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Investigation of Thermoelectric and Structural Properties of $BeAlH_3$, $BeGaH_3$, and $BeInH_3$ perovskite Hydrides for Energy Applications

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KEYWORDS

DFT; $BeAlH_3$, $BeGaH_3$, and $BeInH_3$; Gravimetric; Hydrogen; Thermal.

ABSTRACT

This study explores the structural, electrical, and thermoelectric properties of crystalline beryllium hydrides $BeXH_3$ (X = Al, Ga, In) using the generalized gradient approximation (GGA) within the framework of density functional theory (DFT). The analysis is performed using the BoltzTrap package, integrated with the Wien2k code, and the Murnaghan equation of state to determine total energy and atomic volume while providing detailed information on band structure and electronic densities of states.

Key thermoelectric properties, including power factor (PF), figure of merit (Zt), thermal conductivity (κ), and electrical conductivity (σ), were investigated over a temperature range from 300 to 900 K. The results show that BeGaH3 exhibits the best thermoelectric performance over the entire temperature range, with a maximum electrical conductivity of $3.5\text{x}10^{20}$ (.s) at 900 K. In contrast, BeAlH3 and BeInH3 show interesting thermoelectric behaviors with an increase in efficiency at higher temperatures. Thermal conductivity increases with temperature, influenced by electron vibrations, while Zt and PF factors show material-specific variations, highlighting the optimization potential of these compounds for thermoelectric devices.

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دراسة الخواص الحرارية الكهربائية والبنيوية لهيدريدات البيروفسكايت لتطبيقات الطاقة $BeInH_3$ و $BeGaH_3$ $BeAlH_3$

أيوب كوفي، يونس زيات، حمزة بلخنشي، عبد الله بوزيد.

ملخص: تستكشف هذه الدراسة الخصائص التركيبية والكهربائية والحرارية الكهربائية لهيدريدات البيريليوم البلورية $BeXH_3$ (X = Al, Ga, In) باستخدام تقريب التدرج المعمم (GGA) في إطار نظرية الوظيفة الكثيفة (DFT). تم إجراء التحليل باستخدام حزمة BoltzTrap المدمجة مع كود Wien2k، ومعادلة الحالة لـ Murnaghan لتحديد الطاقة الكلية وحجم الذرة، مع توفير معلومات مفصلة عن بنية النطاقات وكثافة الحالات الإلكترونية. تم التحقيق في الخصائص الحرارية الكهربائية الرئيسية، بما في ذلك معامل القدرة (PF)، ومعامل الجودة (Zt)، والتوصيلية الحرارية (k)، والتوصيلية الكهربائية (σ) ضمن نطاق درجات حرارة من300 إلى 900 كلفن. أظهرت النتائج أن $BeGaH_3$ يتمتع بأفضل أداء حراري كهربائي عبر نطاق درجات الحرارة بالكامل، حيث يصل الحد الأقصى للتوصيلية الكهربائية إلى 3.5×10^{20} (.s) عند 900 كلفن. في المقابل، أظهر كل من $BeAlH_3$ و$BeInH_3$ سلوكيات حرارية كهربائية مثيرة للاهتمام مع زيادة الكفاءة عند درجات حرارة أعلى. تزداد التوصيلية الحرارية مع ارتفاع درجة الحرارة، متأثرة باهتزازات الإلكترونات، بينما تظهر عوامل Zt وPF اختلافات تعتمد على المادة، مما يبرز إمكانيات تحسين هذه المركبات لتطبيقات الأجهزة الحرارية الكهربائية.

الكلمات المفتاحية: DFT؛ $BeGaH_3$، $BeAlH_3$، و $BeInH_3$؛ الجاذبية النوعية؛ الهيدروجين؛ الحراري .

1. INTRODUCTION

Hydrogen is one of the most abundant elements on Earth [1] and possesses unique properties that make it particularly interesting in the energy field. Compared with traditional fossil fuels, hydrogen releases far more heat when it reacts with oxygen [2, 3, 4]. The gas is considered a clean and sustainable energy source, as it is carbon-free, meaning it emits no CO_2 during combustion [5, 6]. This makes it a promising alternative for environmentally friendly energy solutions [7, 8, 9]. Hydrogen's applications are vast, ranging from fuel cells, employed in vehicles and some power plants, to internal combustion engines, notably in hybrid cars [10]. However, to enable wider adoption of hydrogen, two major challenges remain mass production and storage [11, 12, 13]. Current methods, such as steam methane reforming or electrolysis fueled by non-renewable sources, are proving costly and pose environmental problems [14, 15, 16]. Hydrogen storage also represents a technical challenge, due to its low energy density per unit volume [17, 18, 19]. This calls for specific solutions, such as storage in the form of chemical compounds, at very low temperatures or under high pressure, which entails risks in terms of safety and technological feasibility [20, 21, 22]. To make hydrogen accessible in a safe, economical, and efficient way, advances in production and storage technologies are crucial [23, 24]. With alternative energy sources such as hydrogen, wind, nuclear, and solar power, it becomes possible to mitigate the negative effects associated with fossil fuels and reduce our dependence on them [13, 25, 26].

