Potential High-T_c Superconductivity in La and Y Hydrides

06/2017

Scientific Achievement

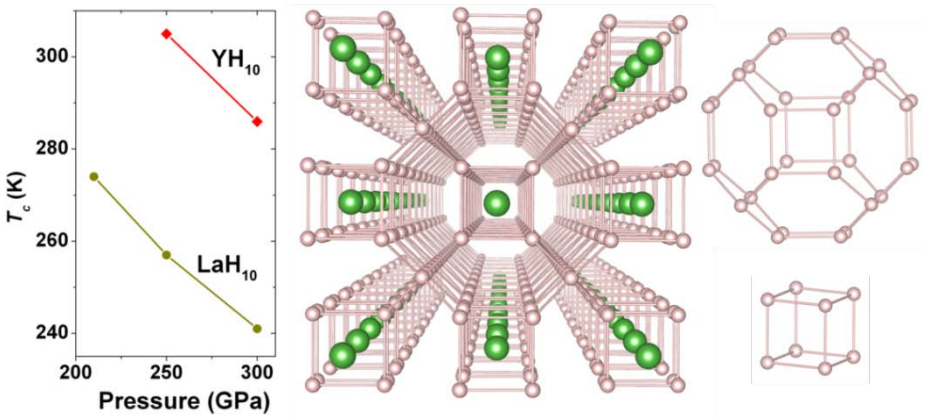
Novel hydrogen-rich lanthanum and yttrium hydride structures are predicted to exhibit superconductivity near room temperature under pressure.

Significance and Impact

First-principles calculations predict that superconductors with T_c's above 300 K could be synthesized in the La-H and Y-H systems at currently accessible laboratory pressures. The results open the prospect for the design, synthesis, and recovery of new high temperature superconductors.

Research Details

- Crystal structure prediction for La-H and Y-H systems at 150 and 300 GPa.
- First-principles calculations of energies, band structures and phonons for LaH_{10} and YaH_{10}.
- Superconducting calculations for predicted structures based on BCS theory.
- BCS calculations suggest that T_c of ~305 K for YH_{10} at 250 GPa, ~274 K for LaH_{10} at 210 GPa.



The predicted structure of LaH_{10} and YH_{10} , with the cube hydrogen units $[4^6 6^{12}]$, and calculated T_c as a function of pressure.

H. Liu, I. I. Naumov, R. Hoffmann, N. W. Ashcroft and R. J. Hemley, Potential high-Tc superconducting lanthanum and yttrium hydrides at high pressure, *Proc. Natl. Acad. Sci. USA, in press*.

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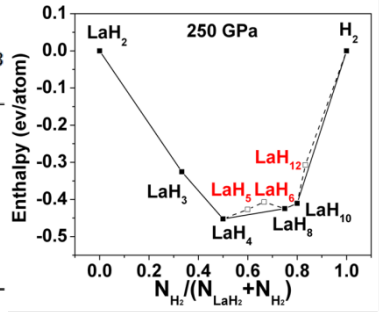
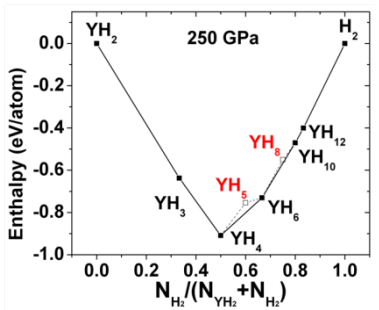
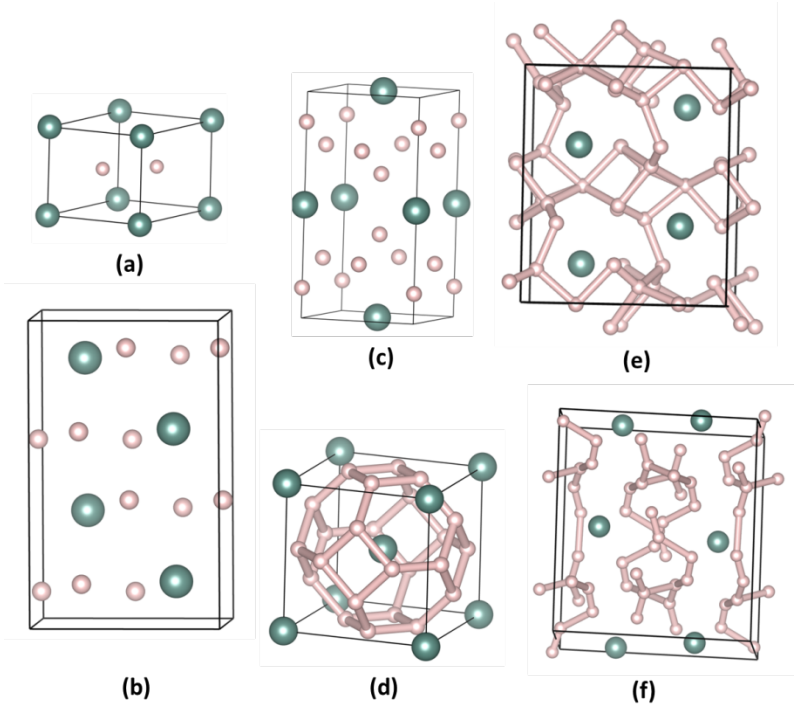
Table S1. T_c of La–H and Y–H systems at different pressures calculated using the McMillan and Eliashberg equations

