnev A.A., Nomerovannaya L.V., Loshkareva N.N., Balbashov A.M. Interplay of p - d and d - d charge transfer transitions in rare-earth perovskite manganites. *Physical Review B*. 2010; 82(3): 035106. <https://doi.org/10.1103/PhysRevB.82.035106>
- Weeks C., Franz M. Topological insulators on the Lieb and perovskite lattices. *Physical Review B*. 2010; 82(8): 085310. <https://doi.org/10.1103/PhysRevB.82.085310>
- Rani M., Kamlesh P.K., Kumawat S., Anuradha, Rani U., Arora G., Verma A.S. *Ab-Initio* calculations of structural, optoelectronic, thermoelectric, and thermodynamic properties of mixed-halide perovskites $\text{RbPbBr}_{3-x}\text{I}_x$ ($x = 0$ to 3): Applicable in renewable energy devices. *ECS Journal of Solid State Science and Technology*. 2023; 12(8): 083006. <https://doi.org/10.1149/2162-8777/acec9c>
- Brenner T.M., Egger D.A., Kronik L., Hodes G., Cahen D. Hybrid organic-inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. *Nature Reviews Materials*. 2016; 1(1): 15007. <https://doi.org/10.1038/natrevmats.2015.7>
- Katan CL, Mercier N., Even J. Quantum and dielectric confinement effects in lower-dimensional hybrid perovskite semiconductors. *Chemical Reviews*. 2019; 119(5): 3140–3192. <https://doi.org/10.1021/acs.chemrev.8b00417>
- Snaith H.J. Perovskites: The emergence of a new era for low-cost, high-efficiency solar cells. *The Journal of Physical Chemistry Letters*. 2013; 4(21): 3623–3630. <https://doi.org/10.1021/jz4020162>
- Meloni S., Moehl T., Tress W., Frankevičius M., Saliba M., Lee Y.H., Gao P., Nazeeruddin M.K., Zakeeruddin S.M., Rothlisberger U. Ionic polarization-induced current-voltage hysteresis in $\text{CH}_3\text{NH}_3\text{PbX}_3$ perovskite solar cells. *Nature Communications*. 2016; 7: 10334. <https://doi.org/10.1038/ncomms10334>
- Kojima A., Teshima K., Shirai Y., Miyasaka T. Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. *Journal of the American Chemical Society*. 2009; 131(17): 6050–6051. <https://doi.org/10.1021/ja809598r>
- Bella F., Griffini G., Correa-Baena J.-P., Saracco G., Grätzel M., Hagfeldt A., Turri S., Gerbaldi C. Improving efficiency and stability of perovskite solar cells with photocurable fluoropolymers. *Science*. 2016; 354(6309): 203–206. <https://doi.org/10.1126/science.aah4046>
- Eames C., Frost J.M., Barnes P.R.F., O'regan B.C., Walsh A., Islam M.S. Ionic transport in hybrid lead iodide perovskite solar cells. *Nature Communications*. 2015; 6: 7497. <https://doi.org/10.1038/ncomms8497>
- Kojima A., Teshima K., Shirai Y., Miyasaka Y. Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. *Journal of the American Chemical Society*. 2009; 131(17): 6050–6051. <https://doi.org/10.1021/ja809598r>
- Berri S. Half-metallic and thermoelectric properties of $\text{Sr}_2\text{EuReO}_6$. *Computational Condensed Matter*. 2021; 28: e00586. <https://doi.org/10.1016/J.COCOM.2021.E00586>
- Berri S. Theoretical study of physical properties of $\text{Ba}_3\text{B}(\text{Nb,Ta})_2\text{O}_9$ ($\text{B} = \text{Mg, Ca, Sr, Cd, Hg, Zn, Fe, Mn, Ni, Co}$) perovskites. *Computational Condensed Matter*. 2021; 29: e00595. <https://doi.org/10.1016/j.cocom.2021.e00595>
