Supplementary materials for "Prediction of high-temperature superconductivity in lithium-doped thorium superhydrides under high pressures"

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SUPPLEMENTARY TABLE AND FIGURES

TABLE S1. Structural parameters of various structures studied in this work.

Pressure (GPa)	System	Space group	Lattice Parameters (Å)	Atom	Atomic coordinates (fractional) x	y	z
300	Li_2ThH_{17}	$Fd\bar{3}m$	$a = 7.07440$	Li ($16c$)	0.12500	0.12500	0.12500
			$b = 7.07440$	Th ($8b$)	0.00000	0.00000	0.50000
			$c = 7.07440$	H ($96g$)	0.19988	0.19988	0.48550
				H ($32e$)	0.33938	0.33938	0.33938
				H ($8a$)	0.25000	0.25000	0.25000
300	Li_2ThH_{16}	$Fd\bar{3}m$	$a = 7.00640$	Li ($16c$)	0.12500	0.12500	0.12500
			$b = 7.00640$	Th ($8b$)	0.00000	0.00000	0.50000
			$c = 7.00640$	H ($32e$)	0.42197	0.92197	0.42197
				H ($96g$)	0.19883	0.19883	0.48228
300	$LiTh_2H_{12}$	$C2/m$	$a = 6.00390$	Li ($2d$)	0.50000	0.00000	0.50000
			$b = 3.48620$	Th ($4i$)	0.78406	0.00000	0.21705
			$c = 4.68090$	H ($8j$)	0.58284	0.30530	0.39108
				H ($4i$)	0.27773	0.00000	0.39268
				H ($4i$)	0.89640	0.00000	0.84750
				H ($4i$)	0.44640	0.00000	0.18355
				H ($4g$)	0.50000	0.74364	0.00000
300	Li_2ThH_{12}	$P2_1/m$	$a = 3.53200$	Li ($2e$)	0.01847	0.75000	0.11250
			$b = 3.54680$	Li ($2e$)	0.99558	0.75000	0.45257
			$c = 5.98380$	Th ($2e$)	0.49888	0.75000	0.75121
				H ($4f$)	0.99768	0.95329	0.69057
				H ($4f$)	0.00303	0.87567	0.88432
				H ($4f$)	0.27349	0.48543	0.99365
				H ($4f$)	0.70931	0.48883	0.50365
				H ($2e$)	0.28923	0.75000	0.28268
				H ($2e$)	0.72427	0.75000	0.26008
				H ($2e$)	0.55511	0.25000	0.90935
				H ($2e$)	0.40291	0.25000	0.58995
300	Li_2ThH_{13}	$C2/c$	$a = 7.96520$	Li ($8f$)	0.76931	0.91589	0.48553
			$b = 6.05190$	Th ($4e$)	0.50000	0.75362	0.75000
			$c = 3.56000$	H ($8f$)	0.42445	0.91230	0.19375
				H ($8f$)	0.38924	0.75413	0.14395
				H ($8f$)	0.24986	0.87176	0.41265
				H ($8f$)	0.24758	0.19975	0.20649
				H ($8f$)	0.62773	0.99737	0.61433
				H ($8f$)	0.89668	0.00856	0.37397
				H ($4e$)	0.50000	0.58474	0.25000

TABLE S2. The superconducting parameters for Li_2ThH_{17} without/with SOC effect under 300 GPa.

	λ	$\omega_{\log}$ (K)	T_c^{ADM} (K)
Without SOC	1.55	1135	154
With SOC	1.54	1137	153

TABLE S3. The value of the H-derived electronic density of states at the Fermi level (states/eV f.u.) its proportion of the total density of states for Li_2ThH_{17} and Li_2ThH_{16} under different pressures.

Phase	Pressure (GPa)	DOS_H	Total DOS	Proportion
Li_2ThH_{17}	250	0.45	1.00	45.0 %
	300	0.47	1.07	43.9 %
	350	0.43	0.99	43.4 %
Li_2ThH_{16}	180	0.43	0.85	50.6 %
	300	0.42	0.87	48.3 %

TABLE S4. Calculated electron–phonon coupling related parameters for Li_2ThH_{17} under different pressures.

