

Supplementary Information

First-principles investigation of pressure-induced variation in the structural and physical properties of ternary high- T_c superconductor LaBeH_8

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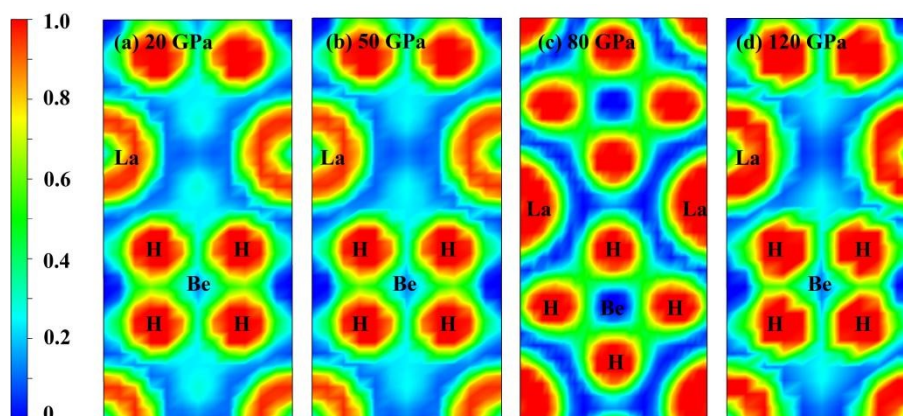


Fig. S1 The 2D electron localization function (ELF) in the (1 1 0) plane for the $Fm\bar{3}m$ - LaBeH_8 phase at 20, 50, 80 and 120 GPa.

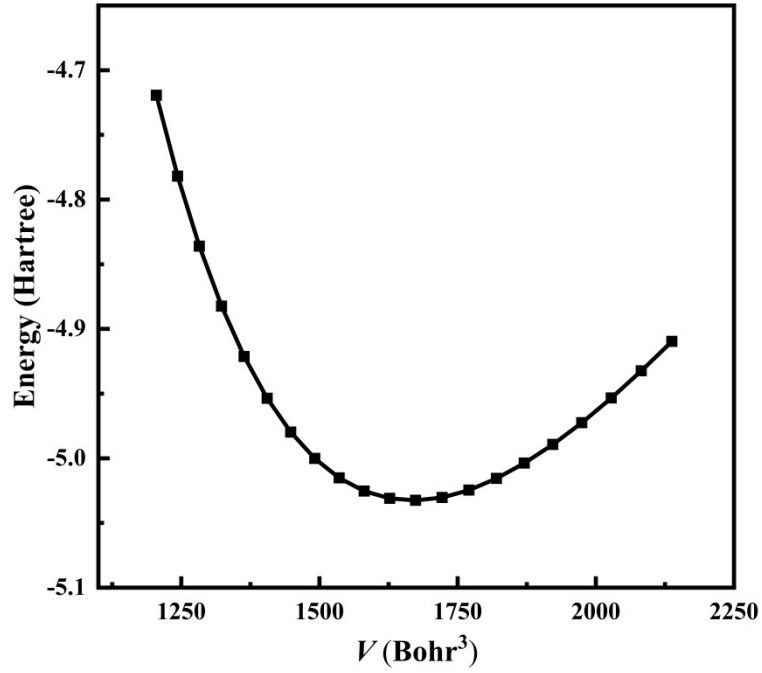


Fig. S2 The calculated total energies of $Fm\bar{3}m$ -LaBeH₈ as function of volume.

