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Structural, Electronic, Mechanical, and Optical Properties of the Li_2CaCdH_6: A First-Principles Study with Gravimetric Hydrogen Storage Capacity

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Abstract

The potential application of hydride perovskite in hydrogen storage, a critical aspect of sustainable energy sources, has gained great attention. This work uses Density Functional Theory to analyze the structure, mechanical, electronic, optical, and hydrogen storing capability of the Li_2CaCdH_6 hydride complex. The investigation of its structural properties indicate that Li_2CaCdH_6 crystallizes in space group #225 (Fm-3m), from its ideal lattice constant and volume calculated. The gravimetric hydrogen storage capacity of Li_2CaCdH_6 was determined to be 3.51 wt%. Electronic property calculations, including band gap and density of states, suggest that the material is a semi-conductor of indirect bandgap (M-G) 1.95 eV calculated by GGA-PBE approximation. Additionally, the research estimated Young's modulus, shear modulus, bulk modulus, Poisson's ratio, Pugh's ratio and anisotropy for Li_2CaCdH_6, verifying its mechanical stability based on Born's stability criterion (C_{ij}). The positive Cauchy's pressure (15.24 GPa) suggests its ductile behavior. The value of B/G = 3.22, also indicates that the examined material has ductile nature. It is found that the studied compound has a Poisson's ratio of 0.36 which confirms that there is a predominant bonding character which is ionic. Furthermore, Density Functional Theory was utilized to predict optical properties that are dielectric function, reflectivity, refractive index, conductivity, absorption, and energy loss function. The present study explores Li_2CaCdH_6 as a potential hydride perovskite for hydrogen storage applications.

1. Introduction

Energy storage is a critical component of contemporary energy systems, especially as the world gradually shifts from fossil fuels to green energy sources [1-3] . Our energy needs are always rising and we use natural gas, coal, and petroleum resources to meet them. As fossil fuels get depleted, their costs rise, prompting the search for alternative energy sources. It is feasible to satisfy routine energy demands using energy generated from renewable sources. The usage of clean energy is rapidly rising while the usage of fossil fuels is being reduced in order to comply with worldwide treaties on carbon dioxide emissions. As a result, the usage of renewable energy sources has been encouraged [4] . Hydrogen applications entail industrial uses like ammonia production and low-carbon steel manufacture, as well as residential heating and transportation, notably in fuel cell electric cars and hydrogen combustion engines, which help to achieve current

energy policy objectives [5]. Hydrogen therapy is being investigated as a cancer treatment owing to its antioxidant, anti-inflammatory, and anti-apoptotic qualities [6]. Hydrogen use in agriculture, notably via H_2-saturated water, improves plant growth, stress tolerance, and post-harvest durability [7]. Energy storage materials, especially solid-state nanoparticles, improve device efficiency by increasing surface area and facilitating charge transfer. Solid-state materials have revolutionized energy conversion and storage processes [8, 9] .

Hydrogen storage problems restrict broad use of hydrogen energy, since old approaches are expensive in terms of energy and resources [10] . There is growing interest in perovskite hydride materials for hydrogen storage that is critical for developing sustainable energy systems. This interest originates from the necessity for effective hydrogen storage options to support renewable energy technologies [11] . Perovskite-type structures hold immense promise for advancing hydrogen storage technologies and solar cell applications, establishing a robust foundation for future breakthroughs in these critical areas [12] .

As attainable compounds for hydrogen storage, $KMnH_3$ has a gravimetric hydrogen storage capability of 3.021 wt% while $KFeH_3$ has a capacity of 2.994 wt% [13] . The novel perovskite hydrides $XSnH_3$, wherein X refers to rubidium, cesium, and francium, are being explored with a spotlight on possible uses as hydrogen storage units. $RbSnH_3$, $CsSnH_3$, and $FrSnH_3$ have hydrogen storage capabilities of 1.45 wt%, 1.18 wt%, and 0.87 wt%, respectively, according to calculations [14] . With gravimetric capacities of 3.771, 3.606, and 3.643 wt% respectively, perovskite hydrides, particularly $MgXH_3$ (X = Cr, Fe, Mn), demonstrate encouraging hydrogen storage characteristics, rendering them prospective contenders for use in renewable energy storage mechanisms for hydrogen [15] . $LaCrO_3$, an oxide perovskite, has shown potential as a hydrogen storage material with a capacity of around 4 wt% [16] . Conventional intermetallic alloys are unable to achieve the hydrogen storage capacity for desired outcomes [17] . One of the most essential demands for automobiles is hydrogen energy, which is 100% renewable and environmentally friendly [18] . Finding the sweet spot between gravimetric and volumetric densities, while limiting the massive amount of hydrogen gas, is the challenge of hydrogen storage [19]. Because of its widespread use in metal hydrides and other modified materials, lithium is an important component in hydrogen storage systems. The solid-state uses of Li-based compounds are supported by research that shows they have potential hydrogen storage capabilities [20-22]. Calcium (Ca) has a significant role in hydrogen storage via diversity of compounds and materials, with promising capabilities and stability. Recent research studies encourage calcium's usefulness in improving hydrogen adsorption and storage in various hydride structures making it an appealing constituent in hydrogen storage technologies [23, 24]. However, recent studies indicate that a silver cadmium oxide alloy has been applied in the hydrogen storage device, which possibly contributes to the durability and efficiency of hydrogen storage [25, 26]. Nevertheless, theoretical investigations into the electronic, mechanical, and optical properties of materials remain relatively scarce, despite their critical importance in understanding the interplay between electronic and optical behaviors in double perovskite materials [27].

In this work, we used ab-initio calculations grounded in density functional theory (DFT) to scientifically examine the structural, electronic, mechanical, and optical properties of

Li_2CaCdH_6, with a specific focus on its potential for hydrogen storage applications. This material was chosen due to its limited existing research, high hydrogen storage capacity, favorable formation energy, and mechanical stability. The comprehensive analyses aim to provide deeper insights into the properties of material and its suitability for advanced energy storage technologies.

