Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Supplemental Material

Structural evolution and superconductivity of Thorium under high pressure and its modulation.

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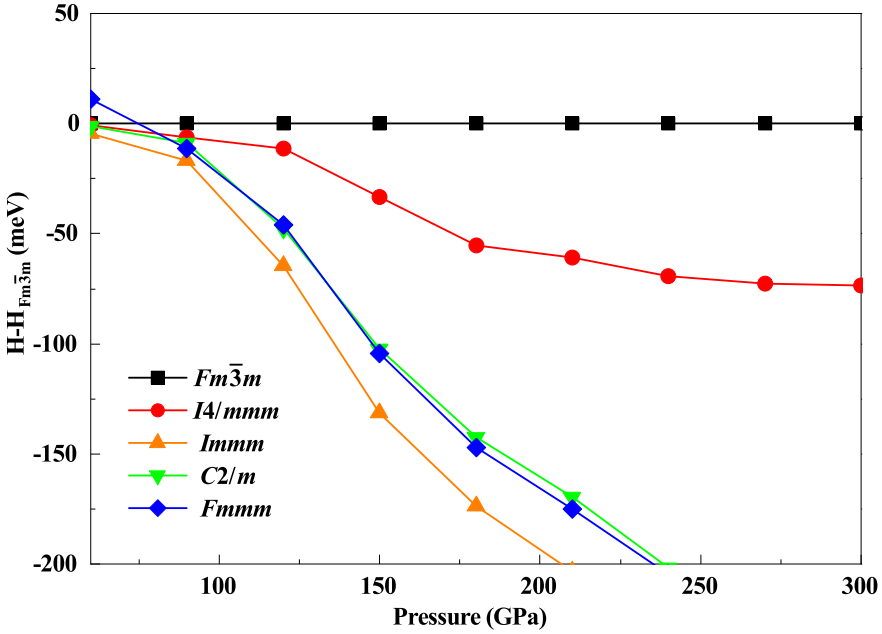

Fig. S1. The enthalpy curves of Th under high pressure from 60 GPa to 300 GPa.

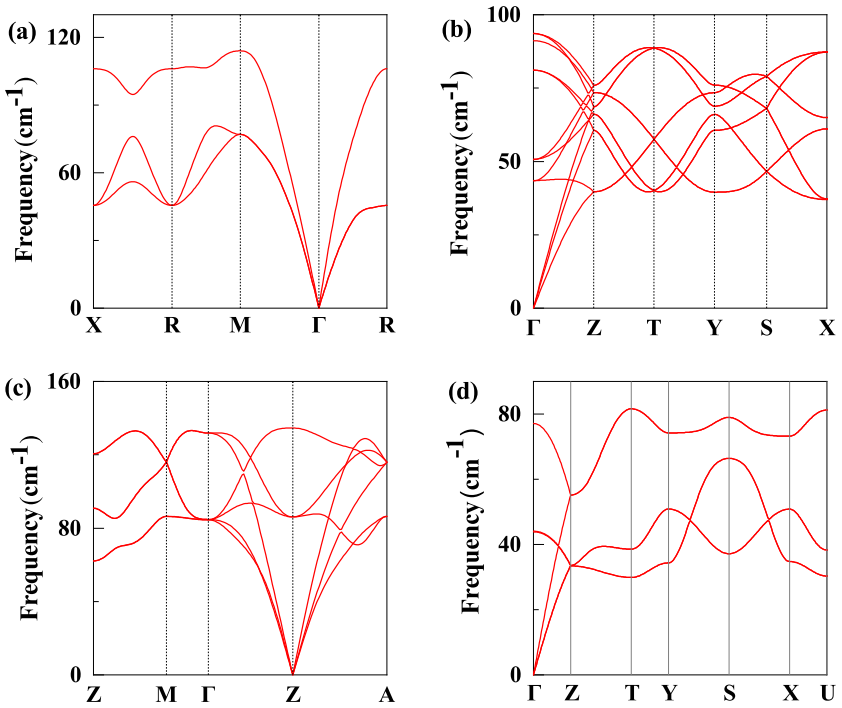

Fig. S2. Phonon dispersion curves of Th under different pressures. (a) $Fm\bar{3}m$ phase at ambient pressure, (b) $Fmmm$ phase at 8 GPa, (c) $I4/mmm$ phase at 10 GPa, (d) $Immm$ phase at 60 GPa.

