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High Pressure Synthesis & Superconductivity of Ytterbium Polyhydrides

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Ytterbium polyhydrides were synthesized through *in-situ* high pressure laser heating techniques utilizing a diamond anvil cell. The temperature dependence of resistance measurement at high pressure demonstrates that the sample undergoes a superconducting transition at 11.5 K at 180 GPa. The investigation of SC under magnetic field indicates that the upper critical field at zero temperature $\mu_0 H_{c2}(0)$ is ~ 5 Tesla. From the analysis of the *in-situ* high pressure X-ray diffraction experiments, the observed superconductivity is proposed to arise from the $Pm\bar{3}n$ Yb_4H_{23} phase. It is speculated that the low superconducting transition temperature T_c in Yb_4H_{23} might be associated with the unusual local magnetic moment in Yb at pressure.

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Introduction. Metallic hydrogen has been proposed to host room temperature superconductivity (SC) because of its light mass and special electron configuration, just one electron outside the nucleus, which are expected to lead to a high Debye temperature and strong electron-phonon coupling, respectively.[1] Although the metallization pressure for hydrogen is predicted to be at least 400 GPa,[2] it is proposed that hydrogen metallization can be realized by compressing polyhydride under reduced pressure due to the chemical pre-compression effect,[3] while SC with high superconducting transition temperature (T_c) can be kept in such a condensed polyhydride.[4–6] Since sulfur hydride of SH_3 was experimentally reported to have SC with T_c above 200 K at 155 GPa,[7] great efforts have been paid to exploring new polyhydride superconductors.[8,9] Up to now, a series of high T_c polyhydride superconductors have been theoretically predicted and experimentally discovered.[10–19] The rare-earth hydride of LaH_{10} was first experimentally reported to have SC with T_c above 250 K at 170 $\sim$ 200 GPa,[13–16] following which yttrium hydride superconductor of YH_9 was discovered with $T_c \sim 243$ K at 201 GPa and YH_6 with $T_c \sim 220$ K at 183 GPa.[17] For the alkali-earth hydrides, CaH_6 was found to host SC with T_c above 210 K at 160–172 GPa.[18,19] In addition, many other binary hydride superconductors with moderate T_c have been experimentally discovered,[20–28] such as the rare-earth hydride of Lu_4H_{23} with T_c of 71 K at 218 GPa,[23] the covalent bonding dominated antimony hydride of SbH_4 with T_c of 116 K at 184 GPa[28] and the transition metal hydrides of ZrH_n with $T_c \sim 71$ K at 220 GPa[24] and HfH_{14} with $T_c \sim 83$ K at 243 GPa.[25]

Magnetism is usually considered to be against to SC. For the light lanthanide polyhydrides, the T_c value decreases when increasing the number of 4f electrons. LaH_{10} with zero f electron has the highest T_c while it goes down to 115 K, 9 K and 5 K in the sequence of CeH_{10},[29] PrH_9[30] and NdH_9.[31] For the heavy lanthanide polyhydride of Lu_4H_{23}, T_c again increases to a moderate value because of the nonmagnetic state for Lu with a full filled f orbital.[23] At ambient pressure Yb metal also has a full filled f shell with $4f^{14}5d^06s^2$ configuration, while under high pressure local magnetic moment would be induced by electron transfer from 4f to 5d orbital.[32] It is expected that the SC in ytterbium polyhydride should be greatly suppressed by the induced magnetic moment. However, YbH_6 and YbH_{10} have been theoretically predicted to have high temperature SC with T_c about 70–90 K at 200 GPa[33] and 102 K at 250 GPa,[34] respectively. To investigate the SC in ytterbium polyhydrides, we synthesized the sample under Megabar pressure. SC was found but with a very low $T_c = 11.5$ K at 180 GPa, and the SC is proposed to be ascribed to the presence of $Pm\bar{3}n$ Lu_4H_{23} phase. Our results suggest that the low T_c value observed in Lu_4H_{23} is closely related with the appearance of magnetic moment induced

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by pressure.

