

## Research Papers

# ab-initio insights of BeXH<sub>3</sub> (X = In, Sn, Sb) hydrides for structural, phonon, electronic, thermodynamic and hydrogen storage properties

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## ARTICLE INFO

## Keywords:

Hydrides

Gravimetric hydrogen storage

ab-initio

Thermodynamic stability

Phonon

## ABSTRACT

The ab-initio investigations have been performed to comprehensively study the structural, electronic, phonon, thermodynamic and the hydrogen storage properties of Beryllium based cubic hydrides, BeXH<sub>3</sub> (X = In, Sn, Sb). The structural optimization was performed first to get the properties of the ground state such as lattice constant, bulk modulus, and its pressure derivative for three materials. The lattice constants are found to be 7.499 (a.u.), 7.599 (a.u.) and 7.622 (a.u.) for BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub> respectively. The structure is also proved stable from formation energy and phonon calculations. The metallic nature of all hydrides is confirmed from the band structure and density of states. The Fermi surfaces are plotted in 3D from the band which cuts the Fermi level. The thermodynamic parameters like specific heat capacities at constant pressure and volume, C<sub>p</sub>, C<sub>v</sub>, entropy (S), thermal expansion (α) coefficient, Debye temperature (Θ<sub>D</sub>), and Grüneisen (γ) parameter have also been investigated for against a range of pressure and temperature. The gravimetric (C<sub>wt%</sub>) hydrogen storage capacity, volumetric (ρ<sub>vol</sub>) hydrogen storage density and desorption (T<sub>des</sub>) temperature are also investigated. The C<sub>wt%</sub> is, 2.33%, 2.26% and 2.21% for BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub> respectively.

## 1. Introduction

The escalating depletion of fossil fuels and rising air pollution levels have necessitated to adopt feasible energy sources [1,2]. To meet growing energy demands and mitigate environmental degradation, it is necessary to reduce reliance on conventional energy sources. The other sources of energy like solar cell and renewable energy [3,4], thermoelectric power generators [5,6] and optoelectronic [7] had been goal of the researchers. In the upcoming decade, the transition to green power will play a major role in reducing the dependence on fossil fuels, preventing environmental degradation and enhancing the overall quality of life. To achieve this goal, effective management and the utilization of non-conventional energy sources have become a top priority. Fortunately, the various alternatives, like wind, solar, geothermal, ocean and hydrogen energy are available [8–10]. Among these options, the hydrogen energy stands up as a superior choice due to its convenience in transportation, efficient, versatile, environmentally compatible and highly utilizable and safe. Zero pollution emissions makes the hydrogen a clean and environmentally

friendly energy source [11,12]. It is the most abundant and lightest element [13]. Hydrogen energy presents as an alternative energy source, the worldwide researchers are involved in making hydrogen energy a commercially viable choice [14,15]. It can be directly converted into mechanical, electrical and thermal energy. Hydrogen energy cannot be used widely before the establishment of hydrogen storage system that is safe, light, sufficient, transportable and clean [16,17]. Perovskite hydrides have a favorable solution for hydrogen storage, that showing great potential in multiple applications [18]. Cations show by A, B and anion shows by X in the ABX<sub>3</sub> formula for perovskite compounds. For X, fluorine, nitrogen, halogen and oxygen are admissible substitutions in ABX<sub>3</sub> formula [19]. When a halide group element is replaced by X in ABX<sub>3</sub>, then the perovskite material is known as halide perovskite. Similarly, when X is replaced by nitrogen, fluorine and oxygen, so, the resulting compounds are called nitride-perovskite (ABN<sub>3</sub>), fluoro-perovskite (ABF<sub>3</sub>) and oxide-perovskite (ABO<sub>3</sub>) respectively [20–23]. When X replaced by hydrogen, the resulting compound called hydride-perovskite having the formula ABH<sub>3</sub> [24,25]. Hydride perovskites,

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<https://doi.org/10.1016/j.est.2025.117817>

Received 29 January 2025; Received in revised form 27 May 2025; Accepted 17 July 2025

Available online 1 August 2025

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having the general formula  $ABH_3$ , featuring a cubic structure, such that  $RbH_3$ ,  $CsCaH_3$  and  $SrLiH_3$ , have significant research attention due to their lightweight composition and low production costs [26]. For the first time,  $NaMgH_3$  along perovskite-type was synthesized by K. Ikeda with others at ambient temperature done by Goldschmidt-tolerance factors. The investigations of hydrogen absorption and desorption properties of the perovskite-type  $NaMgH_3$  hydride were done for the first time [27]. Transition metal hydride perovskites hold significant potential for applications in energy storage and hydrogen [28,29]. The first principles investigations are used to calculate the electronic, structural, optical and thermodynamical properties of  $NaMgH_3$  for hydrogen storage. GGA and LDA both techniques are used to obtained optimized structures [30]. Different physical properties are detailed through first-principles investigations to show the importance of perovskite-type  $CaYH_3$  ( $Y = Mn, Fe, Co$ ) hydrides in hydrogen technology [31]. Chaudhary et al. discussed the causes of destabilization of  $NaMgH_3$  and effects on the hydrogen-storage properties [32]. Lattice dynamics, crystal structures and bonding environments of perovskite-type  $RbMgH_3$  and  $RbCaH_3$  hydrides calculated by NPD, NVS and first-principles investigations [33]. Different properties including hydrogen storage of  $XSrH_3$  ( $X = K, Rb$ ) through DFT within WIEN2k code. Raza et al. investigated the gravimetric-hydrogen storage capacities for  $RbSrH_3$  and  $KSrH_3$  are 2.33 and 1.71 respectively [34]. In-based perovskite  $XInH_3$  ( $X = Li, K$ ) having different properties including hydrogen storage are calculated through first-principles investigations. HSE06 hybrid-functional within CASTEP code was applied to investigate both compounds,  $LiInH_3$  and  $KInH_3$  are thermodynamically and mechanically stable, having metallic behavior with anti-ferromagnetic behavior in magnetic properties [35]. Different perovskite  $XCuH_3$  ( $X = Li, Na, K$ ) [36] and  $LiAH_3$  ( $A = Mn, Fe, Co$ ) [37] hydrides are studied through first-principles investigations for hydrogen storage. With DFT, Xu et al. explored a sequence of cubic  $AVH_3$  ( $A = Na, K, Rb, Cs$ ) [38],  $XTiH_3$  ( $X = K, Rb, Cs$ ) [39] and  $XAlH_3$  ( $X = Na, K$ ) [40] hydrides. The investigated physical properties of these hydrides show that these compounds are thermodynamically, mechanically and dynamically stable respectively. The study of cubic hydrides  $XFFeH_3$  ( $X = Ca, Sr, Ba$ ),  $XPtH_3$  ( $X = Li, Na, K, Rb$ ) and  $XMnH_3$  ( $X = Na, K, Rb$ ) conducted by Song et al. through first-principles investigations. Other physical characteristics, stability and hydrogen storage capacities examined by the comprehensively. The findings results show the promising potential for hydrogen storage demands [41–43]. Y. Du et al. studied the different physical properties of  $RbCuH_3$  and  $KCuH_3$  perovskites through DFT technique. 1.95 wt% and 2.78 wt% are the hydrogen storage capacities are investigated of  $RbCuH_3$  and  $KCuH_3$  respectively [44]. For hydrogen storage technology, different perovskite  $XGaH_3$  ( $X = Rb, Cs, Fr$ ) [45],  $XGeH_3$  ( $X = K, Rb$ ) [46],  $XSrH_3$  ( $X = Cs, Fr$ ) [47],  $XMnH_3$  ( $X = K, Li$ ) [48],  $LiXH_3$  ( $X = Al, Ga, In$ ) [49],  $XGeH_3$  ( $X = Cs, Fr$ ) [50], and  $XPtH_3$  ( $X = Cs, Fr$ ) [51] hydrides are investigated. This motivates us to conduct the physical and hydrogen storage properties of Beryllium based hydrides.

