High-temperature superconductor of sodalite-like clathrate hafnium hexahydride

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Hafnium hydrogen compounds have recently become the vibrant materials for structural prediction at high pressure, from their high potential candidate for high-temperature superconductors. In this work, we predict HfH$_6$ by exploiting the evolutionary searching. A high-pressure phase adopts a sodalite-like clathrate structure, showing the body-centered cubic structure with a space group of $Im\bar{3}$m. The first-principles calculations have been used, including the zero-point energy, to investigate the probable structures up to 600 GPa, and find that the $Im\bar{3}m$ structure is thermodynamically and dynamically stable. This remarkable result of the $Im\bar{3}m$ structure shows the van Hove singularity at the Fermi level by determining the density of states. We calculate a superconducting transition temperature ($T_c$) using Allen-Dynes equation and demonstrated that it exhibits superconductivity under high pressure with relatively high-$T_c$ of 132 K.

Hydrogen–rich materials at high pressure can achieve high-temperature superconductivity because of their outstanding hydrogen properties. Aschroft further proposed that metallic alloys of heavier elements in hydrides besides hydrogen can considerably increase the electron-phonon coupling (EPC). Following this, the heavier elements reduce the pressure required for metallization through chemical pre-compression. Based on the Bardeen-Cooper-Schrieffer (BCS) theory, a high-temperature superconductor can be obtained from a phonon mediated superconductivity because it can open the way to extensive both experimental and theoretical researches. In order to investigate the superconductive properties of metal hydrides, their crystal structures is a crucial information for the study. For instance, LaH$_{10}$ was reported that it is a face-centered cubic structure with a space group of $Fm\bar{3}m$, and later on showing that it has a $T_c$ above 250 K, besides, this material successfully demonstrated the importance of metallic hydrogen, appearing that it has a high potential for superconductivity. Using $ab$ initio calculations, LaH$_{10}$ proposed to be an anharmonic phase because of the quantum effects, leading to reduce pressure for stabilize the structure.

Room temperature superconductor is another holy grail in high-pressure physics, there are several materials which posses high-temperature superconductivity. Among those high promising materials, hydrogen-rich materials emerging as a vibrant candidate. This important feature of metallic hydrogen has proved to be a dominant component for route to high-temperature superconductor. At present, the advancement of the room temperature superconductors can be obtained by materials design. Recently, the superconductivity of metal superhydrides was studied in a binary compound hafnium-hydrogen, it can see hydrogen pentagraphenelike structure, which stabilized by hafnium. Following this case, the hydrogen pentagraphenelike structure is thermodynamically stable by hafnium. The remarkable result showed...
that a value of $T_c$ is around 213–234 K at a pressure of 250 GPa. The solution of this novel structure opened the
door to the exploration of a new class of structure. Interestingly, it is worth to note that this work reported an
energy difference between HfH$_6$ and HfH$_{10}$ which is closed by approximately 1–2 meV at a pressure of 300 GPa.
The high pressure phase of HfH$_6$ is predicted to be a Cmc$_{21}$ structure$^{30,31}$ and found that it is stable structure
among a convex hull diagram. Moreover, the Cmc$_{21}$ structure is reported to be dynamically stable at a pressure of
300 GPa$^{32}$ because it does not indicate any imaginary frequency. Also, the value of $T_c$ of HfH$_6$ is estimated
to be 45.2 K to 55 K. However, there are neither experimentally nor theoretically studies under high-pressure
above 300 GPa.

It is interesting to note that transition metal hexahydride is thermodynamically and dynamically stable, as
being in accordance with the high-$T_c$ such as ScH$_6$, YH$_6$, and ZrH$_6$, respectively. Among the predicted the value
of $T_c$ based on the Allen–Dynes equation$^{32}$. In 2017, ScH$_6$ was predicted the high-$T_c$ above 100 K from 300 to
400 GPa$^{33}$. In the same year, ScH$_6$ was investigated by using the first-principles calculations, carried out the
McMillan formula with Allen-Dynes corrections$^{32,34}$. As result of this, ScH$_6$ displayed superconductivity with $T_c$ of
130 K at 285 GPa. Then, in 2018, ZrH$_6$ was explored the $T_c$, resulting in the estimation $T_c$ to be 114 K at 295 GPa$^{35}$. 
Recently, in 2019, YH$_6$ was determined by using fully anisotropic Migdal-Eliashberg theory. The results on
superconducting properties of YH$_6$ manifested the $T_c$ reads 290 K at 300 GPa$^{33}$. Motivated by the prediction
of $T_c$ of transition metal hexahydride, it is worthy to further explore HfH$_6$ at very high compressed conditions.