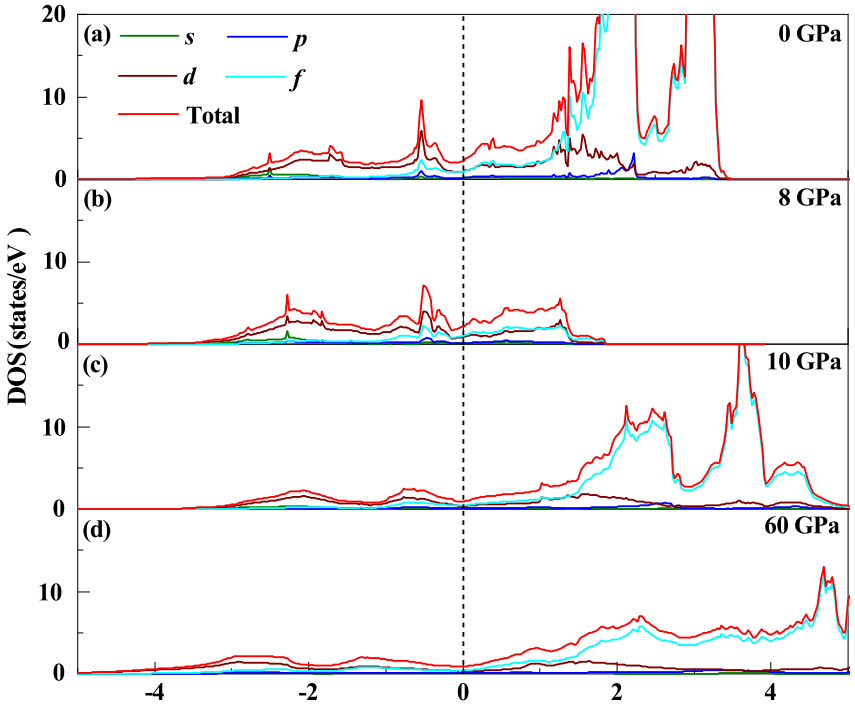

Fig. S3. The PDOS of Th under different pressures. (a) $Fm\bar{3}m$ phase at 0 GPa, (b) $Fmmm$ phase at 8 GPa, (c) $I4/mmm$ phase at 10 GPa, and (d) $Immm$ phase at 60 GPa. The position represented by the dashed line is the Fermi level.

