Supporting Information

Superconductivity in Ce-B-H system at high pressure

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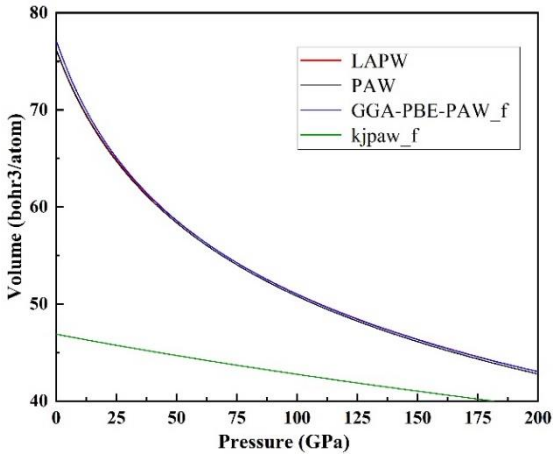

FIG. S1 Pressure-Volume diagrams of Ce element with GGA-PBE-PAW pseudopotential, ultrasoft pseudopotential, and all-electron pseudopotential

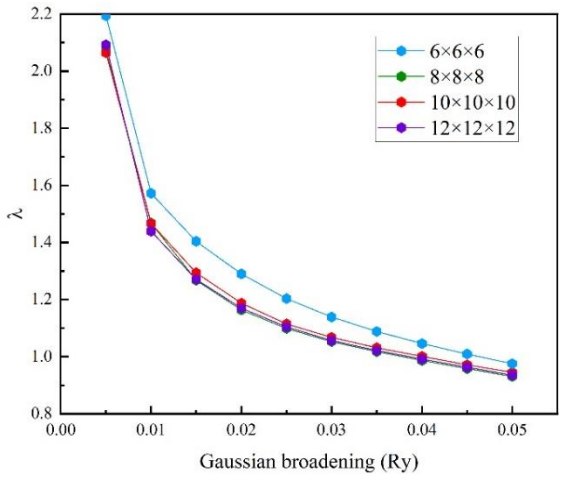

FIG. S2 Energy Electron-phonon· coupling constant λ(q) as a function of the-Gaussian broadening σ for Ce_2BH_{14} at q=0 at 100 GPa. We believe that 12×12×12 k-meshes are converged in Ce_2BH_{14}.

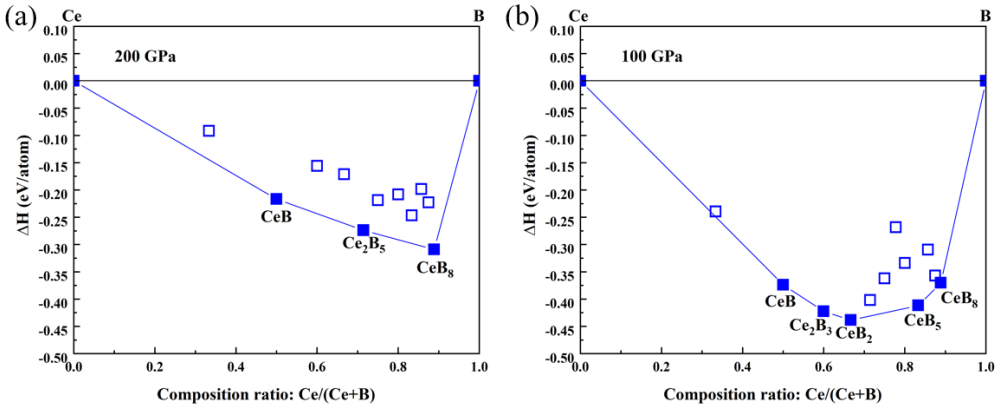

FIG. S3 Convex hull diagrams of Ce-B system at 100 GPa (a) and 200 GPa (b).

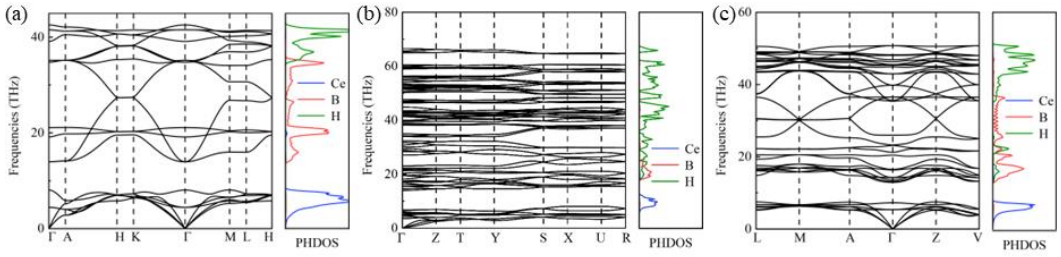

FIG. S4 Phonon dispersions, projected phonon density of states (PHDOS) of (a) CeBH, (b) $CeBH_7$, and(c) CeB_2H_3 at 100 GPa.

