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Research Article

Structural transition of $LiBeH_3$ under high pressure

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ABSTRACT

$LiBeH_3$ has been considered as a solid-state hydrogen storage material. This study investigated Pnma orthorhombic phase of $LiBeH_3$ under pressure. Ab initio constant pressure molecular dynamic simulation under pressure was adopted. The results depicted a phase transition from Pnma orthorhombic phase to $P2_1/m$ monoclinic phase at 270 GPa simulation pressure. The stability of each phase was examined using elastic constants. Based on the well-known Born stability criteria, both phases showed mechanical stability. Several moduli have been computed via elastic constants. The B/G ratios, Cauchy pressures and Poisson's ratios investigation revealed that $LiBeH_3$ is brittle at Pnma phase whereas it is ductile at $P2_1/m$ phase. The electronic band structures and partial and total density of states of phases were also obtained. A 2.058 eV band gap was seen for Pnma phase, and 3 eV band gap was seen for $P2_1/m$ phase.

Keywords: Phase transition, ab initio, elastic properties, stability.

Yüksek basınç altında $LiBeH_3$'ün yapısal faz geçişinin incelenmesi

ÖZ

$LiBeH_3$, katı hal hidrojen depolama malzemesi olarak literatürde çalışılmaktadır. Bu çalışma, basınç altında $LiBeH_3$'ün Pnma ortorombik fazını araştırmaktadır. Ab initio sabit basınç moleküler dinamik simülasyonu kullanılmıştır. Sonuçlar, 270 GPa simülasyon basıncında Pnma ortorombik fazdan $P2_1/m$ monoklinik faza bir faz geçişini göstermektedir. Her fazın kararlılığı, elastik sabitler kullanılarak incelenmiştir. Born stabilite kriterlerine göre, her iki faz da mekanik kararlılık göstermektedir. Elastik sabitler aracılığıyla diğer modüller de hesaplanmıştır. B/G oranları, Cauchy basınçları ve Poisson oranları, $LiBeH_3$'ün Pnma fazında kırılgan yapıya sahip olduğunu, $P2_1/m$ fazında ise sünek yapıya sahip olduğunu göstermektedir. Elektronik bant yapıları incelendiğinde, Pnma fazı için 2.058 eV bant aralığı, $P2_1/m$ fazı için 3 eV bant aralığı görülmektedir.

Anahtar Kelimeler: Faz geçişi, ab initio, elastik özellikler, kararlılık.

1. INTRODUCTION

The continues increase in world population and fast urbanization has caused a dramatic rise in energy consumption and demand. Most of this demand is still met by using hydrocarbon fuels and classic ways of producing electricity which has resulted in an increase in CO_2 emissions and other greenhouse gases. This created climate change crises and global warming. One of the popular options to mitigate climate change is that adopting renewable energy which provides a shift from hydrocarbon-based energy production to clean and sustainable energy production. One challenge with that approach is to store energy to avoid fluctuations and setbacks. Recently, hydrogen has been suggested as a reliable energy carrier to ease the problem of storing and transporting renewable energy safely.[1,2] Hence, there is growing research in literature to shift carbon-free energy generation using hydrogen as a carrier. Hydrogen energy requires four main stages: production, storage, transport, and end use. There are several materials under investigation for each stage. Hydrogen can be stored in different ways, compressed hydrogen storage, liquid hydrogen, metal hydrides and chemical hydrides.[3] The elemental metal hydrides such as magnesium hydride

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(MgH_2) and aluminum hydride (AlH_3) has been studied extensively.[4-6] Due to slow kinetics of hydrogenation and dehydrogenation and strong bond between magnesium and hydrogen MgH_2 is still under investigation. Light metal hydrides are under intense investigation due to their high hydrogen gravimetric density. $LiBeH_3$ is one of the studied materials which exists in different symmetries. The experimental studies are very little since Be is very toxic and requires precautions. Thus, most properties of $LiBeH_3$ were investigated computationally. The elastic properties of cubic and orthorhombic $LiBeH_3$ was studied by Rehmat et al.[7] It was reported that $LiBeH_3$ can be used as active photocatalyst for green hydrogen production.[8] The electronic and mechanical properties of cubic and orthorhombic $LiBeH_3$ have been studied theoretically.[9-11] In this study, elastic and electronic properties of orthorhombic $LiBeH_3$ will be studied by adopting first principles calculations. Also, phase transitions of $LiBeH_3$ will be examined under high pressure. The obtained phases then will be evaluated for phase stability.