Methods. Diamond anvil cell (DAC) technique was used to prepare the ytterbium polyhydride samples. Diamond anvil with culet diameter of 50 μm beveled to 300 μm was adopted for Megabar pressure experiments. The gasket of T301 stainless was prepressed to ∼10 μm thickness and then drilled with a hole of 300 μm in diameter, into which aluminum oxide was filled. A hole of 40 μm in diameter was further drilled on the densely pressed aluminum oxide as a high pressure chamber, after which ammonia borane (AB) was filled into the chamber. AB acts as the hydrogen source as well as the pressure transmitting medium. The inner electrodes with a thickness of 0.5 μm were made by depositing Pt on the surface of the anvil culet. An ytterbium foil (99.9%) with the size of 20 μm × 20 μm and 1 μm in thickness was stacked on the inner electrodes. The pressure was determined by measuring the shift of Raman peak of diamond anvil. The details can be referred to ATHENA procedure reported in Ref. [35].

The samples were heated under high pressure by a YAG laser with a wavelength of 1064 nm and spot size about 5 μm in diameter. The temperature was determined by fitting the black body irradiation spectra. The resistance measurements under high pressure were performed in a MagLab system by using a Van der Pauw method.[36,37] For these measurements an applied electric current of 1 mA was used.

The *in-situ* high pressure X-ray diffraction (XRD) experiments at room temperature were performed at 13-IDD of Advanced Photon Source at the Argonne National Laboratory. For the X-ray beam, the wavelength of is 0.3344 Å and the beam size is ∼ 3 μm in diameter. The rhenium was used as the gasket for the XRD experiments. The pressure calibration was done by using the equation of state from rhenium gasket material.

Results and Discussion. Figure 1 displays the temperature dependence of resistance measured at 180 GPa for the sample synthesized at the same pressure. The resistance shows a sharp drop at ∼ 11 K and goes down to zero below 5 K. Further, this transition can be suppressed by magnetic field as seen in Fig. 2(a). Thus, it is proposed that such an observed sharp drop of resistance should origin from superconducting transition. The resistance derivation over temperature was plotted to determine the transition temperature T_{c}. As seen in the left inset of Fig. 1, T_{c} is determined to be about 11.5 K by the right upturn of dR/dT curve. Another transition occurs at about 7.3 K and can be clearly seen from an enlarged view shown in the right inset of Fig. 1. In fact, before heating the Yb sample to synthesize polyhydride, *in-situ* high pressure resistance measurements have been carried out for the Yb metal under different pressures as seen in Fig. S1. The onset T_{c} at 180 GPa for Yb metal reaches 7.3 K, which is the same as the second transition temperature observed in Fig. 1 and comparable to the reported $T_{\mathrm{c}} \sim 6$ K for Yb metal at 179 GPa,[32] it is suggested that the second transitions in Fig. 1 should arise from Yb superconducting transition. However, we cannot rule out other possibilities that the sample contains hydrides with different hydrogen content and presents multistep superconducting transitions as usually seen in other polyhydride superconductors.[13,18,28]

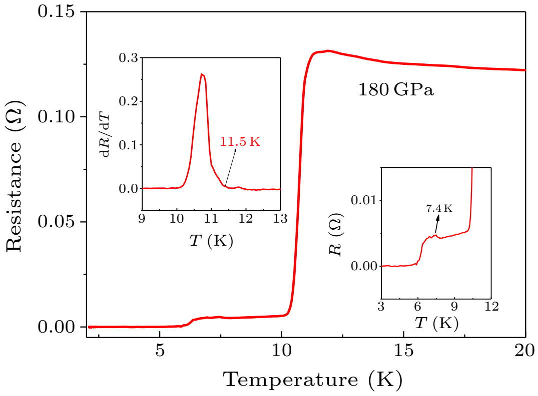

Fig. 1. The temperature dependence of resistance measured at 180 GPa. The left inset is the resistance derivative over temperature to determine the first superconducting transition temperature T_{c}, and the right inset is the enlarged view of $R(T)$ to show the second superconducting transition.

