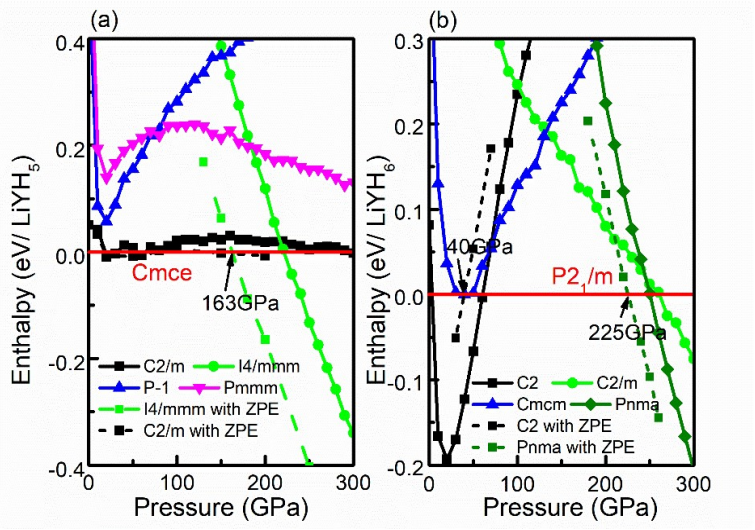
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Material of Predicted Structures and Superconductivity of $LiYH_n$ (n=5-10) under High Pressures

Huan Li[1,2], Tao Gao[1,], Shiyin Ma[1], Xiaoqiu Ye[2,*]*

[1]Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

[2]Science and Technology on Surface Physics and Chemistry Laboratory, Jiangyou, 621908, China



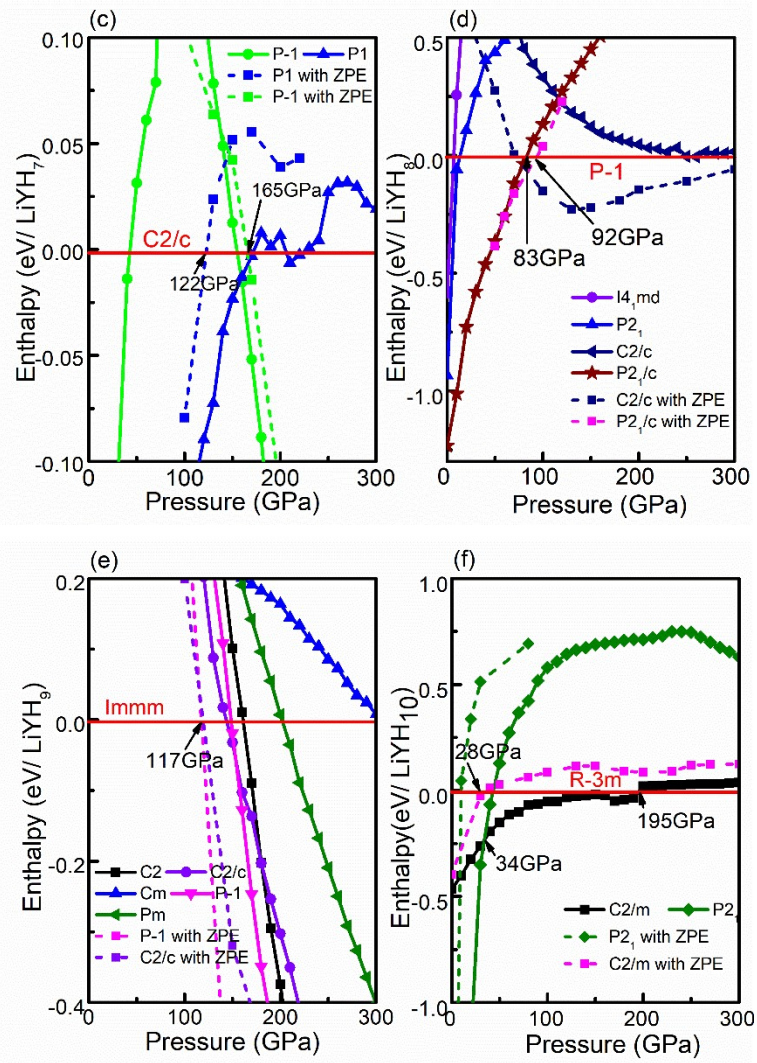


Fig. S1. Ground-state static enthalpy curves per formula units as a function of pressure for $LiYH_n$ (n=5-10) after the correction of zero point energy (ZPE) was considered.