2. METHOD OF COMPUTATION

The ab initio computations were adopted within the density functional theory as implemented in SIESTA method in order to calculate structural, elastic, and electronic properties of $LiBeH_3$.[12] Perdew-Burke-Ernzerhof, generalised gradient approximation (PBE-GGA) was used for the exchange correlation potential.[13] A 8x8x8 k-points mash was taken to sample the Brillouin zone. The electronic wave functions were expanded in plane-wave basis to set up a kinetic energy cut off to 30 Ry, while the cut off energy for the electronic charge density was set to 300 Ry. $LiBeH_3$ was modelled using 2x2x2 cells with periodic boundary conditions for 160 atoms supercells. The Brillouin zones (BZ) were sampled with the 8x6x8 and 8x8x8 Monkhorst-Pack k-point mesh for Pnma and $P2_1/m$ structures, respectively.

3. RESULTS AND DISCUSSION

3.1 Structural evolution

Firstly, the formation energy of $LiBeH_3$ has been computed as -0.221 eV. The negative formation energy indicates synthesizability and dynamic stability. Then pressure was applied to the structure. The volume change under pressure using the simulation cell (160 atoms with a 2x2x2 cells) is shown in **Figure 1**. V/V_o represents a reduction in volume compared to zero pressure volume. The cell parameters at 0 GPa (Pnma phase) are a= 4.6167 Å, b= 6.4320 Å and c = 4.5438 Å. The volume of simulation cell drops at 270 GPa about 3.90 %, and a phase transition from Pnma to $P2_1/m$ is observed. The cell parameters are 4.5217 Å, b= 4.5762 Å and c = 4.7251 Å. The atomic structures at both phases are illustrated in Figure 2.

It is possible to estimate the transition pressure higher than the actual phase transition due to adopting perfect structures and boundary conditions during the simulation[14-18] Hence, the thermodynamic theorem to calculate the transition pressure was also used. The energy-volume calculations have been carried out and presented in Figure 2 and Figure 4. The details of calculation was given in ref.[19] It can be seen from Figure 4 that both phases cross each other at 34 GPa, suggesting that the transition from Pnma phase to $P2_1/m$ phase occurs at 34 GPa.

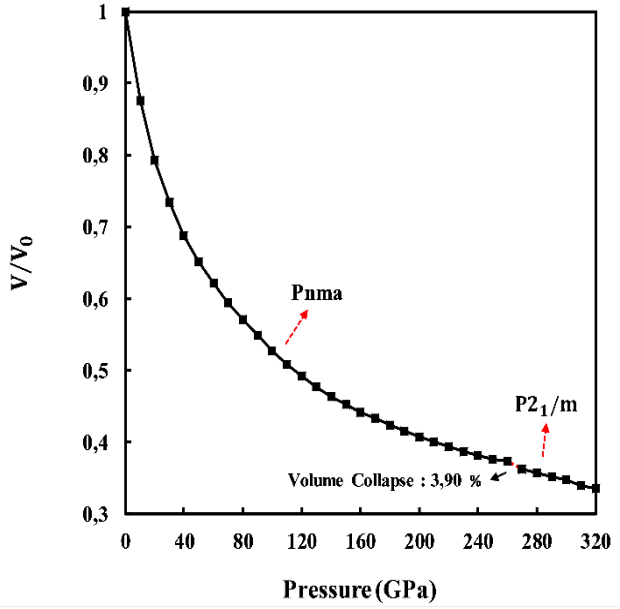

Figure 1. The change in volume of $LiBeH_3$ under hydrostatic pressure.

