SUPPLEMENTARY INFORMATION

Predicted hot superconductivity in $LaSc_2H_{24}$ under pressure

Xin-Ling He[a,b,c,1], Wenbo Zhao[a,c,1], Yu Xie[a,c], Andreas Hermann[d], Russell J. Hemley[e,f,g], Hanyu Liu[a,c,h,2], and Yanming Ma[a,c,h]

[a]Key Laboratory of Material Simulation Methods and Software of Ministry of Education, College of Physics, Jilin University, Changchun 130012, China
[b]Institute of Physics, Henan Academy of Sciences, Zhengzhou, 450046, China
[c]State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun 130012, China
[d]Centre for Science at Extreme Conditions and Scottish Universities Physics Alliance, School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom
[e]Department of Physics, University of Illinois Chicago, Chicago, IL 60607
[f]Department of Chemistry, University of Illinois Chicago, Chicago, IL 60607
[g]Department of Earth and Environmental Sciences, University of Illinois Chicago, Chicago, IL60607
[h]International Center of Future Science, Jilin University, Changchun 130012, China

[1]X.H. and W.Z. contributed equally to this work.
[2]To whom correspondence may be addressed. Email: hanyuliu@jlu.edu.cn.

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Tables S1 and S2

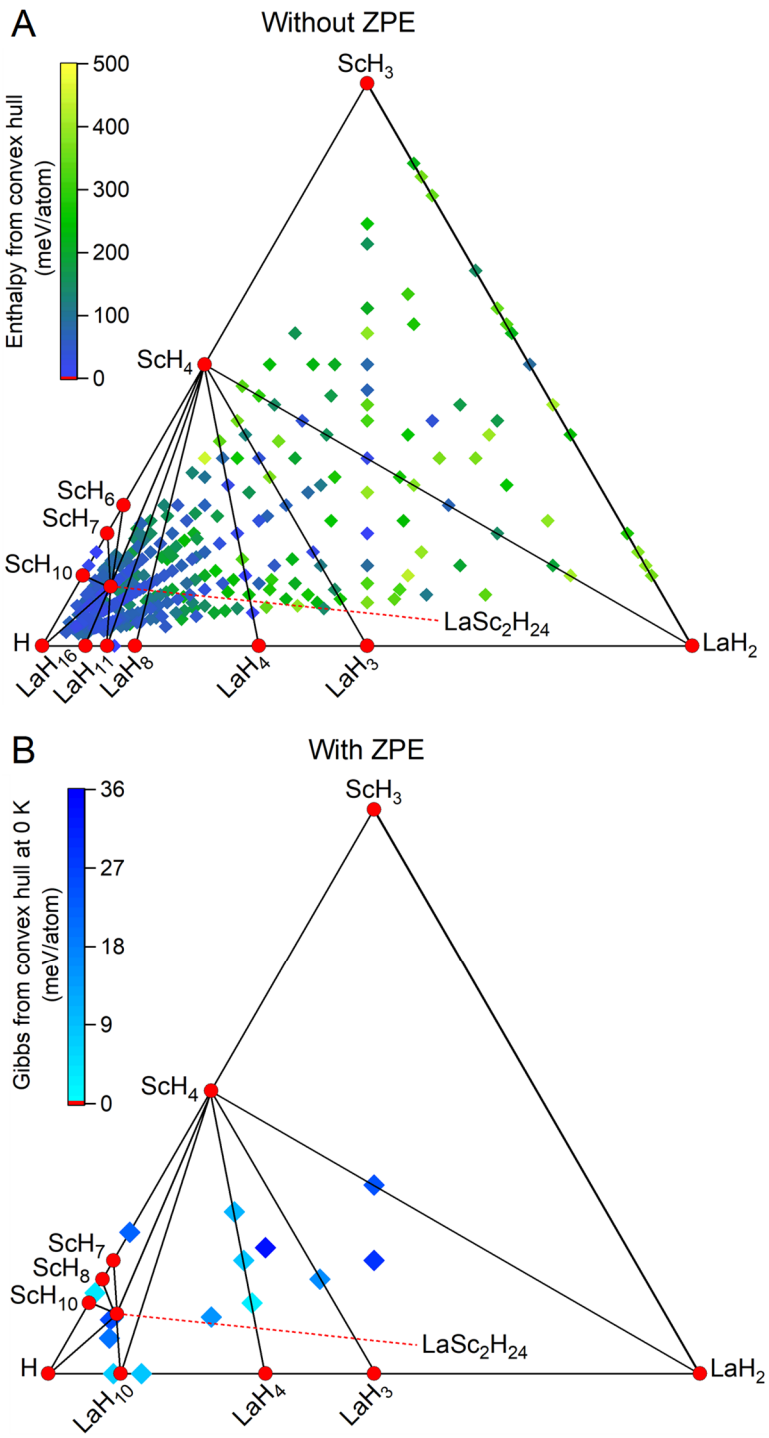

Fig. S1. For clarity, we replotted the ternary phase diagram of La-Sc-H system with LaH_2, ScH_3, and H as corners (*A*) without and (*B*) with inclusion of considering zero-point energy (ZPE) within the harmonic approximation at 300 GPa. Red solid circles and colored squares indicate thermodynamically stable and unstable phases, respectively.

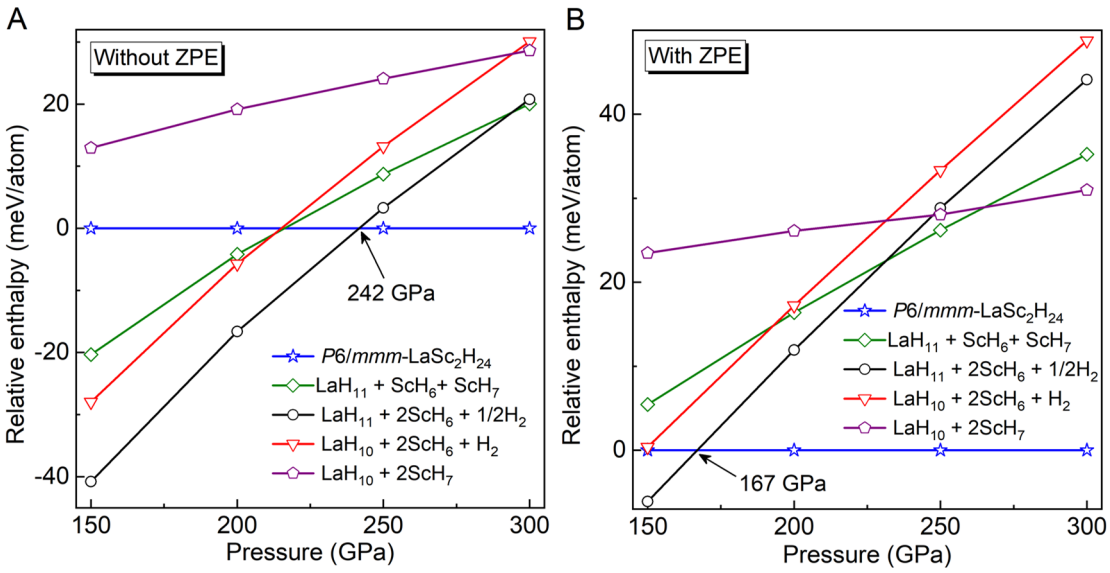

Fig. S2. (*A*) The enthalpy comparison between $LaSc_2H_{24}$ and selected decomposition routes under different pressure without considering zero-point energy (ZPE), in which the enthalpy of $LaSc_2H_{24}$ at each pressure is set to zero. (*B*) Calculated relative enthalpies as a function of pressure with considering ZPE at the anharmonic level by using the stochastic self-consistent harmonic approximation (SSCHA) approach.

