DFT analysis of physical properties and solid-state hydrogen storage potential of Sodium - Based Double Perovskites Na_2XH_6 (X = V, Cr and Co)

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Abstract. This study investigates novel hydrogen storage materials Na_2XH_6 (X = V, Cr and Co) using first-principles density functional theory (DFT) within the GGA-PBE approximation, as implemented in the CASTEP code. The structural, electronic, mechanical, optical and thermal properties are systematically analyzed. Gravimetric capacities (Cwt.%) are 5.88%, 5.81% and 5.45% for Na_2VH_6, Na_2CrH_6 and Na_2CoH_6, respectively. Geometry optimization yields stable structures with lattice constants of 7.65Å, 7.50 Å and 7.24Å. Negative formation enthalpies confirm thermodynamic stability, while band structure analysis reveals metallic character. Mechanical stability is verified by calculated elastic constants (C_{11}, C_{12} and C_{44}) satisfying the Born-Huang criteria.

Keywords: DFT; Sodium-based double perovskites hydrides; Hydrogen storage capacity; Mechanical properties; Optical properties.

1 Introduction

The current global energy context is characterized by a persistent dependence on fossil fuels [1], accompanied by growing concerns related to greenhouse gas emissions and climate change. In this perspective, hydrogen stands out as a promising energy vector due to its high energy density and clean nature, as its combustion produces only water. However, the large-scale development of a hydrogen-based economy remains strongly limited by the challenges associated with its safe, efficient, and cost-effective storage. Recent research has highlighted the advantages of implementing double perovskite hydride materials in advanced solid-state hydrogen storage systems that are safe, efficient and economically viable [2–4]. In this context, the Mg_2AH_x family (with x = 4, 5, or 6 and A representing a transition metal) exhibits remarkable potential for hydrogen storage applications, due to its superior gravimetric and volumetric hydrogen densities (ranging from 3.6–5.4 wt% and 77–150 kg. $H_2.m^{-3}$, respectively). In particular, Mg_2NiH_4 has a significantly enhanced hydrogen absorption and desorption kinetics relative to the widely utilized MgH_2 compound [5,6].
In this respect, a lot of attention has been paid to the development of lightweight complex hydrides based on lithium and magnesium. For instance, Li_2CaH_4 and Li_2SrH_4 [7] have been studied for hydrogen storage applications. In addition, a number of magnesium based compounds such as Mg_2FeH_6, Mg_2NiH_6, Mg_2CoH_6, Mg_2XH_6 (X = V, Cr) [8] and X_2NiH_6 (X = Li, Na, K) have also been extensively studied [9]. The objective of our study is to present and understand structural, thermodynamic, optical, electronic and mechanical properties of sodium-based double perovskite hydride compounds with a cubic structure having the formula Na_2XH_6 (X = V, Cr and Co). These properties are fundamental to the search for new materials for hydrogen storage applications. The reliable solid-state properties achieved in this study are based on employing first principles (ab-initio) quantum simulation methods using the software packages CASTEP and WIEN2k within the framework of density functional theory (DFT).

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2 Numerical Methodology

To optimize the crystal structure and evaluate the properties of Na_2XH_6(X = V, Cr and Co), first-principles calculations were performed within the framework of DFT using the CASTEP software[10] package. The exchange-correlation potential interactions were treated using the GGA-PBE approximation. In this regard, to ensure computational accuracy, the FP-LAPW was employed, with a cutoff energy of 540 eV, whereas the Monkhorst-Pack scheme was adopted for the sampling of the k-point within the first irreducible Brillouin zone (BZ) using a 4 × 4 × 4 grid. To model the interactions between electrons - ions in crystalline materials and to determine their electronic wave functions and charge densities, the BFGS algorithm and ultrasoft pseudopotentials energy minimization methodologies were employed. Finally, the mechanical stability was investigated by calculating the elastic constants (C_{ij}) using CASTEP. The convergence criteria were set to an energy tolerance of 5×10^{-6} eV/atom, a maximum Hellmann Feynman force of 0.01eV/Å and a maximum ionic displacement of 5×10^{-4} Å.