- Berri S. Thermoelectric properties of A_2BCl_6 : A first principles study. *Journal of Physics and Chemistry of Solids*. 2022; 170: 110940. <https://doi.org/10.1016/j.jpcs.2022.110940>
- Berri S. First-principles calculations to investigate structural, electronic, elastic, optical and transport properties of halide double perovskites Cs_2ABF_6 ($\text{AB} = \text{BiAu, AgIr, CuBi, GaAu, InAs, InAg, InAu, InSb}$ and InBi) for solar cells and renewable energy applications. *Chemical Physics Letters*. 2023; 826: 140653. <https://doi.org/10.1016/j.cplett.2023.140653>
- McClure E.T., Ball M.R., Windl W., Woodward P.M. $\text{Cs}_2\text{AgBiX}_6$ ($\text{X} = \text{Br, Cl}$): new visible light absorbing, lead-free halide perovskite semiconductors. *Chemistry of Materials*. 2016; 28(5): 1348–1354. <https://doi.org/10.1021/acs.chemmater.5b04231>
- Berri S., Bouarissa N. *Ab initio* study of fundamental properties of ACdX_3 ($\text{A} = \text{K, Rb, Cs}$; and $\text{X} = \text{F, Cl, Br}$) halide perovskite compounds. *Emergent Materials*. 2023; 6: 1009–1025. <https://doi.org/10.1007/s42247-023-00488-x>
- Mahmood Q., Nazir G., Rahim A., Alzahrani J., Aljameel A.I., Murtaza G., Aldayyat A., Albalawi H., Mera A., Ul Haq B. Impact of $5d$ electrons on half metallic ferromagnetism, and thermoelectric properties of $\text{Cs}_2\text{Z}(\text{Cl/Br})_6$ ($\text{Z} = \text{Os, Ir}$) for spintronic applications. *Materials Chemistry and Physics*. 2022; 288: 126414. <https://doi.org/10.1016/j.matchemphys.2022.126414>
- de Souza G.B.G., Nascimento V.B., de Paiva R., Rappe A.M. Thermoelectric properties of $\text{M}_2\text{AgAlBr}_6$ ($\text{M} = \text{K, Rb, Cs}$) double perovskites: A first principles study. *Solid State Communications*. 2024; 378: 115399. <https://doi.org/10.1016/j.ssc.2023.115399>
- Bouhmaid S., Harbi A., Pingak R.K., Azouaoui A., Moutaabbid M., Setti L. First-principles calculations to investigate lead-free double perovskites CsInSbAgX_6 ($\text{X} = \text{Cl, Br}$ and I) for optoelectronic and thermoelectric applications. *Computational and Theoretical Chemistry*. 2023; 1227: 114251. <https://doi.org/10.1016/j.comptc.2023.114251>
- Harbi A., Bouhmaid S., Pingak R.K., Larbi S., Moutaabbid M. First-principles calculations to investigate optoelectronic, thermoelectric and elastic properties of novel lead-free halide perovskites CsRbPtX_6 ($\text{X} = \text{Cl, Br}$ and I) compounds for solar cells applications. *Physica B: Condensed Matter*. 2023; 668: 415242. <https://doi.org/10.1016/j.physb.2023.415242>

22. Iqbal M.W., Manzoor M., Noor N.A., Rehman I., Mushahid N., Aftab S., Alanazi Y.M., Ullah H., Afzal A.M. Tuning of the electronic bandgap of lead-free double perovskites K_2AgBiX_6 ($X = Cl, Br$) for solar cells applications and their thermoelectric characteristics. *Solar Energy*. 2022; 239(3): 234–241. <https://doi.org/10.1016/j.solener.2022.05.018>
23. Dar S.A., Want B., Khandy S.A. Computer based predictions of structural stability and systematic study of magneto-electronic and optical properties of lead free halide double perovskites: Cs_2KXC_{16} ; $X = Co$ and Ni . *Journal of Magnetism and Magnetic Materials*. 2022; 545: 168603.