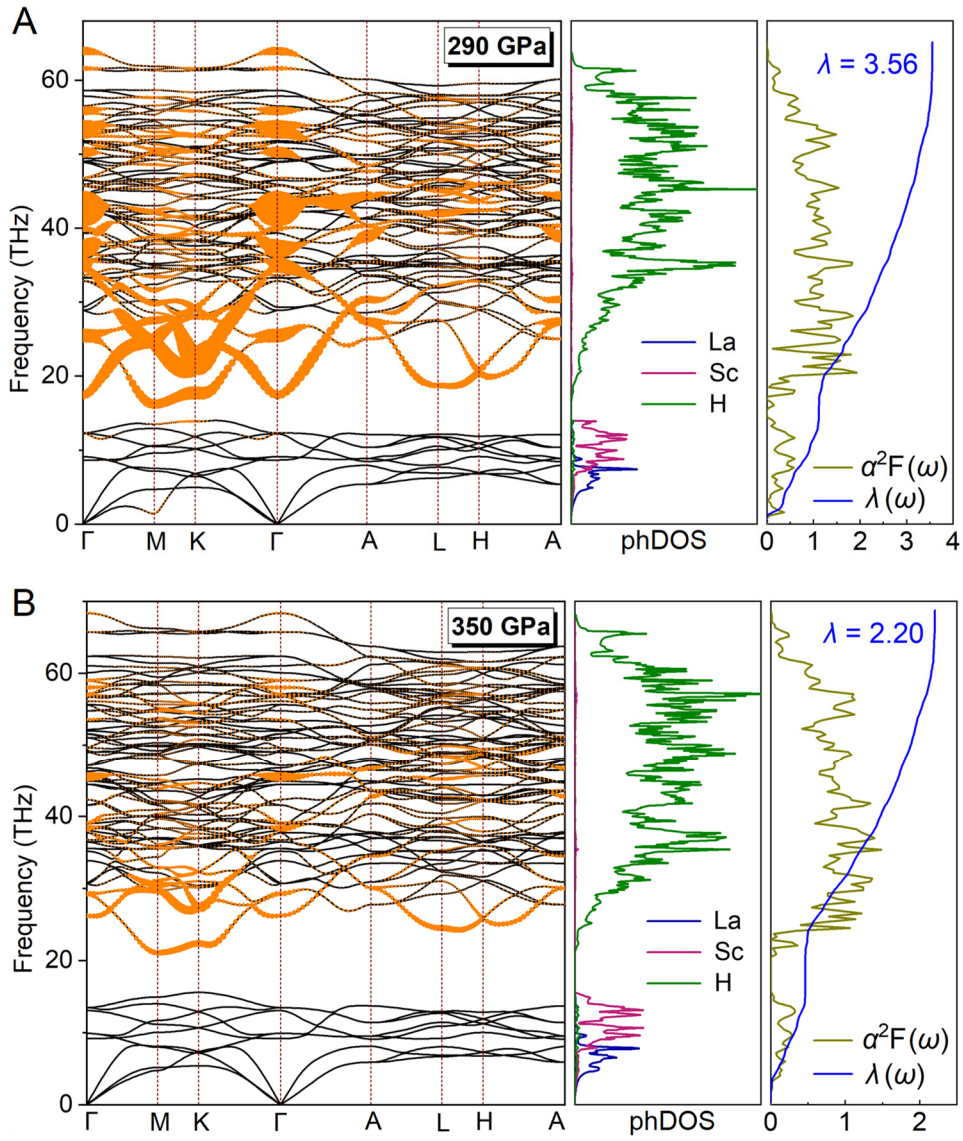

Fig. S3. Harmonic phonon spectra, where orange solid circles show the phonon linewidth with a radius proportional to its strength (left), projected phonon density of states (phDOS) (middle), Eliashberg spectral function $\alpha^2F(\omega)$, and the electron-phonon integral $\lambda(\omega)$ (right) of $LaSc_2H_{24}$ at (*A*) 290 GPa and (*B*) 350 GPa.