## 2. Computational details

The different physical properties of perovskite  $BeXH_3$  ( $X = In, Sn, Sb$ ) hydrides based are investigated within FP-LAPW method executed in Wien2k code [52] based on Density Functional Theory. The exchange and correlation energy is approximated using the famous GGA-PBE, and Tran–Blaha modified Becke Johnson, TB-mBJ functional [53] for accurate results. The mBJ potential is,

$$v_{x,\sigma}^{mBJ}(\mathbf{r}) = c v_{x,\sigma}^{BR}(\mathbf{r}) + 3(c - \frac{2}{3}) \frac{1}{\pi} \sqrt{\frac{5}{12}} \sqrt{\frac{2t_{\sigma}(\mathbf{r})}{\rho_{\sigma}(\mathbf{r})}}, \quad (1)$$

where, electron density,  $\rho_{\sigma}$ , kinetic energy density,  $t_{\sigma}$  and Becke–Roussel  $v_{x,\sigma}^{BR}(\mathbf{r})$  potential [54] given as

$$v_{x,\sigma}^{BR}(\mathbf{r}) = -\frac{1}{b_{\sigma}(\mathbf{r})} \left( 1 - e^{-x_{\sigma}(\mathbf{r})} - \frac{1}{2} x_{\sigma}(\mathbf{r}) e^{-x_{\sigma}(\mathbf{r})} \right) \quad (2)$$

**Table 1**

The optimized structural parameters of  $BeXH_3$  ( $X = In, Sn, Sb$ ).

| Hydride            | a (a.u.) | $V_0$ (a.u.) <sup>3</sup> | $B_0$ (GPa) | $B'$ | $\Delta H_f$ (eV/atom) | $\Delta H_f$ (kJ/mole) |
|--------------------|----------|---------------------------|-------------|------|------------------------|------------------------|
| BeInH <sub>3</sub> | 7.499    | 421.76                    | 46.9        | 4.26 | −0.62                  | −59.824                |
| BeSnH <sub>3</sub> | 7.599    | 438.83                    | 40.8        | 3.65 | −1.14                  | −110.000               |
| BeSbH <sub>3</sub> | 7.622    | 442.79                    | 41.0        | 3.13 | −0.11                  | −10.807                |

In Eq. (1), the choice of  $c$  is made such that it must depend linearly on the square root of the average of  $|\nabla \rho|/\rho$ ;

$$c = \alpha + \beta \left( \frac{1}{V_{\text{cell}}} \int_{\text{cell}} \frac{|\nabla \rho(\mathbf{r}')|}{\rho(\mathbf{r}')} d^3 \mathbf{r}' \right). \quad (3)$$

The Perdew Burke Ernzerhof functional [55] is often regarded as the standard DFT method. Since decades, this method has attained the central importance in the computational material scientist. The added advantage is its availability in the commercial codes. The kinetic cut off energy to separate the core and valance electron is used to be  $-6.0\text{Ry}$  for both the materials. We set  $R_{\text{MT}} \times K_{\text{max}} = 3.0$  and plane-wave expansion cutoff,  $G_{\text{max}} = 16^{-1}(\text{a.u.})$ . For SCF convergence cycle, we set the energy and charge criteria of  $10^{-5}\text{Ry}$  and  $10^{-4}e$  respectively. The denser k-point grid of  $20 \times 20 \times 20$  with Monkhorst Pack [56] mesh sampling is used to study these materials accurately. The thermodynamic parameters are computed using the Gibbs2 code [57] which depends on Quasi-Harmonic approximations.

## 3. Results and discussion

### 3.1. Structural properties

The hydrides  $BeXH_3$  ( $X = In, Sn, Sb$ ) exhibit cubic structure are classified under a specific space group  $Pm\bar{3}m$  (No. 221) [58]. The Beryllium atom located at (0.0, 0.0, 0.0) positions, ( $X = In, Sn, Sb$ ) atoms settled at (0.5, 0.5, 0.5) and three hydrogen atoms  $H_3$  situated at (0.0, 0.5, 0.5), (0.5, 0.0, 0.5), (0.5, 0.5, 0.0) positions respectively. The E-V optimization of present hydrides shown in Fig. 1. These optimized structural parameters, including lattice constants, volume, bulk modulus, and its pressure derivative and formation energy are highlighted in Table 1.