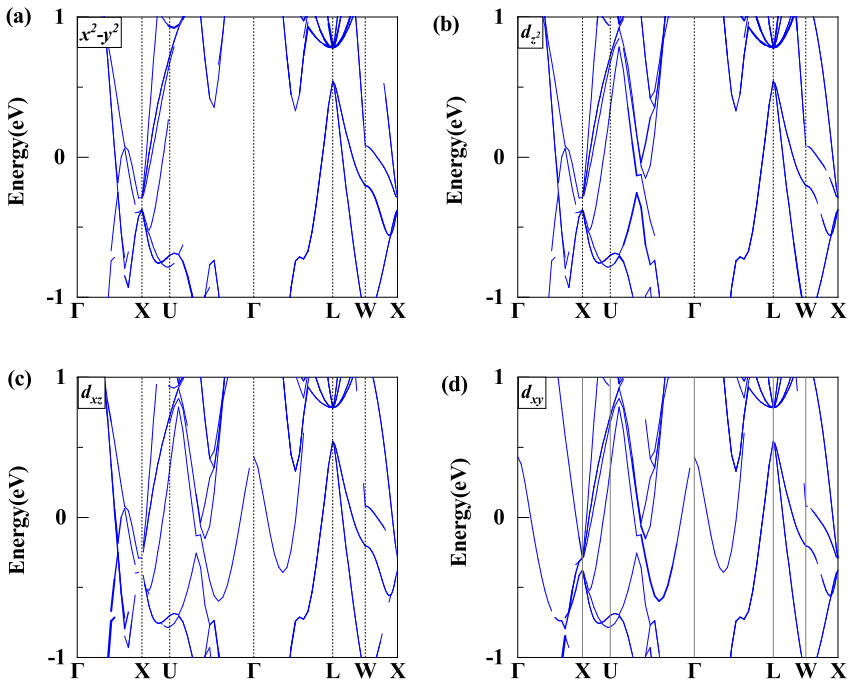

Fig. S4. Calculated orbital-resolved band structures corresponding to different orbitals of the $Fm\bar{3}m$ phase of Th under ambient pressure. (a) $d_{x^2-y^2}$, (b) d_{z^2}, (c) d_{xz}, and (d) d_{xy} orbitals. The thicknesses of curves represent the weight of orbitals in the corresponding band structures.

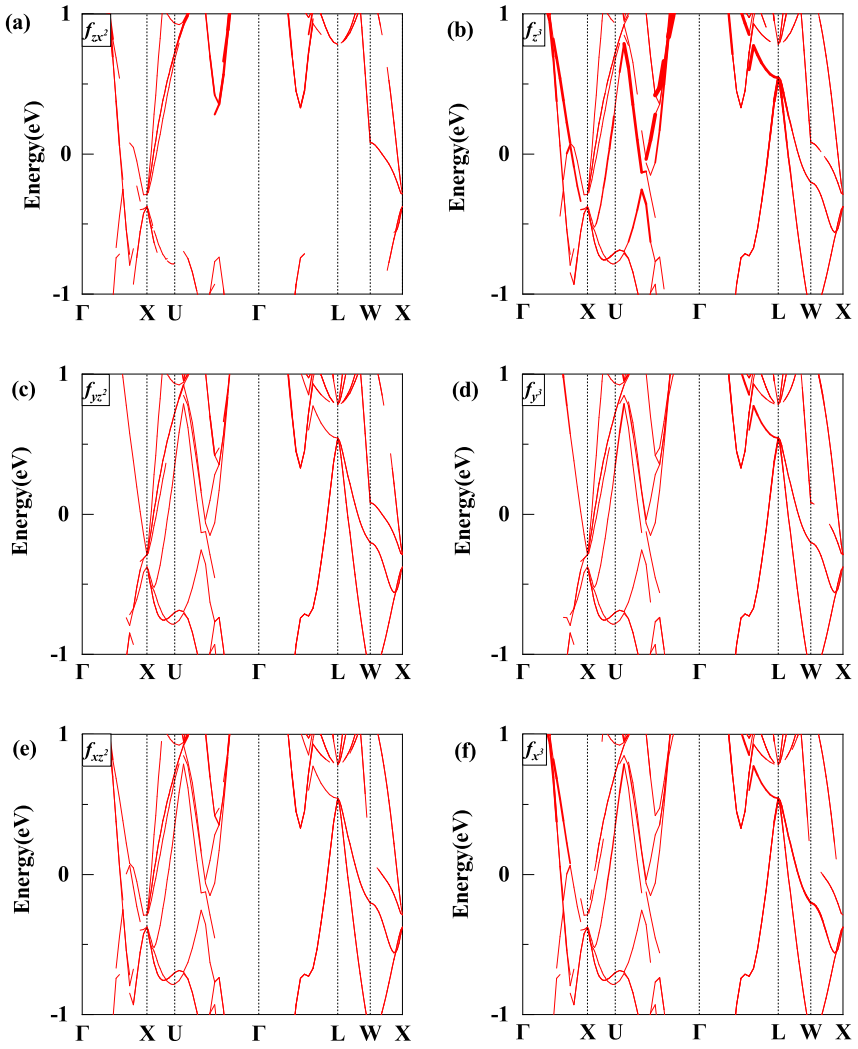

Fig. S5. Calculated orbital-resolved band structures corresponding to different orbitals of the $Fm\bar{3}m$ phase of Th at ambient pressure. (a) f_{zx^2}, (b) f_{z^3}, (c) f_{yz_2}, (d) f_{y^3}, (e) f_{xz^2} and (f) f_{x^3} orbitals. The thicknesses of curves re--present the weight of orbitals in the corresponding band structures.