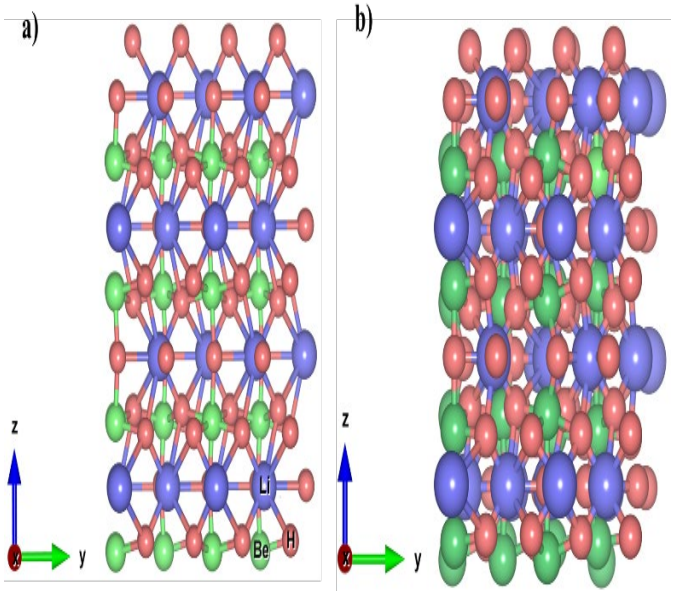

Figure 2. The structure of $LiBeH_3$ at a) 0 GPa (Pnma) b) 270 GPa ($P2_1/m$).

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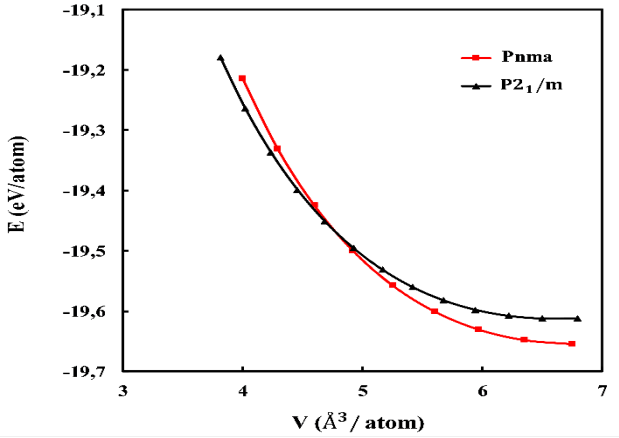

Figure 3. Energy volume of $LiBeH_3$ phases.

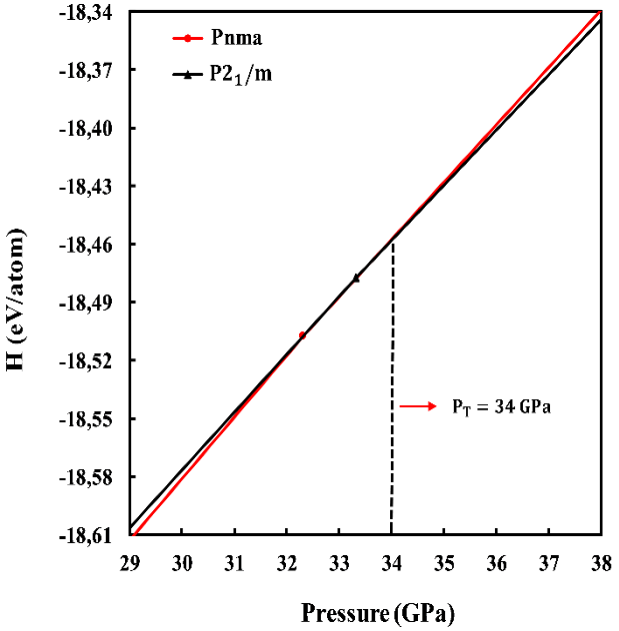

Figure 4. Enthalpy changes of phases under pressure.

3.2 Elastic properties

Elastic constants of materials provide information about materials' response when an external pressure is applied along with mechanical properties.[20,21] For an orthorhombic structure, there are nine elastic constants defined as C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{23}.[22,23] The well-known Born criteria for an orthorhombic structure is given as;[24,25]

$C_{11} + C_{33} - 2C_{13} > 0$, $C_{22} + C_{33} - 2C_{23} > 0$, $C_{11} + C_{22} - 2C_{12} > 0$,
$C_{11} > 0$, $C_{22} > 0$, $C_{33} > 0$, $C_{44} > 0$, $C_{55} > 0$, $C_{66} > 0$,
$C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0$,
$1/3\ (C_{12} + C_{13} + C_{23}) < B < (C_{11} + C_{22} + C_{33})$ (1)

There are thirteen independent elastic constants are defined for a low symmetry monoclinic structure as C_{ij}.[26,27] Born stability criteria is defined as;[28,29]