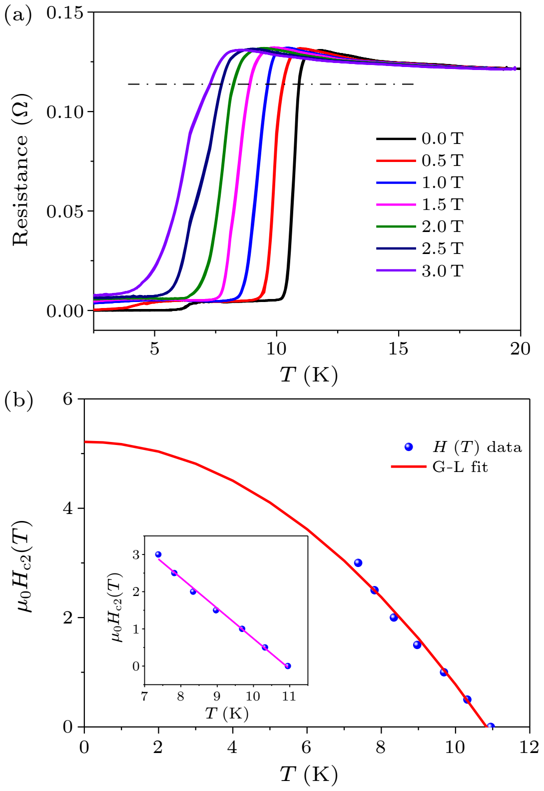

Fig. 2. The SC under magnetic field. (a) The temperature dependence of resistance measured under different magnetic field. The dashed line marks the 90% of resistance of the normal state at onset temperature. (b) The temperature dependence of upper critical magnetic field $\mu_0 H_{\mathrm{c2}}(T)$. The red line is the fitting via GL theory. The inset shows the linear fitting for the $\mu_0 H_{\mathrm{c2}}(T)$ data.

The superconductivity under magnetic field for the generated ytterbium polyhydride has been studied. Figure 2(a) shows the resistance measured under magnetic field (H) at 180 GPa. Both the two superconducting transitions are gradually suppressed by H. It is noted that the second transition is completely suppressed at $H = 1\,\mathrm{T}$, leading to a nonzero resistance at low temperature. The small resistance drop corresponding to the second transition implies that the fist superconducting transition should be the major phase of the sample. For the first superconducting transition, the dashed line in Fig. 2(a) marks the 90% of normal state resistance at onset temperature. The $T_c^{90\%}$ value can be determined by the cross between the dashed line and the resistance curve. The data of magnetic field versus temperature are plotted in Fig. 2(b), from which the upper critical field at zero temperature $\mu_0 H_{c2}(0)$ can be estimated. The inset shows the linear curve of $\mu_0 H(T)$, and a linear fitting leads to a slope of $\mathrm{d}H_{c2}/\mathrm{d}T|_{T_c}$ about $-0.81\,\mathrm{T/K}$. By using the obtained slope value and $T_c^{90\%} = 11\,\mathrm{K}$, the $\mu_0 H_{c2}(0)$ value controlled by orbital deparing mechanism in a dirty limit $[\mu_0 H_{c2}^{\mathrm{Orb}}(0)]$ can be calculated to be about 6 T from the Werthamer-Helfand-Hohenberg (WHH) formula of $\mu_0 H_{c2}(T) = -0.69 \times \mathrm{d}H_{c2}/\mathrm{d}T|_{T_c} \times T_c$. In addition, the $\mu_0 H_{c2}(0)$ value can also be estimated by the Ginzburg Landau (GL) formula of $\mu_0 H_{c2}(T) = \mu_0 H_{c2}(0) \times [1-(T/T_c)^2]$. By using the GL formula to make a fit for the $\mu_0 H(T)$ data, the $\mu_0 H_{c2}^{\mathrm{GL}}(0)$ is obtained to be about 5 T, which is slightly smaller than $\mu_0 H_{c2}^{\mathrm{Orb}}(0)$. The GL coherence length can be calculated to be $\xi = 81\,\text{Å}$ from the formula $\mu_0 H_{c2}(0) = \Phi_0/2\pi\xi^2$, where $\Phi_0 = 2.067 \times 10^{-15}$ Web is the magnetic flux quantum.