The lattice constants of  $BeInH_3$ ,  $BeSnH_3$  and  $BeSbH_3$  are 7.499(a.u.), 7.599(a.u.) and 7.622(a.u.) respectively. The noted thing is, lattice constant increasing from In to Sb due to the difference of atomic mass. The bulk modulus and unit cell volume having an inverse relationship observed in Table 1. This action of both parameters aligns with anterior research on this class of materials. The stability of these hydrides is also evaluated through formation energy calculations. The negative formation energies of  $BeInH_3$ ,  $BeSnH_3$  and  $BeSbH_3$  are  $-0.62\text{ eV/atom}$ ,  $-1.14\text{ eV/atom}$  and  $-0.11\text{ eV/atom}$  respectively indicating their stability and potentials to use in different applications. The formation energy of  $BeInH_3$ ,  $BeSnH_3$  and  $BeSbH_3$  hydrides can be investigated through the following relation

$$\Delta H_f = \frac{E_{\text{total}}^{\text{BeXH}_3(X=In,Sn,Sb)} - x E_{\text{total}}^{\text{Be}} - y E_{\text{total}}^{\text{X}} - z E_{\text{total}}^{\text{H}}}{x + y + z}. \quad (4)$$

### 3.2. Phonon properties

The number of phonon modes are linked with the number of atoms in the unit cell of a material. In a material with five atoms in the unit cell like the under study hydrides, fifteen phonon modes by formula  $3N$  [47,59]. The acoustic phonons are three while optical phonon modes are given by  $3N - 3$  [60,61]. The computed phonon dispersion curves of  $BeInH_3$ ,  $BeSnH_3$ , and  $BeSbH_3$  are shown in Figs. 2(a)–2(c).

In full Brillouin zone, the phonon frequencies are positive for  $BeInH_3$  and  $BeSnH_3$  which depicts the dynamical stability [62–65]. There are small negative frequency in phonon dispersion curves of  $BeSbH_3$  which might be attributed with the phase change. It is interesting to note that the phonon dispersion curves have overwhelming similarity due to the fact that two atoms are same while only In is changed with Sn and Sb.

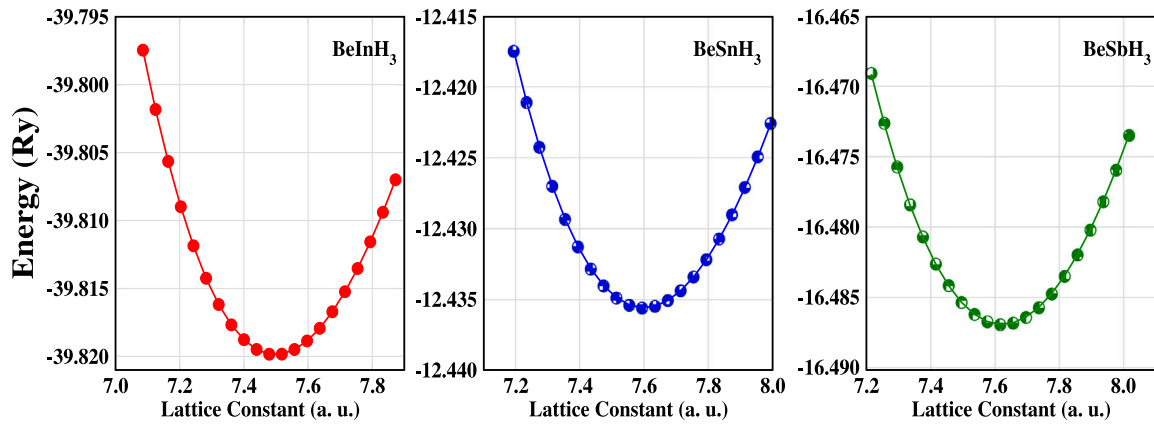


Fig. 1. The energy volume curve of Hydride Perovskites with BeInH<sub>3</sub> (red), BeSnH<sub>3</sub> (blue) and BeSbH<sub>3</sub> (green).

