Pressure-stabilized superconductive yttrium hydrides

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The search for high-temperature superconductors has been focused on compounds containing a large fraction of hydrogen, such as SiH4(H2)2, CaH6 and KH6. Through a systematic investigation of yttrium hydrides at different hydrogen contents using an structure prediction method based on the particle swarm optimization algorithm, we have predicted two new yttrium hydrides (YH4 and YH6), which are stable above 110 GPa. Three types of hydrogen species with increased H contents were found, monatomic H in YH3, monatomic H+ molecular “H2” in YH4 and hexagonal “H6” unit in YH6. Interestingly, H atoms in YH6 form sodalite-like cage sublattice with centered Y atom. Electron-phonon calculations revealed the superconductive potential of YH4 and YH6 with estimated transition temperatures (Tc) of 84–95 K and 251–264 K at 120 GPa, respectively. These values are higher than the predicted maximal Tc of 40 K in YH3.

The study of hydrogen-rich compounds at high pressure is mostly motivated by their potential high-temperature superconductivities at high pressures. In 2004, Ashcroft1 suggested that hydrogen-rich compounds can become metallic and superconducting at lower pressures than hydrogen, presumably because of “chemical compression”. Since then, theoretical studies have revealed a large number of superconducting hydrides (SiH42–4, SnH45,6, GeH47, ScH38, YH39, GaH310, H2S11 et al.) at high pressures with predicted Tc ranging from 17 to 86 K. Remarkably, our previously prediction of high Tc (80 K at 160 GPa) in H2S11 has been proven recently from experiments12. Recently, a new type of hydrogen solvated molecular complex SiH4(H2)2 has been synthesized13,14 and was predicted to have a Tc of ~100 K at 250 GPa15, which is much higher than the 17 K observed in SiH42. The experimental and theoretical studies have led to further investigations on hydrides with large hydrogen fraction that may provide a pathway to better superconductors. Using first-principle structure predictions, Zurek et al.16 first predicted three new lithium hydrides (LiH2, LiH6 and LiH8) above 130 GPa, which are stabilized by charge transfer from Li to H. Subsequent studies have revealed a number of hydrides with large hydrogen fractions at high pressures, such as Na-H17, K-H18, Rb-H20, Cs-H21, Ca-H22, GeH4-H23 and H2S-H24. Remarkably, some hydrides were predicted to possess high Tc, e.g., ~82 K in LiH6 (300 GPa)25, ~70 K in KH6 (166 GPa)18 and strikingly ~235 K in CaH6 (150 GPa)22.

Among the different hydrides, yttrium hydrides (YHn) are of special interest because each Y atom has three valence electrons and, in principle, could be shared with three H atoms. Experimentally, that during the continuous absorption of H atoms, a reversible transition of YH2 between the reflecting YH2 and optically transparent YH3 was observed. This interesting phenomenon offers a great potential for practical application as a “switchable mirror”. Raman26 and infrared27 studies found that the semiconducting YH3 transforms to a metallic fcc structure above 10 GPa. Significantly, fcc-YH3 was predicted to be a superconductor with Tc of 40 K at 17.7 GPa, the lowest reported pressure for hydrides to date. The prediction, however, has not been confirmed by experiment.

At high pressure, it is expected that the valence electronic state of Y atom will change and therefore provides a possibility of bonding with more H atoms. Here, we focus on the formation of Y hydrides with larger H concentration at high pressures of YHn (n = 2, 3, 4, 5, 6, 8). Two new thermodynamically stable...
Results