3 Results and discussions

3.1 Stability of the Cubic Crystal Structure

The three-dimensional crystal structure of the Na_2XH_6 (X=V, Cr and Co) compounds were visualized using the VESTA software [11]. These hydrides perovskites adopt a cubic crystal structure with the space group Fm-3m (No. 225). As illustrated in **Fig.1**, the Na atoms occupy the (0.250, 0.250, 0.250) positions, the X atoms are situated at (0.00, 0.00, 0.00), while the hydrogen (H) atoms are located at (0.25, 0.00, 0.00).

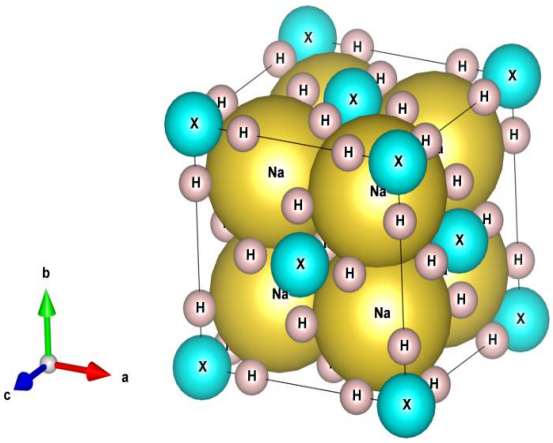

Fig. 1. Representation of the cubic crystal structure of the Na_2XH_6 (X = V, Cr and Co) double perovskites.

The thermodynamic stability of the studied structures was evaluated by computing their formation energies (ΔH_f) using the following expression [12,13]:

$$\Delta H_f = \frac{E((Na_2XH_6)-(2E(Na)+E(X)+6E(H))}{p} \quad (1)$$

In this equation, E(X), E(Na) and E(H) represent the ground state energies of isolated atoms of X, Na and H, respectively. While $E(Na_2XH_6)$ denotes the total energy of the Na_2XH_6 hydrides, and p is the total number of atoms in the system. The computed formation energies ΔH_f for these materials are summarized in **Table 1**. The negative formation energies (ΔH_f) -2.30, -2.27 and -2.50 (eV/atom) for Na_2VH_6, Na_2CrH_6 and Na_2CoH_6, respectively, confirm their thermodynamic stability

The gravimetric hydrogen storage capacities ($C_{wt\%}$) indicates a material's ability to store hydrogen and is evaluated as follows [14,15]:

$$C_{wt}\% = \left(\frac{\left(\frac{H}{M}\right)m_H}{m_{Host}+\left(\frac{H}{M}\right)m_H}\times 100\right)\% \quad (2)$$

Here, m_{Host} and m_H represent the molar mass of the host compound and hydrogen, respectively, while (H/M) denotes the ratio of hydrogen atoms to host material atoms. According to **Table 1**, Na_2VH_6 exhibits the highest hydrogen storage capacity (5.81 %), making it the most efficient and highly potential candidate among the materials studied.

In order to determine the ground state structural properties, we compute the total energy (E_T) as a function of volume (V) using WIEN2k software [16] through a subsequent fit to the Birch Murnaghan equation of state yielded the equilibrium structural parameters-namely the lattice constant (a_0) and the unit cell volume (V_0). The optimized parameters are summarized in **Table 1**. The governing equation for the total energy is expressed as follows [17]:

$$E_T = E_0 + \frac{B_0 V}{(B'_0(B'_0-1))}\left[B_0\left(1-\left(\frac{V_0}{V}\right)\right) + \left(\frac{V_0}{V}\right)^{B'_0} - 1\right] \quad (3)$$

Here, B_0 and B'_0 correspond to the equilibrium bulk modulus and its pressure derivative, respectively. E_0 and V_0 denote the total energy and equilibrium volume of the unit cell at zero pressure and temperature. The resulting energy - volume curves $E_T(V)$ for the studied perovskite hydride compounds are presented in **Fig. 2**.