Pressure (GPa)	λ	$\omega_{\log}$ (K)	$N_{Ef}(eV^{-1})$	$\langle\omega^2\rangle$ (eV^2)	$\langle I^2\rangle$	T_c^E (K)
250	1.45	1177	1.00	0.0208	13.93	159
300	1.55	1135	1.07	0.0208	15.39	162
350	1.87	975	0.99	0.0188	16.99	187

TABLE S5. Calculated Bader charge (eV/f.u.) and electronic properties at the Fermi level (states/eV f.u.) for Li_2ThH_{17} and $LiLaH_{17}$ at 300 GPa.

Phase	atom	Bader charge	DOS	Total DOS	Proportion
Li_2ThH_{17}	Li	+1.63	0.12	1.07	11.2 %
	Th	+1.44	0.48		44.9 %
	H	-3.07	0.47		43.9 %
Li_2LaH_{17}	Li	+1.63	0.01	0.91	1.1 %
	La	+1.03	0.34		37.4 %
	H	-2.66	0.56		61.5 %

TABLE S6. $N(E_f)$ (states/Ry/f.u.), electron–phonon coupling constant λ, logarithmic average phonon frequency $\omega_{\log}$ (K), and superconducting transition temperature T_c (K) estimated using $\mu^* = 0.13$ for Li-RE-H compounds at different pressures (GPa). Superhydrides marked with (M) indicate metastable phases at 300 GPa.

Compound	Pressure (GPa)	$N(E_f)$	λ	$\omega_{\log}$ (K)	T_c (K)
Li_2YH_{17}	300	2.99	0.69	1758	50
Li_2LaH_{17}	300	4.87	0.86	1854	99
Li_2LaH_{17} (this work)	300	4.52	0.85	1856	94
Li_2ScH_{17} (M)	300	3.94	1.11	941	80
Li_2ThH_{17} (this work)	300	7.43	1.55	1135	162

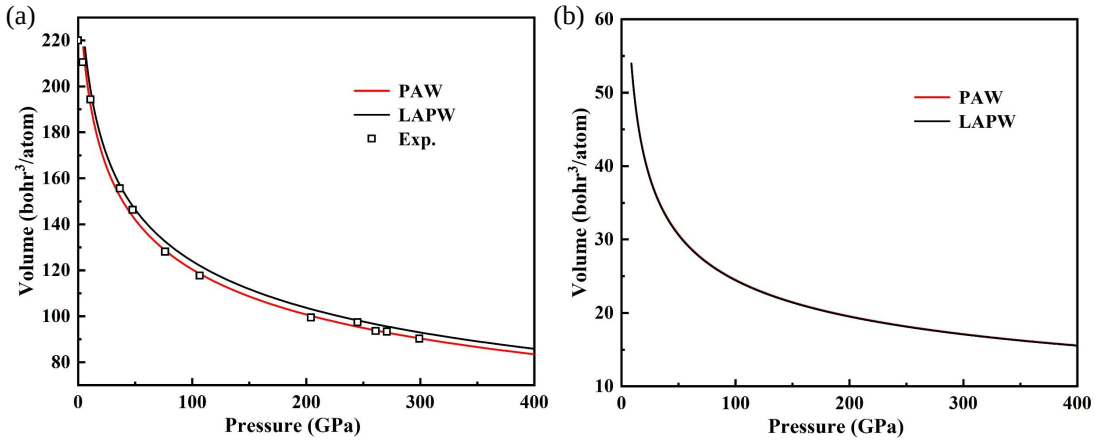

FIG. S1. Comparison of the fitted Birch-Murnaghan equation of states for (a) $Fm\bar{3}m$ Th and (b) LiH using calculated results with the PAW pseudopotentials, full-potential LAPW methods and experimental data. The results further validate the reliability of the adopted PAW pseudopotentials under pressure.