24. Nawaz P.A., Mustafa G.M., Iqbal S.S., Noor N.A., Ahmad T.S., Mahmood A., Nefati R. Theoretical investigations of optoelectronic and transport properties of Rb_2YInX_6 ($X = Cl, Br, I$) double perovskite materials for solar cell applications. *Solar Energy*. 2022; 231: 586–592. <https://doi.org/10.1016/j.solener.2021.11.076>
25. Sakintuna B., Lamari-Darkrim F., Hirscher M. Metal hydride materials for solid hydrogen storage: A review. *International Journal of Hydrogen Energy*. 2007; 32: 1121–1140. <http://dx.doi.org/10.1016/j.ijhydene.2006.11.022>
26. Bouhadda Y., Boudouma Y., Fennineche N.E., Bentabet A. *Ab initio* calculations study of the electronic, optical and thermodynamic properties of $NaMgH_3$, for hydrogen storage. *Journal of Physics and Chemistry of Solids*. 2010; 71(9): 1264–1268. <https://doi.org/10.1016/j.jpcs.2010.05.007>
27. Nicholson K.M., Sholl D.S. First-principles prediction of new complex transition metal hydrides for high temperature applications. *Inorganic Chemistry*. 2014; 53: 11849–11860. <https://doi.org/10.1021/In501992X>
28. Boudrifa O., Bouhemadou A., Uğur Ş., Khenata R., Bin-Omran S., Al-Douri Y. Structural, electronic, optical and elastic properties of the complex K_2PtCl_6 -structure hydrides $ARuH_6$ ($A = Mg, Ca, Sr$ and Ba): first-principles study. *Philosophical Magazine*. 2016; 96(22): 2328–2361. <https://doi.org/10.1080/14786435.2016.1198874>
29. Souadia Z., Bouhemadou A., Boudrifa O., Bin-Omran S., Khenata R., Khenata R., Al-Douri Y. Hydrostatic pressure effects on the structural, elastic and thermodynamic properties of the complex transition metal hydrides A_2OsH_6 ($A = Mg, Ca, Sr$ and Ba). *High Pressure Research*. 2017; 37(4): 558–578. <https://doi.org/10.1080/08957959.2017.1383408>
30. Bouras S., Ghebouli B., Benkerri M., Ghebouli M.A., Bouhemadou A. First-principles calculations on elastic, electronic and optical properties for the alkaline platinum hydrides A_2PtH_6 ($A = K, Rb$ and Cs). *Materials Science in Semiconductor Processing*. 2013; 16(3): 940–946. <https://doi.org/10.1016/j.mssp.2013.01.024>
31. Parker S.F., Bennington S.M., Ramirez-Cuesta A.J., Auffermann G., Bronger W., Herman H., Williams K.P.J., Smith T. Inelastic neutron scattering and Raman spectroscopies and periodic DFT studies of $Rb(2)PtH(6)$ and $Rb(2)PtD(6)$. *Journal of the American Chemical Society*. 2003; 125(38): 11656–11661. <https://doi.org/10.1021/ja034323h>
32. Bouras S., Ghebouli B., Benkerri M., Ghebouli M.A., Choutri H., Louail L., Chihi T., Fatmi M., Bouhemadou A., Khenata R., Khachai H. Theoretical characterization of quaternary iridium based hydrides $NaAeIrH_6$ ($Ae = Ca, Ba$ and Sr). *Materials Chemistry and Physics*. 2015; 87: 149–150. <https://doi.org/10.1016/j.matchemphys.2014.09.040>
33. Ghebouli M.A., Choutri H., Bouarissa N., Ghebouli B., Bouhemadou A., Soyalt F., Ucgun E., Ocak H.Y. Theoretical prediction of the fundamental properties for the ternary Li_2PtH_6 and Na_2PtH_6 . *Journal of Solid State Chemistry*. 2012; 196: 498–503. <https://doi.org/10.1016/j.jssc.2012.06.044>
34. Engel E., Dreizler R.M. Density functional theory. An advanced course. Berlin; Heidelberg: Springer-Verlag; 2011. 548 p.
35. Vanderbilt D. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Physical Review B*. 1990; 41(11): 7892(R). <https://doi.org/10.1103/PhysRevB.41.7892>
36. Pedroza L.S., da Silva A.J.R., Capelle K. Gradient-dependent density functionals of the Perdew–Burke–Ernzerhof type for atoms, molecules, and solids. *Physical Review B*. 2009; 79: 201106(R). <https://doi.org/10.1103/PhysRevB.79.201106>
37. Perdew J.P., Burke K., Ernzerhof M. Generalized gradient approximation made simple. *Physical Review Letters*. 1996; 77(18): 3865–3868. <https://doi.org/10.1103/PhysRevLett.77.3865>
38. Chen H.C. The mechanical and thermodynamic properties of $\alpha\text{-Na}_3(U_{0.84(2)}, Na_{0.16(2)})O_4$: A combined first-principles calculations and quasi-harmonic Debye model study. *Nuclear Engineering and Technology*. 2021; 53(2): 611–617. <https://doi.org/10.1016/j.net.2020.07.027>
39. Kuzmenko A. Kramers–Kronig constrained variational analysis of optical spectra. *Review of Scientific Instruments*. 2005; 76(8): 083108. <https://doi.org/10.1063/1.1979470>