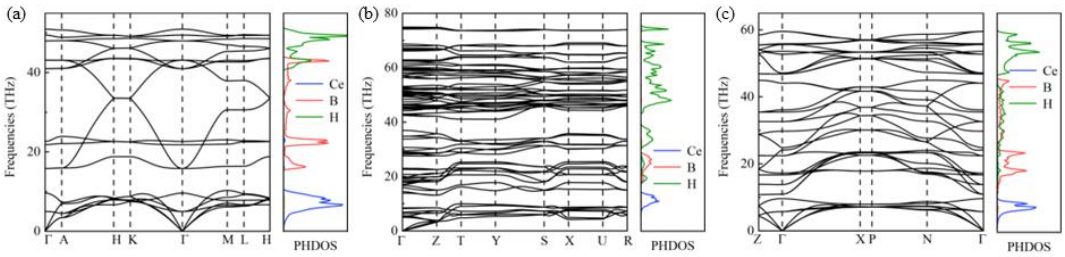

FIG. S5 Phonon dispersions, projected phonon density of states (PHDOS) of (a) CeBH, (b) $CeBH_7$, and (c) CeB_2H_3 at 200 GPa.

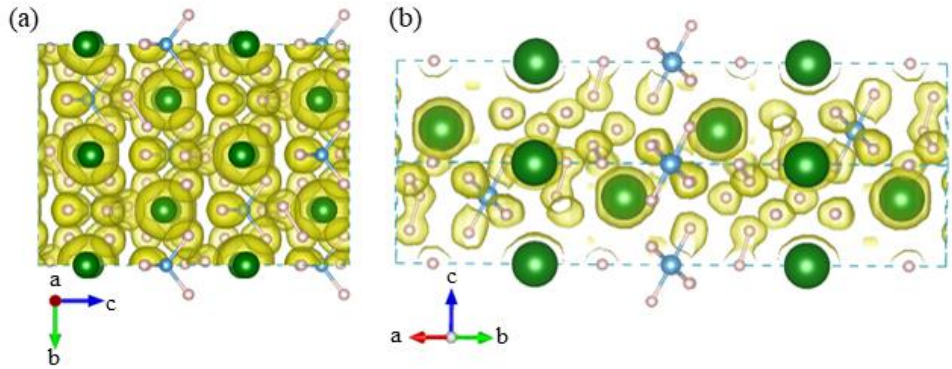

FIG. S6 Electron localization function (ELF) maps of (a) Ce_2BH_{14} (100 GPa), and (b) Ce_2BH_{16} (100 GPa).