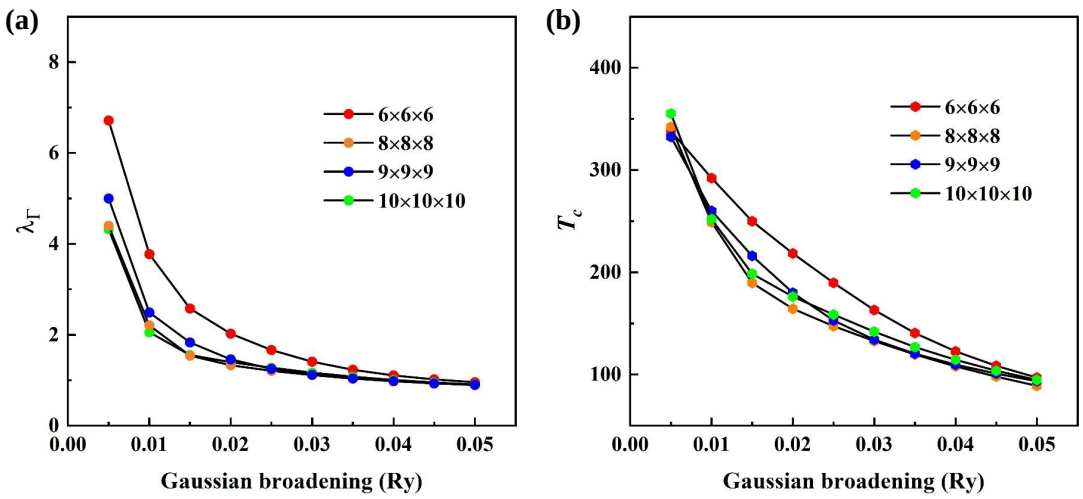

FIG. S2. (a) Electron-phonon constant λ(q) and (b) T_c at q = (0, 0, 0) as a function of the Gaussian broadening σ for $Fd\bar{3}m$ Li_2ThH_{17} at 300 GPa for different k-point grids. The $9 \times 9 \times 9$ is considered to be converged to the required accuacy.

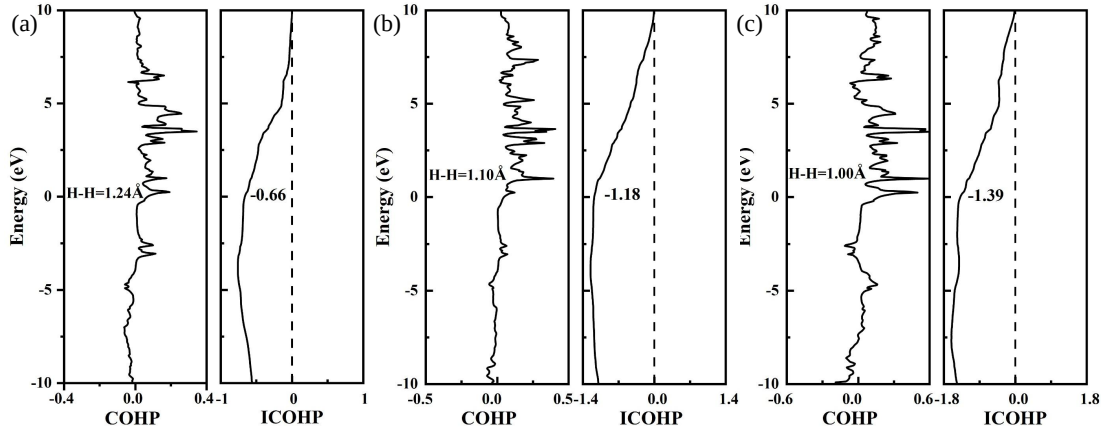

FIG. S3. The COHP and ICOHP of Li_2ThH_{17} at 300 GPa for different H-H bonds from H_{28} calthrate. The negative COHP indicates bonding and positive COHP indicates antibonding.

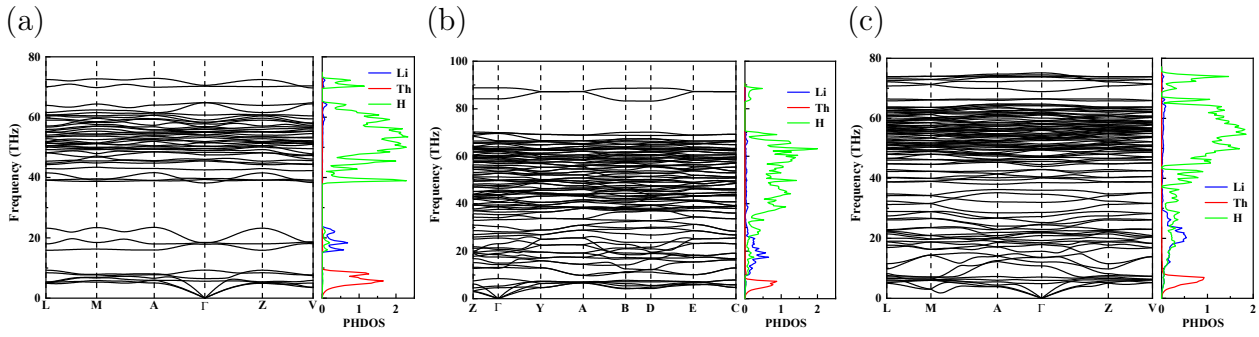

FIG. S4. Phonon dispersions, projected phonon density of states (PHDOS) of (a) $C2/m$ $LiTh_2H_{12}$, (b) $P2_1/m$ Li_2ThH_{12} and (c) $C2/c$ Li_2ThH_{13} at 300 GPa.