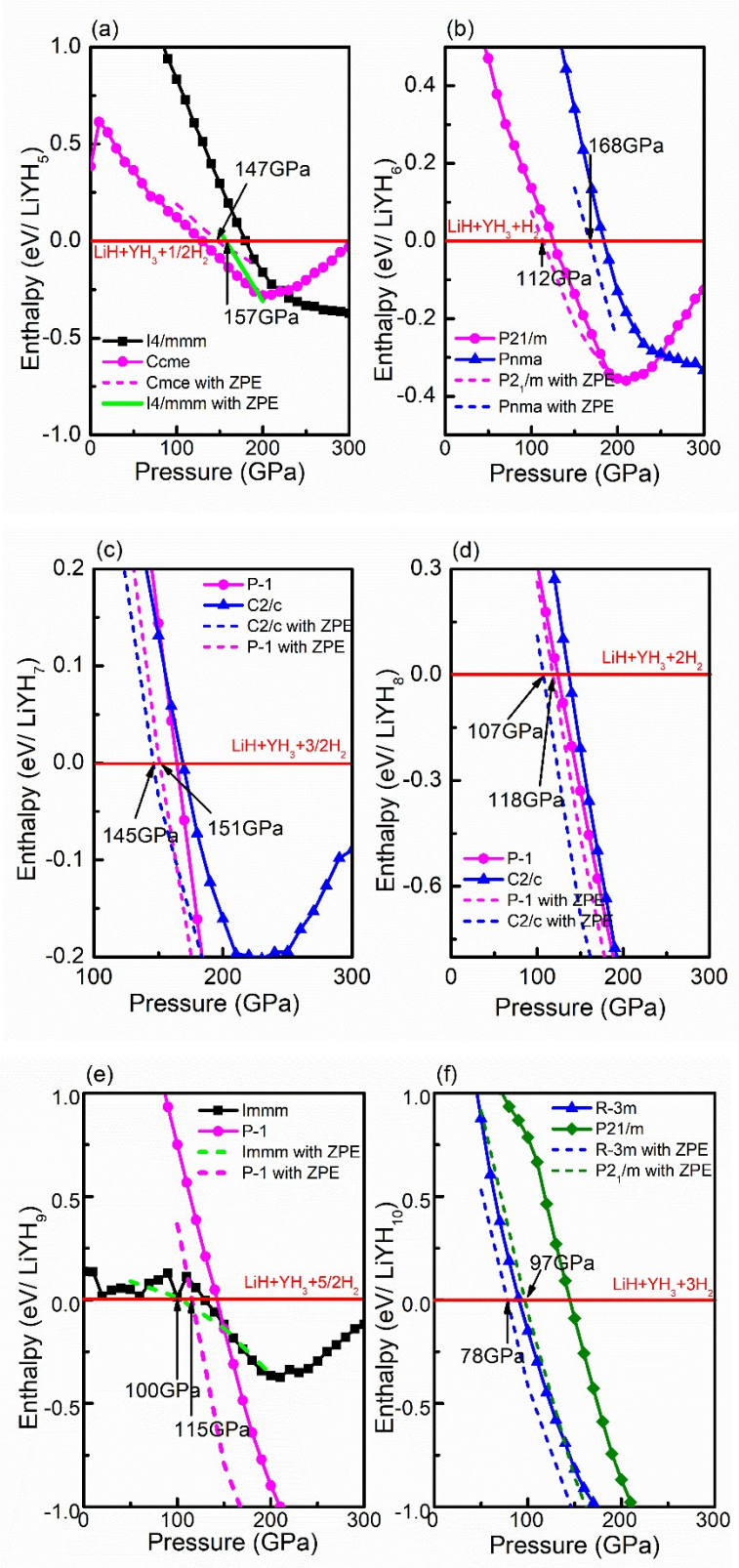


Fig. S2. Enthalpy curves of various structures of $LiYH_n$ (n=5-10) relative to

$LiH+YH_3+nH_2$ (n=0.5-3) as functions of pressure, ZPEs included. We have considered the most stable structures of $LiYH_n$ (n=5-10) in their respective pressure ranged, as shown in Fig. S1.