To check the superconducting phase, *in-situ* high pressure XRD experiments have been performed on a new sample under 190 GPa, of which the synthesis conditions are similar to that of the sample for resistance measurements. Figure 3(a) displays the typical XRD pattern, from which the peaks from the gasket of Re can be easily identified, and the majority of the remainder peaks can be indexed by a cubic lattice with $a = 5.3265\,\text{Å}$ with the space group of $Pm\bar{3}n$. The lattice constant is comparable with that of $Pm\bar{3}n$-$\mathrm{Lu_4H_{23}}$ at 185 GPa. Thus, the structure of $\mathrm{Lu_4H_{23}}$ was used as an initial mode to carry out the refinement for the XRD data of ytterbium polyhydride by using the Rietveld method,[23] where the contribution to the diffraction from hydrogen atoms is ignored. The refinement smoothly converges with $R_{\mathrm{wp}} = 9.8\%$ and $R_{\mathrm{p}} = 6.9\%$, which suggests that the initial structural model is reasonable and the observed ytterbium polyhydride should be $\mathrm{Yb_4H_{23}}$. Therefore, it is proposed that observed SC should arise from $\mathrm{Yb_4H_{23}}$. The crystal structure of $\mathrm{Yb_4H_{23}}$ is sketched as shown in Fig. 3(b). where the Wyckoff positions of hydrogen atoms in $\mathrm{Eu_4H_{23}}$ are used.[38] In the structure of $\mathrm{Yb_4H_{23}}$, there are two kinds of hydrogen cages: $\mathrm{H_{20}}$ and $\mathrm{H_{24}}$ cages with the central Yb atoms located at $\mathrm{Yb_1}$ (0, 0, 0) and $\mathrm{Yb_2}$ (0.25, 0, 0.5) sites, respectively. The H–H bond length in $\mathrm{Yb_4H_{23}}$ ranges from 1.208 Å to 1.275 Å at 190 GPa and is comparable to that in typical high T_c superconducting polyhydrides.[5,9,10,12]

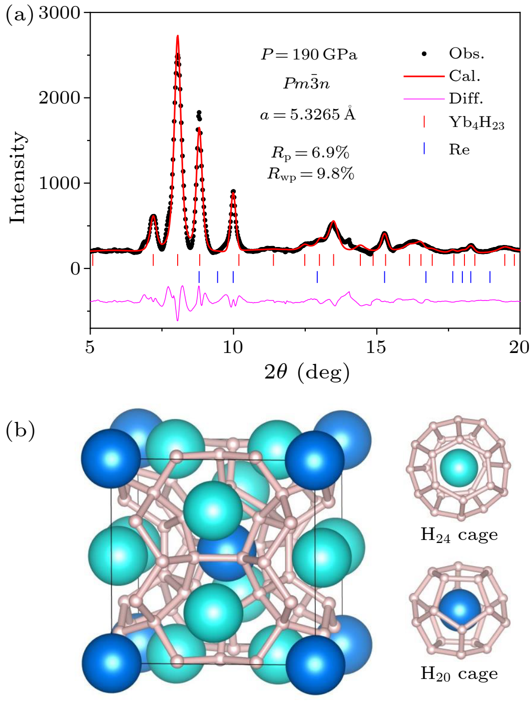

Fig. 3. (a) The X ray diffraction pattern collected under 190 GPa and the refinement. (b) The sketch of the crystal structure of $Pm\bar{3}n$-$\mathrm{Yb_4H_{23}}$ and the $\mathrm{H_{20}}$ and $\mathrm{H_{24}}$ cages.