2. Computational Method

The geometry of the hydride perovskite Li_2CaCdH_6 was optimized in Density Functional Theory (DFT) calculations using the Cambridge Serial Total Energy Package (CASTEP) [28, 29]. Exchange correlation was treated within the Generalized Gradient Approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) functional (While GGA/PBE underestimates band gaps and van der Waals interactions, but it remains highly efficient for large systems due to its low computational cost and rapid band structure prediction, including valence band (VB) and conduction band (CB) density of states.) [30-33] , and electron ion interactions were defined retaining the Projector Augmented Wave (PAW) method [34, 35] with a cut-off of 598 eV for kinetic energy. Brillouin zone was sampled using a 4×4×4 Monkhorst-Pack k-point grid [36, 37] and Vanderbilt ultrasoft pseudopotentials [38] were applied for the electron ion potential. Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm with Pulay density mixing scheme was used to perform energy minimization [39, 40] . The maximum force was set to 0.03 eV/Å, the maximum ionic displacement to 0.001 Å and the total energy/atom to 1.0 $\times 10^{-5}$ eV. Elastic constants were used to evaluate mechanical stability and material properties [41] . We employed computational details and theoretical approximations to systematically evaluate the material's structural stability, mechanical behavior, and optical characteristics.

3. Results and Discussion

3.1 Structural Properties

Figure 1 depicts the face-centered cubic crystal structure of the double hydride-perovskite Li_2CaCdH_6, which belongs to space group Fm-3m (#225).

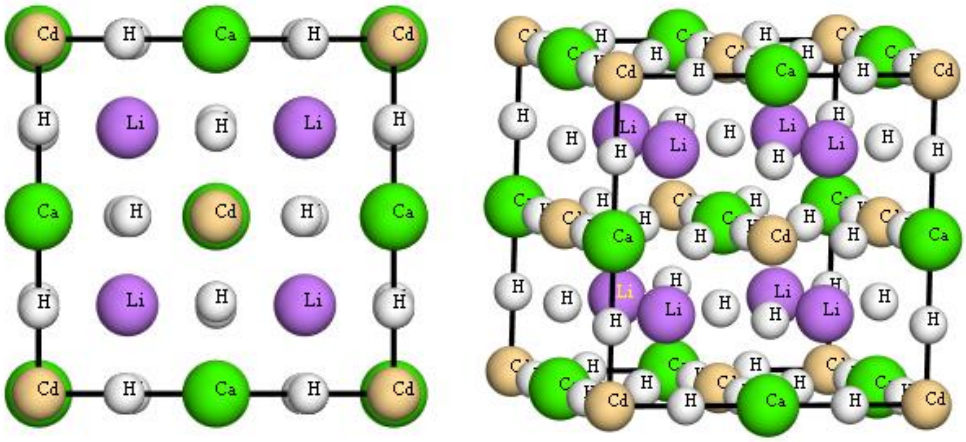


Fig. 1. Equilibrium crystal structure of double perovskite Li_2CaCdH_6

During optimization process of the cubic phase structure of compound, the Wyckoff positions of the atoms in Li_2CaCdH_6 were detailed in table 1: Calcium (Ca) atoms were positioned in the center of the unit cell; Cadmium (Cd) atoms were positioned at the; and Hydrogen (H) and Lithium (Li) atoms were situated at coordinates shown in table 1.

Table 1. Wyckoff position of Li, Ca, Cd and H

Element	Wyckoff position
Li	0.25, 0.25, 0.25
Ca	(0.5, 0.5, 0.5
Cd	0.0, 0.0, 0.0
H	0.25, 0.0, 0.0

The optimized lattice-constant for the structure was determined to be 8.271 Å, with the corresponding volume of the optimized unit cell calculated as 565.85 $Å^3$. This volume is associated with a final minimum energy of -1.105×10^4 eV. The density of the Li_2CaCdH_6 compound was found to be 2.024 g/cm³. Additionally, the final enthalpy was calculated by using equation 1, and its negative value strongly indicates the thermodynamic stability of the Li_2CaCdH_6 compound.

$$\boldsymbol{\Delta H_f = \frac{E_{total}^{Li_2CaCdX_6} - \left[2\,E_{total}^{Li_2} + E_{total}^{Ca} + E_{total}^{Cd} + 6E_{total}^{H_6}\right]}{N}} \quad \textbf{(1)}$$

The formation energy per atom (ΔH_f) for the Li_2CaCdH_6 perovskites is calculated using the above relation. Where E_{tot} (Li_2CaCdH_6) is the total energy of the optimized compound, E_{tot}(Li), E_{tot}(Ca), E_{tot}(Cd) and E_{tot}(H) represent the energies of the isolated constituent atoms in the material, and N is the total number of atoms in the unit cell.

The computed ΔH_f values is −1.104 eV/atom. The negative formation energies confirm thermodynamic stability, suggesting that the synthesis of studied hydride perovskites is energetically favorable and proceeds via an exothermic reaction. This stability arises from the strong bonding interactions between the constituent elements in the perovskite structure.

3.2 Hydrogen storage capacity

A theoretical equation is applied to estimate the gravimetric hydrogen storage capacity Cwt% of Li_2CaCdH_6 hydride-perovskite, assessing their viability for hydrogen storage appliances. The $C_{wt\%}$ metric quantifies the mass of deposited hydrogen relative to the host perovskite's mass, as defined by the following equation 2a [42, 43]:

$$\mathbf{C_{wt\%} = \left(\frac{\left(\frac{H}{M}\right)m_{Hydrogen}}{m_{Host} + \left(\frac{H}{M}\right)m_{Hydrogen}}\right)} \quad \textbf{(2a)}$$

In the equation, $m_{Hydrogen}$ represents the hydrogen molar mass, m_{Host} denotes the host compound molar-mass, and H/M is the ratio of hydrogen atoms to compound atoms. The $C_{wt\%}$ values, accessible in Table 2, indicate the hydrogen's gravimetric storage capacity of Li_2CaCdH_6

perovskite. With a $C_{wt\%}$ value of 3.51, Li_2CaCdH_6 demonstrates significant potential as a capable candidate for hydrogen (H_2) storage applications.