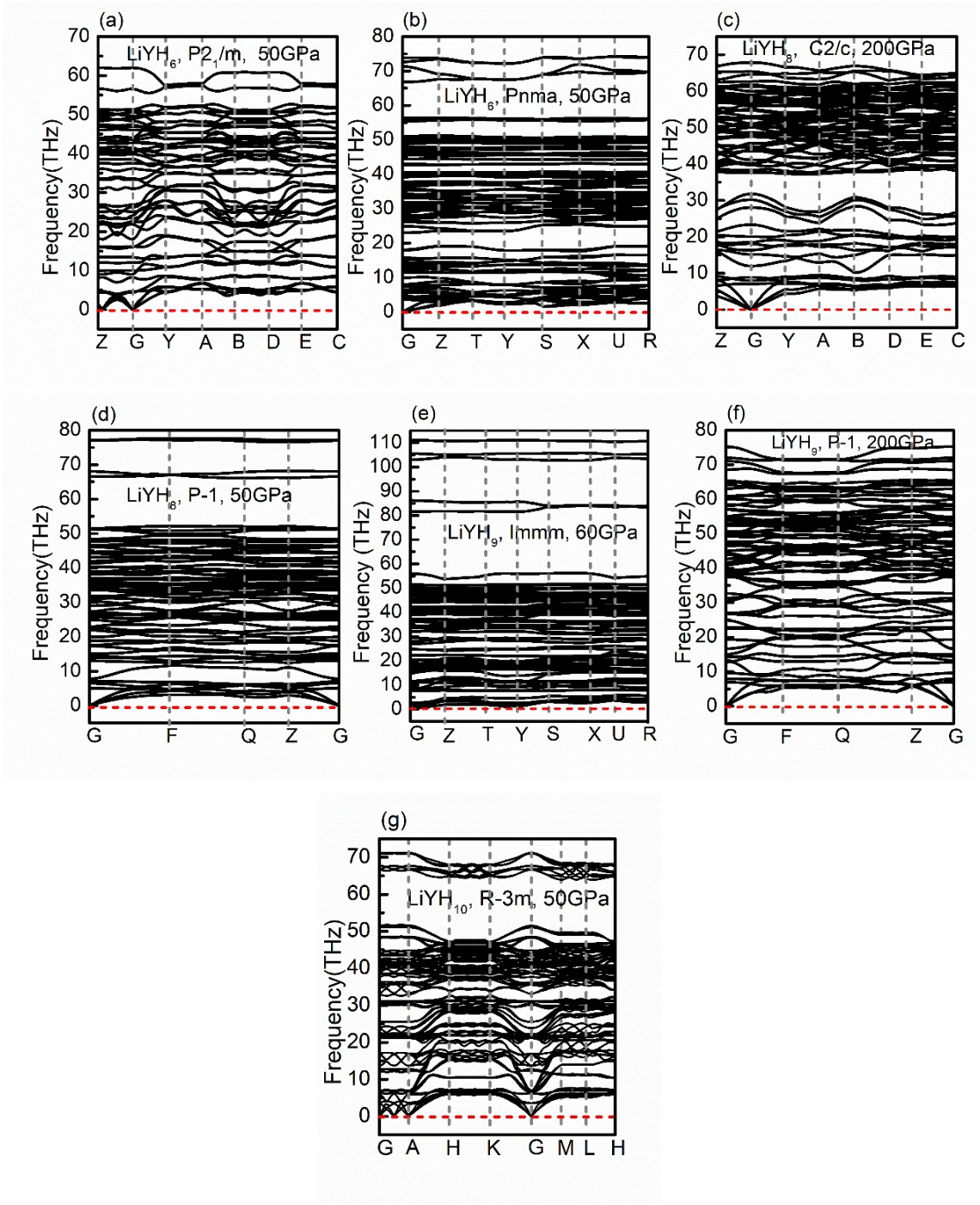


Fig. S3. Phonon dispersion curves of stable or metastable phases of $LiYH_n$ (n=5-10).