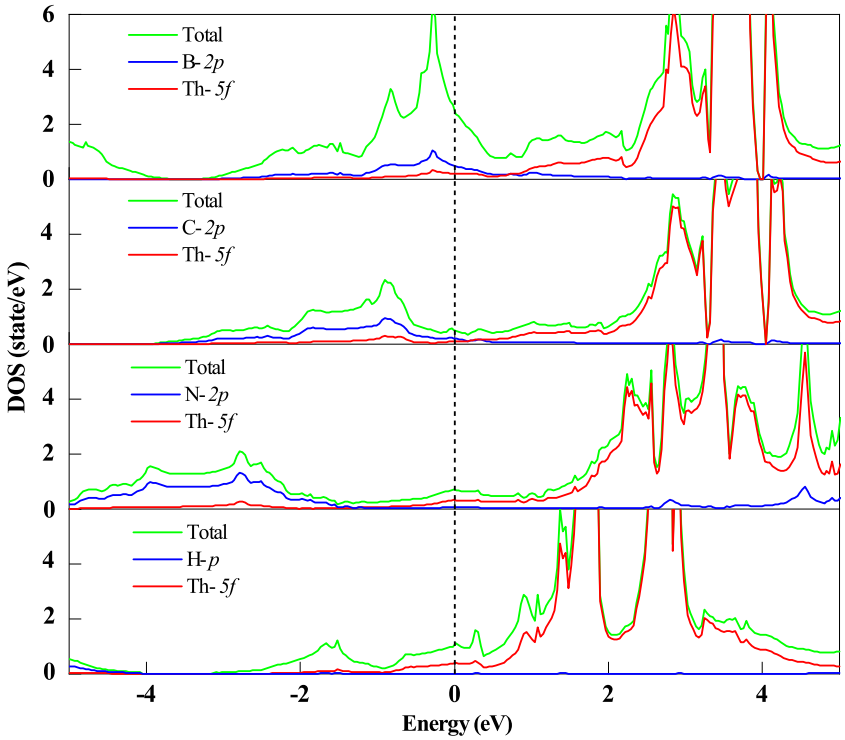

Fig. S6. The $5f$ bands of Th and the $2p$ bands of light elements at ambient pressure. (a) The $5f$ bands of Th and the $2p$ bands of boron. (b) The $5f$ bands of Th and the $2p$ bands of carbon. (c) The $5f$ bands of Th and the $2p$ bands of nitrogen. (d) The $5f$ bands of Th and the p bands of hydrogen.