Table 2. Optimized compounds parameter and compression with Li_2CaCdH_6

Compounds	a (Å)	V (Å^3)	E_g (eV)	λ (nm)	$C_{wt\%}$	Ref.	
$LiCaH_3$	4.29	78.953	2.37	523.206	4.40	[44]	DFT
K_2NaScH_6	8.62	640.503	4.41	281.179	5.08	[45]	DFT
$NaCaH_3$	4.35	82.312	2.23	563.636	4.38	[44]	DFT
Ca_2FeH_6	4.87	115.50	1.67	742.514	4.28	[46]	DFT
K_2LiAlH_6	7.93	498.677	2.82	439.716	3.771	[45]	DFT
$KCaH_3$	3.92	60.45	2.71	457.56	3.67	[43]	DFT
Li_2CaCdH_6	8.27	565.85	1.95	635.82	3.51	This work	
Na_2CaCdH_6	8.405	593.764	2.08	596.153	2.956	[11]	DFT
$KSrH_3$	4.77	108.50	1.41	879.432	2.33	[47]	DFT
Rb_2CaCdH_6	8.76	674.07	2.30	539.130	1.69	[27]	DFT

Li_2CaCdH_2 demonstrates a hydrogen storage capacity of 3.51 wt%, achieving 64% of the U.S. DOE's 2025 interim target (5.5 wt%) and 54% of the ultimate storage goal (6.5 wt%) [48]. While this performance places it below the highest-capacity complex hydrides like $LiBH_4$ (18 wt% theoretical) [49]. The studied material shows significant advantages over conventional metal hydrides in terms of operating conditions with predicted theoretically calculated desorption temperatures. The hydrogen desorption temperature is defined as the temperature needed to release hydrogen (H) from the material. This value can be derived from Equation 2b, which incorporates the formation enthalpy (ΔH_f) and the entropy change (ΔS) of hydrogen taken as 130.7 J/mol·K [50].

$$T_{des} = \frac{\Delta H_f}{\Delta S} \quad \textbf{(2b)}$$

Applying this equation, the desorption temperature for Compound is to be 815.3 K.

Table 3 Desorption temperature of the compound.

Materials	Desorption temperature T_{des} (K)	Ref.
$LiCrH_3$	3055.48 K	[50]
$KCrH_3$	2865.02 K	[50]
$CsCrH_3$	2610.34 K	[50]
CaTiO3H6	827.1 K	[51]
Li_2CaCdH_6	815.3 K	This work

3.3 Electronic properties

The bands structure determines the available energy levels where electrons can exist to control the electrical behavior of compounds. An inspection of band structure enables materials classification into insulator, semiconductor and conductor. The electronic band structure calculation of Li_2CaCdH_6 appears in Fig. 2a. A horizontal red line marks the Fermi level at 0.0 eV position. The materials framework consists of two energy portions that include the valence band (V.B) lower and the conduction band (C.B) higher in energy. The band gap of the compound reveals an indirect Band gap (M-G) of 1.95 eV because valence and conduction bands throughout the structure do not merge together. It confirmed that Li_2CaCdH_6 shows semiconducting behavior according to its band gap analysis [52] .

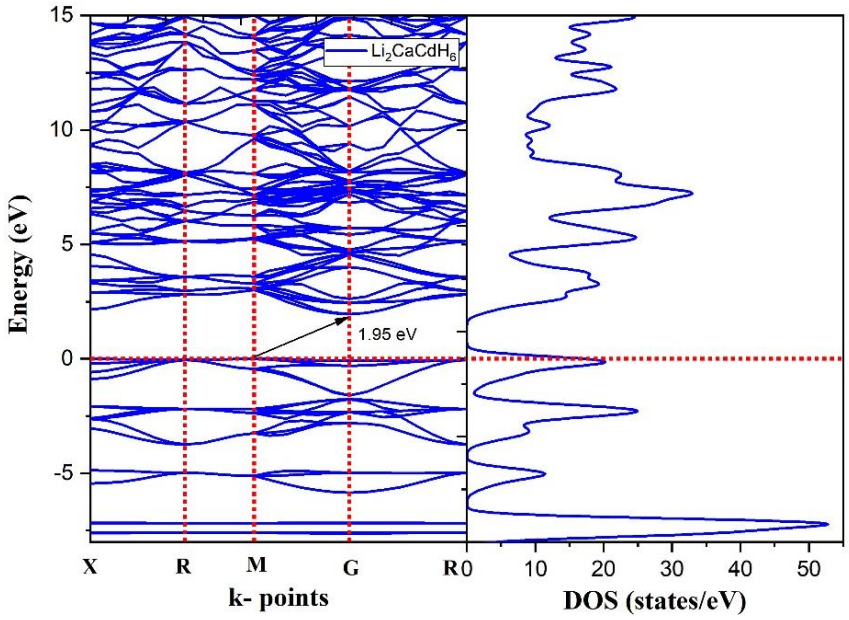


Fig. 2. Electronic properties of Li_2CaCdH_6 (a) Band structure and, (b) DOS.

Figure 2(b) shows the Density of States (DOS) curve that illustrates how individual elements affect the entire band structure. Both bands in Li_2CaCdH_6 reach their maximal density of states at 32.91 states/eV (7.26 eV) in C.B and 52.94 states/eV (-7.21 eV) in V.B., while the Fermi level intersects (20.16 eV/states, -0.11 eV). The C.B contains 2.0 to 4.0 eV occupancy from s-states but the p-state stands out within 6.0 to 10.0 eV. The C.B contains the d-state and extends from 2.0 eV through 4.0 eV where multiple states including d- and p-states affect both C.B and V.B regions. The majority of s-states and d-states exist in the vicinity of the Fermi level and within the V.B. Both DOS analysis and PDOS analysis of Li_2CaCdH_6 were performed over different energy ranges that extended from (-8 to 8) eV and (-8 to 20) eV respectively. The PDOS measurement around the Fermi level identifies 20.45 states/eV in Li_2CaCdH_6 together with the separate PDOS values of 3.84 states/eV for Li, 7.99 states/eV for Ca, 3.85 states/eV for Cd and 5.84 states/eV for H respectively. The partial density of states for Li_2CaCdH_6 receives major support from the elements H, Li and Ca. The C.B region shows Li and Ca are the principal elements in Figure 3a–d where Li

s- and p-orbital peaks are seen at (3.31 eV, 6.19 states/eV) and (7.32 eV, 16.28 states/eV) and Ca exhibits prominent d-orbital peaks at (3.75 eV, 7.70 states/eV) and (7.18 eV, 10.36 states/eV).