The enthalpies of the candidate structures of YH₄ found in structure predictions relative to the products of dissociation into Y + solid H₂ and YH₃ + solid H₂ at selected pressures are summarized in Fig. 1 (a,b), respectively. Fig. 1 (a) shows all the stoichiometries considered here possess negative formation enthalpies with respect to Y + solid H₂. Among those, YH₃ has the lowest energy. Two thermodynamically stable polymorphs, YH₄ and YH₆, are to be thermodynamically more stable than the decomposition into YH₃ + solid H₂ were found at 140 and 160 GPa (Fig. 1b). Although YH₂, YH₅ and YH₈ have negative formation enthalpies with respect to Y + solid H₂, they are expected to decompose at all pressure. For example, YH₂ decomposes into YH₃ + Y since the enthalpy is above the tie-line connecting YH₃ and Y. Similarly, YH₅ and YH₈ decompose into YH₄ + YH₆ and YH₆ + H₂, respectively (Fig. 1b). Therefore, YH₂, YH₅ and YH₈ are excluded in the discussions hereafter.

So far, YH₃ is the only experimentally known yttrium hydrides at high pressure. The structure search readily reproduced the observed fcc structure at 100 and 150 GPa. As can be seen from Fig. 2 (a), there exist only one type of Y atom occupying the fcc site and two nonequivalent, H1 and H2, atoms at the octahedral and tetrahedral sites. The H-H separation is of 1.9 Å at 120 GPa, clearly indicates no interaction between the H atoms (Fig. 2d). Therefore, the H atoms in fcc-YH₃ are monoatomic. fcc-YH₃ was previously predicted to be stable in a large pressure region of 20 GPa to 197 GPa and undergo a superconductor – metal – superconductor transition under pressure⁹.

Figure 1 (c,d) show the formation enthalpies of YH₄ and YH₆ with respect to YH₃ + solid H₂ as functions of pressure. The formation enthalpy of YH₄ becomes negative relative to YH₃ + solid H₂ near 128 GPa (Fig. 1c). It is important to include the quantum nuclear zero-point energies (ZPE) when considering the energetics of systems containing light atoms. We therefore calculated the ZPEs of YH₄, YH₅, and H₂ phases within the quasi-harmonic approximation. When ZPE corrections are included, the predicted pressure for the onset of stability of YH₄ is lowered to 112 GPa (inset in Fig. 1c). The stable YH₄ has a tetragonal structure (space group I₄/mmm, denoted tI₁₀ hereafter, Fig. 2b) with two formula units per unit cell. We found that the tI₁₀-YH₄ has the same structure type with tI₁₀-CaH₂²². The tI₁₀ structure at 120 GPa consists of body-centered arranged Y atoms and two nonequivalent H1 and H2 atoms with H1-H2 and H2-H2 distances of 1.58 and 1.33 Å, respectively. Valence electrons localization was found...
between the two neighbouring H2 atoms while absent between H1 and H2 atoms (Fig. 2e). This indicates the presence of both molecular “H 2” and monoatomic H in tI10-YH 4.

YH 6 becomes thermodynamically more stable than YH 3 + solid H 2 above 122 GPa (Fig. 1d). The onset pressure of the stability of YH 6 is reduced to 110 GPa when considering the ZPE effect (inset in Fig. 1d). In the thermodynamically stable pressure region, YH 6 adopts a cubic structure with space group Im 3m (2 f.u./unit cell, denoted cI14 hereafter, Fig. 2c). The “H 6” hexagons are forming a corner-shared sodalite-like cage with a Y atom at the center, the same sodalite structure found in CaH 6 above 150 GPa22. In this case, the H-H distance of 1.31 Å at 120 GPa is longer than in CaH 6. Despite the longer distance, covalent interaction between H atoms is clearly visible from the localized valence electrons between the H atoms (Fig. 2f).