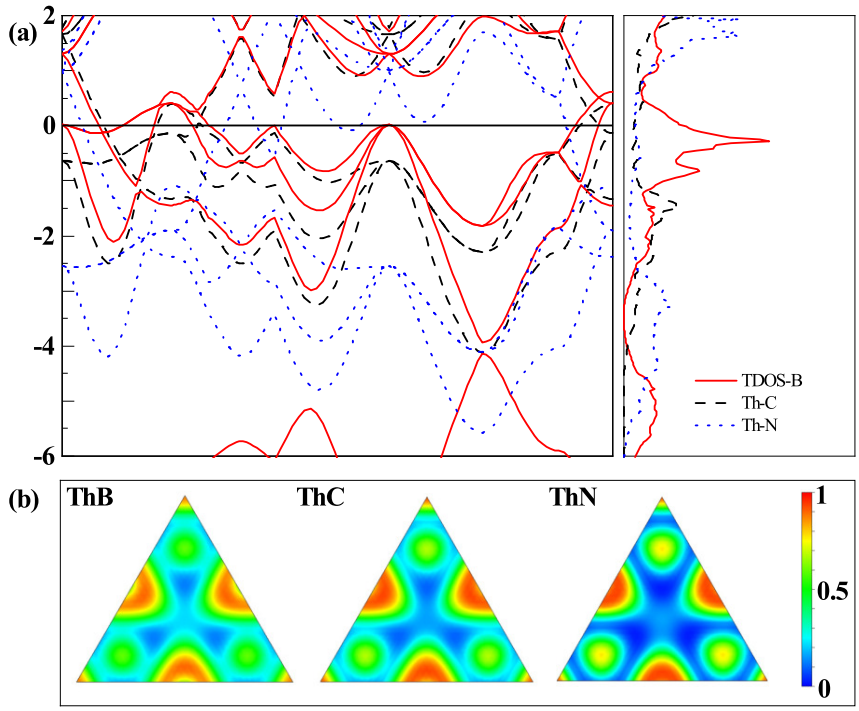

Fig. S7. (a) The energy bands of Th based light element compounds at ambient pressure. The red solid line represents the energy band of ThB, the black dashed line represents the energy band of ThC, and the blue dashed line represents the energy band of ThN. (b) ELF diagrams of the (111) plane of ThB, ThC, and ThN.

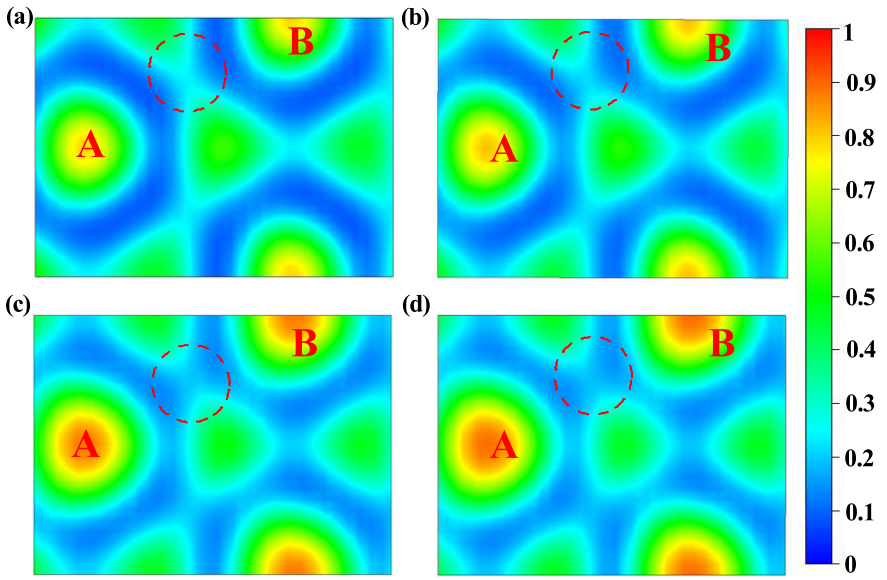

Fig. S8. The ELF diagrams of the $I4/mmm$ phase of Th in (111) plane under high pressure. (a)10 GPa, (b)20 GPa, (c)30 GPa, and (d)40 GPa. The atoms marked by "A" and "B" are the nearest-neighbor atoms.