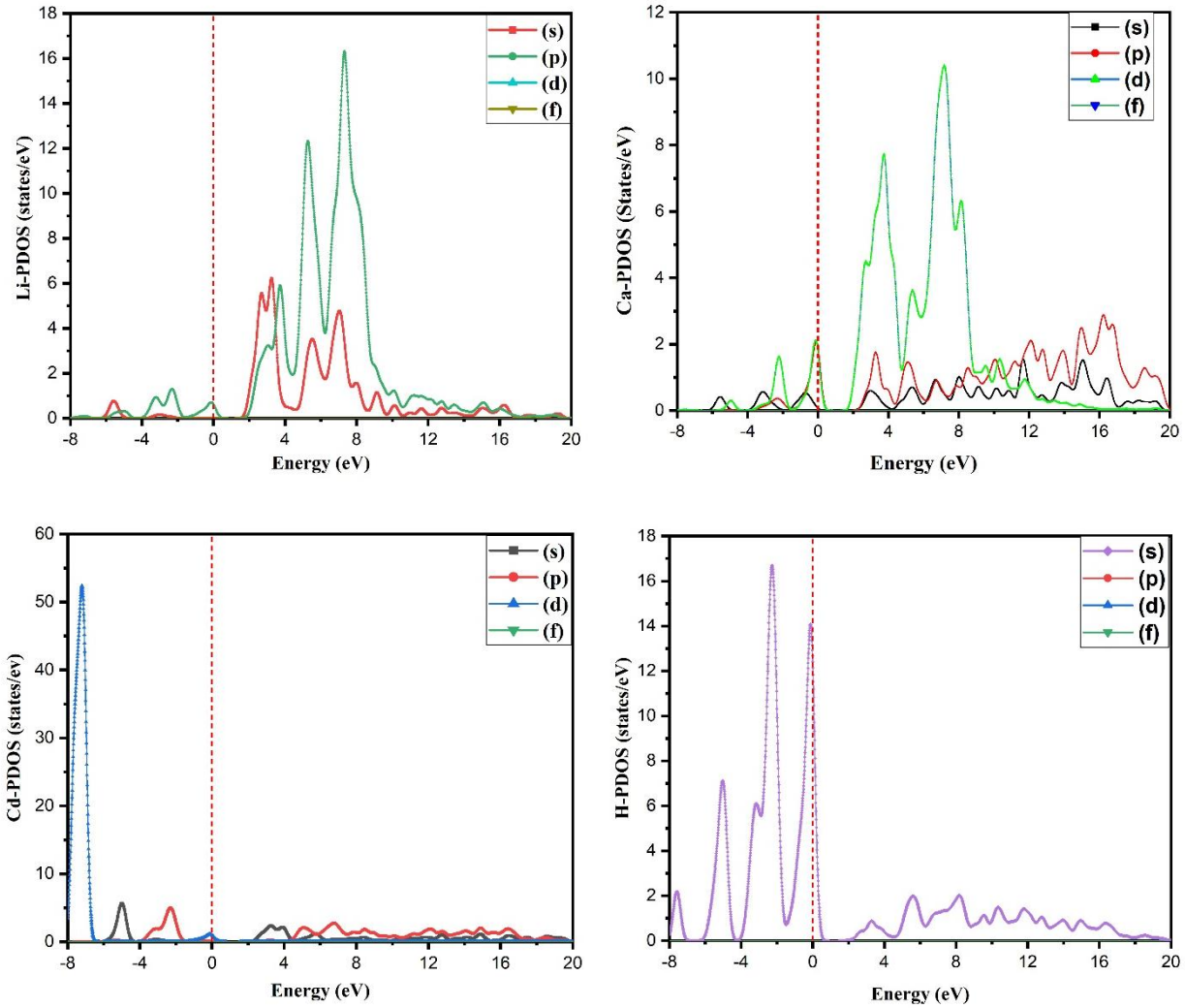


Fig. 3. Partial density of states of Li_2CaCdH_6 (**a**) Li- (**b**) Ca- (**c**) Cd- (**d**) H-PDOS.

In contrast, cadmium (Cd) primarily contributes through its d-orbital in the valence band, with a prominent peak at (-7.28 eV, 52.20 states/eV). The s orbitals and p-orbitals of Cd show minimal contribution, while the f-orbital plays no role. The s-orbital of hydrogen (H) significantly contributes to the valence band, with one of its peaks (-0.10 eV, 14.01 states/eV) crossing the Fermi level and partially contributing to the conduction band's minima. Other peaks for the H-atom are observed at (-2.24 eV, 16.63 states/eV), (-4.99 eV, 7.00 states/eV), and (-7.59 eV, 2.10 states/eV). The red dotted line at 0 eV denotes the Fermi-level. The curves collectively indicate that the f-orbital has no contribution to either the DOS or PDOS.

Li_2CaCdH_6 works based on how hydrogen (H), lithium (Li), calcium (Ca), and cadmium (Cd) interact with each other at the orbital level. The main role of the hydrogen 1s orbital is to form the valence band as a hydride ion (H^-) and to bond by ionic and polar covalent methods with lithium (Li^{2+}), calcium (Ca^{2+}), and cadmium (Cd^{+2}). Molecular orbitals of the H-s states are found mostly in the valence band (VB), while some also overlap with the conduction band due to weak

antibonding effects. The 2s orbital of lithium is closed, which allows it to donate electrons strongly and play a deep role in the CB, but without much hybridization or ability to conduct electricity. In its Ca^{2+} form, calcium has strong bonds with H^- and uses both its 4s and part of its 3d orbitals in the lower CB.

The covalent bond between cadmium and hydrogen is caused by mixing of the outermost orbitals of cadmium and hydrogen atoms. The weak effect of Cd-d on the VB is important to note, while the 5s/p orbitals may be close to the CB, but have a very little effect on conductivity. From the overall electron structure, it is clear that the compound acts as a semiconductor, with the valence band having localized H and Cd states, and the conduction band filled by Ca and Li states, and minor H states

3.4 Mechanical and anisotropic elastic properties

The material's mechanical stability - and consequently its industrial performance is fully described through its elastic constants (C_{ij}). These constants were calculated using CASTEP. For cubic structures, the essential elastic constants are C_{11}, C_{44} and C_{12}, which are provided in Table 4 for Li_2CaCdH_6. The estimated values meet the well-established Born stability criteria [53, 54] , as given in Eq. (3). Consequently, the material is confirmed to be mechanically stable, with C_{11} - C_{12} = 23.11558 and C_{11} + 2C_{12} = 94.75435, making them suitable for further mechanical property calculations.