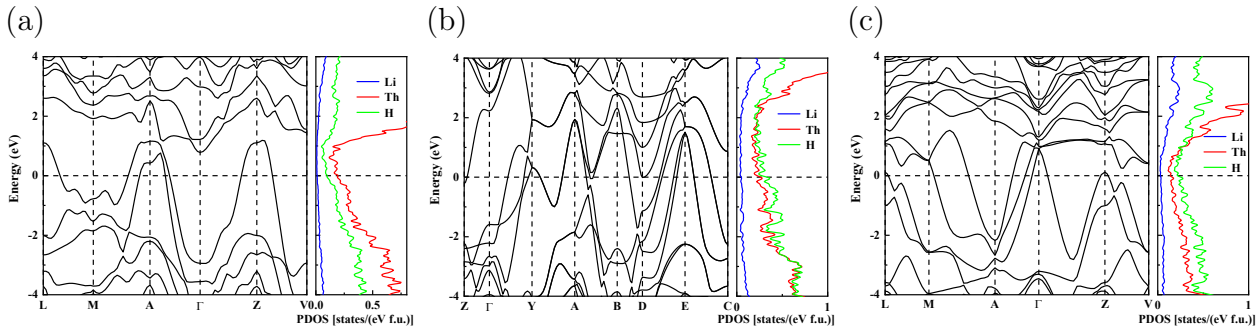

FIG. S5. Electronic band structure and atom-projected density of states near the Fermi level for (a) $C2/m$ $LiTh_2H_{12}$, (b) $P2_1/m$ Li_2ThH_{12} and (c) $C2/c$ Li_2ThH_{13} at 300 GPa.

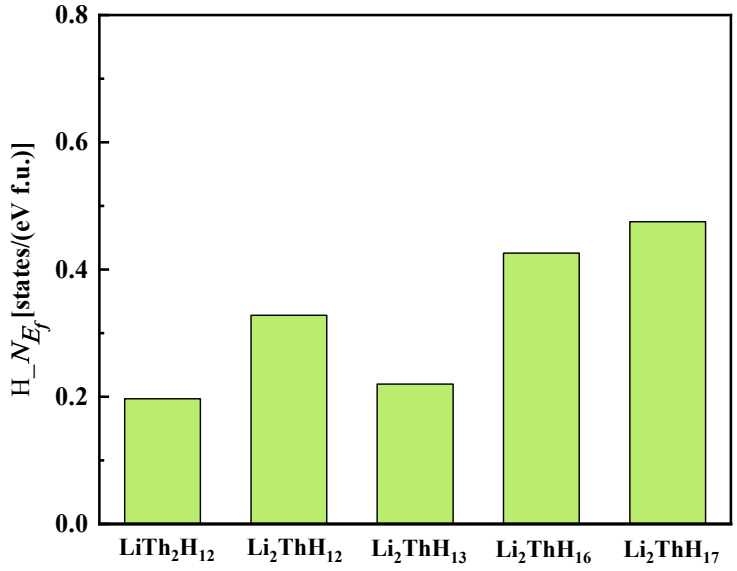

FIG. S6. The calculated values of DOS_H (eV^{-1} per formula unit) at the Fermi level N_{Ef} in Li-Th-H system at 300 GPa.