In this work, we provide a potential high pressure candidate structure of HfH$_6$, leading to scientific leap frog
of high pressure superconductivity. We explore the high-pressure phase of HfH$_6$ under pressure from 300 GPa to
600 GPa by first-principles evolutionary techniques. Moreover, we aim to predict the value of $T_c$ by performing
a candidate structure of HfH$_6$. Regarding its potential for superconductivity, the electronic properties shown to
propound a possibility of the value of $T_c$ such as a band structure, a density of states, and a nature of chemical
bonding. Particularly, the electronic properties play an important role in support the value of $T_c$.

**Methods**

The searching for the structures of the clathrate hafnium hexahydride HfH$_6$ was performed by the Universal
Structure Predictor: Evolutionary Xtallography (USPEX)$^{36}$. In all subsequent generations, the random symmetric
algorithm employed 40% heredity, 20% random symmetric, 20% soft mutation, and 20% transmutation operators
in the pressure range from 200 to 600 GPa with structures containing up to four formula units. A plane-wave
basis set up to cutoff energy of 700 eV and an initial Brillouin-zone (BZ) sampling grid of spacing $2\pi \times 0.02 \AA^{-1}$
were used for this calculation as well as a plane-wave basis set up to cutoff is guaranteed to be converged within
an accuracy of 3 meV per atom. All structures were fully relaxed using the generalized gradient approximation
of the Perdew–Burke–Ernzerhof (GGA-PBE) functional$^{37}$ for the exchange-correlation functional. We used the
projector augmented wave (PAW) method$^{38}$ and the conjugate gradient scheme, as implemented in the Vienna
ab inito simulation package (VASP)$^{39}$. For electron-phonon and the spectral function calculations, a plane-wave
cutoff energy of 80 Ry was used. The dense k-points mesh contained all k and k+q grid points were used. The
subsequent electron-phonon and spectral function calculations depended on the k-point part due to it covered
the grid of q-point. The calculations were computed in the first BZ on $24 \times 24 \times 24$ k-points mesh and $2 \times 2 \times 2$
q-meshes, showing that it is sufficient to produce accurate electron-phonon coupling. Computational details of
the electron-phonon and spectral function calculations were successfully reported in the theoretical studies$^{16,17}$

The Allen-Dynes equation$^{32}$ was exploited with the effective Coulomb pseudopotential parameter, $\mu^* = 0.10.$
as follows:

$$T_c = \alpha_{\log} \frac{1.2}{\lambda} \exp \left[ -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right],$$

(1)

where $\alpha_{\log}$ is the logarithmic average of the spectral function. $\lambda$ is the total electron-phonon coupling strength.
The projected crystal orbital Hamilton population$^{40}$ (pCOHP) used to explain the chemical bonding of the
sodalite-like clathrate hafnium hexahydride structure, as implemented in LOBSTER code$^{41}$.

**Results and discussion**

Regarding ground-state structure in HfH$_6$, we aimed to identify the unknown structure of HfH$_6$ above 300 GPa
due to theoretical predictions is a crucial key to the exploration of a candidate structures at high pressure. First of
all, we predicted the high-pressure phase using USPEX code, it shows that our main structural prediction
revealed low-enthalpy structures, showing an orthorhombic structure with a space group of Cmc$_{21}$ and a body
centered cubic with a space group of Im3m.

For the first step in the structural predictions, a structural sequence showed that the Cmc$_{21}$ structure transformed
into the Im3m structure at a pressure of 543 GPa. Under higher pressure, it found that the Im3m structure
declined steadily up to 600 GPa, as showed in Fig. 1a. Moreover, we analyzed the further stable structure of HfH$_6$
with respect to the elemental hafnium (the Im3m structure) and hydrogen (the Cmc$_{12}$-12 structure). Considering
the relative enthalpy, one can see that the Cmc$_{21}$ structure is thermodynamically stable favored over the Im3m
structure at a pressure of 300 GPa. On further compression to 600 GPa, the Im3m structure is apparently stable
(Fig. 1b). Following this, we further investigated to the structural stability by the incorporation of the zero-
point energy (ZPE) of the nuclei estimation, indicating that the Im3m structure is thermodynamically stable
throughout the whole studied pressure range, as showed in Fig. 1c. It should be mentioned that our calculations
performed the DFT at 0 K, we therefore investigated by considering at elevated temperatures. As a result, the
Im3m structure is thermodynamically more stable than the Cmc$_{21}$ structure with increasing temperature up
to at least 300 K, depicting in the convex hull envelopes at a pressure of 600 GPa of Fig. S1 in the Supplemental
Material. This further implies the Im3m structure probably occurs at room temperature. Furthermore, we
investigated further study of the stable structure of HfH\textsubscript{6} at a pressure of 300 GPa. As a result, we pointed out that the Cmc\textsubscript{21} structure is a potential candidate. Our calculations are in good agreement with those recently reported in the theoretical works\textsuperscript{30,31}.