$$C_{11} > 0; \qquad C_{44} > 0;$$

$$C_{11} - C_{12} > 0; \qquad C_{11} + 2C_{12} > 0 \qquad (3)$$

The computed elastic constants can be used to derive various physical parameters, like Young's modulus, shear modulus and bulk modulus, which are accessible in Table 4. These moduli were determined using the Voigt [55] , Reuss [56] , and Hill [57] approximations. The Voigt method gives the maximum value of the modulus, the Reuss method provides the minimum value, and the Hill approximation is the arithmetic mean of the two.

$$G = \frac{1}{2}(G_V + G_R) \qquad (4a)$$

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \qquad (4b)$$

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

The bulk modulus (B) quantifies a material's resistance to volume change under applied pressure. As evident from Table 4, Li_2CaCdH_6 shows the highest bulk modulus of 31.585 GPa. The shear modulus (G), estimated by the ratio of shear-stress to shear-strain, is a critical parameter for assessing hardness, with higher values indicating greater opposition to plastic deformation. In contrast, the bulk modulus (B) reflects the material's opposition to fracture. Young's modulus (Y) represents the ratio of tensile stress to strain and aids as an important estimate of the material's

stiffness. A material having a higher estimate of Young's modulus (E) will be stiffer. These properties collectively provide essential understandings into the mechanical behavior of the compound. The equations used for mechanical properties are:

$$A = \frac{2C_{11}}{C_{11} - C_{12}} \quad \textbf{(5a)}$$

$$Y = \frac{9GB}{3B+G} \quad \textbf{(5b)}$$

$$\nu = \frac{3B - 2G}{2(2B+G)} \quad \textbf{(5c)}$$

The factor "A" in anisotropy is the degree of elastic anisotropy in cubic crystals so that A = 1 means consistent isotropy. The studied material, has an anisotropy factor of A = 4.07 and that is why material has anisotropic nature. Poisson's ration (ν) indicates to some extent about the nature of the bonding in the material, as it indicates how much perpendicular expansion or contraction will occur during compression or expansion. The Poisson's ratio of the order of 0.1 might indicate covalent bonding and 0.25, 0.3 value for ionic bonding. It is found that the studied compound has a Poisson's ratio of 0.36 which confirms that there is a predominant bonding character which is ionic.

Another critical parameter for the brittle or ductile behavior of a material is the B/G ratio (Pugh's modulus). A B/G ratio greater than 1.75 specifies ductility, while B/G ratio less than this means that material is brittle conferring to the Pugh's criterion. The value of B/G = 3.22, indicates that the examined material has ductile nature. Furthermore, the Cauchy pressure (C_P) = $C_{12} - C_{44}$ is a solid indicator of material's behaviour. A positive C_P value produces ductility; a negative C_P value constitutes brittleness. It is further confirmed that the studied compound has ductile characteristics for the studied compound, as the positive C_P values.

Anisotropic elastic properties and the Debye temperature were determined to analyze the material further. The ELATE code was used to create 2D and 3D visualizations [58] of the directional dependence of Young's modulus (Y), shear modulus (G), linear compressibility (β) and Poisson's ratio (υ) at specific conditions for Li_2CaCdH_6, as illustrated in Fig. 4. Three-dimensional spherical plots represent isotropy, while non-spherical shapes indicate anisotropy. The 3D contour plots for the studied compound reveal non-spherical shapes, confirming elastic anisotropy in all directions. However, the linear compressibility of the compound is isotropic across all directions [59] . For Li_2CaCdH_6, the parameters E, G, β, and υ exhibited consistent behavior across the xy, yz, and zx planes, further highlighting its anisotropic elastic properties.

Table 4. The computed elastic parameters: [C_{11}, C_{12}, C_{44}] (GPa), Bulk modulus B (GPa), Shear modulus G (GPa), Young's modulus Y (GPa), Poisson's ratio (υ), Pugh ratio (B/G), anisotropy factor (A) and Cauchy pressure (C_P)

Compound	C_{11}	C_{12}	C_{44}	B	G	Y	υ	B/G	A	C_P
Li_2CaCdH_6	46.995	23.879	8.641	31.585	9.808	26.665	0.36	3.22	4.07	15.24

3.4.1 Debye temperature

The Debye temperature (T_D) is strictly associated with various other properties of material, including melting temperature and heat capacity. A greater Debye temperature typically implies better thermal conductivity and a higher melting point for the material. The computed values of the velocity of longitudinal-wave (V_l), velocity of transverse-wave (V_t), average wave velocity (V_m), and T_D are presented in Table 5. T_D, V_m, V_l, and V_t were determined by the below equations [60, 61] . In Equation (6), h represents Planck's constant, n (No. of atoms per unit cell), k (Boltzmann constant), ρ (density), M (unit cell atoms mass), and NA (Avogadro's number).

$$T_D = \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_a\rho}{M}\right)\right]^{1/3} v_m \qquad (6)$$

where

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_l^3} + \frac{1}{v_t^3}\right)\right]^{-1/3} \qquad (6a)$$

Utilize the G and B values, to get the values of υ_l and υ_t.

$$v_l = \sqrt{\frac{3B + 4G}{\rho}} \qquad and \qquad v_t = \sqrt{\frac{G}{\rho}}. \qquad (6b)$$

The melting temperature (T_m) has also been calculated by using the Equation (7) [62] .

$$T_m(K) = [553(K) + 5.911C_{11}] \pm 300K \qquad (7)$$

Table 5. Computed Debye temperatures point (T_D), transverse (υ_t), longitudinal (υ_l) and average (υ_m) wave-velocities and melting points (T_m) for Li_2CaCdH_6

Compound	T_D (K)	υ_t (m/s)	υ_l (m/s)	υ_m (m/s)	T_m (K)
Li_2CaCdH_6	303.20	2021.3	8136.3	2886.0	830.79 ± 300

