First-principles study of a hydrogen storage material Beryllium borohydride

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Abstract

First-principles calculations were performed to investigate the structural, electronic, and hydrogen storage properties of $Be(BH_4)_2$ using density functional theory (DFT). First, we evaluate the structural stability of $Be(BH_4)_2$ hydrides using formation enthalpy calculations. The calculated lattice parameter of the $Be(BH_4)_2$ compound is in good agreement with the available experimental parameters. The study of the electronic band structure and density of states of this compound reveals that $Be(BH_4)_2$ is an insulator. In this regard, $Be(BH_4)_2$ has demonstrated its interest in hydrogen storage applications, despite its high hydrogen volume density of 125.13 g/L and a gravimetric hydrogen density of 20.83 wt %, exceeding that of the U.S. Department of Energy for 2025. Our study predicts the applicability of $Be(BH_4)_2$ hydride as promising solid-state hydrogen storage materials.

Keywords: $Be(BH_4)_2$; Density functional theory; Hydrogen storage.

1. Introduction

Any nation's economy can grow significantly through energy. Currently, electricity and energy storage are the biggest challenges facing scientists. The development of lithium-ion batteries and super-capacitors in recent decades has significantly contributed to solving energy storage problems [1]. With increasing energy demand, the search for alternatives to conventional fossil fuels has become more urgent. Solar radiation, as abundant and important energy source, offers a promising solution for electricity generation [2]. Materials scientists are primarily focused on finding innovative materials with improved properties. Therefore, they prioritize the creation of materials that can convert solar energy into useful electricity in a cost-effective, reliable, and highly efficient manner [3]. The most popular energy source is solar energy, sometimes referred to as "green energy," and its sperformance depends on the ingredients used to manufacture optoelectronic devices [4]. In recent decades, different energy storage methods have been studied on different materials belonging to different compound groups [5-9]. There are various ways to save energy, from superconductivity to super-capacitance, including thermoelectric, photo-catalytic, and photovoltaic applications of materials. Moreover, finding a low-cost and environmentally friendly process to manufacture devices that provide optimal energy storage for different applications is a major concern of many materials science researchers [10-19].

Thermoelectric materials and devices have undergone considerable development over the past few decades [20-22]. Despite extensive studies, current state-of-the-art thermoelectric studies are not viable for large-scale commercial application due to their low efficiency or dependence on rare or hazardous materials such as lead and tellurium [21-25]. Moreover, materials with excellent optical properties and high absorption rates have potential applications in the field of renewable energy as they can serve as absorbers in photovoltaic (PV) devices. Silicon (Si) is commonly used as a photovoltaic absorber due to its abundance, cost-effectiveness, and potential application in advanced processing technologies [26].

Hydrides are the most important structures that can be applied to the use of hydrogen storage utilization [27]. Theoretically and experimentally predicted candidates include $Mg(B_3H_8)_2$ [28], $BeH_8(H_2)_2$[29], $LiBH_4$ [30], $C_6O_6Li_6/C_6O_6Na_6$ [31], Mg_2FeH_6 [32], Li_2CaH_4 [33], and $La_{1-x}Y_xMgNi_{3.8}Al_{0.2}$ ($x = 0, 0.1, 0.2, 0.3, 0.4$) [34] have been studied so far.

In our current study, we conducted a comprehensive analysis of the structural, mechanical, electronic and hydrogen storage of $Be(BH_4)_2$. To the best of our knowledge, this material has only been studied by van Setten and de Wijs [35]. In fact, $Be(BH_4)_2$ differs from other boranates and alanates in that its dehydrogenation to elements is thermodynamically slightly more favorable than dehydrogenation via the simple hydride BeH_2. The different behaviors of $Be(BH_4)_2$ are mainly due to the high stability of bulk beryllium metal [35]. The novelty of the present work in light of the previous study is that $Be(BH_4)_2$ has demonstrated its interest in hydrogen storage applications, despite its high hydrogen volume density of 110.13 g/L and a gravimetric hydrogen density of 20.83 wt %, exceeding that of the U.S. Department of Energy for 2025.