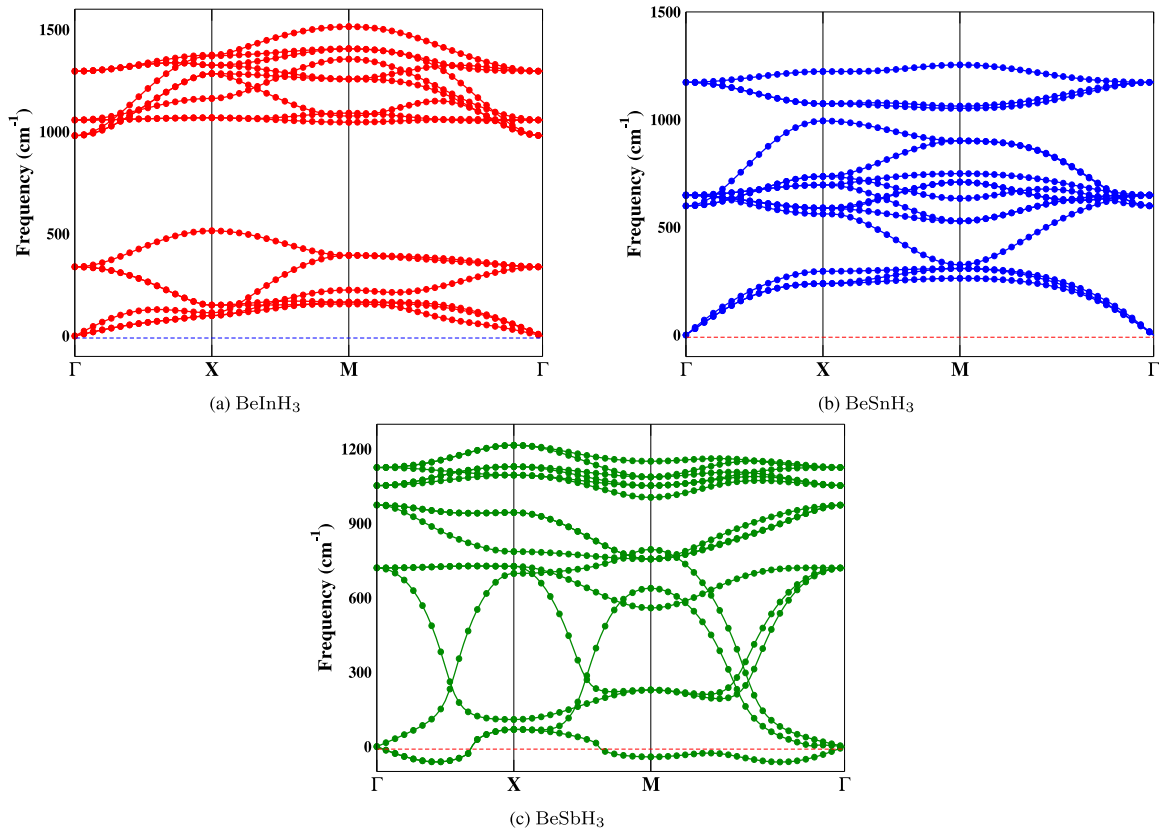


Fig. 2. The computed phonon dispersion curves of (a) BeInH<sub>3</sub>, (b) BeSnH<sub>3</sub> and (c) BeSbH<sub>3</sub>.

### 3.3. *ab-initio* molecular dynamics simulations

The *ab-initio* molecular dynamic simulations (AIMD) can be used to check the thermodynamic stability at finitely large temperature. The Andersen thermostat [66] is used to control the ionic temperature with 1 fs time step. The mean squared displacement (MSD), total energy fluctuations and radial distribution function (RDF) are different key indicators for stability check. The atomic diffusion for structure stability is tested by the MSD as

$$MSD(t) = \frac{1}{N} \sum_{i=1}^N \langle |\mathbf{r}_i(t) - \mathbf{r}_0(t)|^2 \rangle. \quad (5)$$

The number of atoms of the system are represented by  $N$ , the initial atomic positions is  $\mathbf{r}_0$  and the atomic position at time  $t$  of the  $i$ th atom is  $\mathbf{r}_i$ .  $\langle |\mathbf{r}_i(t) - \mathbf{r}_0(t)|^2 \rangle$  gives the ensemble average. The varying MSD gives

the atomic movement while it is constant value predicts the stability. The coefficient of self diffusion,  $D$  (in units,  $\text{\AA}^2/\text{fs}$  or  $\text{cm}^2/\text{s}$ ) is obtained from the slope of linear behavior of MSD against the time as,

$$D = \frac{1}{6} \frac{d(MSD)}{dt}. \quad (6)$$

The factor six comes due to three dimensional space due to the fact that MSD grows as  $MSD(t) = 6Dt$ . The MSD against time is shown in Fig. 3. The variation of pressure, temperature and total energy of the system has also been recorded against time (see Figs. S1–S6 of the [Supplementary Material](#)). Further, the diffusion coefficient and fluctuation in the total energy is listed in Table 2. The higher stability is predicted by the lower diffusion coefficient because of the strong binding of hydrogen in the host materials. The BeSnH<sub>3</sub> is the tightly bound and has the higher stability due to the lowest diffusion coefficient. The diffusion coefficient for BeSbH<sub>3</sub> is the highest which cause the more

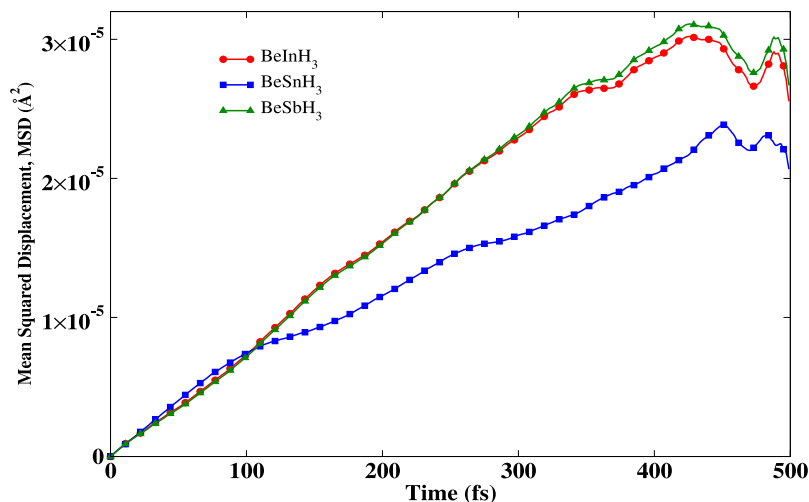


Fig. 3. The MSD of  $\text{BeXH}_3$  ( $X = \text{In, Sn, Sb}$ ).

**Table 2**

The diffusion coefficient,  $D$  (in unit  $\text{cm}^2/\text{s}$ ) and fluctuation in energy (in unit Ry) of  $\text{BeXH}_3$  ( $X = \text{In, Sn, Sb}$ ).

| Material          | $\text{BeInH}_3$        | $\text{BeSnH}_3$       | $\text{BeSbH}_3$        |
|-------------------|-------------------------|------------------------|-------------------------|
| $D$               | $1.068 \times 10^{-16}$ | $7.54 \times 10^{-17}$ | $1.113 \times 10^{-16}$ |
| Fluctuated energy | 231.411                 | 243.039                | 254.747                 |

mobile hydrogen and its easy release eventually make it less stable. The fluctuation energy for  $\text{BeSbH}_3$  is the highest while  $\text{BeInH}_3$  has the lowest fluctuation energy.