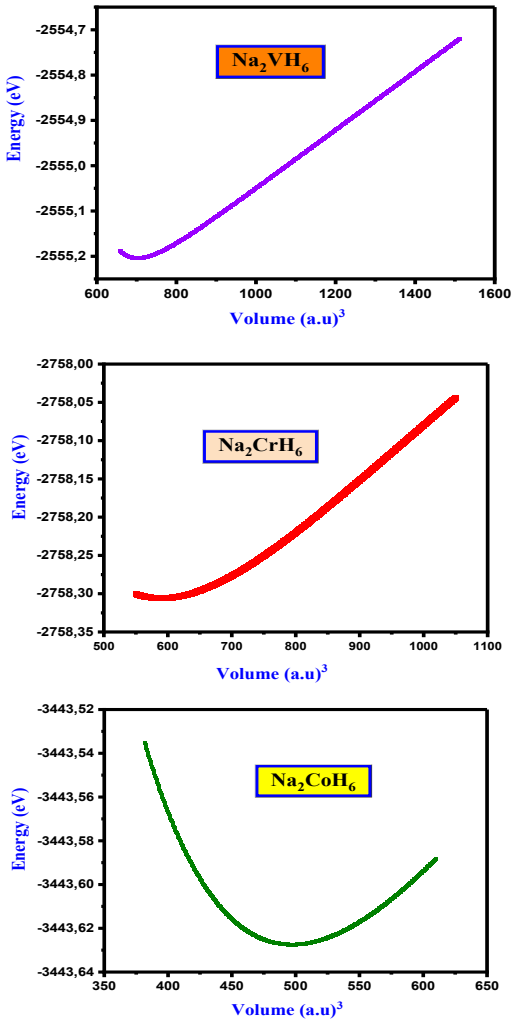

Fig. 2. Total energy as a function of volume for Na_2XH_6 (X = V, Cr and Co) double perovskites.

Table 1. The optimized values of lattice constants a_0 (Å), volumes V_0(Å^3), gravimetric capacities (C_{wt}%) and formation energies ΔH_f (eV/atom) of Na_2XH_6 (X = V, Cr and Co) compared with some previously studied compounds.

Materials	a_0	V_0	Cw %	ΔH_f	reference
Na_2VH_6	7.65	448.62	5.88	-2.30	Present study
Na_2CrH_6	7.50	423.16	5.81	-2.27	
Na_2CoH_6	7.24	380.46	5.45	-2.50	
Mg_2VH_6	6.75	307.99	5.73	-2,48	Previous study [8]
Mg_2CrH_6	6.60	288.56	5.67	-2,40	

The volumetric capacity (ρ_v) denotes volumetric density represents the amount of hydrogen that may be stored per unit volume of storage material. It can be calculated using the following expression [18,19]:

$$\rho_v = \frac{N_H \cdot m_H}{V \cdot N_A} \quad (4)$$

Here N_H, m_H, V and N_A denote the number of hydrogen atoms, the molar mass of hydrogen atoms, the volume of hydrogen per litre and the Avogadro's number, respectively.

Desorption Temperature T_{des} is linked to the amount of energy required to release hydrogen from that material. In the case of a metal hydride, it is intrinsically related to its thermodynamic stability, which can be studied by calculating the standard Gibbs free energy of formation (ΔG). For the perovskite hydrides investigated in our study namely Na_2XH_6 (X = V, Cr and Co), the hydrogen release process occurs through the following decomposition reaction [20]:

$$Na_2XH_6 \rightarrow 2\,Na + X + 3.H_2 \quad (5)$$

whose associated change in Gibbs free energy (ΔG) for this reaction can be determined using the following relation [21]:

$$\Delta G = \Delta E_f - T_{des} \cdot \Delta S \quad (6)$$

Here, ΔE_f, ΔS and T_{des} denote the formation energy, the entropy changes and the desorption temperature, respectively. Under standard ambient conditions and by setting $(\Delta G = 0)$, the system attains equilibrium at the temperature (T) given by the following formula [22]:

$$T_{des}\,(K) = \frac{\Delta E_f}{\Delta S} \quad (7)$$

Here, the entropy change is taken as ($\Delta S = -130.7$ J.mol^{-1}.K^{-1}) [23].
The determined desorption temperatures T_{des} (K) and the volumetric capacity of the Na_2XH_6 (X= V, Cr and Co) hydrides are presented in **Table 2**.

Table 2. Analysis of the properties density (ρ), volumetric capacity (ρ_v), enthalpy of dehydrogenation (ΔH) and desorption temperature (T_{des}) of Na_2XH_6 (X = V, Cr and Co).