Beryllium borohydride is an inorganic compound with the formula $Be(BH_4)_2$ (sometimes written BeB_2H_8), it is a white crystalline solid, at 180 °C, the purest beryllium hydride is obtained by the reaction:

$$BeCl_2 + 2\,Li(BH_4) \rightarrow Be(BH_4)_2 + 2LiCl \tag{1}$$

The calculation details will be presented in the next section. In addition, the behavior of the electronic band structure, mechanics, desorption temperature, and volumetric and gravimetric storage of hydrogen will be analyzed in detail.

2. Computational method

The present work used the Materials Studio system to calculate the mechanical, electrical, and structural characteristics of the TSF. The software called CASTEP is considered before the calculations by applying the principles of plane wave pseudo-potential technique and density functional theory (DFT) [36]. The Kohn-Sham equations [37–39] should be used for the calculations. To explore the connection between electron transfers, Perdew–Burke–Ernzerhof (PBE) proposed the generalized gradient approximation (GGA) method [40]. The current GGA-PBE functional is the exchange-correlation. It is assumed that the ion-electron connection can be measured by using the Vanderbilt-type ultra-soft pseudo-potentials (USP) with a cutoff energy of 380 eV [41]. Pseudo-atomic calculations have been performed for: B : $2s^2$ $2p^1$, Be : $2s^2$ and H : $1s^1$. Using the Monkhorst-Pack grid, the Brillion zone model is run on 15 × 15 × 12 k-point mesh sets. For example, to achieve a maximum displacement of 0.00001 Å, a residual force less than 0.001 V/Å, a self-consistent convergence accuracy of 5×10^{-5} eV/atom, and a self-consistent field of 1.0×10^{-6} Å, the geometry is augmented during single-point energy calculation using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method [42].

3. Results and discussion

3.1. Structural Properties

$Be(BH_4)_2$ crystallizes in the tetragonal space group $I4_1cd$. The results of X-ray diffraction (XRD) experiments revealed that $Be(BH_4)_2$ is a structure (See Figure 1.).

Figure 1: The crystal structure of $Be(BH_4)_2$.