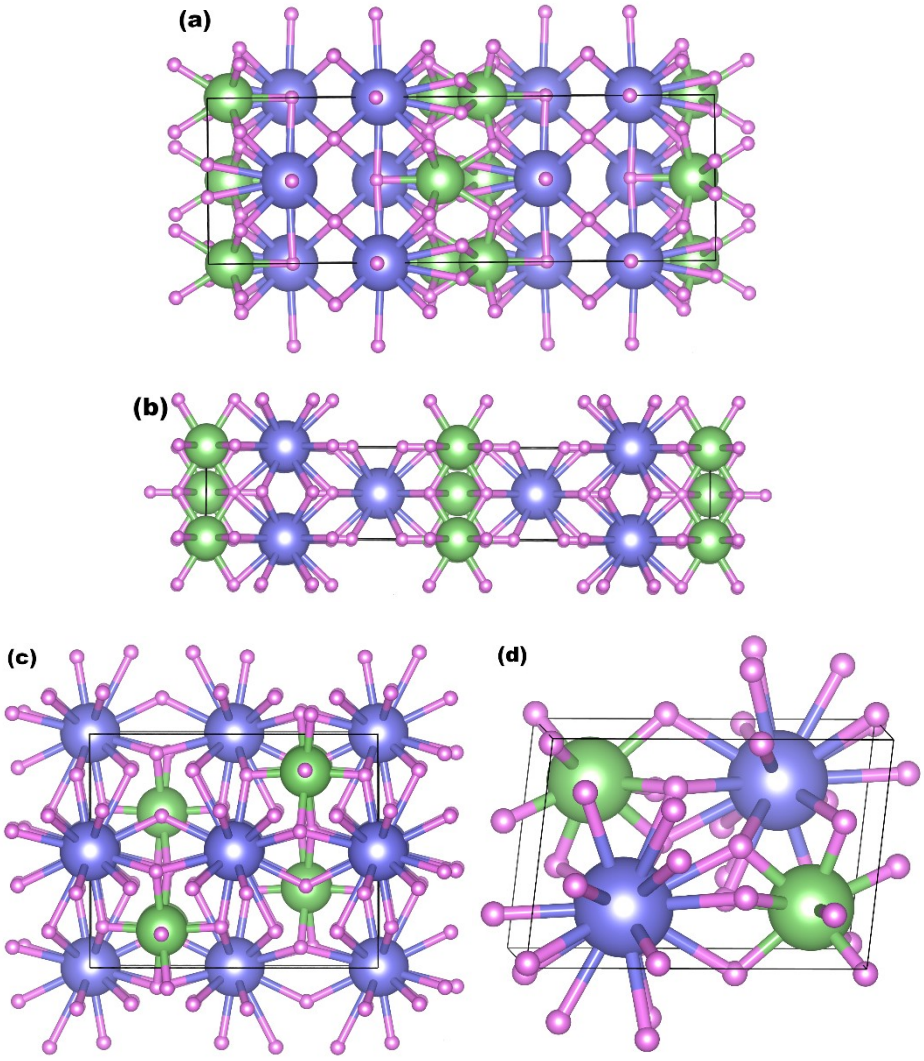


Fig. S4. Predicted ground-state static structures of $LiYH_5$ and $LiYH_7$ ((a) Cmce $LiYH_5$ at 150 GPa, (b) I4/mmm $LiYH_5$ at 200 GPa, (c) C2/c $LiYH_7$ at 150 GPa and (d) P-1 $LiYH_7$ at 200 GPa). The green, purple and pink spheres represent Li, Y and H atoms, respectively. Lines are drawn for Li-H, Y-H separations shorter than 1.70 Å and 2.2 Å.

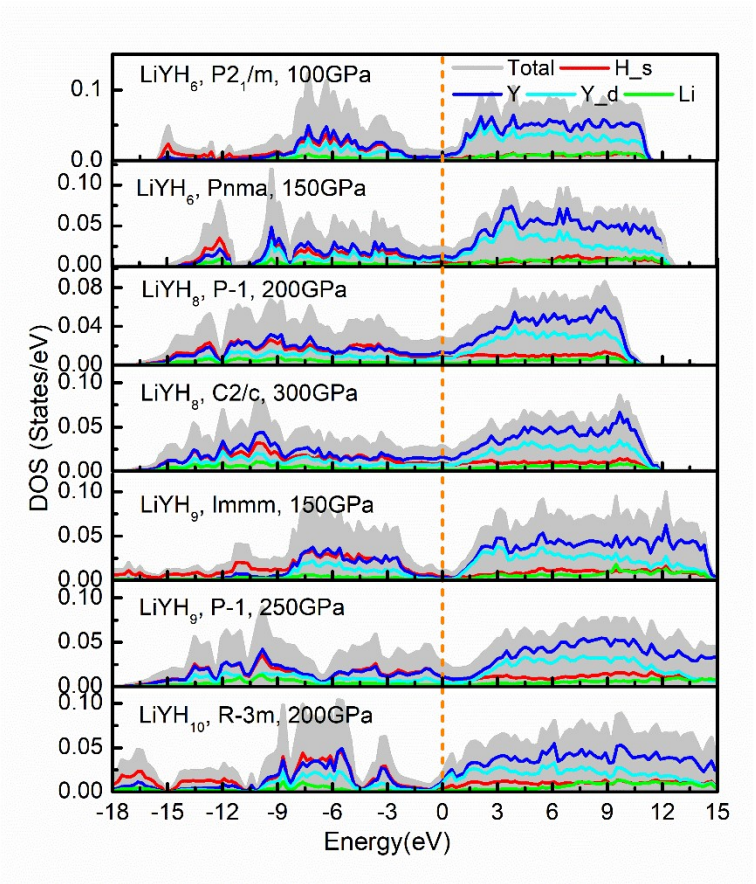
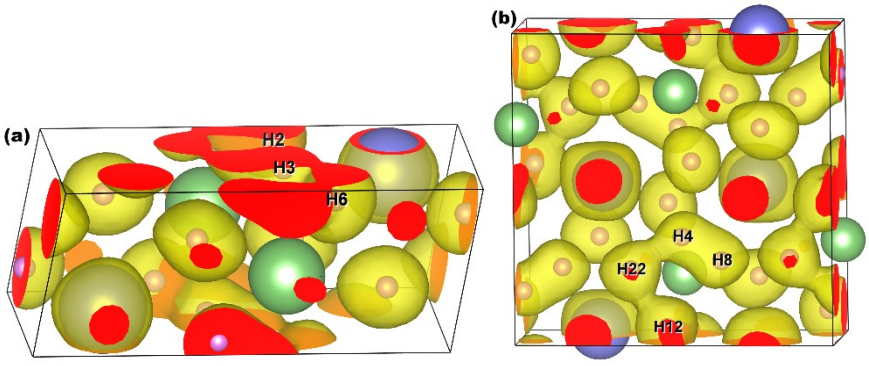


Fig. S5. Total DOS, local DOS and partial DOS of $LiYH_n$ (n=5-10). Energy is shifted so that the Fermi level E_F equals zero.