Following the discovery of $\mathrm{Lu_4H_{23}}$,[23] $\mathrm{Eu_4H_{23}}$,[38] $\mathrm{La_4H_{23}}$[39] and $\mathrm{Y_4H_{23}}$,[40] $\mathrm{Yb_4H_{23}}$ is another example experimentally reported polyhydride with such a stoichiometry. $\mathrm{La_4H_{23}}$ and $\mathrm{Y_4H_{23}}$ have not been experimentally reported to host high T_c SC although they were highly expected.[39] For $\mathrm{Eu_4H_{23}}$, it was suggested to have a ferromagnetic ground state due to the local moment.[38] In our previous work, $\mathrm{Lu_4H_{23}}$ was found to be superconducting with $T_c \sim 70\,\mathrm{K}$ at 218 GPa.[23] Here, the T_c of $\mathrm{Yb_4H_{23}}$ is 11.5 K, much lower than $\mathrm{Lu_4H_{23}}$. Generally, magnetic moment tends to form a magnetic state and is considered to be against SC. For the hydride of $\mathrm{LaH_{10}}$ without f electron, it has a high T_c above 250 K, while the T_c value dramatically drops to 9 K in $\mathrm{PrH_9}$ because of the existence of magnetic moment from local f electrons.[30] Yb has a full filled 4f shell at ambient pressure and is a non-magnetic metal with a $\mathrm{4f^{14}5d^06s^2}$ configuration. By applying pressure the f electron would transfer to 5d orbital, and it has been revealed that at 125 GPa such an electron transfer leads to a mixed configurations of $\mathrm{4f^{14}5d^06s^2}$ and $\mathrm{4f^{13}5d^16s^2}$ by high pressure X-ray absorption experiments.[32] That is for Yb metal magnetic moment would be induced by pressure, which might explain why $\mathrm{Yb_4H_{23}}$ has a very low T_c value relative to $\mathrm{Lu_4H_{23}}$.

Conclusion. In summary, ytterbium polyhydride has been successfully synthesized at Megabar pressure and found to host SC with $T_c = 11.5\,\mathrm{K}$ at 180 GPa. The $\mu_0 H_{c2}(0)$ was estimated to be $\sim 5\,\mathrm{T}$. The result of *in-situ* high pressure X-ray experiments reveals that the SC might arise from $Pm\bar{3}n$-$\mathrm{Yb_4H_{23}}$ phase. It is suggested that the very low T_c in $\mathrm{Yb_4H_{23}}$ should be closely related with the appearance of local magnetic moment in Yb induced by pressure.

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References

[1] Ashcroft N W 1968 *Phys. Rev. Lett.* **21** 1748

[2] McMahon J M, Morales M A, Pierleoni C, and Ceperley D M 2012 *Rev. Mod. Phys.* **84** 1607

[3] Xu J A and Zhu Z W 1977 *Physics* **6** 296 (in Chinese)

[4] Ashcroft N W 2004 *Phys. Rev. Lett.* **92** 187002

[5] Duan D F, Liu Y X, Tian F B, Li D, Huang X L, Zhao Z L, Yu H Y, Liu B B, Tian W J, and Cui T 2014 *Sci. Rep.* **4** 6968

[6] Li Y W, Hao J, Liu H Y, Li Y L, and Ma Y M 2014 *J. Chem. Phys.* **140** 174712

[7] Drozdov A P, Eremets M I, Troyan I A, Ksenofontov V, and Shylin S I 2015 *Nature* **525** 73

[8] Flores-Livas J A, Boeri L, Sanna A, Profeta G, Arita R, and Eremets M 2020 *Phys. Rep.* **856** 1

[9] Semenok D V, Kruglov I A, Savkin I A, Kvashnin A G, and Oganov A R 2020 *Curr. Opin. Solid St. M* **24** 100808

[10] Wang H, Tse J S, Tanaka K, Iitaka T, and Ma Y M 2012 *Proc. Natl. Acad. Sci. U. S. A.* **109** 6463