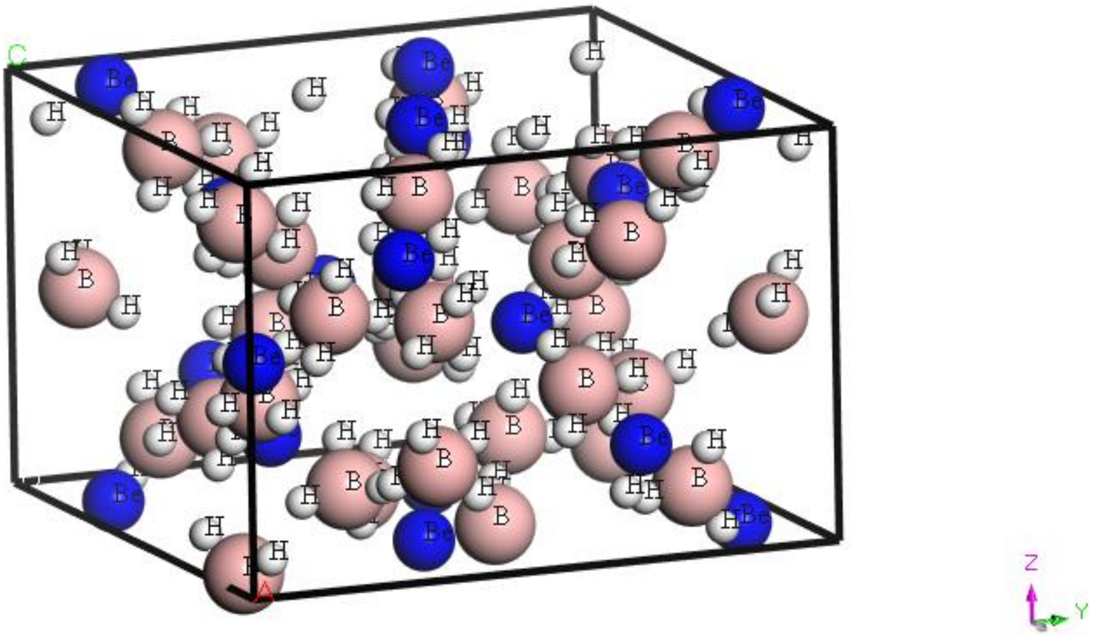

Table 1 presents the calculated structural properties of Be$(BH_4)_2$, along with other experimental data. The lattice parameters of Be$(BH_4)_2$ at 0 GPa are a = b = 13.86 Å and c = 9.40 Å. The previously recorded lattice parameters of Be$(BH_4)_2$ are a = b = 13.62 Å and c = 9.100 Å. The optimized structures are relatively reliable, as the discrepancy between the lattice parameters and those measured experimentally [43] is less than 0.2 Å.

Table 1 . Lattice constants a (Å) and c (Å) for Be$(BH_4)_2$.

	a (Å)	b (Å)	c (Å)
PBE	13.86	13.86	9.40
EXP. [43]	13.62	13.62	9.100

3.2. Electronic Structure

The band gap of a compound, which provides a detailed description of its optical and electronic character s, is one of the most important electronic features that help in understanding its device applications. To examine the electronic structure attributes shown in

Figure 2, we estimated the band structure of $Be(BH_4)_2$ using PBE-GGA. The calculated band structure and total density of states for $Be(BH_4)_2$ are shown in Figure 2, which has a large energy gap of approximately 7.815 eV, indicating that $Be(BH_4)_2$ is a wide-gap insulator. There is no data on the amount of band gap in the literature to contrast with our results. A larger band-gap generally corresponds to a higher intrinsic carrier concentration, while a smaller band-gap results in a higher intrinsic carrier concentration. This relationship is due to the energy required to promote electrons from the valence band to the conduction band [44-51]. Wide band gap (WBG) semiconductors are a broad class of materials widely used in commercially produced electronic devices as well as emerging energy applications, such as photovoltaic (PV) solar cells , energy splitting devices, and photo-electrochemical (PEC) water splitting devices [52-56].The investig ation of the electronic band structure and density of states of this material reveals that $Be(BH_4)_2$ is an insulator. This indicates $Be(BH_4)_2$ has a high hydrogen storage capacity. Solar energy can be stored as hydrogen through a process called electrolysis, where electricity from solar panels splits water into oxygen and hydrogen gas. The hydrogen gas can then be stored under pressure, or in a metal hydride, and converted back into electricity when needed through fuel cells. The results of the total and partial density of states are analyzed and these results can help understand how the constituent atoms shape the electronic structure. Moreover, the optical features of these materials highlight their importance for hydrogen storage, electronic devices, and sophisticated optoelectronic materials. These results indicate that $Be(BH_4)_2$ may be suitable for high energy applications such as photo-voltaics.

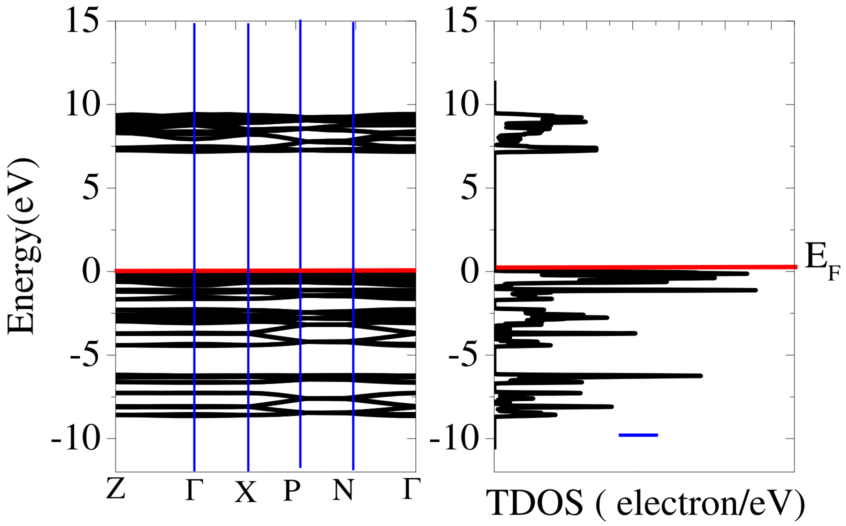

Figure 2. The calculated electronic band structure and TDOS for $Be(BH_4)_2$.