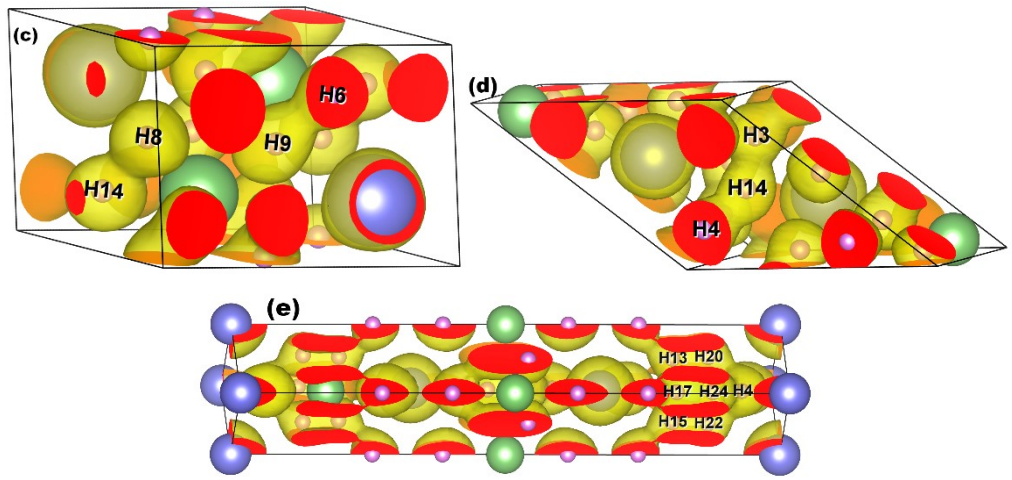
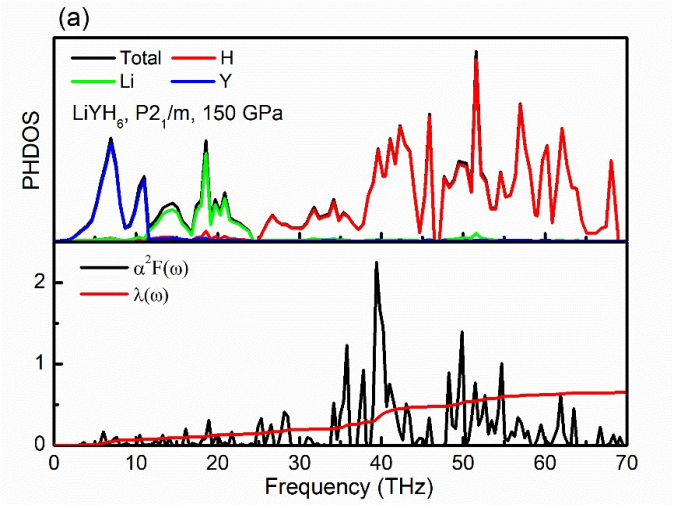
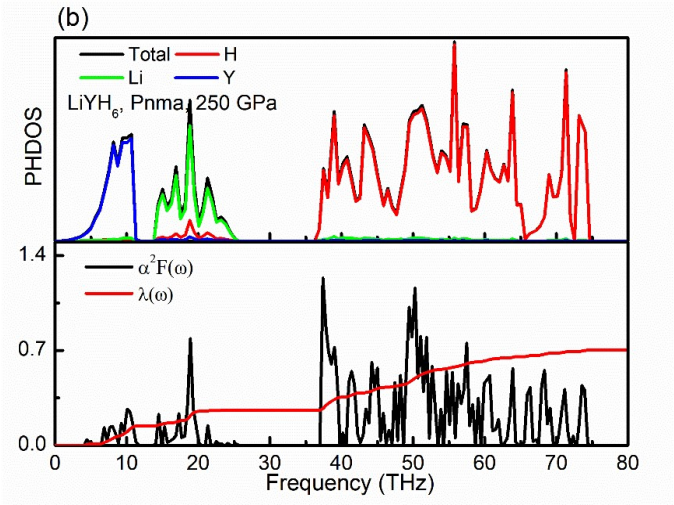
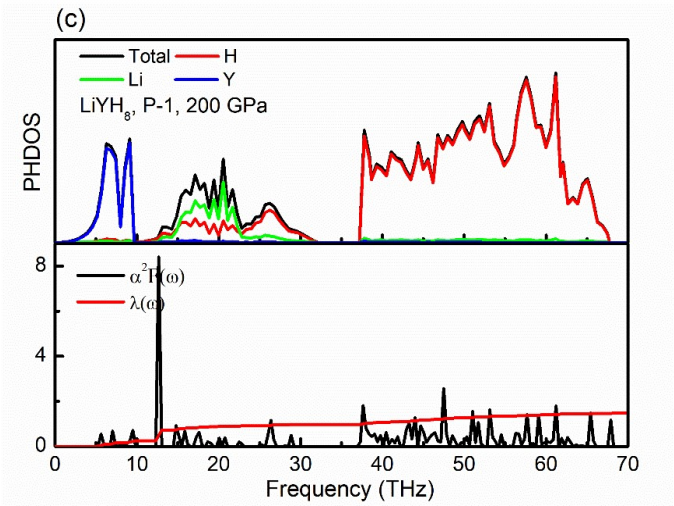
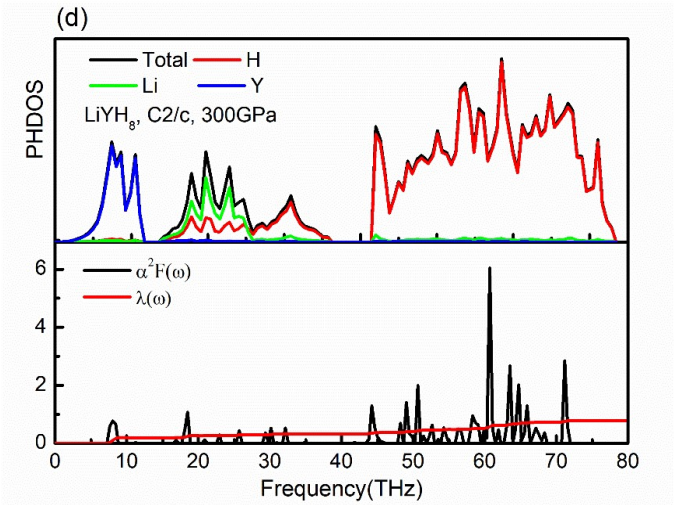