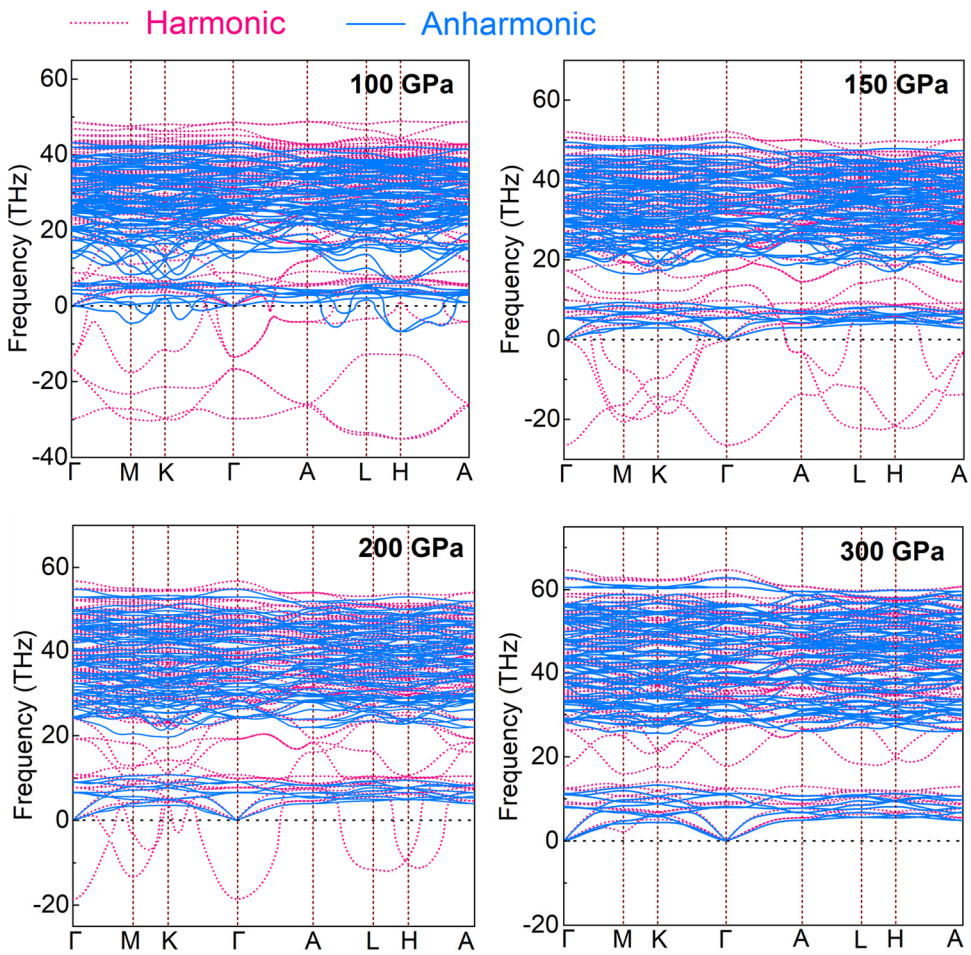

Fig. S4. Phonon spectra of $LaSc_2H_{24}$ at different pressures both at the harmonic and anharmonic levels. The area under the black dotted line marks the region with imaginary phonon frequencies, which are depicted as negative frequencies.