$C_{33}C_{55} - C^2_{35} > 0$, $C_{44}C_{66} - C^2_{46} > 0$,
$C_{22} + C_{33} - 2C_{23} > 0$ $C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0$
$C_{22}(C_{33}C_{55} - C^2_{35}) + 2C_{23}C_{25}C_{35} - C^2_{23}C_{55} - C^2_{25}C_{33} > 0$,
$2[C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - C_{12}C_{23}) + C_{25}C_{35}(C_{11}C_{23} - C_{12}C_{13})] - [C^2_{15}(C_{22}C_{33} - C^2_{23}) + C^2_{25}(C_{11}C_{33} - C^2_{13}) + C^2_{35}(C_{11}C_{22} - C^2_{12})] + gC_{55} > 0$,
With $g = C_{11}C_{22}C_{33} - C_{11}C^2_{23} - C_{22}C^2_{13} - C_{33}C^2_{12} + 2C_{12}C_{13}C_{23}$ (2)

As can be seen from Table 1 that both Pnma and $P2_1/m$ phase is mechanically stable. In order to investigate mechanical properties of phases, other crucial parameters have been calculated using elastic constants and presented in Table 2. Bulk modulus of $LiBeH_3$ was found to be 54 GPa in this study which is in a good agreement with ref.[11] (59.82 GPa) and ref.[7] (68.17 GPa). There is no data found in literature to compare bulk modulus of $P2_1/m$ phase of $LiBeH_3$.

Table 1. The obtained elastic constants (GPa) of phases of $LiBeH_3$.

Phases	C_{11}	C_{12}	C_{13}	C_{15}	C_{22}	C_{23}	C_{25}	C_{33}	C_{35}	C_{44}	C_{46}	C_{55}	C_{66}	Refs.
Pnma	96.41	38.13	32.41	-	100.05	27.73	-	93.78	-	52.34	-	36.46	60.65	This study
$P2_1/m$	685.49	252.96	414.79	58.11	757.95	297.67	-4.72	680.11	-83.74	238.18	-8.01	113.94	217.97	This study

Table 2. The calculated Bulk modulus (*B*,GPa), Shear modulus *G* (GPa), Young's modulus *E* (GPa) , *B/G and G/B* ratios, and Poisson's ratios (σ) of phases of $LiBeH_3$.

Phases	B	G	E	B/G	G/B	σ	Refs.
Pnma	54.00	41.17	98.49	1.31	0.76	0.196	This study
$P2_1/m$	449.75	162.65	435.47	2.77	0.36	0.339	This study

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Brittleness and ductility of $LiBeH_3$ was examined using B/G, G/B and Cauchy pressures. It was stated that a B/G ratio higher than 1.75 indicates ductility and a B/G ratio lower than 1.75 indicates brittleness.[30,31] In addition, Pettifor[32] stated that Cauchy pressure can also provide information about ductility/brittleness and bonding characteristics. Negative Cauchy pressure implies brittleness and directional angular or covalent bondingwhereas positive Cauchy pressure indicates ductility and predominance of ionic bonding characteristics. For an orthorhombic structure, Cauchy pressure is C_{23}-C_{44} for (100) plane, C_{13}-C_{55} for (010) plane and C_{12}-C_{66}) for (001) plane.[33] Pnma phase of $LiBeH_3$ has a B/G ratio of 1.31 which lower than 1.75, thus Pnma phase of $LiBeH_3$ is brittle. Cauchy pressures are -24.61 for (100) plane, -4.05 for (010) plane and -22.52 for (001) plane. The negative values of Cauchy pressures also suggest brittleness and angular/covalent nature. On the other hand, $P2_1/m$ phase of $LiBeH_3$ shows ductile nature since its B/G ratio is higher than 1.75. Cauchy pressures for $P2_1/m$ phase is calculated similar to Pnma phase.[34] It is found as 59.49 GPa for (100) plane, 300.85 GPa for (010) plane and 34.99 GPa for (001) plane. The positive values of Cauchy pressure confirm ductile nature of $P2_1/m$ phase of $LiBeH_3$.

Frantsevich et al.[35] also stated that Poisson's ratio (σ) can be used to determine ductility and brittleness of materials by the ratio of 0.26. If the Poisson's ratio is less than 0.26, the material is brittle, if it is higher than 0.26, it is classified as ductile. By evaluating, Poisson's ratios of phases, it can be confirmed that Pnma phase of $LiBeH_3$ is brittle and $P2_1/m$ phase of $LiBeH_3$ is ductile.
Shear modulus (G) of materials describe materials response against shape change. Young modulus (E) gives information about stiffness. By comparing two phases, it is seen that $P2_1/m$ phase will show higher resistance towards shape change and stiffer compared to Pnma phase.