Fig. S6. Three-dimensional electron localization functions (ELF) with an isosurface value 0f 0.5 (a) $P2_1/m$ $LiYH_6$ at 150 GPa, (b) Pnma $LiYH_6$ at 250 GPa, (c) P-1 $LiYH_8$ at 200 GPa, (d) C2/c $LiYH_8$ at 300 GPa, and (e) R-3m $LiYH_{10}$ at 200 GPa. The green, purple and pink spheres represent Li, Y and H atoms, respectively.




(b)
Total
H
Li
Y
LiYH6, Pnma, 250 GPa
PHDOS
α²F(ω)
λ(ω)
1.4
0.7
0.0
0
10
20
30
40
50
60
70
80
Frequency (THz)


(c)
Total
H
Li
Y
LiYH8, P-1, 200 GPa
PHDOS
α²F(ω)
λ(ω)
8
4
0
0
10
20
30
40
50
60
70
Frequency (THz)


(d)
Total
H
Li
Y
LiYH8, C2/c, 300GPa
PHDOS
α²F(ω)
λ(ω)
6
4
2
0
0
10
20
30
40
50
60
70
80
Frequency(THz)

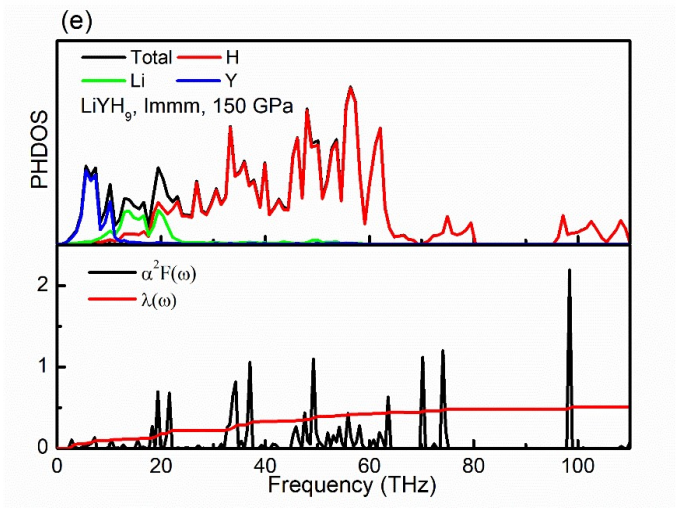


Fig. S7. Projected phonon density of states (PHDOS), Eliashberg spectral function $\alpha^2F(\omega)$, and EPC coupling $\lambda(\omega)$ of $LiYH_n$ (n=5-10).