This scientific discussion aims to highlight the growing importance of perovskite-type hydrides, emphasizing their unique properties and crucial role in the search for new materials for energy storage [27]. The crystalline structure of perovskite, with its ABH3 composition, is renowned for its malleability and modification potential, making it an ideal material for a variety of applications [28, 29]. In particular, perovskite hydrides show great promise as high-capacity hydrogen storage materials [30]. Thanks to the hydride ions embedded in their lattice, these materials enable reversible absorption and release of hydrogen, a valuable feature for meeting storage challenges in clean energy technologies [31, 32]. Interactions between hydride ions and the intrinsic structure of perovskites pave the way for advanced energy conversion technologies, including catalytic functions that could enhance electrochemical and photoelectrochemical processes [33, 34]. A study of perovskite hydrides, including $MgCrH_3$ and $MgFeH_3$, revealed that $MgFeH_3$ is a very promising candidate due to its balance between conductivity, storage capacity, and stability [35]. Storage capacity is decreased when transition metal dopants are added, even though this speeds up processes and lowers desorption temperatures [36]. Density functional theory (DFT)-based methods are crucial for optimizing these materials because they allow for the prediction of structural and optoelectronic properties [37, 38]. Researchers can predict important characteristics, including thermal and electrical conductivity, Seebeck coefficient, and thermoelectric figure of merit by using DFT to simulate perovskites at the atomic scale [39]. New opportunities for thermal energy conversion and the creation of more efficient and sustainable energy technologies are made feasible by these developments, which enable the design of materials with the best thermoelectric qualities. In this work on the electronic gravimetric and thermoelectric properties of beryllium hydrides $BeXH_3$ (X = Al, Ga, and In) based on DFT, we use the generalized gradient approximation (GGA) integrated into the BoltzTrap program. This approach enables us to model atomic interactions and assess the ability of these materials to convert thermal energy into electrical energy. The following sections describe in detail the computational techniques deployed, present the data obtained, and discuss conclusions regarding the thermoelectric performance of beryllium hydrides as a function of temperature. This work thus contributes to our understanding of the potential of thermoelectric materials and their optimization for advanced energy applications. $BeXH_3$ compounds, particularly those with Al, Ga, and In, are of interest for a variety of applications. For instance, these hydrides could have potential uses in hydrogen storage, catalysis, or even in the development of novel materials for energy-related technologies. Their properties may also be relevant in the development of new types of batteries, sensors, and other electronic devices, owing to their lightweight nature and possible stability in specific conditions.

2. CALCULATION METHOD

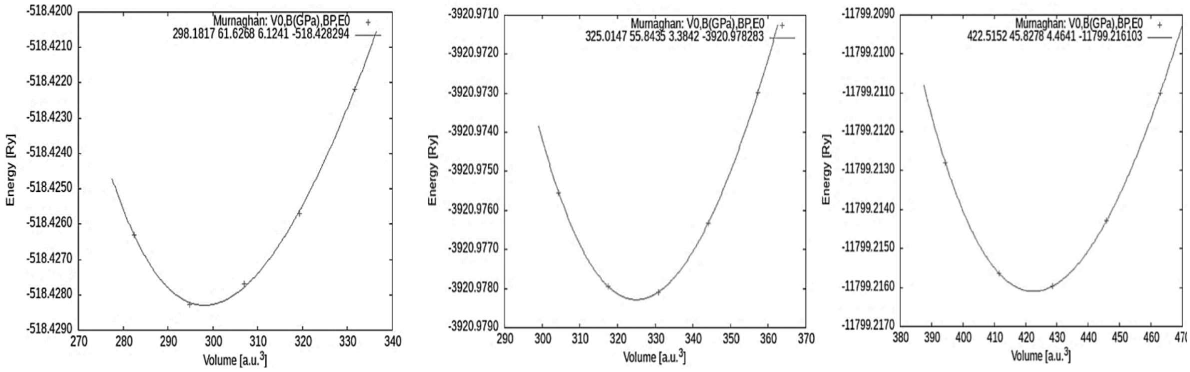
This study utilizes theoretical calculations to evaluate the hydrogen storage capabilities and other properties of $BeXH_3$ (X = Al, Ga, and In) using the GGA, within the framework of DFT [40, 41], which elucidates the exchange and correlation potentials in these calculations. To do this, we use the BoltzTrap package implemented in the Wien2k code [42, 43]. Birch Murnaghan's equation of state is used for structural optimization [44]. During the self-consistent field (SCF), the convergence of total energy and charge was set at 0.0001 (Ry) and 0.001 (e). Using octahedral integration, a 1000 k-point mesh is used to sample the Brillouin zone in detail.