Here, we introduce sodalite-like clathrate at extremely high-pressure, showing the stabled bcc with the Im\textbar 3m space group. To further describe this structure, the H atoms which is in the form of a sodalite-like cage, consisting of eight H-hexagons and six H-squares, and Hf atoms crystallize into a lattice site of body-centered cube. The structural morphology showed in Fig. 1d, which resembles the structures of MgH\textsubscript{6}, CaH\textsubscript{6} and YH\textsubscript{6}\textsuperscript{9,23}.

For the electronic property in the Im\textbar 3m structure, it is clearly demonstrated in Fig. 2a. The band structure manifested a metallic state because a conduction band and a valence band crossed at the Fermi level. Besides, we found that the density of states (DOS) exhibited van Hove singularities (vHs) at the Fermi level, indicating a large electron-phonon coupling (EPC). Interestingly, it is worth noting that the vHs is dominated by a d-electron of Hf. As depicted in the DOS, the characteristics of the vHs play an important role in superconductivity. For example, H\textsubscript{3}S\textsubscript{4}\textsuperscript{2,43}, YH\textsubscript{6}\textsuperscript{23}, and LaH\textsubscript{10}\textsuperscript{44} systems, leading to the possibility of achieving high values of T\textsubscript{c}. To further explore the electronic structure, the Fermi surface is described, as shown in Fig. 2b. It can see that the Fermi surfaces around the P-point exhibited the Fermi nesting because several Fermi surfaces are parallel to each other. It can thus enhance the EPC and the value of T\textsubscript{c}.

According to Fig. 1, we computed phonon dispersions and phonon density of states (PhDOS) of the Im\textbar 3m structure at a pressure of 600 GPa. As a result, we found that the Im\textbar 3m structure is dynamically stable because it does not exhibit the imaginary frequency. Also, the phonon dispersions displayed acoustic modes and optical modes, as can be seen from Fig. 3, where the acoustic modes are the vibrations of the Hf atom and the optical modes are the vibrations of the H atoms. Moreover, the optical branches showed that there was an abundantly spread, showing the stretching and bending modes. These vibrations associated with the electron-phonon interaction and it yielded the high-T\textsubscript{c}. Also, these characteristics corresponded with the PhDOS. It is interesting to note that the H atoms exhibited large vibrations by approximately from 1138 to 2918 THz. A remarkable solution is shown to propound a possibility of the high-T\textsubscript{c}, as will be discussed later.
The spectral function $\alpha^2 F$ of the $\text{Im}\overline{3}m$ structure is calculated at a pressure of 600 GPa, as shown in Fig. 3. The Allen–Dynes equation\(^3\) carried out for the estimation $T_c$. It showed that the Eliashberg spectral function contributed slightly by approximately 0 cm\(^{-1}\) to 324 cm\(^{-1}\) and it contributed mainly by approximately 1120 cm\(^{-1}\) to 2918 cm\(^{-1}\). The solution of the integrating of lambda displayed that it climbed dramatically from 147 cm\(^{-1}\) to 249 cm\(^{-1}\). After that, it remained stable between 247 cm\(^{-1}\) and 1149 cm\(^{-1}\). Then, it increased moderately up to 2918 cm\(^{-1}\), showing the integrating of lambda is 1.06. Here, we found that $\omega_{\log}$ is 1741 K and the $T_c$ is 132 K, using $\mu^*$ = 0.10. Additionally, the $T_c$ is estimated by directly solving the McMillan formula with Allen-Dynes corrections $\mu^* = 0.13$\(^4\). The calculated result shows that the estimated $T_c$ is 114 K. As a possible cause of this, one might think that the H atoms contributed a large frequency. Here again, we have already mentioned the DOS, it can see that an s-electron of H showed a large contribution to the DOS in comparison to s and p-electron of Hf, showing that it supported the existence of the $T_c$. As a result of this, we suggested that the existence of an unforeseen the $\text{Im}\overline{3}m$ structure with remarkably high-$T_c$ can pave the way for further studies on the trend of the high-temperature superconductors.