Table S1. Zero point energies (ZPE) of $LiYH_n$ (n=5-10), LiH, YH_3 and H_2 at different pressures.

System	Space Group	Pressure (GPa)	ZPE (eV/atom)
$LiYH_5$	C2/m	10	0.300
		20	0.322
		50	0.376
		100	0.437
		150	0.479

		200	0.513
	Cmce	10	0.302
		20	0.323
		50	0.378
		100	0.439
		130	0.466
		150	0.482
		180	0.504
		200	0.516
		250	0.543
	I4/mmm	130	0.417
		150	0.436
		180	0.460
		200	0.476
		250	0.504
		300	0.532
$LiYH_6$	$P2_1/m$	100	0.433
		150	0.471
		180	0.492
		200	0.503
		220	0.515
		240	0.527
		250	0.533
		260	0.538
	Pnma	150	0.456
		180	0.477
		200	0.490
		220	0.503
		240	0.515
		250	0.520
		260	0.526
		300	0.547
$LiYH_7$	P-1	100	0.430
		130	0.456
		150	0.473
		170	0.487
		200	0.507
		220	0.520
		250	0.535
		300	0.560
	C2/c	100	0.438

		130	0.457
		150	0.470
		170	0.483
		200	0.501
		220	0.511
$LiYH_8$	P-1	20	0.367
		50	0.409
		60	0.419
		70	0.430
		100	0.452
		120	0.465
		130	0.472
		150	0.482
		180	0.497
		200	0.505
		250	0.536
		300	0.561
	C2/c	20	0.303
		50	0.352
		70	0.376
		100	0.403
		130	0.431
		150	0.447
		180	0.473
		200	0.489
		250	0.525
		300	0.553
$LiYH_9$	Immm	100	0.463
		150	0.498
		180	0.515
		200	0.525
	P-1	100	0.427
		150	0.440
		180	0.466
		200	0.480
$LiYH_{10}$	R-3m	1atm	0.308
		30	0.361
		40	0.374
		50	0.387
		80	0.424
		100	0.445

		130	0.471
		150	0.485
		180	0.519
		200	0.534
		230	0.550
		250	0.562
		270	0.573
		300	0.589
YH_3	C2/m	50	0.365
		100	0.426
		150	0.470
	$P6_3/mmc$	200	0.494
	Cmcm	250	0.508
		300	0.533
H_2	$P6_3/m$	50	0.478
		100	0.521
	C2/c	150	0.549
		200	0.574
	Cmca	250	0.590
		300	0.607
LiH	Fm-3m	50	0.329
		100	0.389
		150	0.431
		200	0.464
	Pm-3m	250	0.338
		300	0.363

Table S2. Structural parameters of $LiYH_n$ (n=5-10) system under different pressures.

System	Space Group	Structural Parameter (Å,°)	Atom	Atomic Coordinate (Å)		
				X	Y	Z
$LiYH_5$ (150 GPa)	Cmce	a=4.19080	Li (8f)	-0.50000	0.16164	0.45769
		b=4.08830	Y (8f)	-0.00000	0.90224	-0.34035
		c=12.81360	H (16g)	-0.29716	0.13897	-0.43581
		α=β=γ=90	H (8f)	-0.50000	0.90137	-0.33341
			H (8d)	-0.09844	-0.00000	-0.50000
			H (8e)	-0.25000	0.34237	0.25000
$LiYH_6$ (150	$P2_1/m$	a=2.84460	Li (2e)	0.61889	0.75000	0.59365
		b=3.02270	Y (2e)	0.81013	0.75000	0.16811