3.3. Hydrogen storage properties

The gravimetric density of hydrogen is an important parameter for the research of hydrogen storage materials, before studying the prediction of atomic structure and mechanical stability. The gravimetric density of hydrogen of the compound $Be(BH_4)_2$ is estimated using the following equation [57],

$$C_{wt\%} = \left(\frac{nM_H}{nM_H + M_{com}} * 100\right)\% \qquad (2)$$

where n represents the ratio of hydrogen to material atoms, and M_H and M_{Com} represent the molar masses of hydrogen and the compound, respectively. The gravimetric density of hydrogen for $Be(BH_4)_2$ compounds was calculated to be 20.83 wt %, which is higher than that set by the U.S. Department of Energy of 5.5 wt% for practical applications [58]. Furthermore, we calculated the volumetric hydrogen storage capacities (V_{sc}) of $Be(BH_4)_2$ to better understand their hydrogen storage potential [53]. It turns out that BeB_2H_8 has the GHD (20.83 wt% H_2) and volumetric capacity (125.13 g/L), which is in line with the target set by the United States Department of Energy for 2025.

The volumetric hydrogen storage capacity (V_{sc} ($Kg.H_2/m^3$)) is given by the following formula [59]:

$$V_{sc} = \frac{m_{H_2} - m_{H_2}^0}{V} \tag{3}$$

where m_{H_2} is the total mass of hydrogen contained in the calculated volume, $m_{H_2}^0$ is the mass of hydrogen in the bulk phase, and V is the effective volume. $Be(BH_4)_2$ is found to have the the highest GHD (20.83 wt%) and the highest volumetric capacity (125.13 g/L).

The thermodynamic stability of $Be(BH_4)_2$ compound is evaluated by examining their formation energies at absolute zero. Generally, materials are deemed stable if they display negative formation energy; conversely, they are regarded as unstable if their formation energy is positive.

The following equation is employed to calculate the formation energy of $Be(BH_4)_2$:

$$Be + 2B + 4H_2(g) \rightarrow Be(BH_4)_2 \quad [60] \tag{4}$$

The formation of the hydride $Be(BH_4)_2$ is obtained by the following reaction:

$$\Delta H = E_{\mathrm{Be(BH4)2}}^{total} - 4E_{\mathrm{H_2}}^{total} - 2E_{\mathrm{B}}^{total} - E_{\mathrm{B}}^{total} \tag{5}$$

The calculated energy value of the H_2 molecule is 31.70 eV, which is equal to 31.70 eV as reported by Abdellaoui et al. in their work [61]. The ΔH value calculated for the hydride $Be(BH_4)_2$ is -11.09 KJ/mol. The results are confirmed in Table 1. Its negative value as shown in Table 1 confirms the stability of the studied compound in the tetragonal phase. The evaluation of these parameters allows optimizing the choice of materials and improving the design of systems that rely on efficient hydrogen storage solutions. In addition, the desorption temperature, T_{de}, is a critical parameter in the evaluation of materials for hydrogen storage. This temperature represents the threshold at which hydrogen is released from the material when it is subjected to heating. This is a key factor in assessing the practicality of the material for hydrogen storage applications, as it affects the efficiency and safety of hydrogen release. The desorption temperature can be calculated using the Gibbs-Helmholtz equation, which relates the temperature to the enthalpy and entropy changes of the desorption process. This equation, detailed in equation (5) of reference [62], provides a quantitative measure of the influence of temperature on hydrogen release from the material.

$$\Delta G = \Delta H - T\Delta S \tag{6}$$

ΔG represents the standard Gibbs free energy change for the hydrogen dehydrogenation reaction, ΔH denotes the enthalpy change (more precisely, the enthalpy of formation), and ΔS the entropy change associated with the reaction. At equilibrium, the Gibbs free energy change (ΔG) is zero, indicating that there is no net change in the free energy of the system and that the reaction has reached its equilibrium state.