### 3.4. Electronic attributes

The electronic band profiles fitted with electronic density of states of  $\text{BeXH}_3$  ( $X = \text{In, Sn, Sb}$ ) are illustrated in Fig. 4(a) 4(c) 4(e). The high symmetry points are selected in the 1st BZ, to explore the band structures [67]. The study to precise the conducting, insulating and semi-conducting nature of any material is done by these properties [68,69]. Dotted lines representing the Fermi level, above Fermi level, conduction band is present, while, the valence band lies below it [70]. The investigation of energy difference among the minima of conduction band and the maxima of the valence band evoked the band gap energy. The results show that there is no band gap, due to the overlap of band curves in both the valence and the conduction bands, so the hydrides  $\text{BeXH}_3$  ( $X = \text{In, Sn, Sb}$ ) show the metallic nature. The DOS of  $\text{BeInH}_3$ ,  $\text{BeSnH}_3$  and  $\text{BeSbH}_3$  hydrides are illustrate in Fig. 4(a), 4(c), 4(e), show the number of available electronic states for the occupation against energy. Fermi surfaces formation depends on those bands which cross the Fermi level and viewed in three dimensional BZ. The Fermi surfaces of  $\text{BeInH}_3$ ,  $\text{BeSnH}_3$  and  $\text{BeSbH}_3$  are shown in Fig. 4(b), 4(d), 4(f). Band structure of  $\text{BeInH}_3$  shown in Fig. 4(a), with a violet band which cuts the Fermi level at  $\Gamma$ -symmetry point and flatten in the  $\Gamma - X$  direction. Therefore the Fermi surface of  $\text{BeInH}_3$  show the large cylindrical area in  $\Gamma - X$  direction Fig. 4(b). This flat band give rise to the value of density of states at Fermi level which seems to be around somewhat 0.5 states/eV for  $\text{BeInH}_3$ . In  $\text{BeSnH}_3$  band structure Fig. 4(c), three bands are merged at R symmetry point. Therefore, the Fermi surface shows the large area in R direction as shown in Fig. 4(d). Band structure of  $\text{BeSbH}_3$  shows two bands, violet and blue band cut the Fermi level at  $\Gamma$  symmetry point but only blue band flatten in the  $\Gamma - X$  direction. So, in Fermi surface of  $\text{BeSbH}_3$ , cylindrical area shown in this direction with wider outer surface area near X point as shown in Fig. 4(f). Violet band flatten in  $\Gamma - X$  direction in conduction band for  $\text{BeInH}_3$ , but after crossing the two band violet and blue for  $\text{BeSbH}_3$ , only blue band

flatten in the X symmetry direction in valence band. Therefore,  $\text{BeInH}_3$  has larger cylindrical area in  $\Gamma - X$  direction as compare with  $\text{BeSbH}_3$  cylindrical area in this direction. This can clearly be seen in Fig. 4(b), 4(f). Interestingly, TB-mBJ does not affect much except a constant shift in the Fermi energy and bands (see Figs. S7–S9 of the [Supplementary Material](#)).

### 3.5. Thermodynamic properties

The study of various thermodynamic parameters which including entropy ( $S$ ), thermal expansion coefficient ( $\alpha$ ), specific heat capacity at constant volume ( $C_V$ ), specific heat capacity at constant pressure ( $C_P$ ), Debye temperature ( $\Theta_D$ ) and Grüneisen parameter ( $\gamma$ ) of  $\text{BeInH}_3$ ,  $\text{BeSnH}_3$  and  $\text{BeSbH}_3$  hydrides under the influence of different ranges of pressure (0 Pa, 5Pa, 10Pa) and extensive range of temperature (0–600 K) is done via Quasi-Harmonic Debye Approximation executed in Gibbs2-codes [71]. Both pressure and temperature are applied and created the disorder inside crystal structure is symbolized by Entropy ( $\alpha$ ) [72]. The entropy of  $\text{BeXH}_3$  ( $X = \text{In, Sn, Sb}$ ) hydrides is illustrated in Fig. 5(a).

Entropy and temperature having the direct relation, with increasing temperature, entropy also increases. Entropy decreasing with the increasing pressure, because the unit cell volume reduces when pressure goes up and motion of particles will be constrained. The variation of thermal expansion coefficient ( $\alpha$ ) with temperature and pressure is shown in Fig. 5(b). The thermal expansion ( $\alpha$ ) coefficient has the direct relation with temperature and inverse relation with pressure, as  $\alpha$  rises when temperature goes up and decreases as pressure increases respectively. The Debye temperature ( $\Theta_D$ ) has separate importance in thermodynamic parameters because it shows the interlink of thermodynamic characteristics with elastic characteristics.  $\Theta_D$  against temperature and pressure shown in Fig. 6(a).  $\Theta_D$  has the indirect relation with temperature, at rising temperature,  $\Theta_D$  going down and has the direct relation with pressure, when pressure goes up then  $\Theta_D$  also goes up. The Grüneisen parameter ( $\gamma$ ) plays a main role to understand the vibrational characteristics of a substance.  $\gamma$  has the same relation with temperature and pressure, similar as the other parameters have the relation with both temperature and pressure shown in Fig. 6(b). Specific heat capacity at constant volume ( $C_V$ ), specific heat capacity at constant pressure ( $C_P$ ) are display in Fig. 7. Both  $C_V$  and  $C_P$  increase and decrease when temperature and pressure increase respectively.  $C_V$  and  $C_P$  obey the Dulong–Petit-Rule [73] at high temperature but at low temperature,  $C_V$  obeys the Debye-Model.