[11] Liu H Y, Naumov I I, Hoffmann R, Ashcroft N W, and Hemley R J 2017 *Proc. Natl. Acad. Sci. U. S. A.* **114** 6990

[12] Peng F, Sun Y, Pickard C J, Needs R J, Wu Q, and Ma Y M 2017 *Phys. Rev. Lett.* **119** 107001

[13] Drozdov A P, Kong P P, Minkov V S, Besedin S P, Kuzovnikov M A, Mozaffari S, Balicas L, Balakirev F F, Graf D E, Prakapenka V B, Greenberg E, Knyazev D A, Tkacz M, and Eremets M I 2019 *Nature* **569** 528

[14] Somayazulu M, Ahart M, Mishra A K, Geballe Z M, Baldini M, Meng Y, Struzhkin V V, and Hemley R J 2019 *Phys. Rev. Lett.* **122** 027001

[15] Hong F, Yang L X, Shan P F, Yang P T, Liu Z Y, Sun J P, Yin Y Y, Yu X H, Cheng J G, and Zhao Z X 2020 *Chin. Phys. Lett.* **37** 107401

[16] Geballe Z M, Liu H Y, Mishra A K, Ahart M, Somayazulu M, Meng Y, Baldini M, and Hemley R J 2018 *Angew. Chem. Int. Edit* **57** 688

[17] Kong P P, Minkov V S, Kuzovnikov M A, Drozdov A P, Besedin S P, Mozaffari S, Balicas L, Balakirev F F, Prakapenka V B, Chariton S, Knyazev D A, Greenberg E, and Eremets M I 2021 *Nat. Commun.* **12** 5075

[18] Li Z W, He X, Zhang C L, Wang X C, Zhang S J, Jia Y T, Feng S M, Lu K, Zhao J F, Zhang J, Min B S, Long Y W, Yu R C, Wang L H, Ye M Y, Zhang Z S, Prakapenka V, Chariton S, Ginsberg P A, Bass J, Yuan S H, Liu H Z, and Jin C Q 2022 *Nat. Commun.* **13** 2863

[19] Ma L, Wang K, Xie Y, Yang X, Wang Y Y, Zhou M, Liu H Y, Yu X H, Zhao Y S, Wang H B, Liu G T, and Ma Y M 2022 *Phys. Rev. Lett.* **128** 167001

[20] Semenok D V, Kvashnin A G, Ivanova A G, Svitlyk V, Fominski V Y, Sadakov A V, Sobolevskiy O A, Pudalov V M, Troyan I A, and Oganov A R 2020 *Materials Today* **33** 36

[21] Salke N P, Davari Esfahani M M, Zhang Y, Kruglov I A, Zhou J, Wang Y, Greenberg E, Prakapenka V B, Liu J, Oganov A R, and Lin J F 2019 *Nat. Commun.* **10** 4453

[22] Hong F, Shan P F, Yang L X, Yue B B, Yang P T, Liu Z Y, Sun J P, Dai J H, Yu H, Yin Y Y, Yu X H, Cheng J G, and Zhao Z X 2022 *Mater Today Phys.* **22** 100596

[23] Li Z W, He X, Zhang C L, Lu K, Min B S, Zhang J, Zhang S J, Zhao J F, Shi L C, Peng Y, Feng S M, Deng Z, Song J, Liu Q Q, Wang X C, Yu R C, Wang L H, Li Y Z, Bass J D, Prakapenka V, Chariton S, Liu H Z, and Jin C Q 2023 *Science China-Physics Mechanics & Astronomy* **66** 267411

[24] Zhang C L, He X, Li Z W, Zhang S J, Feng S M, Wang X C, Yu R C, and Jin C Q 2022 *Sci. Bull.* **67** 907

[25] Zhang C L, He X, Li Z W, Zhang S J, Min B S, Zhang J, Lu K, Zhao J F, Shi L C, Peng Y, Wang X C, Feng S M, Yu R C, Wang L H, Prakapenka V B, Chariton S, Liu H Z, and Jin C Q 2022 *Mater. Today Phys.* **27** 100826