Parameters	Na_2VH_6	Na_2CrH_6	Na_2CoH_6
ρ (g/cm^3)	1.55	1.66	1,93
ρ_v ($g \cdot H_2/L$)	91.1	96.5	105.2
ΔH(KJ/mol. H_2)	68.5	66.2	72.0
T_{des} (K)	527	509	554

3.2 Electronic property

In this section, we analyze the densities of states (DOS) and the electronic band structures of Na_2XH_6 (X = V, Cr and Co) hydrides. The calculation of their electronic structure reveals that all hydrides exhibit a metallic character due to the absence of band gap as shown in **Fig.3.**

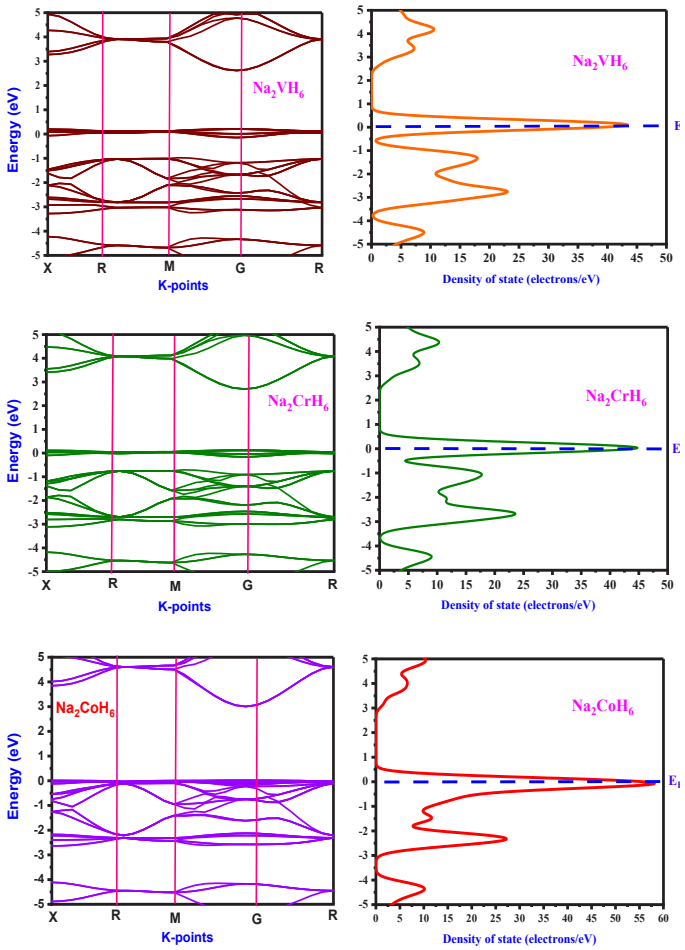

Fig. 3. Band structures and (DOS) of Na_2XH_6 (X = V, Cr and Co) double perovskites.

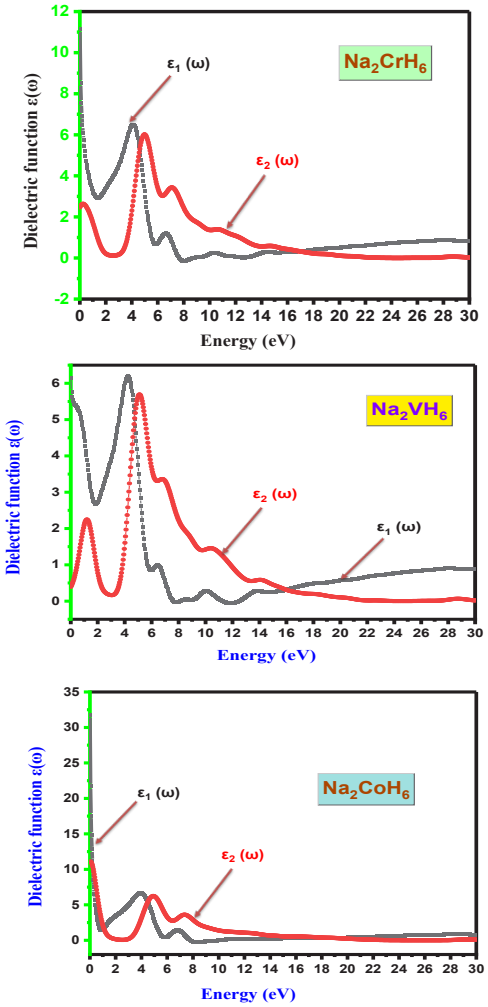

Fig. 4. Dielectric function ε(ω) for Na_2XH_6 (X = V, Cr and Co) double perovskites.