Discussion
We found three types of H species in YH n compounds, monatomic H in YH 3, monatomic H+molecular “H 2” in YH 4 and hexagonal “H 6” in YH 6. Since molecular H 2 has a filled covalent σ bond, the additional electrons donated from Y will occupy the antibonding σ* bond, resulting in a stretched or even dissociated H-H bond. For example, the formation of YH 3 can be described by the reaction 2Y + 3H 2 → 2YH 3. Assuming all 6 valence electrons (3 from each Y atom) were transferred to the H 2, then, each H 2 would accommodate two additional electrons into the σ* orbital and, thus, breaking the H 2 molecule into monatomic H. Integration of the electron density shows that each H1 (H2) atom in fcc-YH 3 have accommodated an additional 0.54 (0.47) electrons. A similar description can be used for the formation of YH 4. In this the reaction is Y + 2H 2 → YH 4. There are three electrons available to two H 2 molecules. Therefore, one H 2 bond is completely broken into two monoatomic H and the remaining electron occupied the σ* one the second H 2, thereby weakening the bond and resulted in a longer H-H distance of 1.33 Å. The additional charge of the monatomic H in tI10-YH 4 is calculated to be 0.42 electrons. Only 0.29 electrons were added to H2 in tI10-YH 4. Finally, the formation of YH 6 can be described as Y + 3H 2 → YH 6. In this case only, one electron is added to each H 2 and the H-H bond is elongated to 1.31 Å, in close agreement with the “molecular” H 2 in YH 4. In cI14-YH 6, each H atom has accepted 0.25 electrons, which is not enough to dissociate the H 2 molecule.

A previous study22 has shown that 4s-3d charge transfer turns Ca from s-dominant into s-δ dominant at high pressure, similar to the electronic configuration of Y atom. Therefore, the presence of same structure types in YH 4 (YH 6) and CaH 4 (CaH 6) is not accidental. However, the H-H distance of “H 2” molecule...
in YH$_6$ ($1.33 \text{ Å}$) is much longer than that (0.81 Å) in CaH$_4$ at 120 GPa as Y transfer one more valence electron to H$_2$ than Ca resulting in a longer H-H distance in YH$_4$ (YH$_6$). The empirical consideration is support from quantitative calculations of the difference of the electron density of tI10-YH$_4$ to that of a hypothetical structure consisting only H sublattice. It is clearly shown in Fig. 3(a,b), that there is no electron density (covalent bond) between the two H$_2$ atoms in the pure H structure. However, when the Y atoms were present, localized electrons are found between two H$_2$ atoms. Therefore, the charge transfer from Y to H2 is responsible to the formation of molecular “H$_2$” in YH$_4$. Similarly, the formtion of “H$_6$” hexagons in YH$_6$ results from the accommodation by H of excess electrons from Y atom (Fig. 3c,d). For comparison, a survey of molecular “H$_2$” in most hydrogen-rich compounds only show a slightly elongated H-H bond length than pure solid H$_2$. Examples are 0.87 Å in GeH$_4$, 0.79 Å in SnH$_4$, 0.84 Å in SiH$_2$(H$_2$)$_2$, 0.76 Å in LiH$_2$, and 0.8 Å in NaH$_2$.

The electronic properties, lattice dynamical and electron-phonon coupling parameter (EPC) of tI10-YH$_4$ and cI14-YH$_6$ have been calculated. Both tI10-YH$_4$ and cI14-YH$_6$ are found to be metals from the band structures presented in Fig. 4. We found three features common to tI10-YH$_4$ and cI14-YH$_6$: (i) the large density of states at the Fermi level ($N_F$), 0.44 eV$^{-1}$ per f.u. in tI10-YH$_4$ and 0.6 eV$^{-1}$ per f.u. in cI14-YH$_6$ at 120 GPa; (ii) the concurrence of flat and steep electronic bands near the $N_F$ providing a possibility of the pairing of eletrons at the $N_F$; (iii) strong Y-H hybridization derived from the significant overlap of Y- and H-DOS. Note that in a previous study it was demonstrated that the Y-H hybridization is responsible for the superconductivity in YH$_3$.