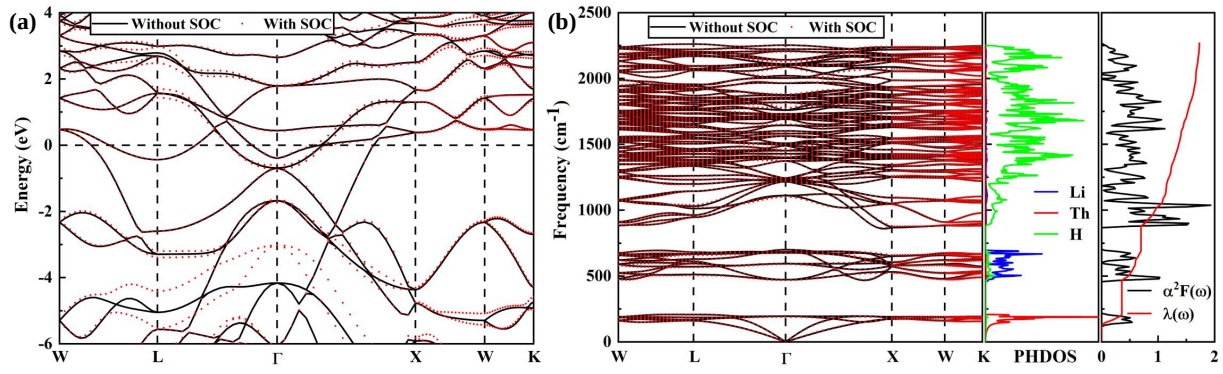

FIG. S7. Calculated (a) electronic structure and (b) superconducting properties with SOC of Li_2ThH_{17} at 300 GPa.

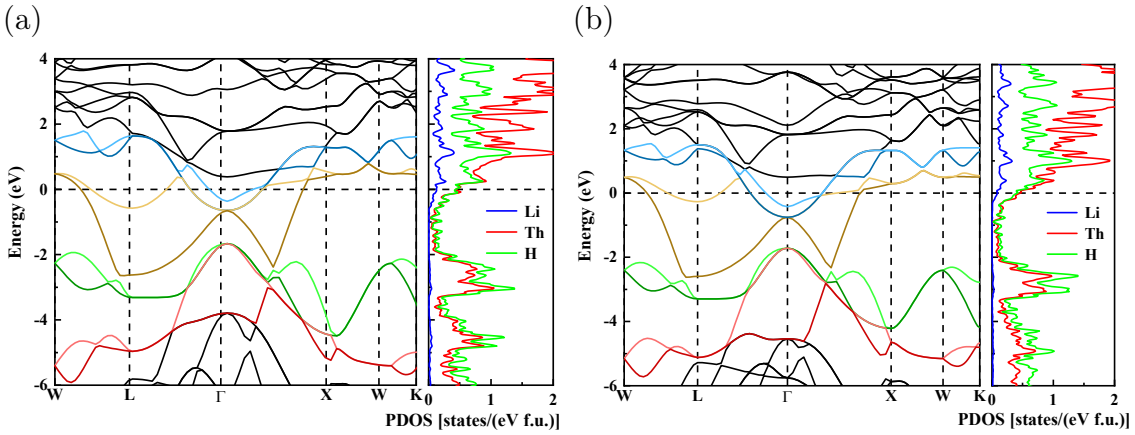

FIG. S8. Calculated electronic band structure and density of states (states/eV/cell) for Li_2ThH_{17} at (a) 350 GPa and (b) 250 GPa, respectively.