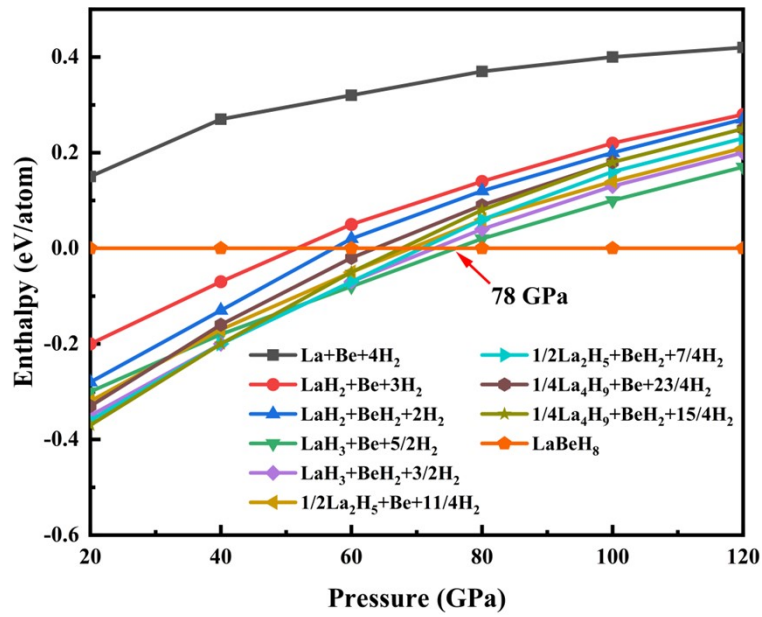


Fig. S3 Static ground-state enthalpy curves as a function of pressure with respect to $Fm\bar{3}m$ -LaBeH₈.

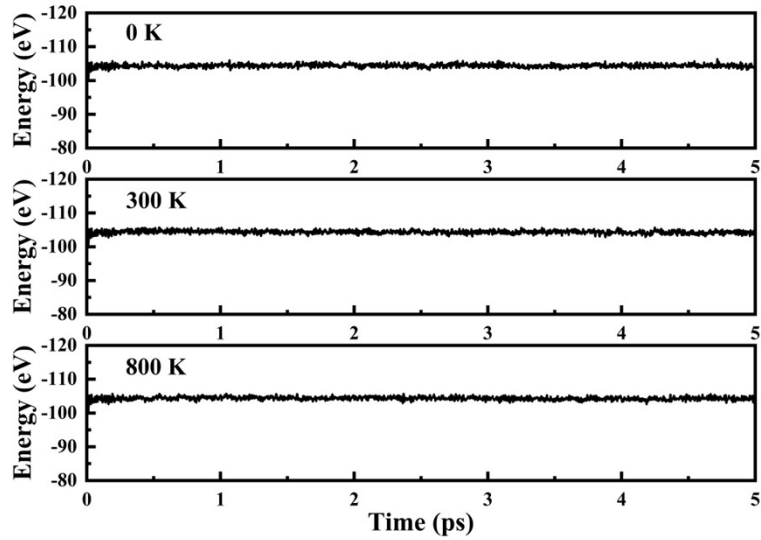


Fig. S4 Free energy as a function of MD time at the temperatures of 0, 300 and 800 K for $Fm\bar{3}m$ -LaBeH₈ at 20 GPa.