To calculate the desorption temperature (T_{de}), the formula used is given by [63]:

$$T_{de} = -\frac{\Delta H}{\Delta S} \tag{7}$$

This formula is derived from the Gibbs-Helmholtz equation, which relates the desorption temperature to the enthalpy and entropy changes of the dehydrogenation reaction. By applying this formula, it is possible to determine the temperature at which hydrogen is released from the material, thus providing a key parameter for assessing the material's suitability for hydrogen storage applications. Here, ΔH generally represents a positive value, as hydrogen dehydrogenation reactions are often endothermic, meaning they require heat input to occur. ΔS represents the entropy change associated with the dehydrogenation reaction. This formula, derived from the Gibbs-Helmholtz equation, relates the desorption temperature to the enthalpy and entropy changes of the reaction, providing a crucial parameter for assessing the material's performance in hydrogen storage applications. The production of hydrogen gas (H_2) is the main factor influencing the entropy change during the decomposition process. According to the prevailing opinion among scientific experts, as shown in the scientific literature, the entropy ΔS of the H_2 molecule is approximately -130.7 J/mol.K when evaluated under standard temperature and pressure conditions [63]. The calculated desorption temperatures for $Be(BH_4)_2$ are 84.90 K. These calculated desorption temperature values are significantly good compared to the critical point of hydrogen (33.20 K). Overall, understanding these specific values allows researchers to better evaluate the potential of this material in hydrogen storage applications, especially in the context of sustainable and clean energy technologies. Materials with appropriate desorption temperatures and entropy changes are essential for optimizing hydrogen storage systems to meet the energy demands of future clean energy solutions. It is essential to mention that hydrogen storage methods are varied, ranging from physical methods such as compressed gas and liquid hydrogen to chemical and hybrid systems, each with its advantages and disadvantages [64]. Although compressed gas storage is common due to its ease of use and low cost, its low energy density highlights the need for other replacement methods [65]. Liquid hydrogen compensates for this increased energy density with more stringent cryogenic requirements, but these also impose significant economic and technical restrictions [66]. Solid-state and chemical storage technologies hold great promise due to their potential to increase storage capacity, especially with new advances in materials science, such as metal hydrides and MOFs [67]. However, the trade-offs between safety, cost, and performance remain significant. Addressing these commercial and technological gaps will be essential to accelerate the actual deployment of hydrogen storage solutions.

4. Conclusions

In this paper, we conducted a detailed study of the structural, electronic, and hydrogen storage properties of the compound $Be(BH_4)_2$.The relaxed unit-cell constant (a =b= 11.11 Å and c=9.40Å) agrees well with the experimental data from the PBE functional. Our calculated band-gap values revealed that $Be(BH_4)_2$ is a wide band-gap insulating material. In this regard, $Be(BH_4)_2$ showed promise for hydrogen storage applications due to its high volume hydrogen density (125.13 g/L) and gravimetric hydrogen density of 20.83 wt%, thus exceeding the 2025 target of 5.5 wt% set by the U. S. Department of Energy. Hydrogen has the potential to play a significant role in the global energy mix and the transition toward a low-carbon economy. The key actions to accelerate decarbonization between now and future are: (1) Using renewable energy sources for electricity generation. (2) Accelerating renewable energy generation (which will further reduce the already low cost of renewable electricity). (3) Expanding the scope of sustainable, modern bio-energy, which is needed—among other things—to produce green fuels that require carbon dioxide, toward the goal of achieving net-zero emissions by 2050. However, the current state of hydrogen development is still in its early stages, and significant investment and advancements in hydrogen production, infrastructure, and technology are necessary for it to reach its full potential.

Conflict of interest

The authors declare that they have no conflict of interests.

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