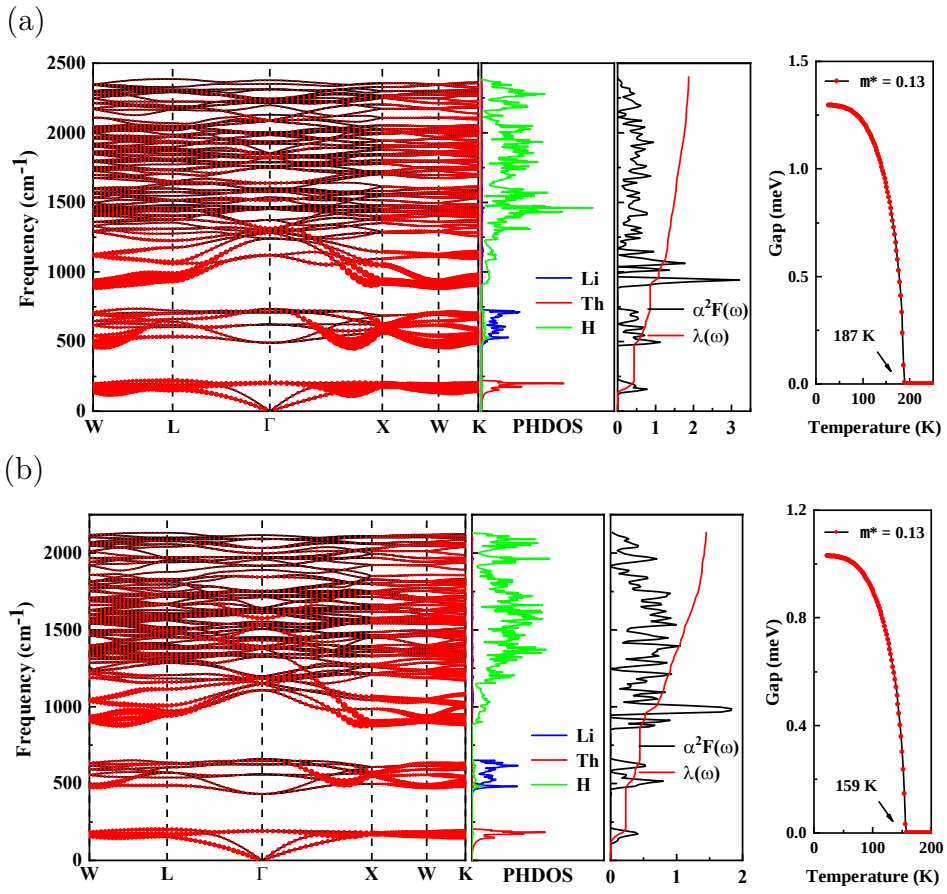

FIG. S9. Phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, EPC parameter $\lambda(\omega)$ and Superconducting energy gap for Li_2ThH_{17} at (a) 350 GPa and (b) 250 GPa, respectively.

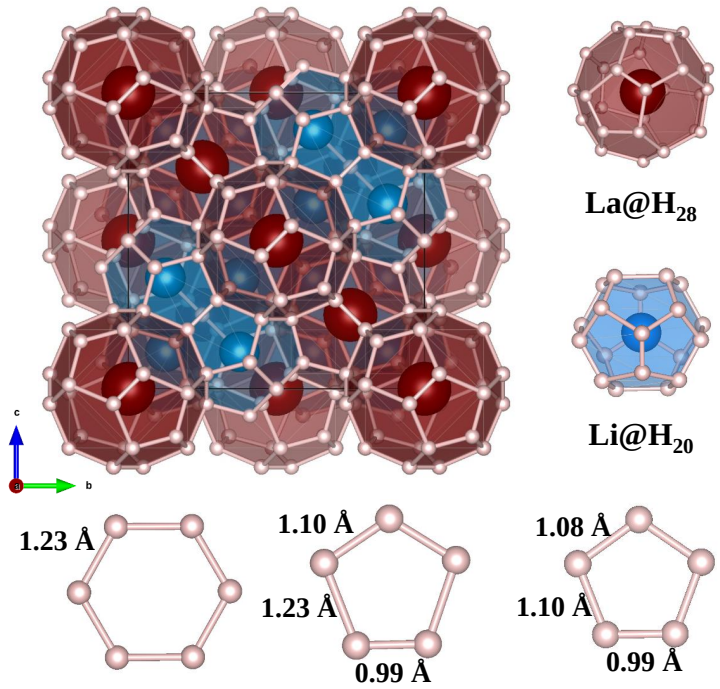

FIG. S10. The structure of $Fd\bar{3}m$ Li_2LaH_{17} at 300 GPa.