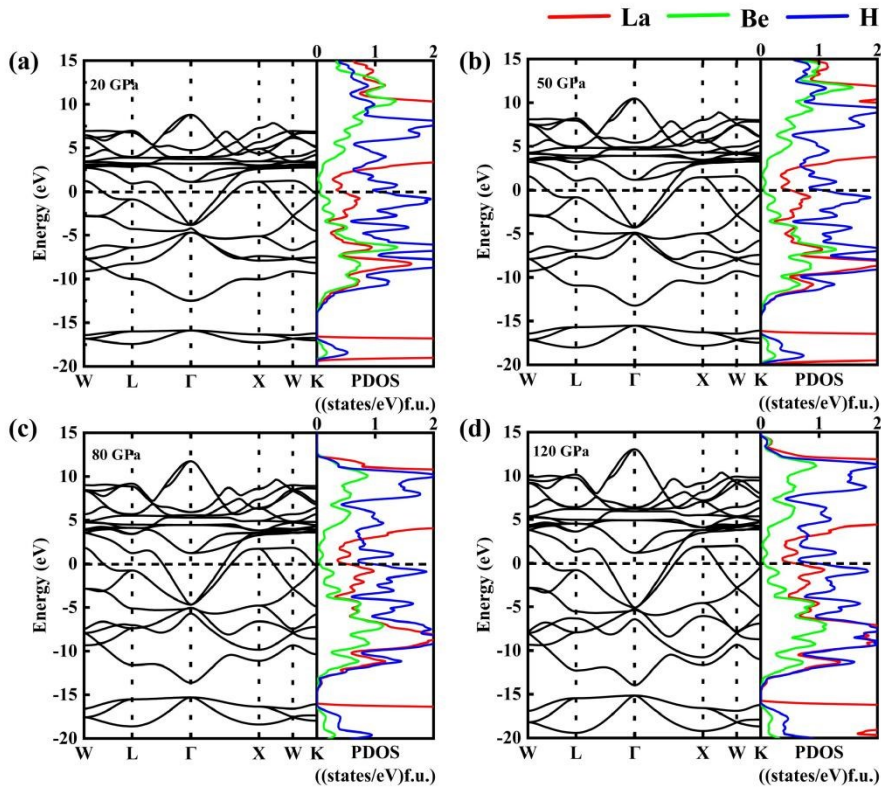


Fig. S5 The predicted electronic energy band structure and projected density of states (PDOS) of $Fm\bar{3}m$ -LaBeH₈ through the HSE06 functional under the pressures of 20, 50, 80 and 120 GPa.

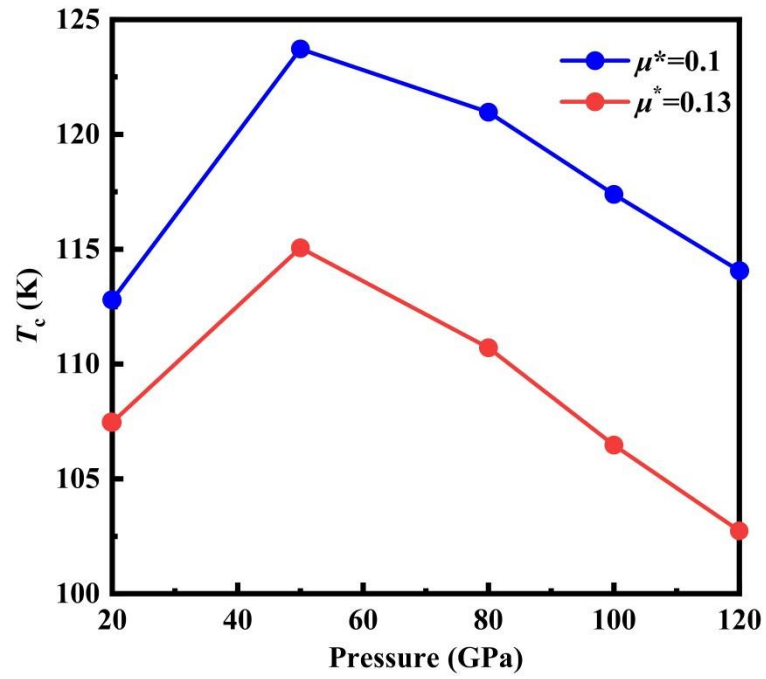


Fig. S6 The T_c values of $Fm\bar{3}m$ -LaBeH₈ as a function of pressure with the μ^* values of 0.1 and 0.13.

Table S1 The computed Bader charges of La, Be and H atoms in the $Fm\bar{3}m$ -LaBeH₈ configuration at 20, 50, 80 and 120 GPa. δ represents the quantitative charge transferred from the La or Be atom to the H atom.

Pressure (GPa)	Atom	Charge value (e)	δ (e)
20	La	9.46	1.54
	Be	0.49	1.51
	H1	1.34	-0.34
	H2	1.42	-0.42
50	La	9.61	1.39
	Be	0.47	1.53
	H1	1.32	-0.32
	H2	1.40	-0.40
80	La	9.62	1.38
	Be	0.52	1.48
	H1	1.35	-0.35
	H2	1.39	-0.39
120	La	9.75	1.25
	Be	0.48	1.52
	H1	1.33	-0.33
	H2	1.39	-0.39

Table S2 The lattice parameters, a , b and c (\AA), cell volume V (\AA^3), atomic cohesive energy E_{coh} (eV/atom) and formation enthalpy ΔH (eV/atom) for $Fm\bar{3}m$ -LaBeH₈ under different pressures.