3.3 Optical properties

To understand how materials interact with electromagnetic radiation, we study their optical properties. These latters are necessary to distinguish between materials and their potential uses in solar panels, optical layers, reflectors, electronic devices and particularly in certain hydrogen storage applications. In this context, we evaluate several optical parameters of Na_2XH_6 (X = V, Cr and Co) perovskite hydrides namely: the complex dielectric function ε(ω), absorption coefficient α(ω), reflectivity R(ω).

The complex dielectric function ε(ω) describes the optical characteristics of a material. Its real part $\varepsilon_1(\omega)$ and imaginary part $\varepsilon_2(\omega)$ are given by equation (8) [24]:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega) \tag{8}$$

The absorption coefficient α(ω) corresponds to the energy absorbed per unit length and characterizes the attenuation of electromagnetic radiation intensity as it propagates through a material. It is expressed as follows:

$$\alpha = \frac{4\pi k}{\lambda} = \frac{2\pi\varepsilon_2}{\lambda n} = \frac{2\omega k}{c} \tag{9}$$

Here, c, k, λ and ω denote the speed of light, the wave number, the wavelength, the angular frequency, respectively.

Reflectivity R(ω) of a material is one of the important optical parameters which depends strongly on its electronic structure. It measures the proportion of reflected light. This latter is related to the extinction coefficient (k) and the refractive index (n) by the following relation [25]:

$$R(\omega) = \frac{(1-n)^2 + k^2}{(1+n)^2 + k^2} \tag{10}$$

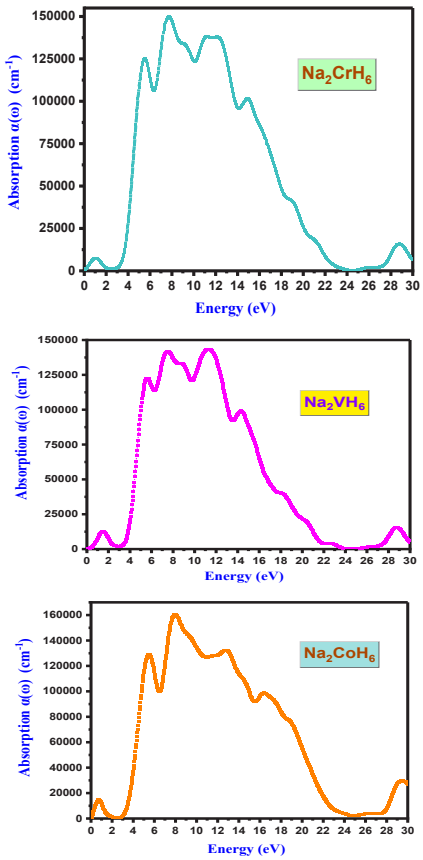

Fig. 5. Absorption coefficient for Na_2XH_6 (X = V, Cr and Co) double perovskites.

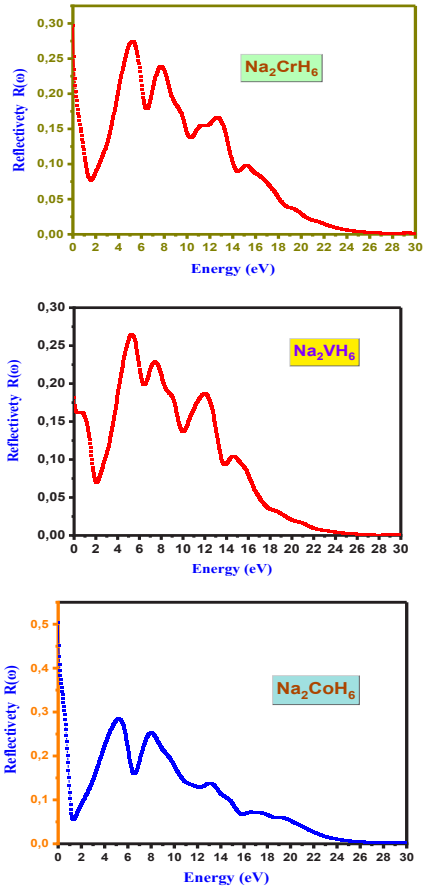

Fig. 6. Reflectivity for Na_2XH_6 (X = V, Cr and Co) double perovskites.