GPa)		c=6.87410	H (4f)	0.07316	0.03695	0.56013
		α=γ=90	H (2e)	0.15725	0.75000	0.67473
		β=98.6134	H (2e)	0.69457	0.75000	0.83977
			H (2e)	0.39096	0.75000	0.36094
			H (2e)	0.24830	0.75000	0.99309
$LiYH_6$	Pnma	a=6.24220	Li (4c)	-0.00078	0.75000	-0.30343
(250		b=2.52950	Y (4c)	-0.26919	0.75000	-0.48398
GPa)		c=6.11210	H (4c)	-0.01613	0.75000	-0.83698
		α=β=γ=90	H (4c)	-0.13997	0.75000	-0.76054
			H (4c)	-0.96775	0.75000	-0.54568
			H (4c)	-0.73378	0.25000	-0.81280
			H (4c)	-0.95056	0.25000	-0.92156
			H (4c)	-0.64573	0.25000	-0.23072
$LiYH_7$	C2/c	a=3.13050	Li (4e)	0.00000	0.16047	0.75000
(150		b=5.64840	Y (4b)	0.50000	-0.00000	1.00000
GPa)		c=7.01850	H (8f)	0.92538	0.15573	1.35788
		α=γ=90	H (8f)	0.02232	0.17553	0.54550
		β=96.3883	H (8f)	0.26111	0.08547	1.23096
			H (4e)	0.00000	0.35106	1.25000
$LiYH_8$	P-1	a=3.43510	Li (2i)	0.55638	0.25431	0.65401
(200		b=3.48600	Y (2i)	-0.15579	0.27334	0.20858
GPa)		c=5.12940	H (2i)	-0.05933	0.18543	0.87132
		α= 86.103	H (2i)	0.22470	0.98966	0.45352
		β=107.8251	H (2i)	0.04327	0.23302	0.60927
		γ=97.4157	H (2i)	-0.66365	0.46907	0.12738
			H (2i)	-0.24962	0.51364	0.48130
			H (2i)	-0.60139	0.18431	0.36278
			H (2i)	-0.38445	0.75800	0.10672
			H (2i)	-0.73604	0.00959	0.11349
$LiYH_8$	C2/c	a=3.31080	Li (4e)	0.00000	0.92155	0.75000
(300		b=9.43890	Y (4e)	0.50000	0.14527	0.75000
GPa)		c=3.27950	H (8f)	0.25048	0.01785	1.48875
		α=γ=90	H (8f)	0.77743	0.69052	1.28818
		β=81.1170	H (8f)	0.53711	0.69092	0.52864
			H (4e)	0.50000	0.05344	1.25000
			H (4e)	0.00000	0.93250	1.25000
$LiYH_9$	Immm	a=15.31190	Li (4f)	0.41737	-0.00000	0.50000
(150		b=3.06180	Y (4f)	0.32091	0.50000	0.00000
GPa)		c=2.99300	H (4f)	0.31311	0.00000	0.50000
		α=β=γ=90	H (8l)	-0.00000	0.76568	0.12912
			H (8m)	0.05533	-0.00000	0.36069

			H (4e)	0.25185	0.00000	0.00000
			H (4e)	0.47467	0.00000	0.00000
			H (4e)	0.10301	0.00000	0.00000
			H (4e)	0.10712	0.50000	0.50000
$LiYH_9$ (250 GPa)	P-1	a=3.41990 b=3.43010 c=5.10130 α= 109.3956 β=89.4492 γ=90.3359	Li (2i)	0.75719	-0.93456	-0.86880
			Y (2i)	0.75291	-0.64232	-0.28451
			H (2i)	0.29874	-0.92085	-0.84970
			H (2i)	0.00887	-0.81917	-0.63560
			H (2i)	0.49863	-1.18652	-0.36896
			H (2i)	0.25570	-0.43554	-0.36153
			H (2i)	0.74709	-1.07013	-0.63479
			H (2i)	0.49934	-0.25909	-0.00318
			H (2i)	0.74559	-1.25270	-0.50539
			H (2i)	0.00021	-1.26344	-0.99904
			H (2i)	0.75160	-1.41828	-0.89341
$LiYH_{10}$ (200 GPa)	R-3m	a=b=2.99220 c=12.72110 α=β=90 γ=120	Li (3b)	0.00000	0.00000	0.50000
			Y (3a)	0.00000	0.00000	0.00000
			H (6c)	0.00000	0.00000	0.25791
			H (6c)	0.00000	-0.00000	0.61411
			H (18h)	0.82935	0.65870	0.199931

Table S3. The average number of remaining valence electrons per Li, Y and H atom in $LiYH_n$ (n=5-10) was obtained by Bader charge analysis under selective pressure. σ(e) represents the number of valence electrons gained or lost (positive values indicate electrons lost, negative values indicate electrons gained).

System	Pressure (GPa)	Atomic Species	Average number of remaining valence electrons (e)	Average number of electrons gained or lost σ(e)
$P2_1/m$ $LiYH_6$	150	Li	0.27445	0.72555
		Y	9.59500	1.40500
		H	1.35510	-0.35510
Pnma $LiYH_6$	250	Li	0.30666	0.69334
		Y	9.80700	1.19300
		H	1.31439	-0.31439
P-1 $LiYH_8$	200	Li	0.32218	0.67782
		Y	9.69874	1.30126

		H	1.24738	-0.24738
C2/c $LiYH_8$	300	Li	0.35377	0.64624
		Y	9.83081	1.16919
		H	1.18728	-0.18728
Immm $LiYH_9$	150	Li	0.27313	0.72687
		Y	9.56170	1.43831
		H	1.24057	-0.24057
P-1 $LiYH_9$	250	Li	0.34823	0.65177
		Y	9.62279	1.37721
		H	1.22544	-0.22544
R-3m $LiYH_{10}$	200	Li	0.29473	0.70527
		Y	9.67335	1.32665
		H	1.20319	-0.20319