Compound	Pressure, GPa	λ	ω_{log}, K	T_c, K; μ* = 0.1 McMillan	T_c, K; μ* = 0.13 McMillan	T_c, K; μ* = 0.1 Eliashberg	T_c, K; μ* = 0.13 Eliashberg
LaH_4	300	0.43	1,624	10	5	10	5
LaH_8	300	1.12	1,591	131	114	150	138
LaH_{10}	210	3.41	848	238	219	286	274
LaH_{10}	250	2.29	1,253	232	212	274	257
LaH_{10}	300	1.78	1,488	215	196	254	241
YH_{10}	250	2.58	1,282	265	244	326	305
YH_{10}	300	2.06	1,511	255	233	308	286

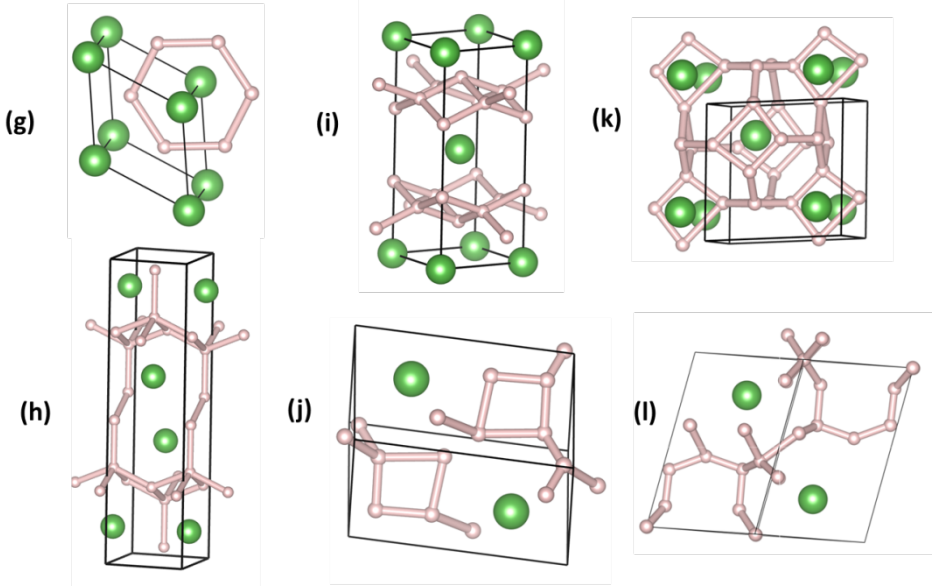




Formation enthalpy for La-H and Y-H.



(a) YH_2, (b) YH_3 (c) YH_4, (d) YH_6, (e) YH_8 and (f) YH_{12}. Large and small spheres represent Y and H atoms at 250 GPa.



(f) LaH_2, (h) LaH_3 (i) LaH_4, (j) LaH_5, (k)LaH_6 and (l) LaH_8. Large and small spheres represent La and H atoms at 250 GPa.