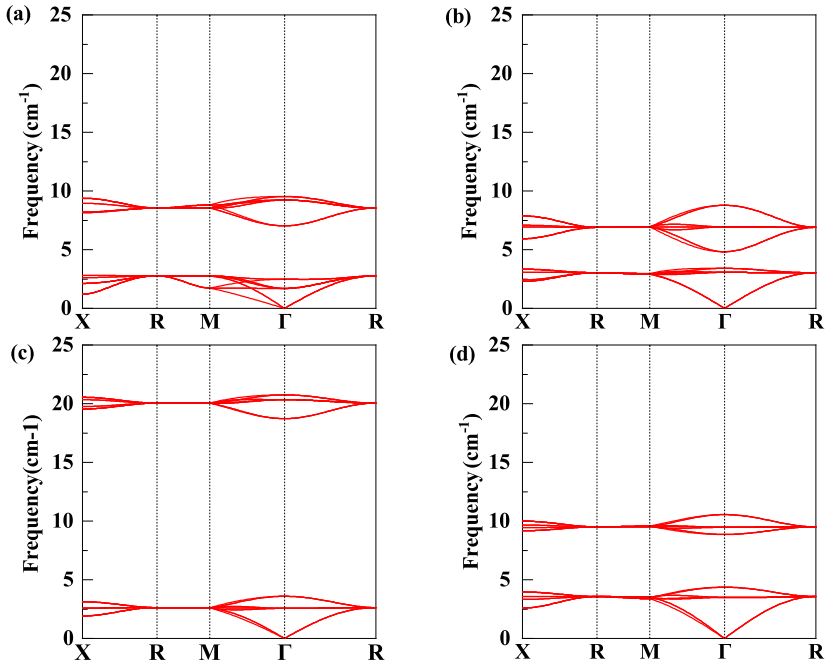

Fig. S9. Calculated phonon dispersion curves of Th based light element compounds at ambient pressure. (a) ThB, (b) ThC, (c) ThH, and (d) ThN.

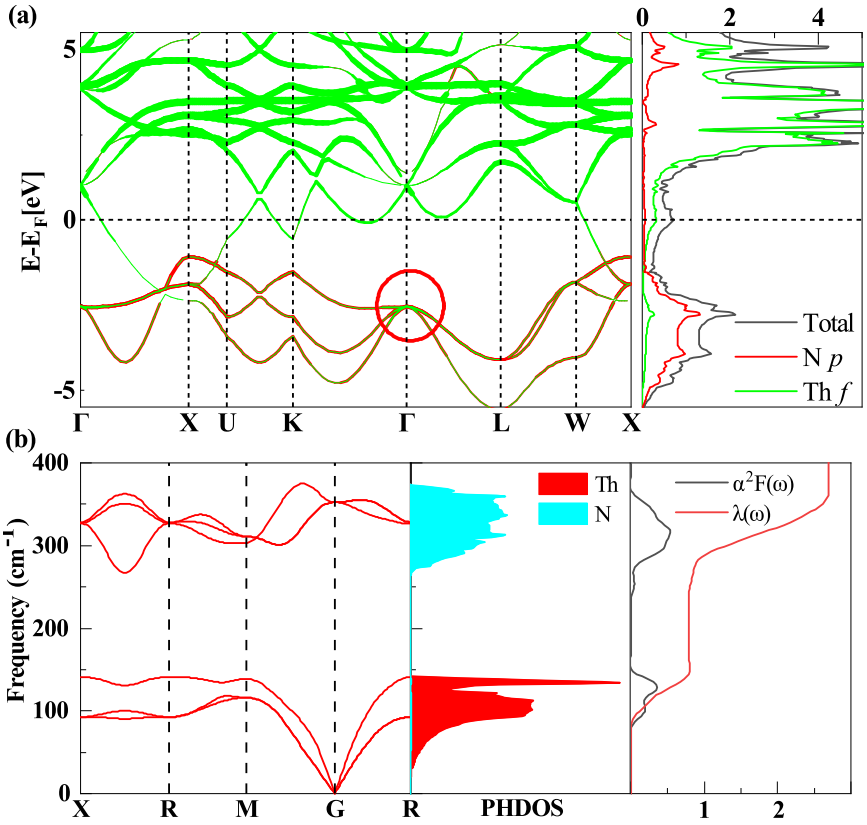

Fig. S10. (a) Electronic band structure and DOSs of ThN. The green orbital represents the $5f$ bands of Th atoms. The red orbital represents the $2p$ bands of N atoms. (b) Phonon dispersion curves, PHDOSs, Eliashberg function $\alpha^2F(\omega)$ and EPC parameter λ of the $Fm\bar{3}m$ phase of ThN under ambient pressure. The relative intensities of the EPC parameters λ_{qv} are represented by the thickness of the red line.