In addition to polycrystal elastic constants, Vickers hardness and melting point of $LiBeH_3$ is also computed. Vickers hardness is obtained from $H_V^G = 0.1769G-2.899$ and $H_V^E = 0.0608E$ relation and melting point is computed using $Tm = 354 + 4.5 (2C_{11}+C_{33})/3$ relation.[36,37] From our calculations, $H_V^G = 4.38$ GPa and $H_V^E = 5.98$ GPa are obtained for Pnma phase. Both values are less than 10 GPa, thus Pnma phase of $LiBeH_3$ cannot be classified as a hard material. The melting point of Pnma phase of $LiBeH_3$ is obtained as 783.9 K. For $P2_1/m$ phase of $LiBeH_3$, $H_V^G = 25.87$ GPa and $H_V^E = 26.47$ GPa are obtained. It is seen that $P2_1/m$ phase of $LiBeH_3$ is a hard material. The melting point is computed as 3430 K for $P2_1/m$ phase.

3.3 Electronic properties

In order to investigate electronic properties of phases, the electronic band structures and partial and total density of states have been computed and presented in Figure 5 and Figure 6 for both phases. 0 eV was determined as Fermi energy level. As can be seen from Figures that band gaps are present for both phases. Pnma phase has 2.058 eV band gap whereas $P2_1/m$ phase has 3 eV band gap. The band gap seems to increase with pressure. H-1s states seem to contribute to the valence band for both phases. Be-2s states seem to contribute to the conduction band along with H-1s states.

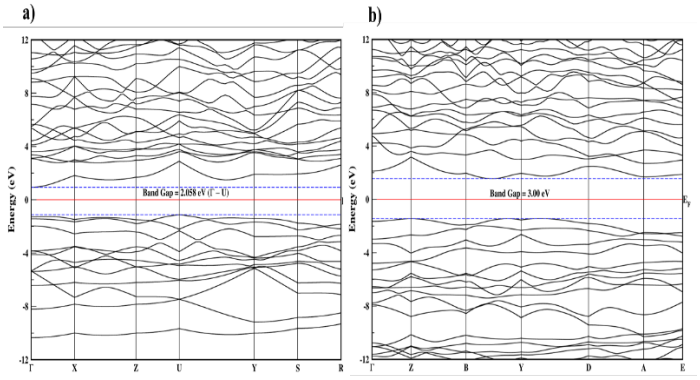

Figure 5. The calculated electronic band structures of $LiBeH_3$ at 0 GPa and at 270 GPa.

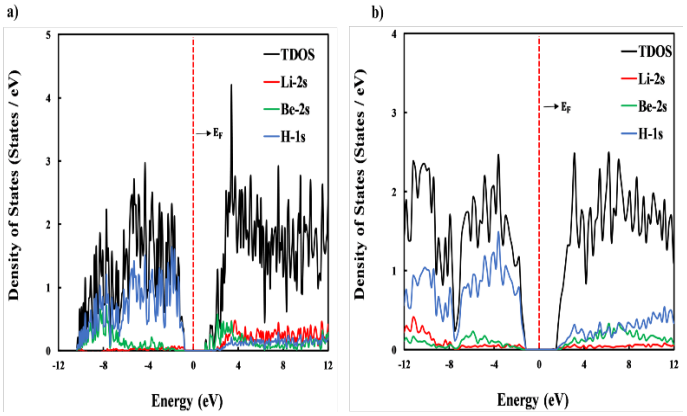

Figure 6. The partial and total DOS of $LiBeH_3$ at 0 GPa and at 270 GPa

4. CONCLUSION

This study investigated the structural, mechanical and electronic properties of $LiBeH_3$ under pressure. A phase transition from Pnma phase to $P2_1/m$ phase was observed at 34 GPa. The elastic constants evaluation depicted that both phases are mechanically stable. The B/G ratio, Cauchy pressure and Poisson's ratio of Pnma phase implied that Pnma phase of $LiBeH_3$ is brittle which might require extra attention when handling it. On the other hand, $P2_1/m$ phase was found to be ductile. The electronic band structure of phases showed band gap, indicating that both phases of $LiBeH_3$ is insulating.

Conflict of interests

I declares that there is no a conflict of interest with any institute, person, company, etc.

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