40. Liu X., Wu W., Zhang Y., Li Y., Wu H., Fan J. Critical roles of high- and low-frequency optical phonons in photodynamics of zero-dimensional perovskite-like $(C_6H_{22}N_4C_{13})SnCl_3$ crystals. *Journal of Physical Chemistry Letters*. 2019; 10(24): 7586–7593. <https://doi.org/10.1021/acs.jpclett.9b03153>
41. Mouhat F., Coudert F.-X. Necessary and sufficient elastic stability conditions in various crystal systems. *Physical Review B*. 2014; 90: 224104. <https://doi.org/10.1103/PhysRevB.90.224104>
42. Irfan H., Mohamed Racik K., Anand S. X-ray peak profile analysis of $CoAl_2O_4$ nanoparticles by Williamson–Hall and size-strain plot methods. *Modern Electronic Materials*. 2018; 4(1): 31–40. <https://doi.org/10.3897/j.moem.4.1.33272>
43. Hill R. The elastic behaviour of a crystalline aggregate. *Proceedings of the Physical Society. Section A*. 1952; 65(5): 349–354. <https://doi.org/10.1088/0370-1298/65/5/307>
44. Faber F.A., Lindmaa A., von Lilienfeld O.A., Armiento R. Machine learning energies of 2 million elpasolite (ABC_2D_6) crystals. *Physical Review Letters*. 2016; 117(113): 135502. <https://doi.org/10.1103/PhysRevLett.117.135502>
45. Kirklin S., Saal J.E., Meredig B., Thompson A., Doak J.W., Aykol M., Rühl St., Wolverton Ch. The open quantum materials database (OQMD): assessing the accuracy of DFT formation energies. *npj Computational Materials*. 2015; 1(1): 1–15. <https://doi.org/10.1038/npjcompumats.2015.10>
46. Gao Q., Opahle I., Zhang H., High-throughput screening for spin-gapless semiconductors in quaternary Heusler compounds. *Physical Review Materials*. 2019; 3(2): 024410. <https://doi.org/10.1103/PhysRevMaterials.3.024410>
47. Azmat A.M., Dar S.Ah., AlObaid A.A., Al-Muhimeed T.I., Hegazy H.H., Nazir Gh., Murtaza G. Appealing perspectives of structural, electronic, mechanical, and thermoelectric properties of $Tl_2(Se, Te)C_{16}$ vacancy-ordered double perovskites. *Journal of Physics and*

- Chemistry of Solids*. 2021; 159: 110258. <https://doi.org/10.1016/j.jpcs.2021.110258>
48. Bobrov V., Borisovich S.A., Trigger G.J.F., Van Heijst, Schram P.P.J.M. Kramers-Kroning relations for the dielectric function and the static conductivity of Coulomb systems. *Europhysics Letters*. 2010; 90(1): 10003. <https://doi.org/10.1209/0295-5075/90/10003>
 49. Hichem El.M., Rached H., Rached D. The half metallic feature at high temperature of the novel half-Heusler alloys and their [100] oriented layered superlattices: A DFT investigations. *Materials Chemistry and Physics*. 2021; 267: 124712. <https://doi.org/10.1016/j.matchemphys.2021.124712>
 50. Berri S., Bouarissa N. Density functional theory calculations of electronic structure and thermoelectric properties of K-based double perovskite materials. *Energy Storage*. 2023; 5(1): e400. <https://doi.org/10.1002/est2.400>
 51. Saeed M., Haq I.U.I., Rehman Sh.Ur., Ali A., Shah W.A., Ali Z., Khan Q., Khan I. Optoelectronic and elastic properties of metal halides double perovskites $\text{Cs}_2\text{InBiX}_6$ ($X = \text{F}, \text{Cl}, \text{Br}, \text{I}$). *Chinese Optics Letters*. 2021; 19(3): 030004. <https://doi.org/10.3788/COL202119.030004>
 52. Frantsevich I.N., Voronov F.F., Bokuta S.A. Elastic constants and elastic moduli of metals and insulators. In: Frantsevich I.N. (ed.). *Handbook on elastic constants and moduli of elasticity for metals and nonmetals*. Kiev: Naukova Dumka; 1982.
 53. Fine M.E., Brown L.D., Marcus H.L. Elastic constants versus melting temperature in metals. *Scripta Metallurgica*. 1984; 18: 951–956. [https://doi.org/10.1016/0036-9748\(84\)90267-9](https://doi.org/10.1016/0036-9748(84)90267-9)
 54. Brik M.G. First-principles calculations of electronic, optical and elastic properties of ZnAl_2S_4 and ZnGa_2O_4 . *Journal of Physics and Chemistry of Solids*. 2010; 71(10): 1435–1442. <https://doi.org/10.1016/j.jpcs.2010.07.007>
 55. Li J., Chen H. First-principles investigation of the mechanical and thermodynamic properties of the antiperovskite centrosymmetric platinum-based superconductors APt_3P ($A = \text{Ca}, \text{Sr}, \text{La}$ and Ce). *Physica B: Condensed Matter*. 2020; 577: 411791. <https://doi.org/10.1016/j.physb.2019.411791>
 56. Gao L.K., Zhao X.H., Diao X.F., Tang T.Y., Tang Y.L. First-principles study of photoelectric properties of CsSnBr_3 under hydrostatic pressure. *Acta Physica Sinica*. 2021; 70(15): 158801. <https://doi.org/10.7498/aps.70.20210397>