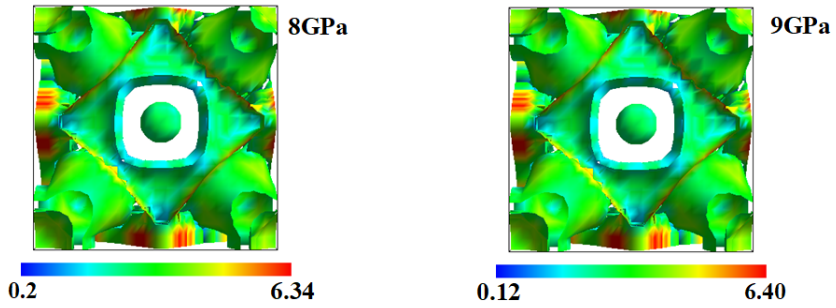

Fig. S11. The bands crossing the FEL of Th at 8GPa and 9GPa in Fmmm structure

Table S1. The calculated lattice parameters of Th at ambient pressure.

Space group	Lattice parameters	Atomic coordinates (fractional)
$Fm\bar{3}m$	$a = b = c = 4.3975$ Å	0.500 0.000 0.500
	$\alpha = \beta = \gamma = 90°$	0.500 0.500 0.000
		0.000 0.500 0.500
		0.000 0.000 0.000
$Fmmm$	a= 4.1616 Å,b= 4.6751 Å,c= 4.2708 Å	0.000 0.000 0.500
	$\alpha = \beta = \gamma = 90°$	0.000 0.500 0.000
		0.500 0.000 0.000
		0.500 0.500 0.500
$I4/mmm$	$a = b = 3.1249$ Å,$c = 4.0399$ Å	0.500 0.500 0.000
	$\alpha = \beta = \gamma = 90$ °	0.000 0.000 0.500
$Immm$	$a = 2.9065$ Å,$b = 3.0234$ Å,$c = 4.7951$ Å	0.500 0.500 0.000
	$\alpha = \beta = \gamma = 90°$	0.000 0.000 0.500

Table S2. The calculated EPC strength λ, the logarithmic average phonon frequency ω_{log}, and the T_c values of Th based light element compounds at ambient pressure.

Compounds	λ	$\omega_{log}(K)$	μ_*	$T_c(K)$
ThH	0.53	171.053	0.10	2.67K
ThB	1.02	173.626	0.10	12.48K
ThC	0.52	314.989	0.10	4.30K
ThN	0.39	280.175	0.10	1.04K
ThN_2	1.09	134.497	0.10	10.63K
Th_4H	0.64	107.657	0.10	2.99K
Th_4C	0.91	131.150	0.10	7.80K

Table S3. Calculated elastic constants (kbar) for all stable structures under different pressures.

phase	pressure	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
$Fm\bar{3}m$	0GPa	92.27	36.34	-	-	-	-	-	-	62.66
$Fmmm$	8GPa	106.97	52.05	52.38	106.09	52.87	105.29	79.09	80.74	81.91
$I4/mmm$	10GPa	170.86	2.55	62.57	-	-	114.64	87.78	-	29.76
$Immm$	60GPa	415.02	42.82	178.50	413.78	176.19	237.27	166.75	158.50	42.73
$Fm\bar{3}m$(ThB)	0GPa	124.61	84.82	-	-	-	-	39.18	-	-
$Fm\bar{3}m$(ThC)	0GPa	216.78	83.04	-	-	-	-	80.98	-	-
$Fm\bar{3}m$(ThN)	0GPa	344.25	106.30	-	-	-	-	77.42	-	-
$Fm\bar{3}m$(ThH)	0GPa	90.88	69.46	-	-	-	-	35.62	-	-

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