The Murnaghan-equation of state was used to obtain the ground state volume (V_0), mass modulus (B_0), and their derivatives (B'_0) during optimization. Also, the Murnaghan-equation is used to calculate the pressure-dependent volume. To achieve network constants, the bulk modulus (B_0), pressure derivative (B'_0), and structural parameters were optimized over the volume of the unit cell, with the compressibility modulus (B) as a measure of a material's resistance to uniform compression, expressed in terms of change in volume under pressure. It is often used to characterize materials in terms of their ability to resist changes in volume under pressure. The mass modulus (B_0), on the other hand, is a term sometimes used in specific models to describe a relationship between mechanical properties and material density, although it is conceptually similar to the compressibility modulus. The pressure derivative (B') refers to the variation of the compressibility modulus as a function of pressure, providing a measure of the material's sensitivity to increasing pressure. This parameter is crucial to understanding how materials react under different pressure conditions and is commonly used in studies of high-pressure material properties.

The postulated equilibrium lattice constants are obtained by fitting the total energy as a function of the normalized volume to the Murnaghan equation of state (EOS). The equilibrium lattice parameters (a0) that we estimated reasonably agree with the experimental ones. Figure 1 shows the volumes extracted as a function of the expected energy using the Birch-Murnaghan depression.

$$E = E_0 + \frac{B_0}{B_0^{'}}\left(V - V_0\right) - \frac{B_0 V_0}{B_0^{'}\left(1 - B_0^{'}\right)}\left[\left(\frac{V}{V_0}\right)^{1-B_0^{'}} - 1\right] \qquad (1)$$

Where E_0 is taken as the minimum energy, which is the ground state energy corresponding to the volume V_0 of the unit cell.



a) b) c)

Figure 1. Variation of total energy as a function of volume for: a) $BeAlH_3$; b) $BeGaH_3$; and c) $BeInH_3$.

3. RESULTS AND DISCUSSION

3.1. Structural properties

The central element of the $BeXH_3$ hydride perovskite structure (X = Al, Ga, and In) is based on a precise arrangement of atoms: beryllium (Be) atoms are placed at the corners (0, 0, 0) of the cube, while three hydrogen atoms occupy octahedral positions located at the face centers (0, 1/2, 1/2), (1/2, 0, 1/2) and (1/2, 1/2, 0). The X atoms (Al, Ga, and In) are located at the heart of the center (1/2, 1/2, 1/2) [45].

The lattice parameters for $BeXH_3$ (see Table 1) confirm the accuracy of our computations and the reliability of the obtained data. This structure corresponds to a face-centered cubic (fcc) lattice with a space group of $Pm\bar{3}m$ (No. 221).

Figure 2 depicts this arrangement, which is exactly in line with the structures reported in earlier research. Thus, it offers a strong foundation for analyzing this intriguing class of materials.

Table 1. Lattice parameters of $BeXH_3$.

Element	Lattice parameter
$BeAlH_3$	$a_0=b_0=c_0$=3.5353 Å (This work) 3.57 Å [45]
$BeGaH_3$	$a_0=b_0=c_0$= 3.6522 Å (This work) 3.66 Å [45]
$BeInH_3$	$a_0=b_0=c_0$= 3.9708 Å (This work) 3.99 Å [45]