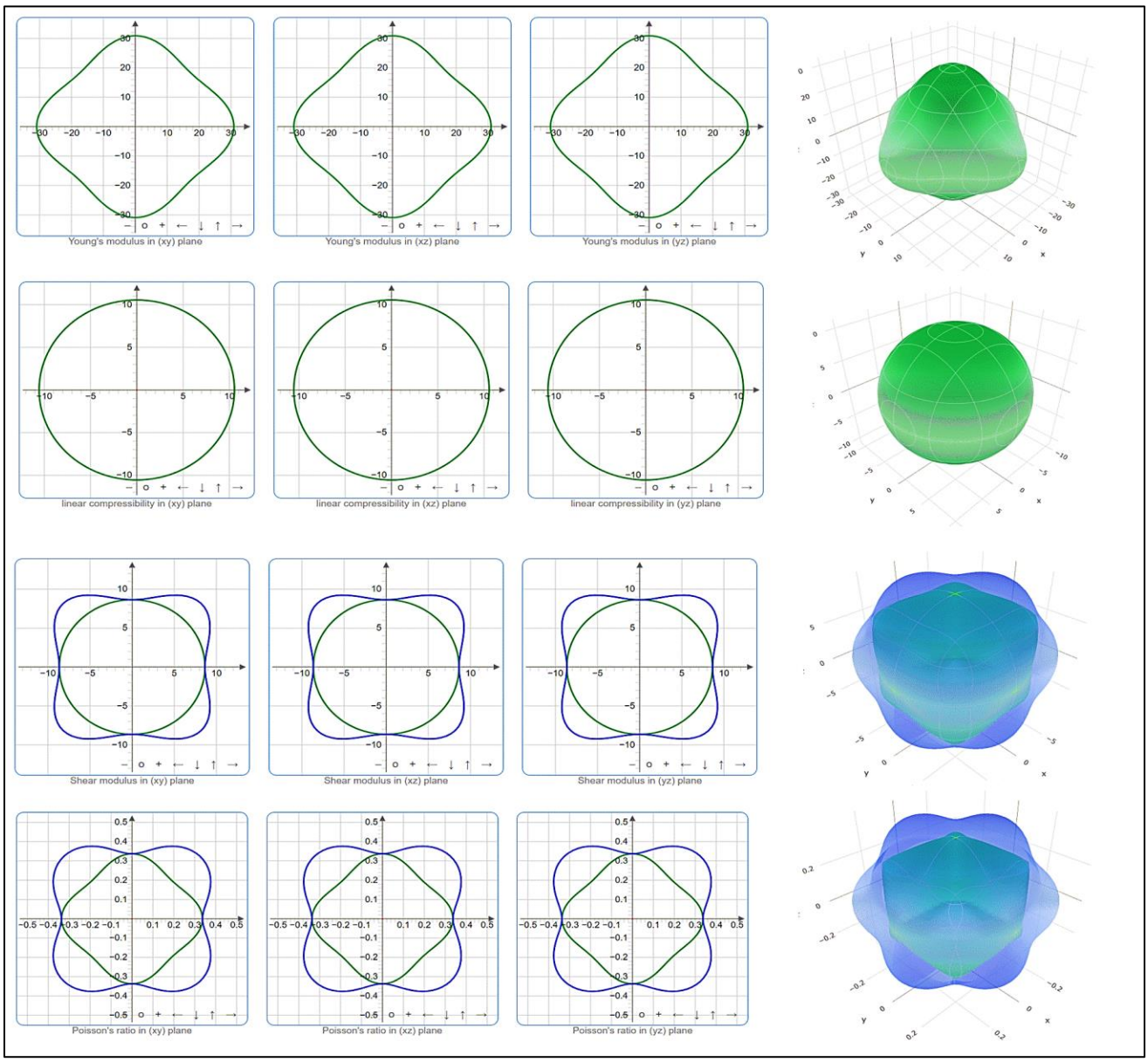


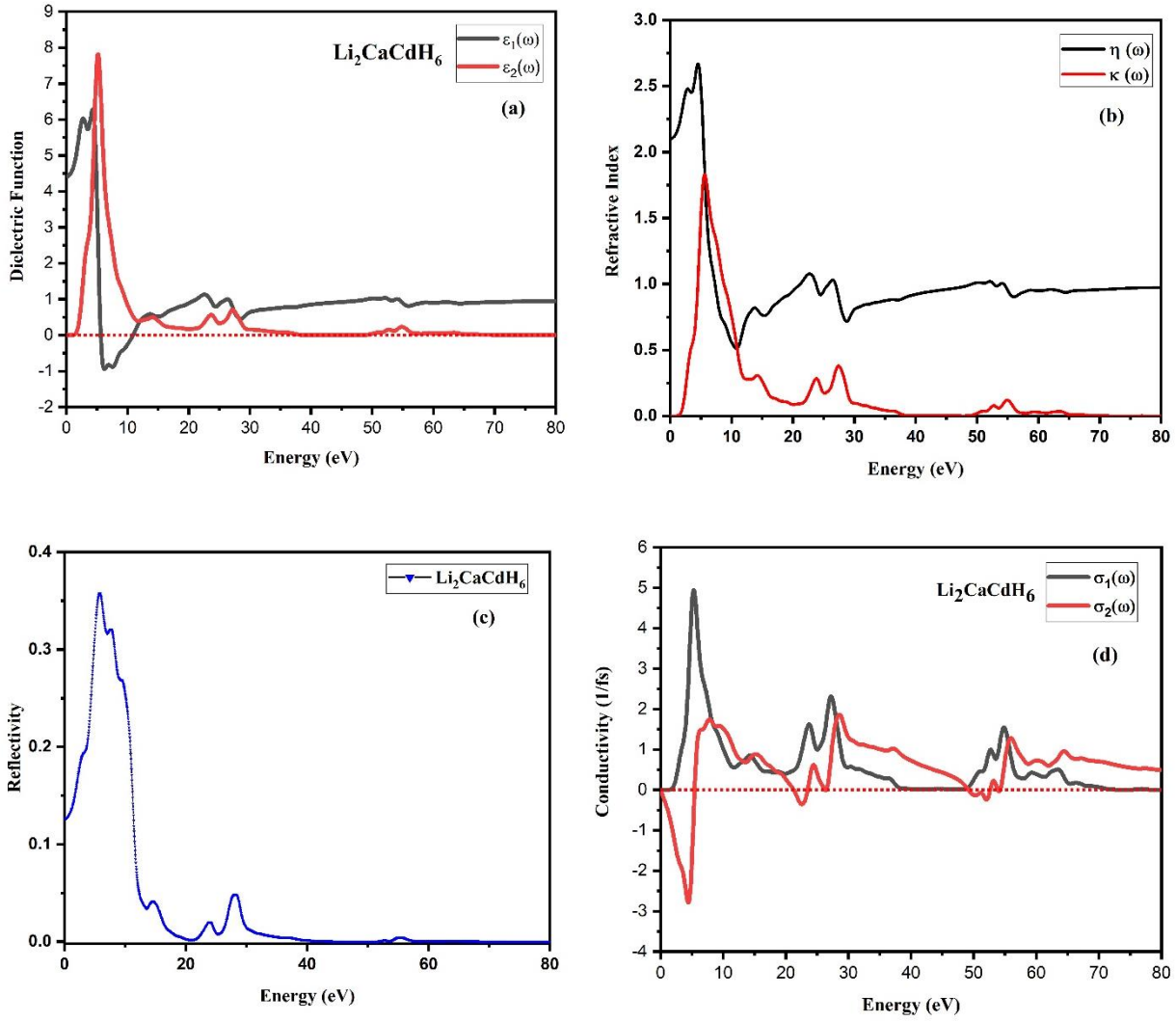
Fig. 4 Anisotropy 2D and 3D plots for Li_2CaCdH_6