Pressure (GPa)	Lattice parameters (\AA) $a = b = c$	V (\AA^3)	E_{coh} (eV/atom)	ΔH (eV/atom)
20	5.93	208.27	3.301	7.767
30	5.82	196.78	3.256	5.940
40	5.72	187.50	3.274	4.659
50	5.64	179.69	3.219	3.510
60	5.57	173.17	3.163	2.291
70	5.51	167.47	3.106	1.172
80	5.46	162.45	3.047	0.083
90	5.41	157.99	2.988	-0.991
100	5.36	153.89	2.927	-2.067
110	5.32	150.27	2.868	-3.074
120	5.28	147.01	2.809	-4.080

Table S3 The lattice parameters, a , b and c (Å), cell volume V (Å³) through the third-order Birch-Murnaghan equation for $Fm\bar{3}m$ -LaBeH₈ under different pressures.

Pressure (GPa)	Lattice parameters (Å) $a = b = c$	V (Å ³)
20	5.93	208.18
30	5.81	196.53
40	5.72	187.28
50	5.64	179.41
60	5.57	173.00
70	5.51	167.32
80	5.46	162.20
90	5.41	157.69
100	5.36	153.60
110	5.32	150.04
120	5.28	146.80

Table S4 The calculated elastic constants C_{ij} (GPa), Cauchy pressure CP (GPa) (C') and tetragonal shear modulus TSM (GPa) (C'') of $Fm\bar{3}m$ -LaBeH₈ under various pressures.

Pressure (GPa)	C_{ij} (GPa)			CP (GPa)	TSM (GPa)
	C_{11}	C_{12}	C_{44}	C'	C''
20	308.22	53.48	36.13	17.3	127.37
30	355.22	61.03	27.35	33.7	147.10
40	403.23	72.89	20.61	52.3	165.17
50	443.04	84.14	17.28	66.9	179.45
60	479.28	96.76	15.55	81.2	191.26
70	512.94	110.86	20.72	90.1	201.04
80	544.05	126.21	31.55	94.7	208.92
90	566.02	141.24	29.77	111.5	212.39
100	597.57	156.33	40.21	116.1	220.62
110	623.16	177.76	49.79	128.0	222.70
120	642.10	188.30	47.43	120.9	226.90

Table S5 The polycrystalline elastic parameters of $Fm\bar{3}m$ -LaBeH₈ under discrete pressures.

Pressure (GPa)	Polycrystalline elastic moduli (GPa)						
	B	G			E		
	B _V =B _R =B _H	G _V	G _R	G _H	E _V	E _R	E _H
20	138.39	72.63	50.65	61.64	185.45	135.43	161.01
30	159.09	75.25	40.57	57.91	195.00	112.17	154.93
40	183.00	78.43	31.72	55.08	205.88	89.96	150.16
50	203.77	82.15	27.07	54.61	217.25	77.77	150.40
60	224.27	85.83	24.59	55.21	228.36	71.17	153.07
70	244.89	92.85	32.32	62.59	247.30	92.87	173.02
80	265.49	102.50	47.77	75.14	272.44	135.20	205.97
90	282.83	102.82	45.38	74.10	275.12	129.23	204.45
100	303.41	112.37	59.74	86.06	300.07	168.18	235.87
110	326.23	118.95	72.21	95.58	318.18	201.74	261.23
120	339.57	119.22	69.37	94.30	320.19	194.84	258.92

Table S6 The calculated Poisson's ratio (ν), Pugh's ratio (G/B) and machinability index (μ_m) for $Fm\bar{3}m$ -LaBeH₈ under various pressures.

Pressure (GPa)	ν	G/B	μ_m
20	0.31	0.45	3.83
30	0.34	0.36	5.82
40	0.36	0.30	8.88
50	0.38	0.27	11.79
60	0.39	0.25	14.42
70	0.38	0.26	11.82
80	0.37	0.28	8.42
90	0.38	0.26	9.50
100	0.37	0.28	7.55
110	0.37	0.29	6.55
120	0.37	0.28	7.16

Table S7 The simulated shear anisotropy factors A_1 , A_2 , A_3 and A^B (in %), A^G (in %), A^U of $Fm\bar{3}m$ -LaBeH₈ under discrete pressures.