In **Figs. 4, 5 and 6**, we plot ε(ω), α(ω) and R(ω) curves for the Na_2XH_6 (X= V, Cr and Co) hydrides in the photon energy span (0 - 30eV). The static dielectric constant $\varepsilon_1(0)$ measures the system ability to polarize under the effect of electric field. According to **Fig.4**, we notice that for Na_2VH_6, Na_2CrH_6 and Na_2CoH_6, its corresponding values are approximately 6.3, 11.3 and 33.2, respectively. Consequently, Na_2CoH_6 exhibits the highest value of $\varepsilon_1(0)$ suggesting enhanced polarization effects compared to the other studied perovskite hydrides. In the ultraviolet (UV) region, especially in the range of energy (3 - 8 eV), we observe absorption peaks of $\varepsilon_2(\omega)$ between 5.0 and 6.5. These features arise from electron transitions from occupied valence states to unoccupied conduction states. For all these compounds, α(ω) is practically zero in the infrared (IR) region, this character can be justified by the negligible optical response in the absence of photons. In the UV region (3-4 eV), a pronounced increase in $\alpha(\omega)$ is observed indicating strong interband electronic transitions to unoccupied conduction states.

At zero photon energy, the calculated static reflectivity R(0) amounts to 0.18, 0.30 and 0.50 for Na_2VH_6, Na_2CrH_6 and Na_2CoH_6 , respectively. In the ultraviolet (UV) region, $R(\omega)$ increases significantly. Finaly, the analysis of the optical properties indicates that Na_2XH_6 (X = V, Cr and Co) hydrides possess a strong (UV) response.

3.4 Mechanical properties

In this section, we investigate the mechanical parameters of Na_2XH_6 hydrides by calculating their elastic constants. Their values are summarized in **Table 3.** For all these compounds, the Born stability criteria $(C_{11} > 0, C_{44} > 0, (C_{11} - C_{12} > 0), (C_{11} + 2C_{12} > 0)$ and $(C_{12} < B < C_{11})$ is satisfied confirming their mechanical stability [26].

The Shear modulus (G), determined using the Voigt, Reuss, and Hill approximation, is given by equation (11):

$$G = \frac{G_V + G_R}{2} \quad \text{where} \quad \begin{cases} G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \\ G_R = \frac{(C_{11} - C_{12})5C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \end{cases} \qquad (11)$$

The Bulk modulus (B) is determined by the following formula:

$$B = \frac{C_{11} + 2C_{12}}{3} \qquad (12)$$

In order to determine whether these compounds have brittle or ductile behavior, we use the following criteria for Pugh's ratio (B/G):

$$\begin{cases} \frac{B}{G} < 1.75 & \text{for brittle behavior} \\ \frac{B}{G} > 1.75 & \text{for ductile behavior} \end{cases} \qquad (13)$$

The other mechanical parameters namely: Young's modulus (E), Poisson's ratio (v), Anisotropy factor (A), Hardness (H) and Machinability index (μ_M) are respectively given by the following equations (14-18) [27]:

$$E = \frac{9GB}{3B+G} \quad (14)$$

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad (15)$$

$$v = \frac{3B-2G}{2(3B+G)} \quad (16)$$

$$H = \frac{E(1-2V)}{6(1+V)} \quad (17)$$

$$\mu_M = \frac{B}{C_{44}} \quad (18)$$

In **Table 3,** the obtained Pugh's ratio (B/G) values are lower than 1.75, indicating a predominantly brittle nature. This conclusion is further supported by the low Poisson's ratio ($v < 0.25$), which is characteristic of brittle materials with limited plastic deformation. Moreover, the anisotropy factor ($A \neq 1$) reveals that these compounds exhibit notable elastic anisotropy, suggesting that their mechanical response is direction-dependent within the crystal lattice. In addition, the relatively low hardness (H) values indicate that Na_2XH_6 compounds can be classified as soft materials. Overall, these findings highlight that Na_2XH_6(X = V, Cr and Co) hydrides are mechanically stable, brittle and anisotropic, which may influence their performance in hydrogen storage applications.