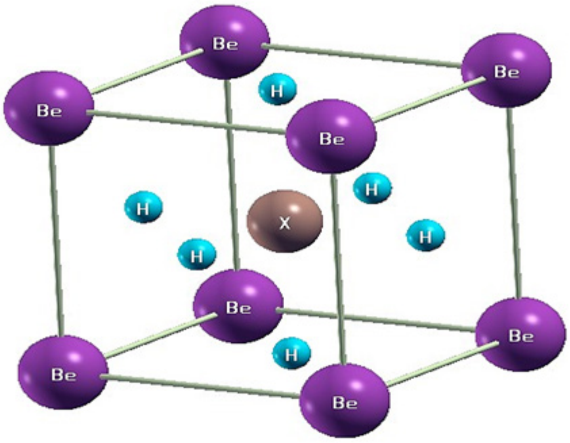
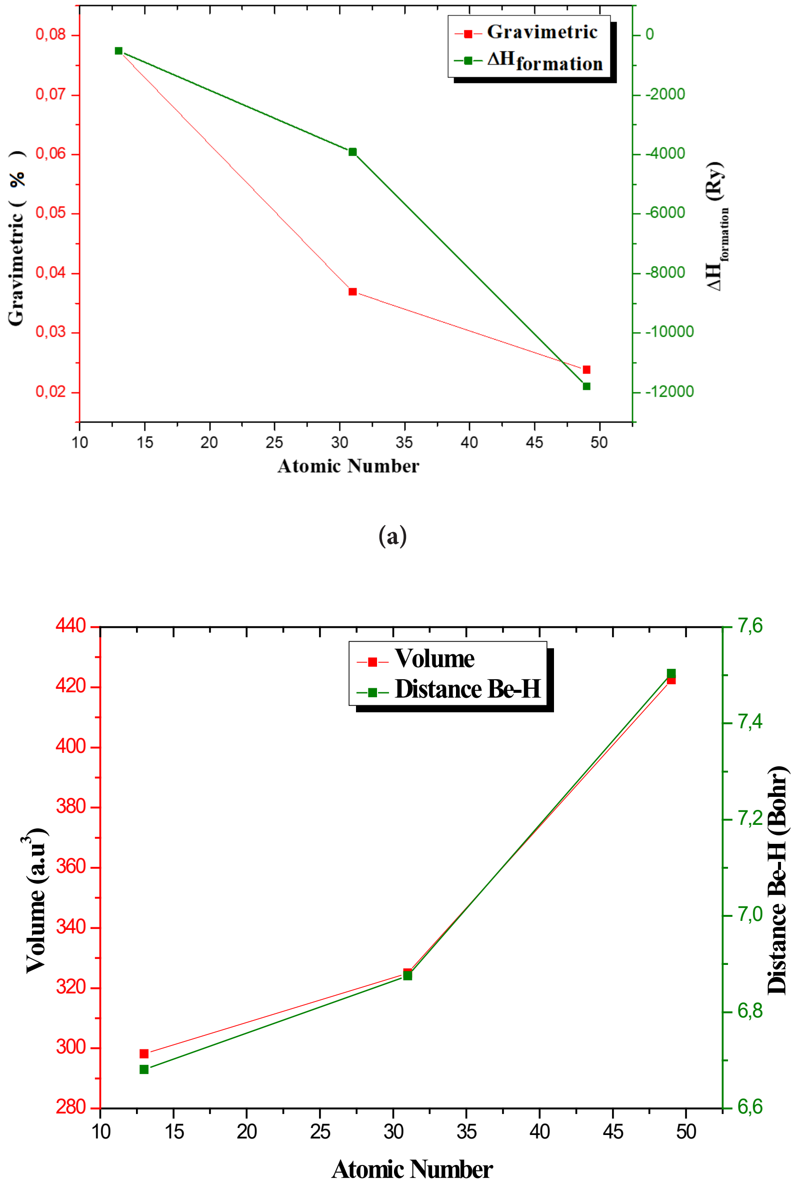


Figure 2. Structure of $BeXH_3$ (X = Al, Ga, and In).



(a)

(b)

Figure 3. a) Gravimetric and $\Delta H_{formation}$ as a function of Atomic Number for $BeXH_3$ (X = Al, Ga, and In); b) Volume and distance Al-H as a function of Atomic Number for $BeXH_3$ (X = Al, Ga, and In).

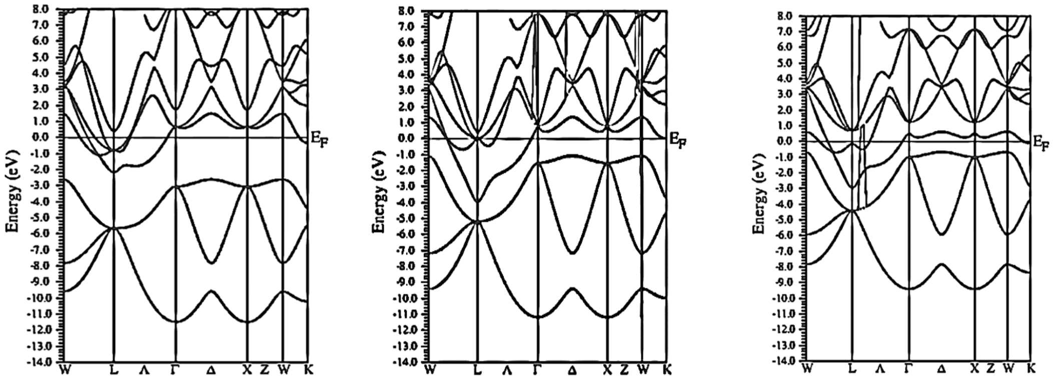
Figure 3(a) illustrates a key observation: the gravimetric values and enthalpy of formation ($\Delta H_{formation}$) of the compounds studied decrease systematically with increasing atomic number of the central element (Al, Ga, In), this decrease in gravimetric values means that, as the central atom becomes heavier, the mass proportion of hydrogen in the compound decreases, directly affecting the energy density of the material. Furthermore, the decrease in $\Delta H_{formation}$ indicates that the thermodynamic stability of compounds is lower for elements with a higher atomic number, an effect attributable to differences in size and nuclear charge between atoms [46, 47]. Aluminum (Al, atomic number 13) has a gravimetric value of 0.077 and a $\Delta H_{formation}$ of -518.42829 Ry, showing good energy density and stability among the three compounds. The element Ga atomic number 31 has a gravimetric value of 0.036 and a $\Delta H_{formation}$ of -3920.9782 Ry. Conversely, indium (In, atomic number 49) displays a gravimetric value of 0.023 and a $\Delta H_{formation}$ of -11799.2161 Ry, signifying lower energy density and stability, making it “softer” than the other compounds. These trends can be partly explained by quantum phenomena such as the electron-shielding effect, which reduces the effective attraction of the nucleus to valence electrons in larger atoms [48, 49, 50]. As a result, bonds are weaker, and less energy is required to form compounds of heavier elements, resulting in a lower enthalpy of formation. This interpretation of the $\Delta H_{formation}$ and gravimetric values suggests that, of the $BeXH_3$ compounds, $BeInH_3$ has the least dense and most malleable structure, while $BeAlH_3$ remains the most stable and dense. Finally, as shown in Figure 3(b), a correlation can be deduced between the atomic number and the physical and chemical properties of these hydrides. The higher the atomic number, the greater the atomic volume, which directly influences the material’s stability and gravimetric density.

