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RESEARCH ARTICLE

High T_c superconductivity in layered hydrides XH_{15} (X = Ca, Sr, Y, La) under high pressures

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Supplementary Matarial

Table S1 The structural parameters of $R\bar{3}$-CaH_{14} at 140 GPa.

Lattice parameters (Å)	Atoms	x	y	z
$a = b$ = 4.88120	H	-0.28237	0.02804	-0.45709
c=5.52890	H	0.21679	0.20047	-0.70519
α=β=90°	H	-0.00000	0.00000	-0.41384
γ=120°	Ca	-0.00000	-0.00000	-1.00000

Table S2 Calculated structural parameters and Bader charge analysis of $P\bar{6}2m$-CaH_{15} at 300 GPa. The $H_{1\text{-}6}$ denotes the H atoms in H_2 units, and the $H_{7\text{-}12}$ demotes the H atoms at the edge of H_3 units, the $H_{13\text{-}15}$ denotes the H atoms at the center of H_3 units. The σ(e) represents the charge transferred from Ca to H.

Lattice parameters (Å)	Atoms	x	y	z	σ(e)
$a = b$ = 3.724	$H_{1\text{-}6}$ (6j)	0.87091	0.43463	0.00000	-0.060
c=2.468	$H_{7\text{-}12}$ (6k)	0.57106	0.73415	0.50000	-0.100
	$H_{13\text{-}15}$ (3g)	0.65438	1.00000	0.50000	-0.016
	Ca	0.00000	0.00000	0.00000	1.008

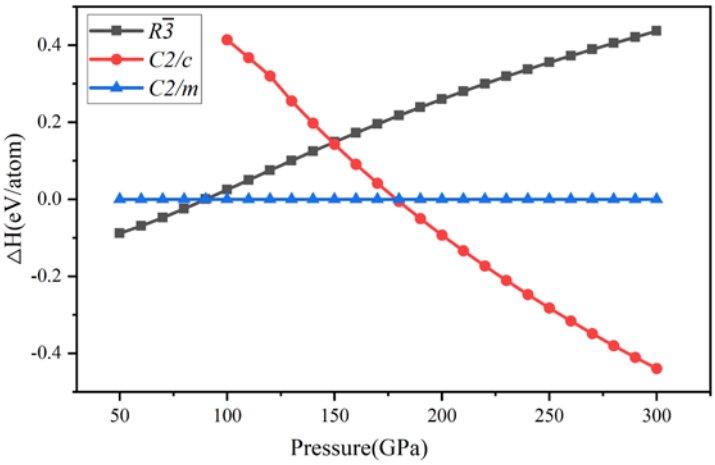

Fig. S1 Calculated enthalpy curves for $R\bar{3}$ and *C*2/*c* relative to *C*2/*m* structure as a function of pressure.

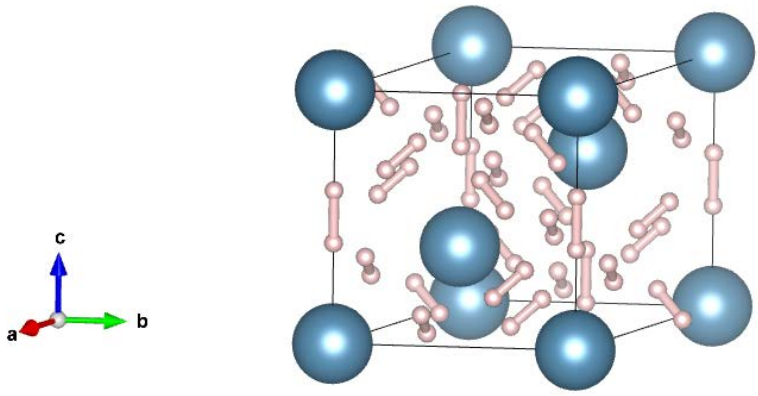

Fig. S2 The structure of $R\bar{3}$-CaH_{14} at 140 GPa containing H_2 molecular units.

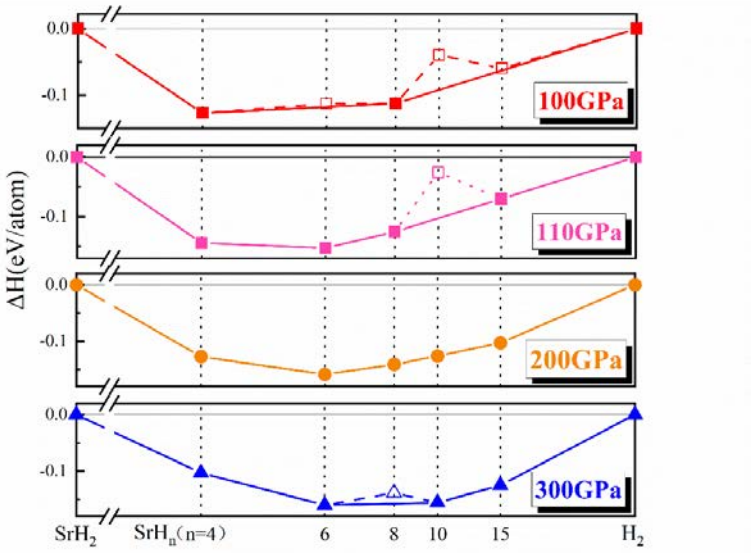

Fig. S3 The convex hull of the Sr–H system at 100, 110, 200 and 300 GPa. The stable structures of element H_2 [1] and binary SrH_n (*n*=2, 4, 6, 8, 10) compounds come from the previous studies [2].