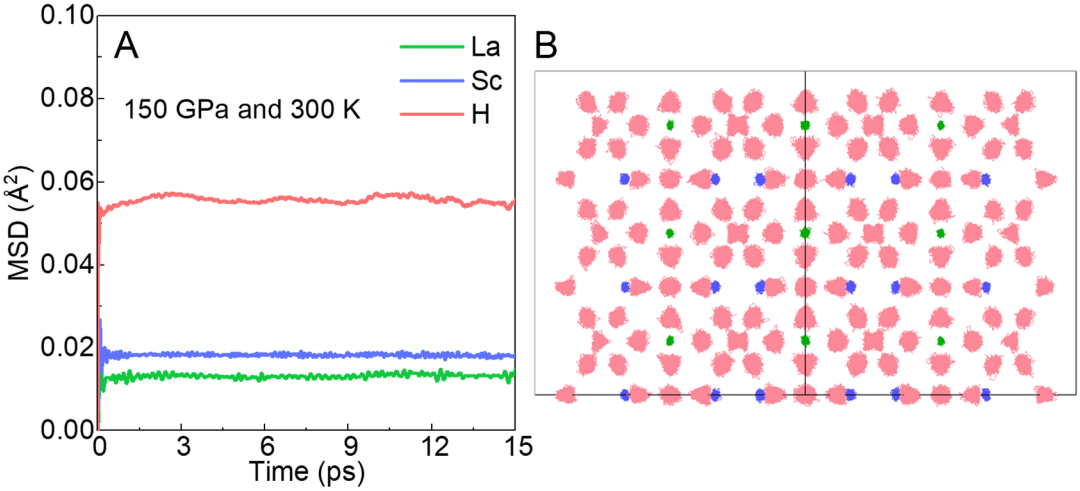

Fig. S5. (*A*) The mean square displacements (MSDs) from ab initio molecular dynamics (AIMD) simulations for the La, Sc and H atoms in $LaSc_2H_{24}$ at 150 GPa and 300 K. (*B*) The projection of atomic trajectories along the [110] direction in $LaSc_2H_{24}$ from the last 15 ps, in which green, blue and pink symbols represent the atomic trajectories of La, Sc and H atoms, respectively.

As shown in Fig. S5, the oscillations of the La, Sc and H atoms with respect to their equilibrium positions indicate that $LaSc_2H_{24}$ is stable at 150 GPa and 300 K, hence it maintains a solid phase without any change. Accordingly, our calculated results show that the stability of our predicted structure is robust.