3.2. Electronic properties

In our study, we used the GGA to analyze the electrical characteristics of $BeXH_3$ perovskite-type hydrides (X = Al, Ga, and In). The results obtained, shown in Figure 4, clearly demonstrate the metallic behavior of these compounds. The crossing of valence band maxima and conduction band minima over the fixed Fermi level (EF) at 0 eV indicates this intermetallic property. This crossover suggests that these materials are very conductive due to their non-zero density of electronic states at the EF.

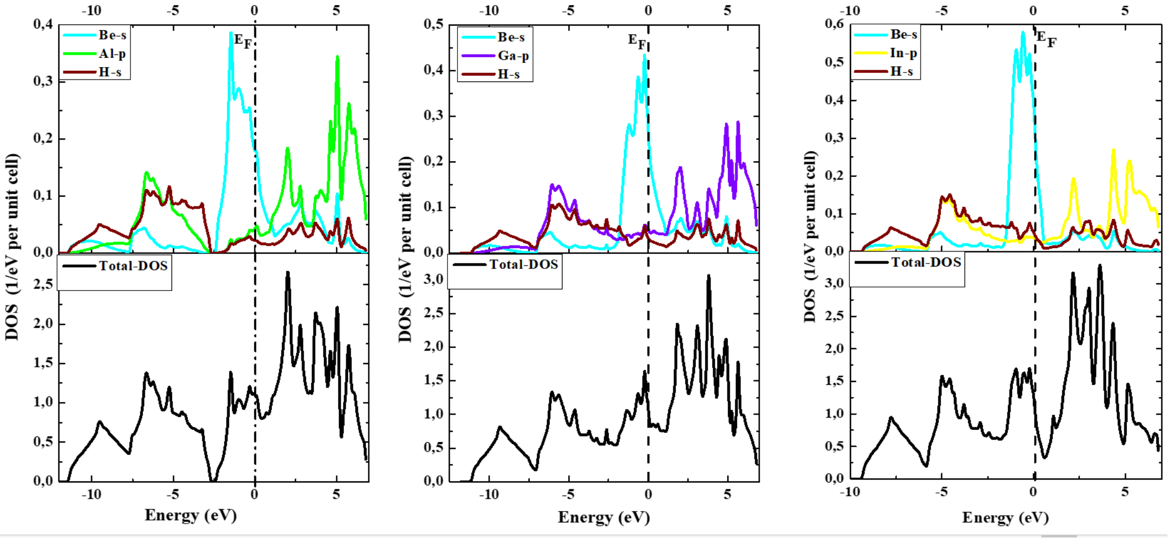
Total density of states (TDOS) and Partial density of states (PDOS) analysis (see Figure 5) explores the individual contribution of each atom type to the overall electronic properties of the compound. Hydrogen s-states (H), X p-states (Al, Ga, and In), and Be s-states play a notable role around the Fermi level, each making significant contributions to the material’s conductivity. However, it is the d states of the X atom (Al, Ga, and In) that dominate the valence band in the energy range between -12 and -6 eV, reflecting a major influence of these elements on the electronic stability of the material. This complex interaction between the electronic states p of X, s of Be, and s of H creates hybridization around the EF, a distinctive feature of metals, which explains their high conductivity. It is also relevant to note that this metallic conductivity confers on perovskite-type hydrides a hydrogen storage capacity superior to that of non-metallic compounds. Indeed, high conductivity facilitates charge transfer during hydrogen absorption and release processes, which is crucial for optimizing hydrogen storage reversibility. Furthermore, owing to their unique electronic structure, metals provide favorable adsorption sites for hydrogen molecules, thereby enhancing their storage capacity [51].