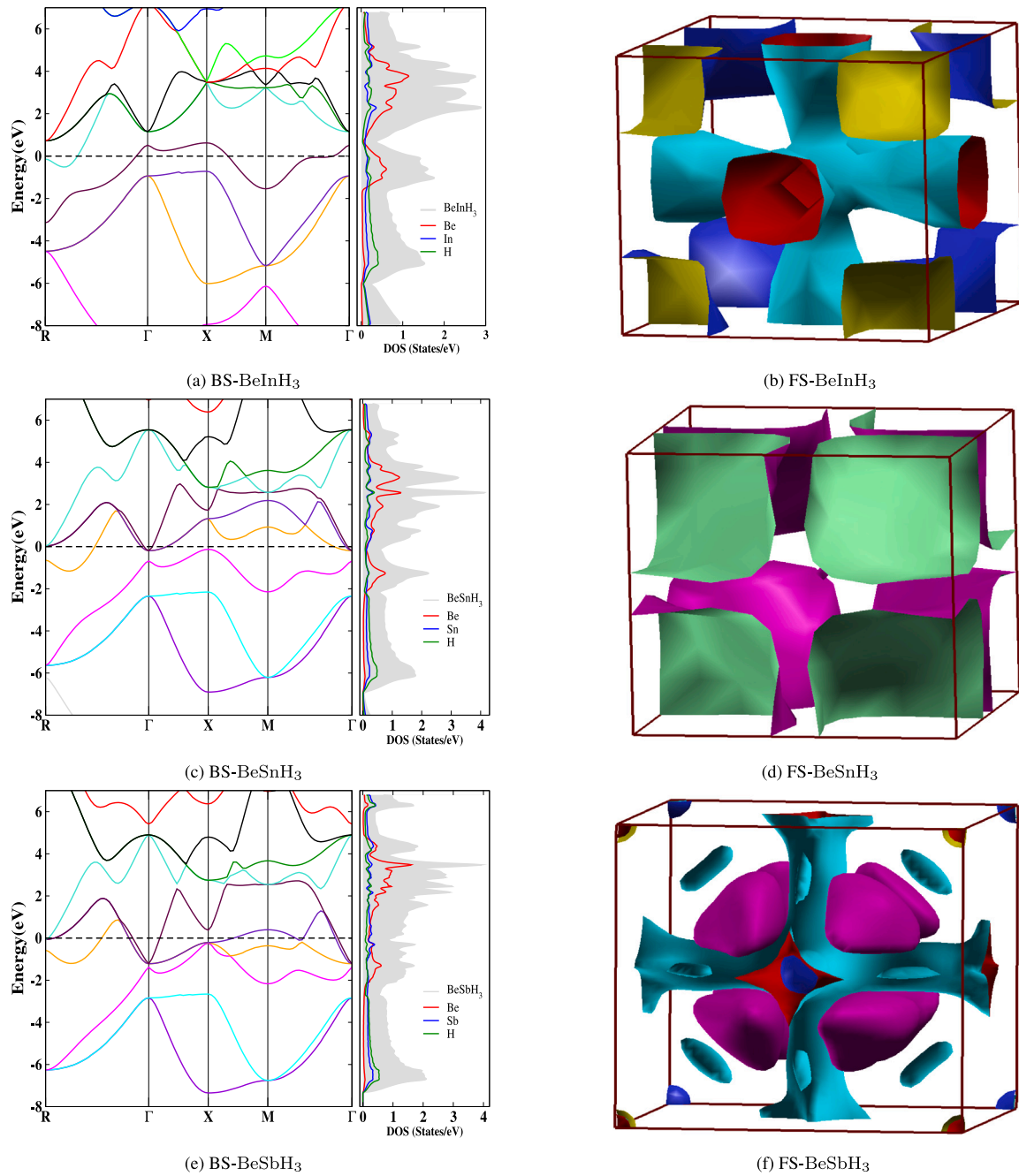


Fig. 4. The band profiles, density of states and Fermi surfaces of BeXH<sub>3</sub> (X = In, Sn, Sb).

### 3.6. Hydrogen storage properties

In present time, the perovskite-type hydrides have emerged as promising materials for hydrogen storage technology due to their simple framework, gravimetric hydrogen storage capacity and manageable desorption temperature. To investigate the hydrogen storage capabilities of under research perovskite BeXH<sub>3</sub> (X = In, Sn, Sb) hydrides, it is essential to evaluate their gravimetric hydrogen storage capacity  $C_{wt}\%$ . A specific formula may be used for their evaluation [74]

$$C_{wt}\% = \frac{(H/M)m_H}{m_{host} + (H/M)m_H} \times 100 \quad (7)$$

where,  $m_H$  is known as hydrogen-mass, while  $m_{host}$  is known as host-mass and  $(H/M)$  represents the (hydrogen-host) atoms ratio. The  $C_{wt}\%$  of BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub> are 2.33%, 2.26% and 2.21% respectively and comparison with others hydrides are listed in Table 3. The

$C_{wt}\%$  of BeXH<sub>3</sub> (X = In, Sn, Sb) has not been previously documented in the literature. Therefore, this research can serve as a useful reference for future research efforts. Moreover, the volumetric hydrogen storage density  $\rho_{vol}$  of BeXH<sub>3</sub> (X = In, Sn, Sb) hydrides is evaluated through the below relation

$$\rho_{vol} = \frac{N_H \cdot m_H}{V(L) \cdot N_A} \quad (8)$$

Here, Avogadro's number, number of hydrogen atom and volume of unit cell shown by  $N_A$ ,  $N_H$  and  $V(L)$  respectively.  $\rho_{vol}$  of under work hydrides BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub> are shown in Table 3. The desorption temperature of perovskite hydrides is evaluated through the following relation [75]