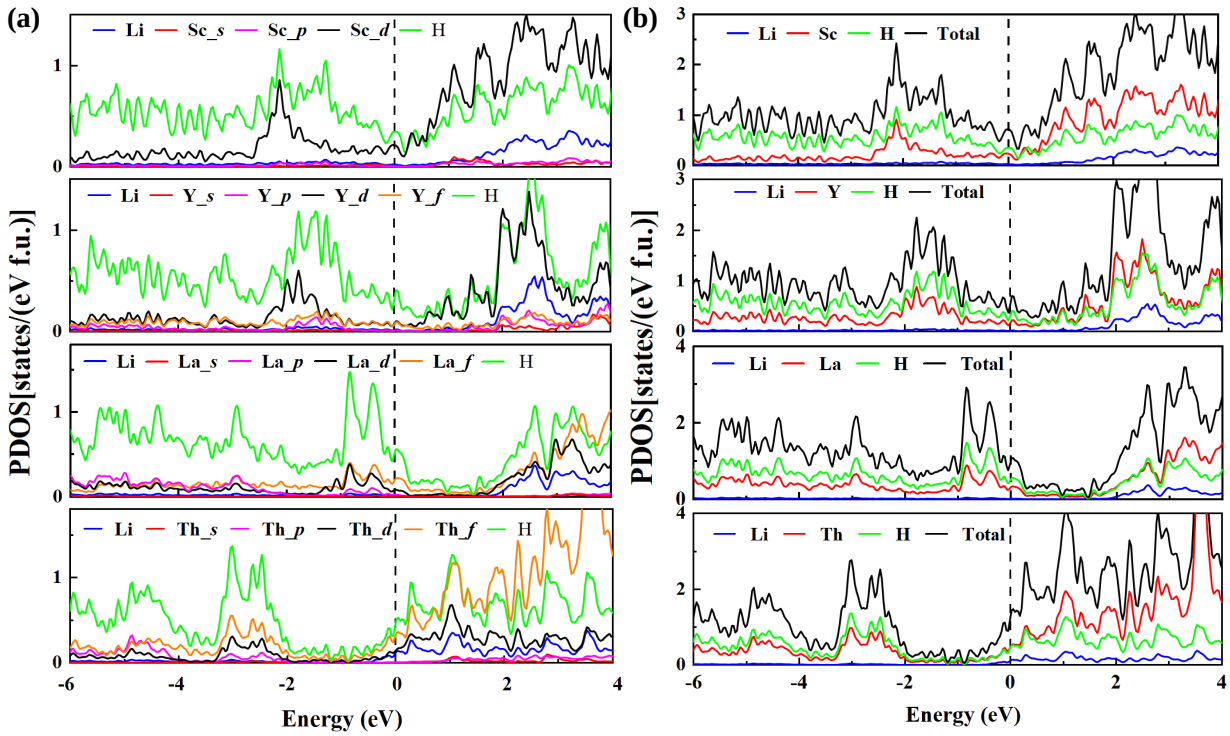

FIG. S11. Calculated orbit-projected and element-projected density of states near the Feimi level for Li_2ThH_{17} and Li_2REH_{17} (RE = Sc, Y and La) at 300 GPa.