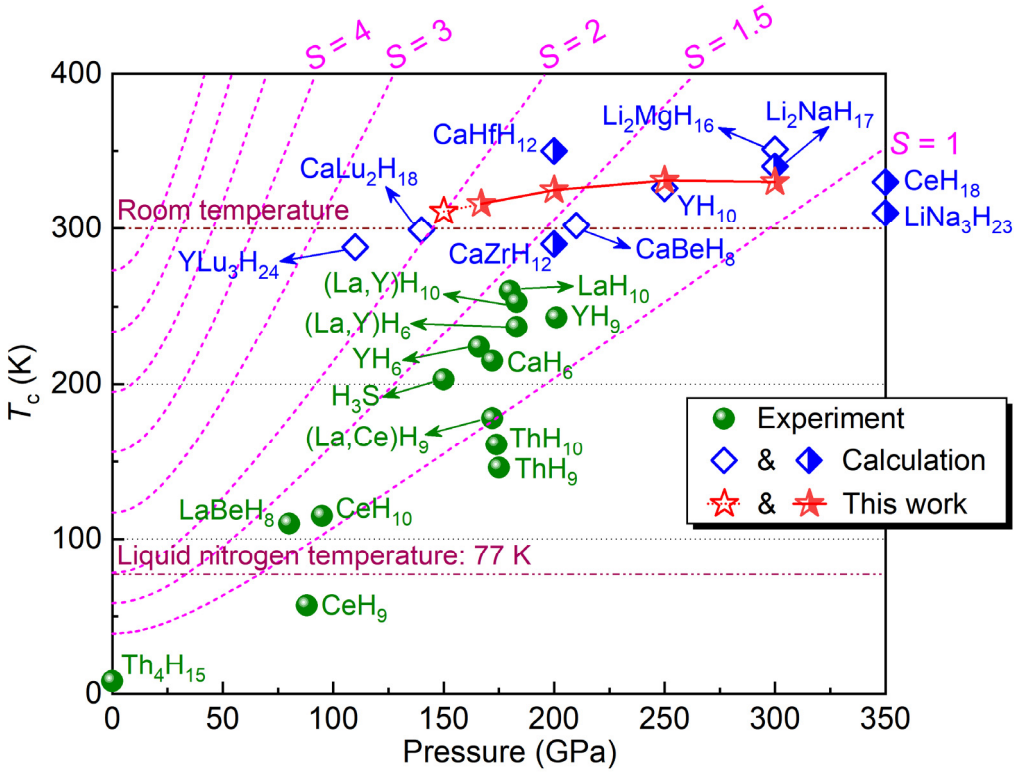

Fig. S6. Pressure dependence of T_c values for typical superconductors. The green filled circles represent the T_c values of well-known superconductors from experiments (1-17). The blue half-filled (unfilled) rhombuses represent the T_c values of the predicted thermodynamically stable (metastable) hydrides (18-25). The red half-filled (unfilled) stars mark the T_c values (with μ^* of 0.1) of the thermodynamically stable (metastable) $LaSc_2H_{24}$ by considering anharmonic effects within a pressure range of 150-300 GPa. The carmine dashed lines are plotted according to the figure of merit $S = (T_c/\sqrt{P^2 + T_{c,MgB_2}^2})$ used to evaluate the significance of a particular superconductor (26).

Table S1. The calculated crystal structural parameters of thermodynamically stable La-Sc and La-Sc-H compounds at 300 GPa.

Compound	Space group	Lattice Parameters (Å, degree)	Atomic coordinates (fractional)			
			Atoms	X	Y	Z
$LaSc_2$	*Fddd*	a = 4.248	La (8b)	0.000	0.000	0.500
		b = 6.845	Sc (16f)	0.000	0.843	0.000
		c = 7.682				
		α = 90				
		β = 90				
		γ = 90				
$LaSc_2H_{24}$	*P*6/*mmm*	a = 4.712	La (1b)	0.000	0.000	0.500
		b = 4.712	Sc (2c)	0.333	0.667	0.000
		c = 3.236	H (6m)	0.759	0.519	0.500
		α = 90	H (6j)	0.762	0.000	0.000
		β = 90	H (12n)	0.614	0.000	0.289
		γ = 120				

Table S2. Calculated structural parameters and H-H bond lengths of the *P6*/*mmm*-$LaSc_2H_{24}$ within the harmonic and annarmonic approximation at different pressures.

Calculation	Pressure (GPa)	Lattice Parameters (Å)		H-H distance (Å)
		$a = b$	c	
Harmonic	290	4.751	3.229	1.068-1.209
	300	4.735	3.216	1.076-1.204
	350	4.659	3.157	1.053-1.183
Anharmonic	150	5.084	3.528	1.156-1.307
	167	5.033	3.490	1.147-1.293
	200	4.943	3.425	1.133-1.268
	250	4.831	3.341	1.113-1.237
	300	4.741	3.271	1.096-1.212