Table 3. Calculated elastic parameters for Na_2XH_6(X = V, Cr, and Co) hydrides at zero pressure and zero temperature.

	Na_2VH_6	Na_2CrH_6	Na_2CoH_6
C_{11}(GPa)	34.99	31.60	38,58
C_{12}(GPa)	9.58	6.74	5,53
C_{44}(GPa)	14.52	16.90	12,89
B(GPa)	18.02	15.03	16,55
β (1/GPa)	0.055	0.067	0,06
G(GPa)	13.76	14.94	14,34
B/G	1.31	1.01	1,36
G_V	13.79	15.11	61,11
G_R	13.73	14.77	61,058
E(GPa)	33.0	33.7	33,39
ν	0.196	0.127	0,16
μ_M	1.24	0.89	1,39
H	2.80	3.71	5,15
A	1.14	1.36	0,074

3.5 Thermodynamic and acoustic properties

We evaluate the thermal and acoustic properties of Na_2XH_6 (X = V, Cr and Co) hydrides by using key parameters mainly Debye temperature (θ_D), sound velocities and melting temperature (Tm). The Debye temperature (θ_D) is calculated through the average wave velocity (v_m) given by the following formula [28]:

$$\theta_D = \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} \times v_m \quad (19)$$

Here, h, k_B, n, N_A , ρ, M and v_m denote the Plank's constant, the Boltzmann's constant, the total atom in the unit cell, the Avogadro's number, the density, the molecular weight, the average sound velocity and the average sound velocity, respectively.
The average sound velocity (v_m) can be determined using the following relation:

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3}+\frac{1}{v_l^3}\right)\right]^{-1/3} \quad (20)$$

where, the longitudinal and transverse wave velocities (v_l) and (v_t), respectively are defined as follows:

$$v_t = \sqrt{\frac{G}{\rho}} \quad (21)$$

$$v_l = \sqrt{\frac{3B+4G}{3\rho}} \quad (22)$$

To determine the melting temperature (T_m) of Na_2XH_6 (X = V, Cr and Co) we employ the following equation (23)[29]:

$$T_m(\text{K}) = [553(\text{K}) + (5.911 \times C_{12})]\ \text{GPa} \pm 300\ \text{K} \quad (23)$$

Table 4. Wave velocities (v_l), (v_t) and (v_m), Debye temperatures (θ_D) and melting temperatures (T_m) for Na_2XH_6 (X = V, Cr and Co) hydrides.

	Na_2VH_6	Na_2CrH_6	Na_2CoH_6
v_t (m/s)	2,97	3	2,72
v_l(m/s)	4,84	4,58	4,29
v_m(m/s)	3319.74	3311.53	2981.45
θ_D(K)	425.885	433.18	404.086
T_m(K)	609,62±300 K	592,84±300 K	585,73 ±300 K

4 Conclusion

In this work, we report a comprehensive investigation of the calcium-based double perovskite hydrides Na_2XH_6(X = V, Cr and Co) conducted within the framework of density functional theory (DFT) employing the GGA-PBE functional. Although Na_2XH_6 exhibits comparatively weaker geometric stability, structural optimization confirms that all compounds

crystallize in a cubic structure with space group Fm3m-(N°225). The obtained gravimetric hydrogen storage capacities (C_w%) range from 7.24 to 7.65 wt%, highlighting the potential of these materials for hydrogen storage applications. Their thermodynamic stability is confirmed by their negative calculated formation enthalpies. The calculation of their electronic structure reveals that all hydrides exhibit a metallic character due to the absence of band gap. The optical analysis of the metal-hydrogen interactions in Na_2XH_6 (X = V, Cr and Co), assesses their stability and performance. In fact, strong ultraviolet (UV) response was manifested for all of them.

Finally, the analysis of their thermal properties shows that Na_2VH_6 has the lowest desorption temperature (527K), whereas Ca_2CoH_6 has the highest one (554K). Overall, these findings demonstrate that Na_2XH_6 (X = V, Cr and Co) hydrides are potential candidates for solid-state hydrogen storage technologies.

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