Pressure (GPa)	A_1	A_2	A_3	A^B	A^G	A^U
20	0.558	0.480	0.194	0	0.178	2.170
30	0.686	0.625	0.381	0	0.299	4.274
40	0.778	0.734	0.559	0	0.424	7.363
50	0.824	0.790	0.659	0	0.504	10.174
60	0.850	0.823	0.723	0	0.555	12.452
70	0.813	0.784	0.685	0	0.484	9.364
80	0.738	0.704	0.600	0	0.364	5.728
90	0.754	0.727	0.652	0	0.388	6.329
100	0.692	0.664	0.591	0	0.306	4.405
110	0.635	0.613	0.562	0	0.245	3.236
120	0.654	0.637	0.598	0	0.264	3.593

Table S8 The calculated transverse sound velocity (v_t), longitudinal sound velocity (v_l), average sound velocity (v_m), Vickers hardness (H_v) and density (ρ) of $Fm\bar{3}m$ -LaBeH₈ under different pressures.

Pressure (GPa)	Sound velocities (m/s)			Hardness (GPa)	ρ (gm/cm ³)
	v_t	v_l	v_m		
20	3519.90	6658.79	3934.71	5.61	4.98
30	3316.20	6699.15	3722.32	3.56	5.27
40	3157.05	6812.30	3555.88	2.10	5.53
50	3077.47	6925.97	3472.77	1.43	5.77
60	3037.85	7056.16	3432.41	1.05	5.98
70	3180.45	7284.80	3591.57	1.54	6.19
80	3432.25	7571.95	3869.79	2.69	6.38
90	3361.37	7628.55	3794.46	2.16	6.56
100	3575.47	7881.12	4031.11	3.18	6.73
110	3723.44	8111.72	4195.70	3.82	6.89
120	3657.84	8125.30	4125.39	3.36	7.05

Table S9 The calculated Grüneisen parameter (γ), Kleinman parameter (ζ), Debye temperature θ_D (K), melting temperature T_m (K) and thermal expansion coefficient α (10^{-5} K^{-1}) of $Fm\bar{3}m$ -LaBeH₈ under various pressures.

Pressure (GPa)	γ	ζ	θ_D (K)	T_m (K)	α (10^{-5} K^{-1})
20	1.81	0.33	675.9	1370.90	25.96
30	2.04	0.32	651.6	1493.23	27.63
40	2.24	0.33	632.6	1634.53	29.05
50	2.38	0.34	626.6	1757.29	29.30
60	2.47	0.35	627.0	1878.18	29.00
70	2.43	0.37	663.4	2000.25	25.57
80	2.32	0.38	722.1	2122.05	21.30
90	2.41	0.40	714.7	2224.54	21.59
100	2.31	0.41	765.9	2346.15	18.59
110	2.28	0.43	803.5	2480.98	16.74
120	2.34	0.44	795.9	2559.82	16.97

Table S10 The calculated contribution proportion (%) for the projected density of states for La, Be, and H to the total density of states around the Fermi level in $Fm\bar{3}m$ -LaBeH₈ under 20, 50, 80, and 120 GPa.

Pressure (GPa)	La	Be	H
20	32.9	3.2	63.9
50	36.6	3.4	60.0
80	36.3	3.8	59.9
120	40.1	3.9	56.0

Table S11 The calculated contribution proportion (%) for the projected density of states for La, Be, and H to the total density of states around the Fermi level within the HSE06 functional in $Fm\bar{3}m$ -LaBeH₈ under 20, 50, 80, and 120 GPa.

Pressure (GPa)	La	Be	H
20	29.9	0.9	69.2
50	32.1	1.7	66.2
80	33.3	4.0	62.7
120	33.7	7.1	59.2

Table S12 The simulated contribution ratios (%) of La, Be, and H atomic vibrations to the electron–phonon coupling (EPC) in $Fm\bar{3}m$ -LaBeH₈ at 20, 50, 80, and 120 GPa.

Pressure (GPa)	La	Be	H
20	27.6	11.6	61.3
50	9.5	5.4	82.7
80	13.4	5.3	81.9
120	14.9	5.4	79.3