References

1. A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, S. I. Shylin, Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system, *Nature* **525**, 73-76 (2015).
2. M. Einaga *et al*., Crystal structure of the superconducting phase of sulfur hydride, *Nat. Phys.* **12**, 835-838 (2016).
3. L. Ma *et al*., High-temperature superconducting phase in clathrate calcium hydride CaH_6 up to 215 K at a pressure of 172 GPa, *Phys. Rev. Lett.* **128**, 167001 (2022).
4. Z. Li *et al*., Superconductivity above 200 K discovered in superhydrides of calcium, *Nat. Commun.* **13**, 2863 (2022).
5. I. A. Troyan *et al*., Anomalous high-temperature superconductivity in YH_6, *Adv. Mater.* **33**, 2006832 (2021).
6. P. Kong *et al*., Superconductivity up to 243 K in the yttrium-hydrogen system under high pressure, *Nat. Commun.* **12**, 5075 (2021).
7. E. Snider *et al*., Synthesis of yttrium superhydride superconductor with a transition temperature up to 262 K by catalytic hydrogenation at high pressures, *Phys. Rev. Lett.* **126**, 117003 (2021).
8. M. Somayazulu *et al*., Evidence for superconductivity above 260 K in lanthanum superhydride at megabar pressures, *Phys. Rev. Lett.* **122**, 027001 (2019).
9. A. P. Drozdov *et al*., Superconductivity at 250 K in lanthanum hydride under high pressures, *Nature* **569**, 528-531 (2019).
10. F. Hong *et al*., Superconductivity of lanthanum superhydride investigated using the standard four-probe configuration under high pressures, *Chin. Phys. Lett.* **37**, 107401 (2020).
11. J. A. Flores-Livas *et al*., A perspective on conventional high-temperature superconductors at high pressure: methods and materials, *Phys. Rep*. **856**, 1-78 (2020).
12. L. Boeri *et al*., The 2021 room-temperature superconductivity roadmap, *J. Phys.: Condens. Matter* **34** 183002 (2022).
13. K. P. Hilleke, E. Zurek, Tuning chemical precompression: theoretical design and crystal chemistry of novel hydrides in the quest for warm and light superconductivity at ambient pressures, *J. Appl. Phys*. **131**, 070901 (2022).
14. Y. Song *et al*., Stoichiometric ternary superhydride $LaBeH_8$ as a new template for high-temperature superconductivity at 110 K under 80 GPa, *Phys. Rev. Lett.* **130**, 266001 (2023).
15. D. V. Semenok *et al*., Superconductivity at 253 K in lanthanum-yttrium ternary hydrides, *Mater. Today* **48**, 18-28 (2021).
16. J. Bi *et al*., Giant enhancement of superconducting critical temperature in substitutional alloy $(La,Ce)H_9$, *Nat. Commun*. **13**, 5952 (2022).
17. W. Chen *et al*., Enhancement of superconducting properties in the La-Ce-H system at moderate pressures, *Nat. Commun.* **14**, 2660 (2023).
18. F. Peng *et al*., Hydrogen clathrate structures in rare earth hydrides at high pressures: possible route to room-temperature superconductivity, *Phys. Rev. Lett.* **119**,

107001 (2017).
19. H. Liu, I. I. Naumov, R. Hoffmann, N. W. Ashcroft, R. J. Hemley, Potential high-T_c superconducting lanthanum and yttrium hydrides at high pressure, *Proc. Natl. Acad. Sci. USA* **114**, 6990-6995 (2017).
20. D. An *et al*., Thermodynamically stable room-temperature superconductors in Li-Na hydrides under high pressures, *arXiv:*2303.09805 (2023).
21. Y. Sun, J. Lv, Y. Xie, H. Liu, Y. Ma, Route to a superconducting phase above room temperature in electron-doped hydride compounds under high pressure, *Phys. Rev. Lett.* **123**, 097001 (2019).
22. Z. Zhang *et al*., Design principles for high-temperature superconductors with a hydrogen-based alloy backbone at moderate pressure, *Phys. Rev. Lett.* **128**, 047001 (2022).
23. M. Du, H. Song, Z. Zhang, D. Duan, T. Cui, Room-temperature superconductivity in Yb/Lu substituted clathrate hexahydrides under moderate pressure, *Research* **2022**, 9784309 (2022).
24. L. Liu *et al*., Generic rules for achieving room-temperature superconductivity in ternary hydrides with clathrate structures, *Phys. Rev. B* **107**, L020504 (2023).
25. X. Zhong et al., Prediction of above-room-temperature superconductivity in lanthanide/actinide extreme superhydrides, *J. Am. Chem. Soc*. **144**, 13394-13400 (2022).
26. C. J. Pickard, I. Errea, M. I. Eremets, Superconducting hydrides under pressure, *Annu. Rev. Condens. Matter Phys.* **11**, 57-76 (2020)