 57. Yacobi B.G. Semiconductor materials: An introduction to basic principles. Springer; 2003. 229 p.
 58. Behram R.B., Iqbal M.A., Alay-e-Abbas S.M., Sajjad M., Yaseen M., Arshad I.M., Murtaza G. Theoretical investigation of mechanical, optoelectronic and thermoelectric properties of BiGaO_3 and BiInO_3 compounds. *Materials Science in Semiconductor Processing*. 2016; 41: 297–303. <https://doi.org/10.1016/j.mssp.2015.09.010>
 59. Aslam F., Sabir B., Hassan M. Structural, electronic, optical, thermoelectric, and transport properties of indium-based double perovskite halides $\text{Cs}_2\text{InAgX}_6$ ($X = \text{Cl}, \text{Br}, \text{I}$) for energy applications. *Applied Physics A*. 2021; 127(2): 1–112. <https://doi.org/10.1007/s00339-020-04178-x>
 60. Liu B.-W., Zhang M.-J., Zhao Z.-Y., Zeng H.-Y., Zheng F.-K., Guo G.-C., Huang J.-S. Synthesis, structure, and optical properties of the quaternary diamond-like compounds $\text{I}_2\text{--II--IV--VI}_4$ ($\text{I} = \text{Cu}$; $\text{II} = \text{Mg}$; $\text{IV} = \text{Si}, \text{Ge}$; $\text{VI} = \text{S}, \text{Se}$). *Journal of Solid State Chemistry*. 2013; 204: 251–256. <https://doi.org/10.1016/j.jssc.2013.05.039>
 61. Penn D.R. Wave-number-dependent dielectric function of semiconductors. *Physical Review*. 1962; 128(5): 2093–2097. <https://doi.org/10.1103/physrev.128.2093>
 62. Gao C., Li R., Li Y., Wang R., Wang M., Gan Z., Bai L., Liu Y., Zhao K., Liu S.F., Cheng Y., Huang W. Direct-indirect transition of pressurized two-dimensional halide perovskite: Role of benzene ring stack ordering. *Journal of Physical Chemistry Letters*. 2019; 10(19): 5687–5693. <https://doi.org/10.1021/acs.jpclett.9b02604>
 63. Shim H., Monticone F., Miller O.D. Fundamental limits to the refractive index of transparent. *Optical Materials Advanced Materials*. 2021; 33: 2103946. <https://doi.org/10.48550/arXiv.2103.15697>
 64. Wei M.-Q., Lai Y.-S., Tseng P.-H., Li M.-Y., Huang C.-M., Ko F.-H. Concept for efficient light harvesting in perovskite materials via solar harvester with multi-functional folded electrode. *Nanomaterials*. 2021; 11(12): 3362. <https://doi.org/10.3390/nano11123362>
 65. Kumar R.V., Varghese J., Varghese J., Unnikrishnan N.V. Structural, optical and dielectric properties of gadolinium incorporated laser ablated ZnO thin films. *Optik*. 2018; 174(2): 274–281. <https://doi.org/10.1016/j.ijleo.2018.08.074>
 66. Soykan C., Gocmez H. First-principles study for comparison of the electronic and optic bandgaps of the $\text{CH}_3\text{NH}_3\text{Pb}_{1-x}\text{Y}_x\text{I}_3$ ($\text{Y} = \text{Bi}, x = 0.00, 0.125$) and $\text{CH}_3\text{NH}_3\text{Pb}_{1-x}\text{Y}_x\text{I}_3$ ($\text{Y} = \text{Ca}, \text{Sr}, x = 0.125, 0.250$) perovskites. *Physica B: Condensed Matter*. 2021; 608: 412897. <https://doi.org/10.1016/j.physb.2021.412897>
 67. Al S., Kurkcu C., Yamcicier C. Structural evolution, mechanical, electronic and vibrational properties of high capacity hydrogen storage TiH_4 . *International Journal of Hydrogen Energy*. 2020; 45(55): 30783–30791. <https://doi.org/10.1016/j.ijhydene.2020.08.108>
 68. Jain I.P., Lal C., Jain A. Hydrogen storage in Mg: A most promising material. *International Journal of Hydrogen Energy*. 2010; 35(10): 5133–5144. <https://doi.org/10.1016/j.ijhydene.2009.08.088>