As a result, $BeXH_3$ perovskite-type hydrides seem to be viable options for storing hydrogen. Their electronic structure ensures high conductivity and favorable interaction with hydrogen molecules, essential qualities for storage technologies. It should also be noted that the subtle differences in electronic structure between the compounds $BeAlH_3$, $BeGaH_3$, and $BeInH_3$, due to the specific properties of the elements Al, Ga, and In, could enable fine-tuning of storage properties, offering additional flexibility in the development of materials optimized for industrial applications [52]. This possibility paves the way for further research into the manipulation of electronic characteristics to further improve hydrogen storage efficiency in perovskites.



a) b) c)

Figure 4. Band Structures of: a) $BeAlH_3$; b) $BeGaH_3$; and c) $BeInH_3$.



a) b) c)

Figure 5. The density of states and partial density of states of a) $BeAlH_3$; b) $BeGaH_3$; and c) $BeInH_3$.

3.3. Thermoelectrical Properties

The behavior of electron transport properties is closely linked to the structure of the electron band, calculated here by applying the semi-classical Boltzmann transport theory and the rigid band model, implemented in BoltzTrap software. Since thermal dissipation is a frequent loss in energy-intensive processes, materials such as $BeXH_3$ (where X = Al, Ga, and In) are of crucial importance in renewable energy devices [53].

The efficiency of thermoelectric devices depends on the ratio between electrical and thermal conductivity, making this a key parameter to optimize [53]. $BeXH_3$ compounds (X = Al, Ga, and In) are of particular interest for their thermoelectric properties, and their electrical conductivity (σ), thermal conductivity (κ), figure of merit (Zt) and power factor (PF) have been studied for temperatures ranging from 300 K to 900 K. Although the electrical conductivity of $BeXH_3$ perovskite, expressed as the flux of free charge carriers, is a fundamental element, it has been little explored in the literature to date. As with most materials, factors such as chemical composition, crystal structure, and impurities significantly influence this conductivity.

The measurements shown in Figure 6(a) demonstrate the evolution of electrical conductivity with temperature: it increases between 300 and 500 K before gradually decreasing from 500 to 900 K. For $BeGaH_3$, conductivity reaches a maximum of 3.5×10^{20} (1/Ω.m.s) at 900 K, while for $BeAlH_3$ and $BeInH_3$ it drops to 2×10^{20} (1/Ω.m.s) and 7.5×10^{20} (1/Ω.m.s) respectively under the same conditions. Furthermore, temperature and pressure conditions during the evaluation of $BeXH_3$ (X = Al, Ga, In) also significantly influence the electronic characteristics and, by extension, the electrical conductivity of these materials. These data highlight the importance of physical properties engineering to improve material performance in thermoelectric applications.

Thermal conductivity, which governs heat transfer in a material, shows a linear increase with temperature in the absence of significant variations. Thermal conductivity values (κ) for $BeXH_3$ compounds (X = Al, Ga, and In) are shown in Figure 6(b): they increase progressively with temperature, reaching 14×10^{15} W/(K.m.s), 7×10^{15} W/(K.m.s), and 3×10^{15} W/(K.m.s) respectively for $BeAlH_3$, $BeGaH_3$, and $BeInH_3$ at 900 K. This increase in thermal conductivity is mainly due to vibrations of free electrons within the compounds, which intensify with increasing temperature. Thus, it can be concluded that temperature increase amplifies molecular vibrations in $BeXH_3$ structures (X = Al, Ga, and In), contributing substantially to the thermal conductivity of these materials. The Seebeck coefficient, thermal conductivity, and electrical resistivity all contribute to the dimensionless merit factor (Zt), which thermoelectric materials use to generate energy from temperature gradients [53]. The merit factor (Zt) is explained by the equation that follows:

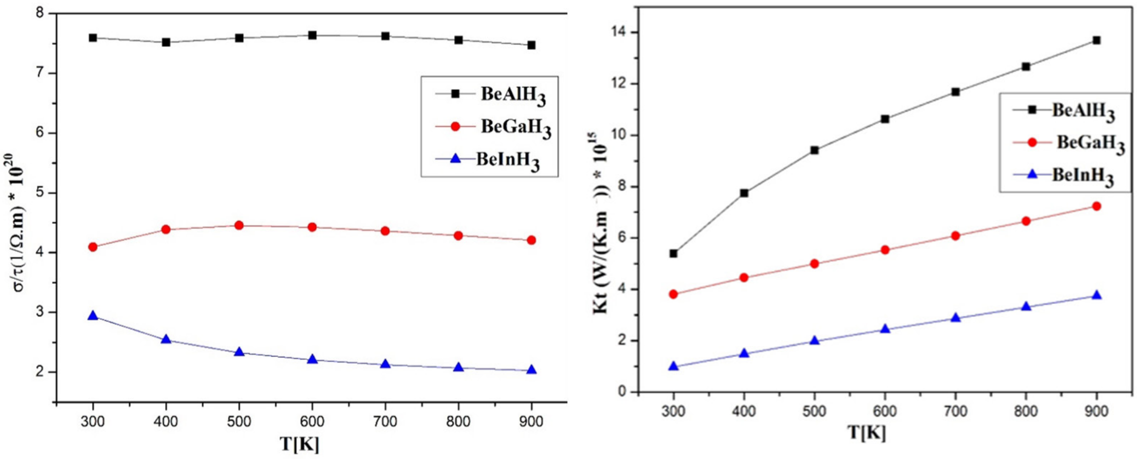
$$Zt = \frac{\sigma S^2 T}{\kappa} \qquad (2)$$

where σ is the electrical conductivity, T is the temperature, S is the Seebeck coefficient, and κ is the thermal conductivity [54]. A high Zt value indicates effective thermoelectric performance in a material with low thermal conductivity, high electrical conductivity, and a significant Seebeck coefficient. The Merit factor (Zt), illustrated in Figure 6(c), shows a distinct variation for each $BeXH_3$ compound (X = Al, Ga, and In) as a function of temperature. For $BeAlH_3$, Zt initially decreases between 300-600 K, then increases from 600 to 900 K with increasing temperature. For $BeGaH_3$, on the other hand, Zt rises steadily over the entire temperature range. For $BeInH_3$, Zt falls slightly between 300 and 400 K before rising steadily from 400 to 900 K. At 900 K, maximum Zt values reach 2.5×10^{-2}, 35×10^{-2}, and 19.8×10^{-2} for $BeAlH_3$, $BeGaH_3$, and $BeInH_3$, respectively. These variations in merit factors highlight the specific thermal responses of each material and their potential for optimization in thermoelectric applications.

The material efficiency in thermoelectric devices is measured by the power factor, which is derived from electrical conductivity and the Seebeck coefficient [53]. For the production of energy, high power factor materials are desired, especially those with a power factor larger than unity, especially in the high-temperature thermoelectric sectors. The following formula explains the PF:

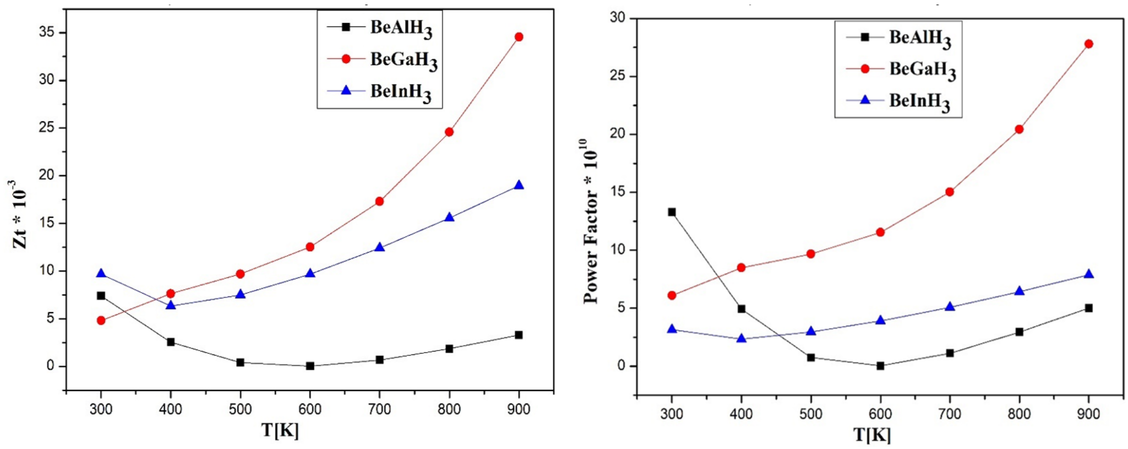
$$Power\ factor(PF) = \sigma S^2 \qquad (3)$$

The power factor (PF), as shown in Figure 6(d), varies differently for each $BeXH_3$ compound (X = Al, Ga, and In) as a function of temperature. For $BeAlH_3$, the power factor first decreases from 300 to 600 K, then increases from 600 to 900 K with rising temperature. For $BeGaH_3$, on the other hand, the power factor rises continuously over the entire temperature range. For $BeInH_3$, the power factor decreases slightly between 300 and 400 K, before resuming an increasing trend from 400 to 900 K. Around 900 K, maximum power factor values reach 2.5×10^{10} W/(K^2.m.s), 27×10^{10} W/(K^2.m.s), and 7×10^{10} W/(K^2.m.s) for $BeAlH_3$, $BeGaH_3$, and $BeInH_3$, respectively. These trends reveal specific variations in each material's response to thermal conditions, highlighting their distinct potential for optimization in thermoelectric applications where a high-power factor is essential. The ability to control and optimize temperature gradients could help maintain the ideal conditions for hydrogen storage, potentially enhancing the performance and efficiency of storage systems. This synergy between thermoelectric properties and hydrogen storage could contribute to more sustainable, energy-efficient solutions for hydrogen-based energy systems.