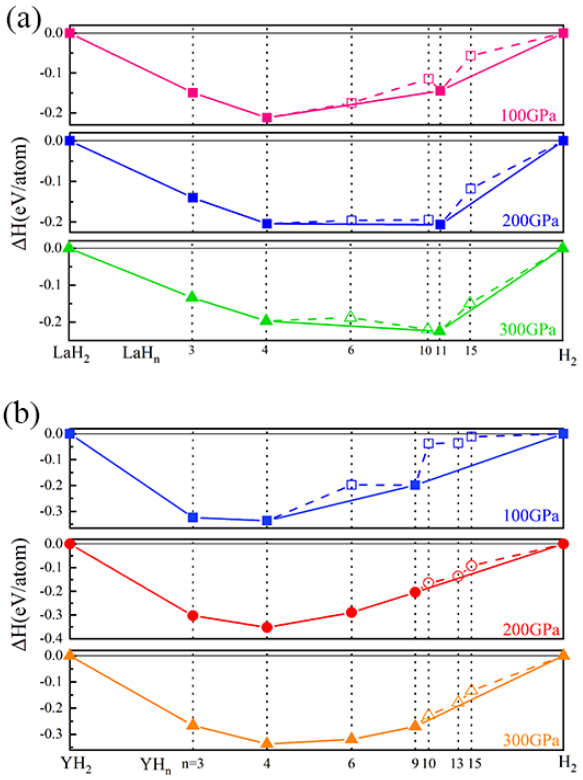

Fig. S4 The convex hull of the **(a)** Y-H and **(b)** La-H system at 100, 200, 300 GPa. The stable structures of element H_2 [1], binary YH_n (*n*=2, 3, 4, 6, 9, 10, 13) compounds [3], binary LaH_n (*n*=2, 3, 4, 6, 10, 11) compounds come from the previous studies [4].

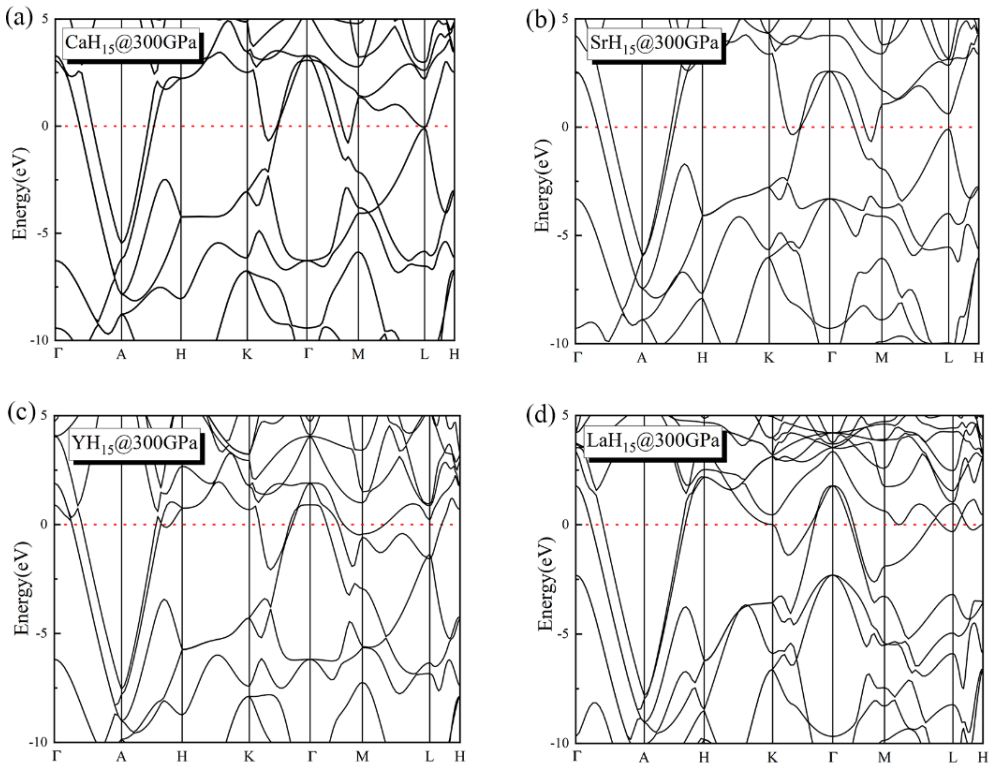

Fig. S5 Electronic band structures of **(a)** CaH_{15}, **(b)** SrH_{15}, **(c)** YH_{15} and **(d)** LaH_{15} at 300 GPa.

References

[1] C. J. Pickard and R. J. Needs, Structure of phase III of solid hydrogen, *Nature Phys.* 3(7), 473 (2007)

[2] Y. Wang, H Wang, J. Tse, T. Iitakad, and Y. Ma, Structural morphologies of high-pressure polymorphs of strontium hydrides, *Phys. Chem. Chem. Phys.* 17(29), 19379 (2015)

[3] F. Peng, Y. Sun, C. J. Pickard, R. J. Needs, Q. Wu, and Y. Ma, Hydrogen clathrate structures in rare earth hydrides at high pressures: Possible route to room-temperature superconductivity, *Phys. Rev. Lett.* 119(10), 107001 (2017)

[4] H. Liu, I. I. Naumov, R. Hoffmann, N. W. Ashcroft, and R. J. Hemley, Potential high-T_c superconducting lanthanum and yttrium hydrides at high pressure, *Proc. Natl. Acad. Sci. USA* 114(27), 6990 (2017)