Figure 5 shows the calculated phonon dispersions, phonon density of states (PHDOS), Eliashberg spectral function ($\alpha^2F(\omega)/\omega$) and EPC integrated ($\lambda(\omega)$) for tI10-YH$_4$ and cI14-YH$_6$ at 120 GPa. The absence of any imaginary phonon modes proves the dynamical stabilities of both compounds. As expected, both phonon spectra are separated into two frequency regions, with the low frequencies (<10 THz) dominated by the vibrations of Y atom while the high end of the spectra by H atoms. In tI10-YH$_4$, the resulting EPC parameter $\lambda$ is 1.01 at 120 GPa, which is comparable to the maximum value (~1.4) predicted for fcc-YH$_3$. Note that the low-frequency vibrations contribute to 18% of the total $\lambda$ while the remaining 82% comes from H vibrations. Circles with radius proportional to the EPC were also plotted in Fig. 6 to illustrate the contributions associated with different phonon modes. One can observe that nearly all phonon modes contribute to the overall $\lambda$, reflecting a three-dimensional nature of the structure.

Surprisingly, according to the calculation, the EPC parameter $\lambda$ of cI14-YH$_6$ reaches 2.93 at 120 GPa, even larger than that (2.69 at 150 GPa) in cI14-CaH$_6$. However, the Eliashberg phonon spectral functions of cI14-CaH$_6$ and cI14-YH$_6$ are quite different. The EPC in cI14-CaH$_6$ was derived primarily from the two phonon modes ($T_{2g}$ and $E_g$) at the zone center Γ point. However, we observed an overall contribution of different modes to $\lambda$ along N-P-Γ-N directions. Moreover, 90% of the total $\lambda$ is contributed by H vibrations. The superconductivity in YH$_6$ is associated with the Kohn anomalies observed in the phonon dispersion of the phonon branch Γ-H and H-N. The calculation of the nesting function (Fig. 5c) confirms this expectation and clearly show strong nesting along Γ-H and H-N directions. Compare to the other 5 bands crossing the Fermi level, the Fermi surface of strongly nested band (Fig. 6c) shows a complex “vase”-like topology with strong nesting along Γ-H.

$T_c$ was estimated from the spectral function ($\alpha^2F(\mu)$) by numerically solving the Eliashberg equations with typical choice of Coulomb pseudopotential $\mu^* = 0.1$–0.13. The Coulomb repulsion is taken into account in terms of the $\mu^*$ scaled to a cutoff frequency. At 120 GPa, the calculated $T_c$ is 84–95 K for...
tI10-YH4, much higher than the maximal 40 K predicted for fcc-YH3. Note that tI10-YH4 has a much larger logarithmic average frequency of 1119 K than fcc-YH3 (350 K) due to the presence of molecular “H2”, which helps to enhance the superconductivity. For cI14-YH6, Tc value of 251–264 K was estimated. This value is comparable to the predicted Tc (220–235 K at 150 GPa) in CaH6. Although, in principle, there is no upper limit to the Tc value within the Midgal-Eliashberg theory, remarks on the very high Tc value of cI14-YH6 must be view with caution. The EPC calculations were based on the harmonic approximation and without the consideration of electron correction effects. A previous study had shown that anharmonicity of atomic motion may reduce or even suppress the superconductivity of AlH3 due to the renormalization of the lower vibration modes by anharmonicity. However, this suggestion is contrary to the observation that anharmonic vibrations will significantly enhance Tc in case of disordered compounds. Another important, but often neglected, situation is that the Fermi level topology may be altered in improved electronic band structure including corrections to self interaction and electron correlation effects. In AlH3, the parallel bands favouring nesting disappeared in the GW calculated band structure. Here, GW band structure calculations were performed for tI10-YH4 and cI14-YH6. No significant change in the band structures, particularly for the bands near or crossing the Fermi level, was found in both case (Fig. 4). Therefore, the discussion presented above will still be valid and we expect YH4 and YH6 are good superconductors.