$$T_{des} = \frac{-\Delta H_f}{\Delta S} \quad (9)$$

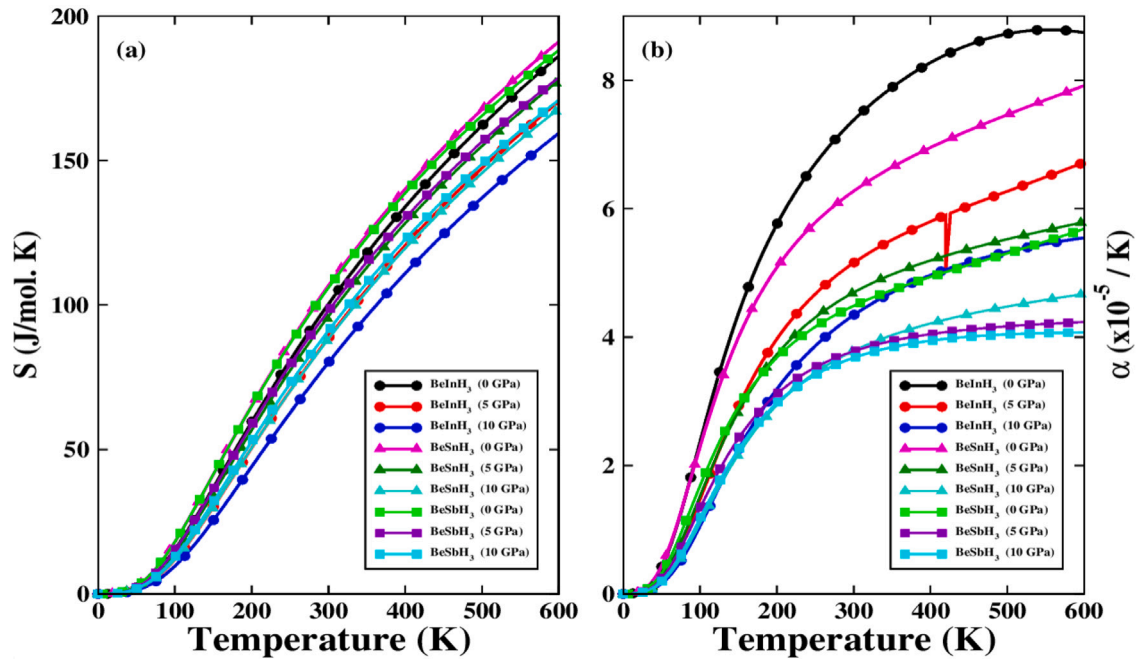


Fig. 5. The change in the thermodynamic parameter (a) entropy ( $S$ ) and (b) thermal expansion ( $\alpha$ ) coefficient against range of pressure and temperature for BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub>.

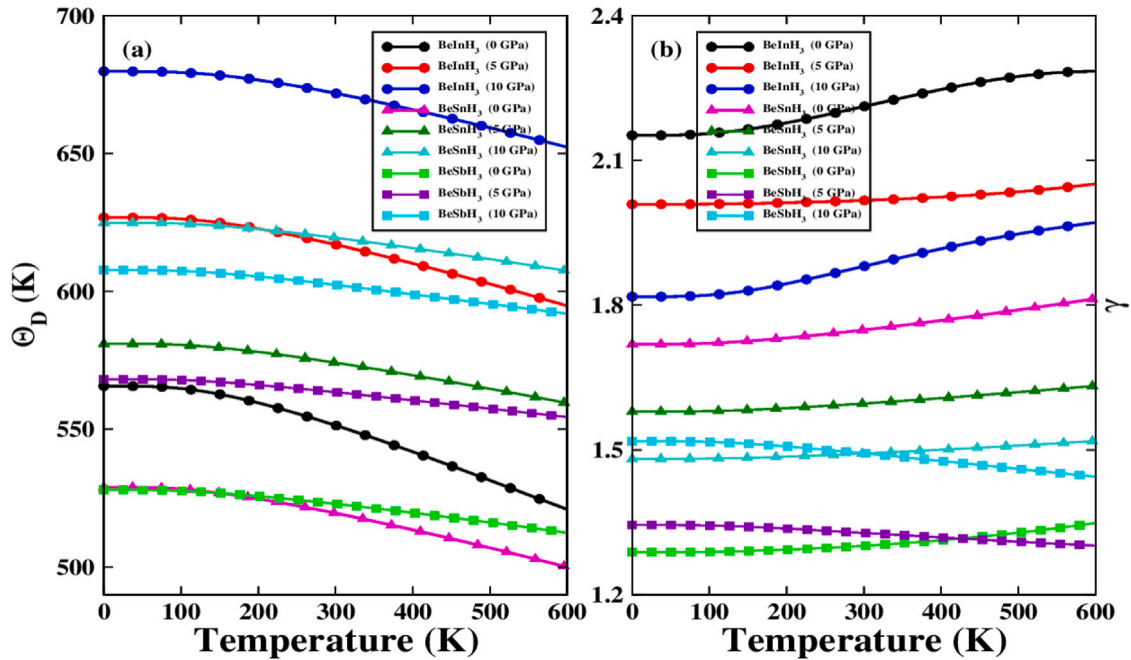


Fig. 6. The change in the (a) Debye temperature and (b) Grüneisen ( $\gamma$ ) parameter against range of pressure and temperature calculated for BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub>.

#### 4. Conclusion

In this study, the ab-initio investigations have been performed to comprehensively study the structural, electronic, thermodynamic, phonon and hydrogen storage properties of Beryllium based cubic hydride perovskites, BeXH<sub>3</sub> (X = In, Sn, Sb). The structural optimization was performed first to get the ground state properties like lattice constant, bulk modulus and its pressure derivative for these materials. The optimized lattice constants are found to be 7.499 (a.u.), 7.599 (a.u.) and 7.622 (a.u.) for BeInH<sub>3</sub>, BeSnH<sub>3</sub> and BeSbH<sub>3</sub> respectively.

The bulk moduli of three hydrides perovskites give values in the range of 40.8 to 46.9 GPa with highest value for BeInH<sub>3</sub>. The change in the bulk modulus against the pressure is minimum for BeInH<sub>3</sub> proves it the most stable material in comparison to BeSnH<sub>3</sub> and BeSbH<sub>3</sub>. The  $B' = \frac{dB}{dP}$  is highest of BeInH<sub>3</sub> and lowest for BeSbH<sub>3</sub>. This low value of  $B'$  for BeSbH<sub>3</sub> predicts its less resistance to pressure. This may also be linked with the slight negative phonon frequencies in BeSbH<sub>3</sub> phonon dispersion curves which is a kind of indication of its phase change. The structural stability is further confirmed from the formation energy. The formation energy ( $-0.11$  eV/atom =  $-10.807$  kJ/mol) is again the lowest for BeSbH<sub>3</sub> as compared with BeInH<sub>3</sub> and BeSnH<sub>3</sub>. The stability against the finite and high temperature is also checked