3.5 Optical properties

Our research in this portion primarily focuses on exploring the material's optical properties to understand their interactions with EM waves (electromagnetic photons). We conducted a comprehensive analysis of the optical properties, emphasizing intraband shifts that show a semiconductor nature, as illustrated in figures 5 (a-f). Our results align with the well-established Drude model, originally proposed by the renowned scientist Drude [63, 64] . By calculating optical parameters, our intention is to evaluate the potential of the studied perovskite compound for hydrogen (H_2) storage purposes.

The solid material's optical properties can be investigated through their electronic dielectric function, which is largely influenced by intra-band and inter-band transitions, as

expressed via Ehrenreich Cohen formulation as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ [65]. Here, $\varepsilon(\omega)$ characterizes the interaction of material with EM waves and is divided into two components: $\varepsilon_1(\omega)$, which indicates polarization, and $\varepsilon_2(\omega)$, which describes energy dissipation within the system [66] . The real and imaginary components of the dielectric function are denoted as $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, correspondingly, as depicted in Fig. 5a.



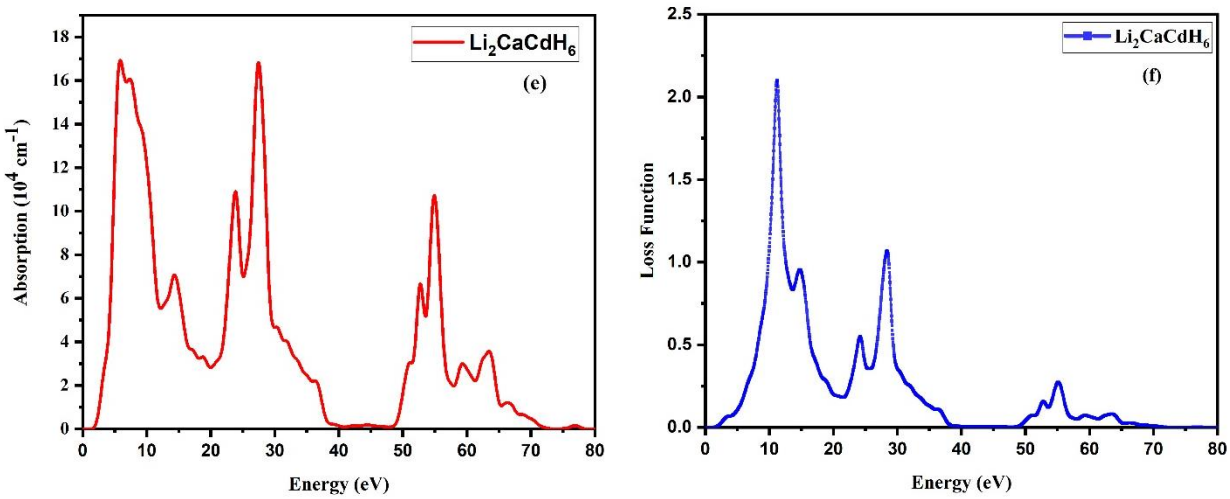


Fig. 5. Optical properties of Li_2CaCdH_6 (**a**) dielectric function (**b**) refractive index (**c**) reflectivity (**d**) conductivity (**e**) absorption and (**f**) loss function.

The imaginary part of the dielectric-function, depending on ($\omega'^2 - \omega^2$), can be utilized to compute the real portion of the dielectric function. Additionally, ω' is directly related to the energy bandgap (E_g). The real part, $\varepsilon_1(\omega)$, can be resulting from the Kramers-Kronig (KK) relation [67] . Conversely, the Kramers-Kronig relation can also be employed to get the imaginary part from the real component, establishing a fundamental connection between the two parts of the dielectric function.

$$\boldsymbol{\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'} \quad \textbf{(8a)}$$

$$\boldsymbol{\varepsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_0^{\infty} \frac{\varepsilon_1(\omega') - 1}{\omega'^2 - \omega^2} d\omega'} \quad \textbf{(8b)}$$

For the compound Li_2CaCdH_6, the real part of the dielectric-function, $\varepsilon_1(0)$ has a value of 4.41. The highest value of $\varepsilon_1(\omega)$ for Li_2CaCdH_6 is 6.27, occurring at 4.29 eV. On the other hand, the imaginary component of dielectric function, $\varepsilon_2(0)$, begins at 1.18 eV with a value of 0.00. The compound Li_2CaCdH_6 exhibits the highest peak in $\varepsilon_2(\omega)$ at 7.81 eV, with a value of 5.17.

The refractive index can be determined by the following equation:

$$\boldsymbol{\eta(\omega) = \left(\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{[\varepsilon_1(\omega)]^2 + [\varepsilon_2(\omega)]^2}}{2} \right)^{1/2}} \quad \textbf{(9a)}$$

$$\boldsymbol{\kappa(\omega) = \left(\frac{\sqrt{[\varepsilon_1(\omega)]^2 + [\varepsilon_2(\omega)]^2}}{2} - \frac{\varepsilon_1(\omega)}{2} \right)^{1/2}} \quad \textbf{(9b)}$$

Figure 5b illustrates the refractive index for both the real (Re) $\eta(\omega)$ and imaginary (Im) $\kappa(\omega)$ components. The maximum (Re) $\eta(\omega)$ for Li_2CaCdH_6 is approximately 2.66 at 4.53 eV, while the imaginary component peaks at 1.89 at 6.03 eV. The static $\eta(0)$ and the imaginary refractive index $\kappa(\omega)$ for Li_2CaCdH_6 are 2.10 and 0, respectively. The real part of the refractive

index reaches 2.65, its highest peak at 4.71 eV. The κ(ω) or extinction coefficient, begins at 1.52 eV with a value of 0.01 and attains its maximum peak of 1.82 at 5.61 eV.