Methods

Structure predictions for YHn were performed using the particle swarm optimization technique implemented in the CALYPSO code. In recent studies, it was shown that the approach was successful on the prediction of high pressure structures on both elemental and binary compounds, such as N33, Ca-H22, H2S11 and BeH239. In this work, systematic structure search were performed on six stoichiometries (YH2, YH3, YH4, YH5, YH6 and YH8) at 100 and 150 GPa. Model cells up to 4 formula units (f.u.) for each stoichiometry were used. The structure search was considered converged when~1000 successive structures were generated after a lowest energy structure was found.

ab initio structure relaxations were performed using density functional theory within the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) as implemented in the Vienna \textit{ab initio} simulation package (VASP)40. The band structures were calculated with both PBE-GGA and GW methods41. The GW interpolated band structures were computed using WANNIER9042. The all-electron projector augmented wave (PAW)43 method was adopted with 1s and 4s4p6d5s2 treated as valence electrons for H and Y, respectively. An energy cutoff of 700 eV and a Monkhorst-Pack Brillouin

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Figure 4. Electronic band structures and projected density of states (PDOS). Electronic band structures and PDOS (in units of eV$^{-1}$ per f.u.) of tI10-YH4 (a) and cI14-YH6 (b) at 120 GPa. Dashed red lines in left pannels are the GW-corrected band structures. The horizontal dashed lines represent Fermi level ($E_F$). The numbers (1–6) in (b) label the six bands accrossing the Fermi energy.
zone sampling grid with a resolution of 0.5 Å⁻¹ were used in the structure searches. Selected low energy structures were then re-optimized with a denser grid better than 0.2 Å⁻¹ and a higher energy cutoff of 1000 eV. Phonon dispersion and electron-phonon coupling (EPC) calculations were performed with density functional perturbation theory using the Quantum-ESPRESSO package. Norm-conserving pseudopotentials for Y and H were considered with a kinetic energy cutoff of 140 Ry. 8 × 8 × 8 (59 q-points) and 10 × 10 × 10 (47 q-points) q-meshes in the first Brillouin zones were used in the EPC calculations for YH₄ and YH₆, respectively. Monkhorst-Pack grids of 32 × 32 × 32 and 40 × 40 × 40 were used to ensure k-points sampling convergence with Gaussians of width 0.03 Ry for YH₄ and YH₆, respectively, in order to approximate the zero-width limit in the calculations of the EPC parameter, λ.

**Conclusion**

In conclusion, structure predictions have demonstrated that yttrium atom can react with more than three hydrogens under pressure. Two high-hydride phases, YH₄ and YH₆, were predicted to be thermodynamically stable relative to YH₃ and H₂ above 110 GPa. At the stable pressure ranges, YH₄ has a bct structure containing both monatomic H and molecular “H₂” while YH₆ adopted a bcc structure with a H sodalite-like cage. Electron-phonon coupling calculations show that both YH₄ and YH₆ are

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**Figure 5. Phonon properties and Eliashberg spectral function.** Phonon dispersions, projected phonon density of states (PHDOS), Eliashberg spectral function ω²F(ω)/ω and EPC integration of λ(ω) of t110-YH₄ (a) and c114-YH₆ (b) at 120 GPa. Red circles in the two left panels indicate the phononline width with a proportional to the strength. (c) The nesting function of c114-YH₆ along several high-symmetry lines of Q calculated at 120 GPa. The present calculation employs 3094 k points and 126 Q points, which result in the evaluation of energy εₖ+Q at 390000 points.
supercodncutive with \( T_c \) higher than YH3. The results presented here support the suggestion that compressing the mixture of elements (compounds) and hydrogen is a way to search high-temperature superconductors. In addition, in principle, YH4 and YH6 can be synthesized by compressing the mixture of YH3 and H2 above 110 GPa.

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Author Contributions
Y. L. and Y. W. conceived the idea. Y.L., J. H. and H. L. performed the calculations. Y L. and J. T. and Y. M. wrote the manuscript with contribution from all.

Additional Information
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