Figure 2. (a) The calculated electronic band structure and projected density of states of the sodalite-like clathrate hafnium hexahydride structure at 600 GPa. (b) Fermi surfaces of the sodalite-like clathrate hafnium hexahydride structure at 600 GPa. (drawn by XCrySDen program (ver. 1.5.60)\(^5\) (URL http://www.xcrysden.org/Download.html#toc_1)).

Figure 3. (Left) The calculated phonon dispersion at 600 GPa. (middle) The calculated projected phonon density of states at 600 GPa. (right) The Eliashberg spectral function and the integrating of lambda at 600 GPa.
To further analyse the spectral function of the $\text{Im}\bar{3}m$ structure, we calculated at a pressure of 550 GPa. Our calculations show that the character of the spectral function is similar at a pressure of 600 GPa, as can be seen in Fig. 4. It exhibited the integrating of lambda is 1.07 and the $\omega_{\log}$ is 1692 K, showing a high-$T_c$ of 130 K.

At this point, as reported above, we found that the high-$T_c$ of the $\text{Im}\bar{3}m$ structure increased with increasing pressure. As a possible, one might think of the $\omega_{\log}$. It showed that at a pressure of 600 GPa is the maximal of the $\omega_{\log}$, which is higher than at a pressure of 550 GPa. We thus can point out that the $\omega_{\log}$ plays an important role in the high-$T_c$ of HfH$_6$.

As mentioned earlier, it is also interesting to answer the question of why the $T_c$ of the $\text{Im}\bar{3}m$ structure is the high-$T_c$. At this point, we perform the electron localization function (ELF) and the projected crystal orbital Hamilton populations (pCOHP) solutions, the ELF method\textsuperscript{45} calculated to investigate bonding. The characteristics of ELF have successfully explained several materials\textsuperscript{14,46–48}.

To begin with, the ELF of the $\text{Im}\bar{3}m$ structure is described a uniform electron gas of the same density in the (001) plane, as shown in Fig. 5a, it can be seen that a contribution of electrons between the H-H bonds are a weak bonding while the distribution of electrons in Hf atoms likely to be lone pairs in that region. Moving on to the pCOHP calculation, we described the character of the nature of a chemical bonding, which further supports the ELF calculation. This method can examine covalent bonding in several materials\textsuperscript{11,49,50}. To further
understand the superconductivity, the influence of bonding plays an important role in considering the value of $T_c$. The pCOHP calculation interprets the wave function into the covalent character. First of all, it can see that the H-H pairs promoted the anti-bonding. Following this, one can see that the H-H pairs were found to be the anti-bonding as well (Fig. 5). As a result of this, one might think that the nature of chemical bonding supported the value of $T_c$. This because the antibonding states in the covalent system led to the way of strong coupling of the EPC, which associated with the large vibration of H-rich.

**Conclusion**

In this work, we identify the high-pressure phases of HH$_6$ by performing an evolutionary searching. Overall, the incorporating of the zero-point energy shows that the Im3m structure is thermodynamically stable favored over the Cmc2$_1$ structure. The sodalite-like clathrate hafnium hexahydride is predicted to be a high-temperature superconductor with estimated $T_c$ of 132 K at a pressure of 600 GPa. The nature of the chemical bonding is associated with the electron localized function, implying that the characteristics of the chemical bonding entail the high-$T_c$. Finally, we point out that the existence of an unexpected the Im3m structure can pave the way for further studies on the development of the high-temperature superconductors.

**Data availability**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Received: 22 May 2021; Accepted: 21 July 2021

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Acknowledgements
We gratefully acknowledge the NSC (National Computer Center, Linköping, Sweden) in Sweden for providing computing time. This research project was supported by the Second Century Fund (C2F), Chulalongkorn University. This project is funded by National Research Council of Thailand (NRCT); (NRCT5-RSA63001-04). This research is partially funded by Chulalongkorn University; Grant for Research. R.A. thanks the Swedish Research Council (VR-2016-06014 & VR-2020-04410) for financial support.

Author contributions
PT, and T.B. designed the research; P.T., P.P., N.P., and T.B. performed the research; P.T., N.P., R.A., and T.B. analysed the data; and P.T., N.P., R.A., and T.B. wrote the paper.

Competing interests
The authors declare no competing interests.

Additional information
Supplementary Information The online version contains supplementary material available at https://doi.org/10.1038/s41598-021-95112-5.

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