a) Electrical Conductivity.

b) Thermal Conductivity.



c) Merit Factor

d) Power Factor

Figure 6. Thermoelectric Properties of $BeXH_3$ (X = Al, Ga, and In).

To evaluate the thermoelectric performance of $BeXH_3$ (X = Al, Ga, In), we compared its properties with those of well-known candidates such as $MgFeH_3$ and $MgCrH_3$ [35]. Our findings reveal that $BeGaH_3$ exhibits significantly superior performance. At 900 K, $BeGaH_3$ shows an electrical conductivity of $3.5\text{x}10^{20}$ (1/Ω.m.s), which is considerably higher than that of $MgFeH_3$ 7.75×10^{19} (1/Ω.m.s) and $MgCrH_3$ 7.74×10^{19} (1/Ω.m.s). Additionally, the figure of merit (Zt) for $BeGaH_3$ reaches 0.35, outperforming $MgFeH_3$ (0.09) and $MgCrH_3$ 0.27 at 300 K. This enhancement is attributed to the unique combination of its high electrical conductivity, moderate thermal conductivity, and a power factor of 27×10^{10} W/(K^2.m.s). These results underline the potential of $BeGaH_3$ as a highly efficient thermoelectric material and hydrogen storage candidate, surpassing the limitations of Mg-based hydrides such as $MgFeH_3$ and $MgCrH_3$, which typically exhibit lower Zt values and higher thermal conductivity.

As a result, metallic behavior, such as that observed in $BeGaH_3$, significantly contributes to hydrogen storage efficiency through improved charge transport and enhanced hydrogen adsorption. High electrical conductivity facilitates the rapid movement of electrons during hydrogen absorption and desorption, improving the kinetics of these processes. This leads to faster hydrogen uptake and release, which is essential for efficient storage. Additionally, the metallic nature of $BeGaH_3$ allows for better hydrogen adsorption at the metal-hydrogen interface, where the availability of delocalized electrons promotes the dissociation and absorption of hydrogen molecules, thus increasing storage capacity. Moreover, the high thermal conductivity of metallic hydrides helps manage the heat generated or absorbed during these cycles, further optimizing the hydrogen storage process. In comparison to non-metallic materials, $BeGaH_3$'s metallic conductivity ensures faster, more efficient hydrogen storage and release, improving both the storage capacity and the overall kinetics of the process.

4. CONCLUSION

In the present study, we have used the BoltzTrap software package, integrated with the Wien2k code, to perform a theoretical analysis and predict the structural, electrical, and thermal properties of $BeXH_3$ (X = Al, Ga, and In) using the (GGA) within the framework of (DFT). Our results reveal that the band structures of $BeAlH_3$, $BeGaH_3$, and $BeInH_3$ behave like conductors, with the valence band and conduction band overlapping with no energy gap (0 eV). Thermoelectric properties, such as electrical conductivity (σ), thermal conductivity (κ), figure of merit (Zt), and power factor (PF), indicate that $BeGaH_3$ outperforms $BeAlH_3$ and $BeInH_3$, particularly in terms of high-temperature stability and efficiency. Thermal conductivity increases linearly with temperature, influenced by electron vibrations, while electrical conductivity and merit and power factors vary with thermal conditions, with distinct optimization potential for each material. These discoveries offer promising prospects, not only for scientific advances but also for practical applications that could transform industry and everyday life, particularly in solid-state energy storage devices. The use of compounds such as $BeXH_3$ metal hydrides (X = Al, Ga, and In) looks promising for more compact and safer energy storage. However, further studies will be needed to improve the kinetics and storage capacity of these materials, supported by rigorous scientific efforts and organizational coordination to maximize their impact in thermoelectric and energy applications. The development of advanced materials for hydrogen storage, including efficient thermoelectric systems, is crucial for improving the performance, energy efficiency, and sustainability of future hydrogen-based energy technologies.

Author Contributions: Ayoub Koufi: Writing – original draft, visualization, validation, investigation, formal analysis, data curation, and conceptualization. Younes Ziat: Supervision. Hamza Belkhanchi: Writing – original draft, visualization, validation, investigation, formal analysis, data curation, and conceptualization. Abdellah Bouzaid: Visualization.

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Conflicts of Interest: The authors declare that they have no conflict of interest.

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