[26] He X, Zhang C L, Li Z W, Zhang S J, Min B S, Zhang J, Lu K, Zhao J F, Shi L C, Peng Y, Wang X C, Feng S M, Song J, Wang L H, Prakapenka V B, Chariton S, Liu H Z, and Jin C Q 2023 *Chin. Phys. Lett.* **40** 057404

[27] He X, Zhang C L, Li Z W, Lu K, Zhang S J, Min B S, Zhang J, Shi L C, Feng S M, Liu Q Q, Song J, Wang X C, Peng Y, Wang L H, Prakapenka V B, Chariton S, Liu H Z, and Jin C Q 2024 *Mater. Today Phys.* **40** 101298

[28] Lu K, He X, Zhang C L, Li Z W, Zhang S J, Min B S, Zhang J, Zhao J F, Shi L C, Peng Y, Feng S M, Liu Q Q, Song J, Yu R C, Wang X C, Wang Y, Bykov M, and Jin C Q 2024 *Natl. Sci. Rev.* **11** nwad241

[29] Chen W H, Semenok D V, Huang X L, Shu H Y, Li X, Duan D F, Cui T, and Oganov A R 2021 *Phys. Rev. Lett.* **127** 117001

[30] Zhou D, Semenok D, Duan D F, Xie H, Huang X L, Chen W H, Li X, Liu B B, Oganov A R, and Cui T 2020 *Sci. Adv.* **6** eaax6849

[31] Zhou D, Semenok D V, Xie H, Huang X, Duan D, Aperis A, Oppeneer P M, Galasso M, Kartsev A I, Kvashnin A G, Oganov A R, and Cui T 2020 *J. Am. Chem. Soc.* **142** 2803

[32] Song J, Fabbris G, Bi W, Haskel D, and Schilling J S 2018 *Phys. Rev. Lett.* **121** 037004

[33] Song H, Zhang Z, Cui T, Pickard C J, Kresin V Z, and Duan D 2021 *Chin. Phys. Lett.* **38** 107401

[34] Sun W, Kuang X, Keen H D J, Lu C, and Hermann A 2020 *Phys. Rev. B* **102** 144524

[35] Jia Y T, He X, Feng S M, Zhang S J, Zhang C L, Ren C W, Wang X C, and Jin C Q 2020 *Crystals* **10** 1116

[36] Zhang J L, Zhang S J, Weng H M, Zhang W, Yang L X, Liu Q Q, Feng S M, Wang X C, Yu R C, Cao L Z, Wang L, Yang W G, Liu H Z, Zhao W Y, Zhang S C, Dai X, Fang Z, and Jin C Q 2011 *Proc. Natl. Acad. Sci. U. S. A.* **108** 24

[37] Zhang S J, Wang X C, Sammynaiken R, Tse J S, Yang L X, Li Z, Liu Q Q, Desgreniers S, Yao Y, Liu H Z, and Jin C Q 2009 *Phys. Rev. B* **80** 014506

[38] Semenok D V, Zhou D, Kvashnin A G, Huang X, Galasso M, Kruglov I A, Ivanova A G, Gavriliuk A G, Chen W, Tkachenko N V, Boldyrev A I, Troyan I, Oganov A R, and Cui T 2020 *J. Phys. Chem. Lett.* **12** 32

[39] Laniel D, Trybel F, Winkler B, Knoop F, Fedotenko T, Khandarkhaeva S, Aslandukova A, Meier T, Chariton S, Glazyrin K, Milman V, Prakapenka V, Abrikosov I A, Dubrovinsky L, and Dubrovinskaia N 2022 *Nat. Commun.* **13** 6987

[40] Aslandukova A, Aslandukov A, Laniel D, Yin Y Q, Akbar F I, Bykov M, Fedotenko T, Glazyrin K, Pakhomova A, Garbarino G, Bright E L, Wright J, Hanfland M, Chariton S, Prakapenka V, Dubrovinskaia N, and Dubrovinsky L 2024 *Sci. Adv.* **10** eadl5416