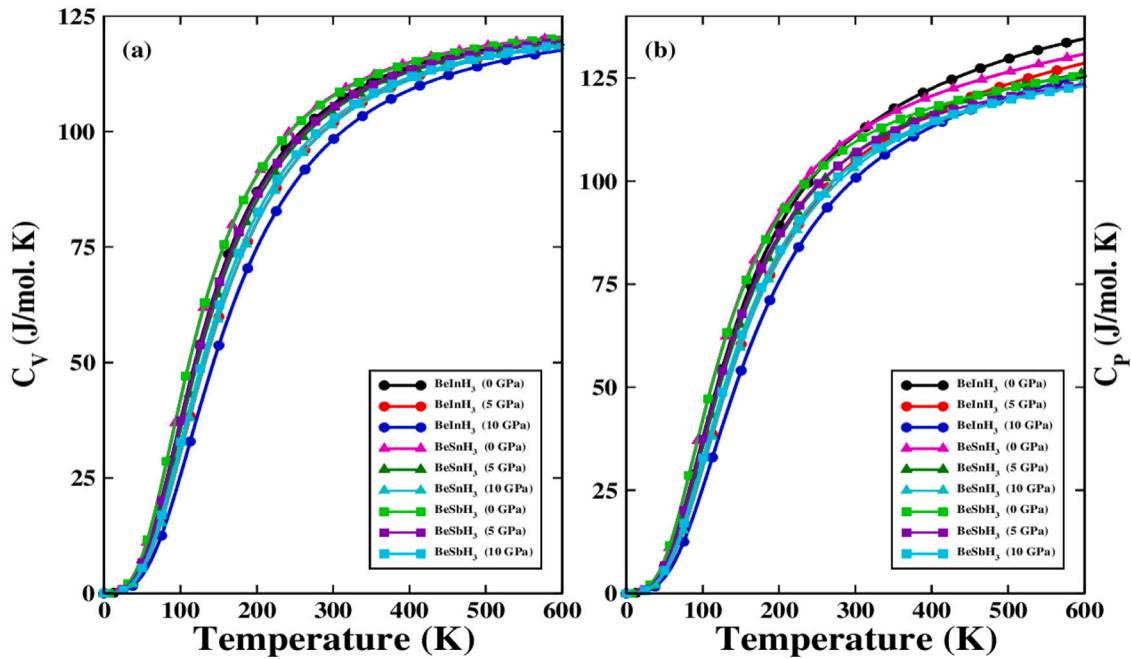


**Fig. 7.** The change in the (a) specific heat capacity,  $C_V$  at constant volume, and (b) specific heat capacity  $C_P$  at constant pressure, against temperature and pressure calculated for  $\text{BeInH}_3$ ,  $\text{BeSnH}_3$  and  $\text{BeSbH}_3$ .

**Table 3**

The hydrogen storage properties,  $C_{wt}\%$ ,  $\rho_{vol}$  and desorption temperature,  $T_{des}$  for  $\text{BeXH}_3$  ( $X = \text{In, Sn, Sb}$ ).

| Material         | $C_{wt}\%$        | $\rho_{vol}(\text{g H}_2/\text{L})$ | $T_{des}(\text{K})$ |
|------------------|-------------------|-------------------------------------|---------------------|
| $\text{BeInH}_3$ | 2.33              | 80.34                               | 458.427             |
| $\text{BeSnH}_3$ | 2.26              | 77.22                               | 842.914             |
| $\text{BeSbH}_3$ | 2.21              | 76.53                               | 82.812              |
| $\text{CsSrH}_3$ | 1.33 <sup>a</sup> | 43.00 <sup>a</sup>                  | —                   |
| $\text{FrSrH}_3$ | 0.95 <sup>a</sup> | 47.08 <sup>a</sup>                  | —                   |
| $\text{CsGeH}_3$ | 1.43 <sup>b</sup> | 72.81 <sup>b</sup>                  | —                   |
| $\text{FrGeH}_3$ | 1.00 <sup>b</sup> | 73.21 <sup>b</sup>                  | —                   |
| $\text{KGeH}_3$  | 2.58 <sup>c</sup> | 74.61 <sup>c</sup>                  | —                   |
| $\text{RbGeH}_3$ | 1.48 <sup>c</sup> | 70.00 <sup>c</sup>                  | —                   |
| $\text{CsPtH}_3$ | 0.90 <sup>d</sup> | 70.21 <sup>d</sup>                  | 826.8 <sup>d</sup>  |
| $\text{FrPtH}_3$ | 0.71 <sup>d</sup> | 77.50 <sup>d</sup>                  | 923.5 <sup>d</sup>  |

<sup>a</sup> Ref [47].

<sup>b</sup> Ref [50].

<sup>c</sup> Ref [46].

<sup>d</sup> Ref [51].

using the ab-initio molecular dynamic calculations.  $\text{BeSnH}_3$  is proved the most stable as compared with  $\text{BeInH}_3$  and  $\text{BeSbH}_3$ . The electronic band structures and density of states confirm the metallic nature of all hydrides. The fermi surfaces are plotted in 3D from the band which cuts the Fermi level. The thermodynamic parameters like heat capacities  $C_V$ ,  $C_P$ , entropy ( $S$ ), thermal expansion ( $\alpha$ ) coefficient, Debye temperature ( $\theta_D$ ), and Grüneisen ( $\gamma$ ) parameter have also been investigated against a range of pressure and temperature. The gravimetric ( $C_{wt}\%$ ) hydrogen storage capacity, volumetric hydrogen storage density and desorption temperature are also investigated. The gravimetric ( $C_{wt}\%$ ) hydrogen storage capacities are, 2.33%, 2.26% and 2.21% and the desorption temperatures are 458.427 K, 842.914 K and 82.812 K for  $\text{BeInH}_3$ ,  $\text{BeSnH}_3$  and  $\text{BeSbH}_3$  respectively.

#### CCrediT authorship contribution statement

**Abu Bakar:** Writing – review & editing, Writing – original draft, Investigation, Software, Data curation, Supervision, Resources, Conceptualization. **Hafiz Muhammad:** Writing – original draft, Formal

analysis, Investigation. **A. Afaq:** Writing – review & editing, Supervision, Resources. **Gulnaz K. Toleubay:** Visualization, Formal analysis, Data curation. **Erik O. Shalenov:** Validation, Methodology, Investigation, Data curation. **H. Elhosiny Ali:** Writing – original draft, Investigation, Formal analysis, Conceptualization.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Acknowledgments

The author (Abu Bakar) extend his appreciation to the Zhejiang Sci-Tech University for the startup funding XJ2025001302. The authors extend their appreciation to the Deanship of Research and Graduate Studies at King Khalid University, Saudi Arabia for funding this work through large Research Project under grant number RGP2/375/46.

#### Appendix A. Supplementary material

The supplementary material can be seen: [Supplementary Data](#)

#### Data availability

Data will be made available on request.

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