Reflectivity measures a material's ability to reflect incoming radiation, providing insights into how light photons interact with its electronic structure. To analyze the frequency-dependent reflectivity R(ω) of the hydride perovskite against incident radiation energy ranging from 0.00 to 80.00 eV, it is plotted in figure 5c. These results offer valuable information about the optical response of material and its prospective applications in various technologies. R(ω) is given by:

$$\boldsymbol{R(\omega) = \frac{n + ik - 1}{n + ik + 1}} \quad \textbf{(10)}$$

At zero energy, the static reflectivity R(0) of the compound is 0.12. The reflectivity peaks at various energies, with the highest peak of 0.35 occurring at 5.94 eV. Other notable reflectivity values include 0.04 at 14.71 eV, 0.01 at 23.81 eV, and 0.05 at 28.07 eV. As the photon energy increases to the high energy values, the reflectance decreases sharply to minimum value of 0.00 at 39.79 eV. Conversely, the highest absorption for Li_2CaCdH_6 was observed in this high energy region.

The research also utilized conductivity σ(ω) to analyze how electrons (incident) interact with the surface of Li_2CaCdH_6 hydride perovskites, leading to bond breaking and conduction due to the photoelectric effect. Figure 5d presents the frequency dependent conductivity of Li_2CaCdH_6 hydride-perovskite in the energy range from 0.0 to 80.0 eV, revealing the influence of incoming photons energy on the real (Re) part of σ(ω). Li_2CaCdH_6 exhibited the maximum conductivity of 4.86 (1/fs) at 5.47 eV. The optical investigation suggests that Li_2CaCdH_6 is a promising candidate for hydrogen storage applications, due to its notable conductivity at specific photon energies. The imaginary component of the compound's conductivity peaks at -2.76 (1/fs) at 4.52 eV.

The absorption coefficient α(ω) has crucial part for finding length to which light travel in material. It depends on the wavelength (or energy, E=hc/λ) of the incident photons. Materials with high absorption coefficients tend to absorb photons more rapidly, exciting electrons into the conduction band. Figure 5e presents the calculated absorption coefficients for the perovskite Li_2CaCdH_6, mapped against incoming photon energy, from 0.0 to 80.0 eV. Notably, the studied material exhibited no absorption α(0). The equation for absorption coefficient [68]:

$$\boldsymbol{\alpha(\omega) = \frac{4\pi}{\lambda} \kappa\,(\omega)} \quad \textbf{(11)}$$

The study highlights a significant and sudden surge in the absorption of Li_2CaCdH_6 as the incident energy rises. The highest absorption for the compound in the ultraviolet region reaches 169,247.33 cm^{-1} at 5.89 eV, as depicted in the graphs. At higher frequencies, the absorption coefficients for all materials examined were found to be nearly zero. Additional absorption peaks were observed at 108,870.97 cm^{-1} (23.94 eV), 167,849.46 cm^{-1} (27.38 eV), and 106,612.90 cm^{-1} (55.19 eV).

The loss-function L(ω), which represents the energy lost by electrons during transitions due to dispersion or scattering, is directly proportional to the inner shell transitions scattering probabilities. Figure 5f illustrates the loss function of Li_2CaCdH_6 plotted against incident energy,

ranging from 0.0 to 80.0 eV. The graph indicates that the loss function remains at 0.00 until the photon energy reaches 1.80 eV, after which distinct peaks are observed.

$$\boldsymbol{L(\omega) = Im\,(\varepsilon(\omega)^{-1}) = \frac{\varepsilon_2(\omega)}{\varepsilon_2{}^2(\omega)} + \varepsilon_2{}^2(\omega)} \qquad \textbf{(12)}$$

Likewise, the curve reveals maximum spike top at 2.10 for radiation energy of 11.20 eV. Similarly, other notable peaks include 0.54 at 24.33 eV, 1.07 at 28.70 eV, and 0.26 at 55.19 eV. The sharp decline in the loss function at higher energies for the examined Li_2CaCdH_6 is expectedly attributed to plasmon emission. The results suggest that Li_2CaCdH_6 is a promising candidate for efficient EM wave absorption, as it exhibits no energy loss by the electrons in infrared range and have least energy L(ω) in the visible range. The release of photoelectrons occurs when E = ħω photon interact with the material's surface. This interaction underscores the potential of Li_2CaCdH_6 in applications requiring effective photon absorption and energy conversion. These findings indicate the potential for photochemical activation of hydrogen storage processes, which could replace conventional thermal methods and significantly reduce energy requirements [69].

4. Conclusion

Perovskite, especially hydride materials have emerged as a focal point in renewable and green energy systems, particularly for their role in H_2-storage. Using the DFT technique, the structural, optical, mechanical, electrical, and hydrogen storage resources of Li_2CaCdH_6 were thoroughly investigated. Structurally, Li_2CaCdH_6 crystallizes in space group 225 (Fm-3m), with optimized lattice constant and volume (V) of 8.27 Å and 565.85 Å³, congruently. The gravimetric hydrogen storage capacity of Li_2CaCdH_6 was calculated to be an impressive 3.51 wt% while desoprtiion temperature of 815.3 K. Electronic band structure and density of states (DOS) analyses revealed a semiconductor nature, characterized by a band gap of 1.98 eV, while structural stability was confirmed by a negative formation enthalpy of -1.104 eV/atom. Mechanical properties were also explored, with elastic constants (C_{11} = 46.995, C_{12} = 23.879, C_{44} = 8.641 GPa), modulus values (B = 31.585, Y = 26.665, G = 9.808 GPa), Pugh's ratio of 3.22, Poisson's ratio (ν = 0.36), anisotropy factor (A = 4.07) calculated for Li_2CaCdH_6. Material shows Ductile behavior. The Cauchy's pressure (C_p = 15.24) and Born stability criteria validated the mechanical stability. The highest absorption for the compound in the ultraviolet region reaches 169,247.33 cm^{-1} at 5.89 eV, this indicate the potential for photochemical activation of hydrogen storage processes. These findings reveal the propensity of Li_2CaCdH_6 perovskite as a promising candidate for hydrogen storage applications, offering a blend of structural integrity, electronic properties, and mechanical stability essential for advancing green energy technologies.

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