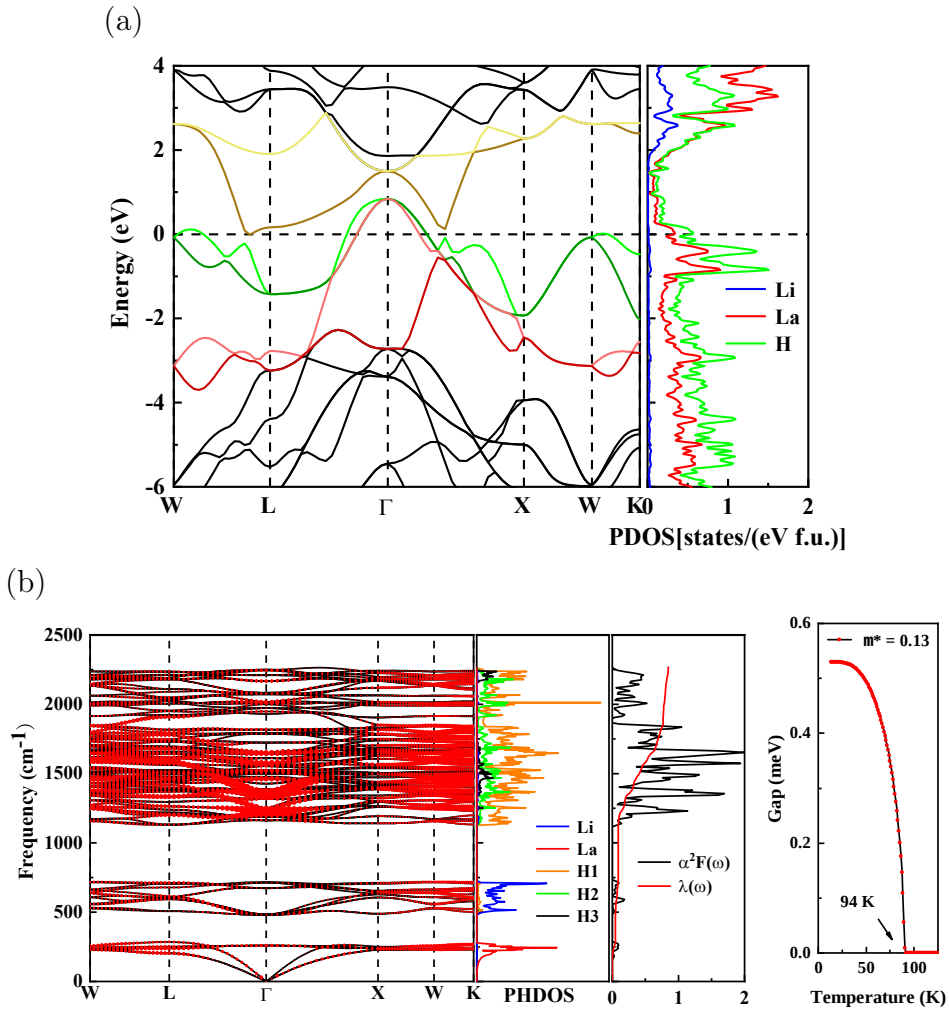

FIG. S12. (a) Calculated electronic band structure, PDOS (states/eV/cell) and (b) Phonon dispersion, PHDOS, $\alpha^2F(\omega)$, $\lambda(\omega)$ and Superconducting energy gap for Li_2LaH_{17} at 300 GPa.

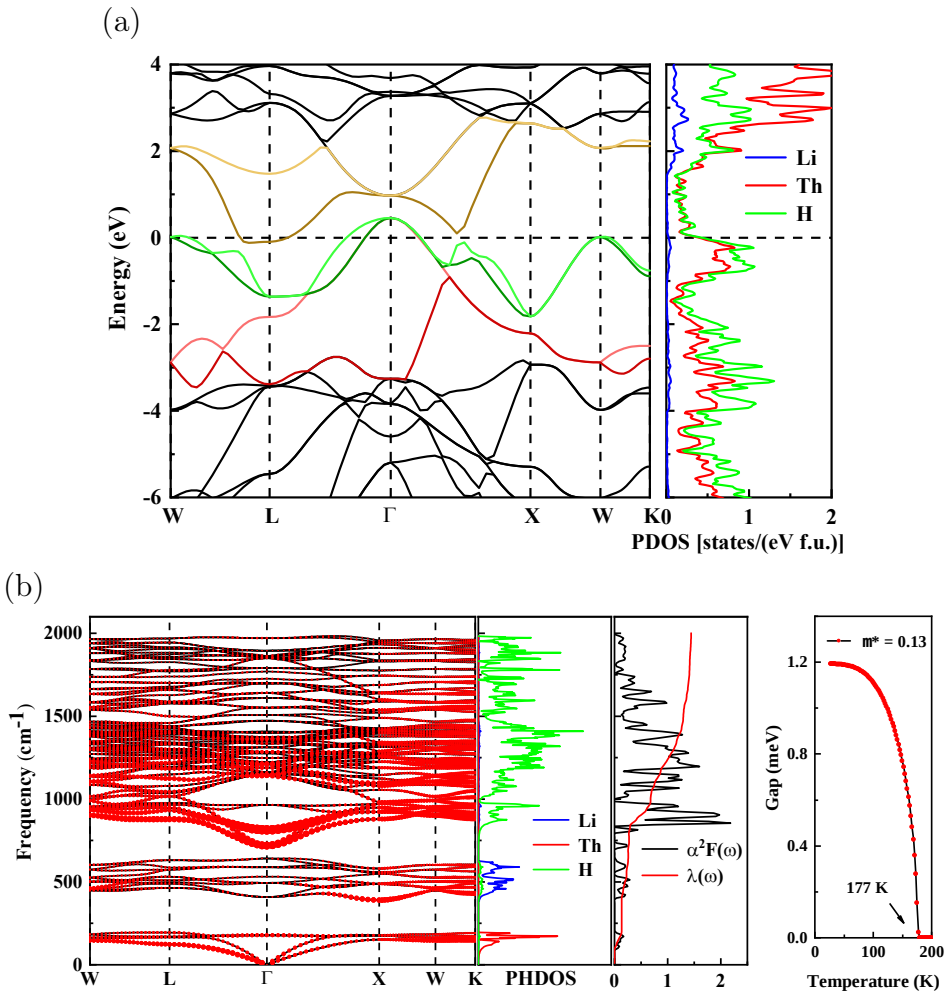

FIG. S13. (a) Calculated electronic band structure, PDOS (states/eV/cell) and (b) Phonon dispersion, PHDOS, $\alpha^2F(\omega)$, $\lambda(\omega)$ and Superconducting energy gap for Li_2ThH_{16} at 180 GPa.