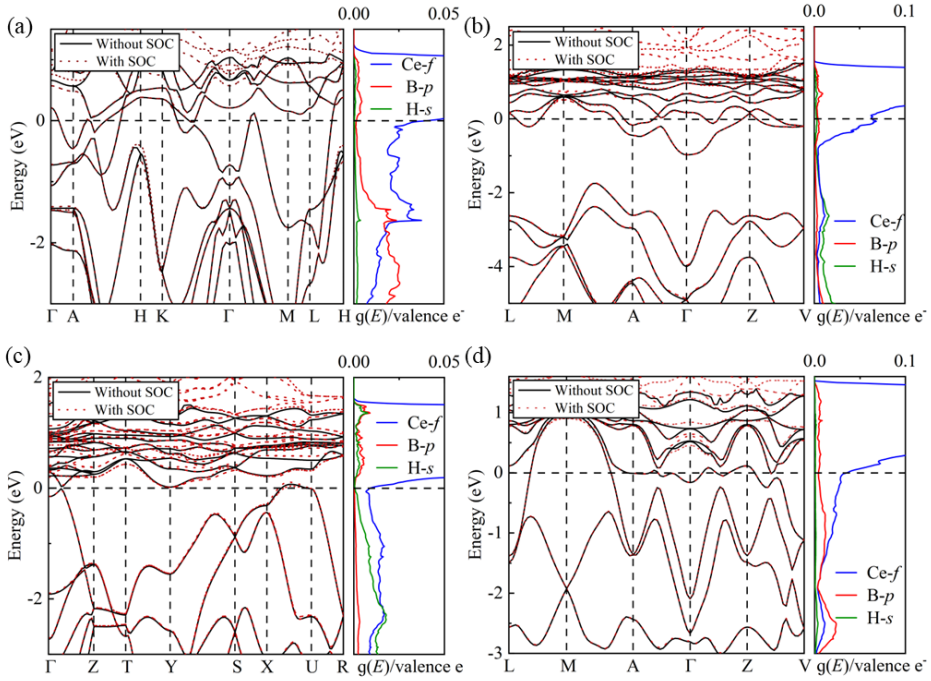

FIG. S7 Energy band, projected electronic density of states (PDOS) of (a) CeBH ,(b) $CeBH_6$,(c) $CeBH_7$, and (d) CeB_2H_3 at 100 GPa.

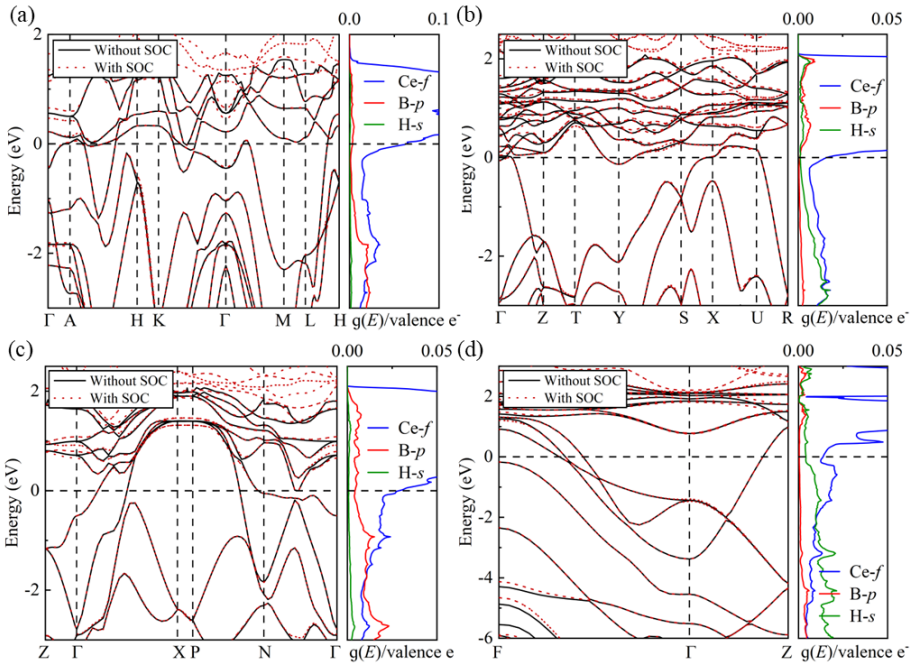

FIG. S8 Energy band, projected electronic density of states (PDOS) of (a) CeBH, (b) $CeBH_7$, (c) CeB_2H_3, and (d) Ce_2BH_{16} at 200 GPa.

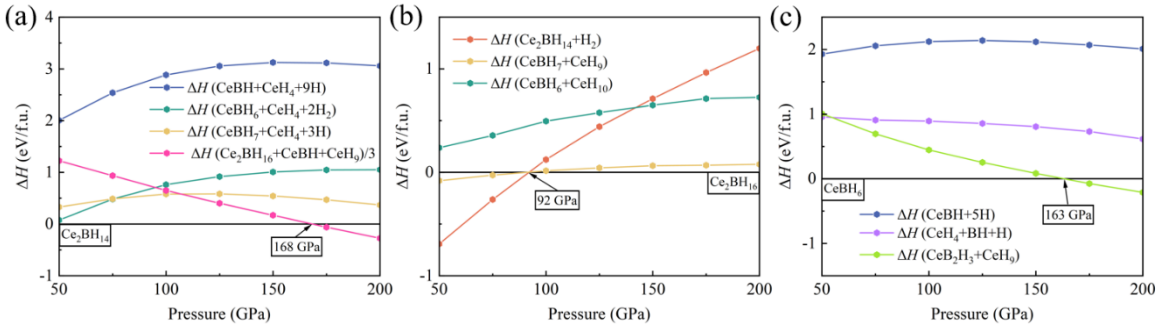

FIG. S9 The enthalpies per formula unit of various structures as a function of pressure for (a) Ce_2BH_{14} (b) Ce_2BH_{16} and (c) $CeBH_6$.

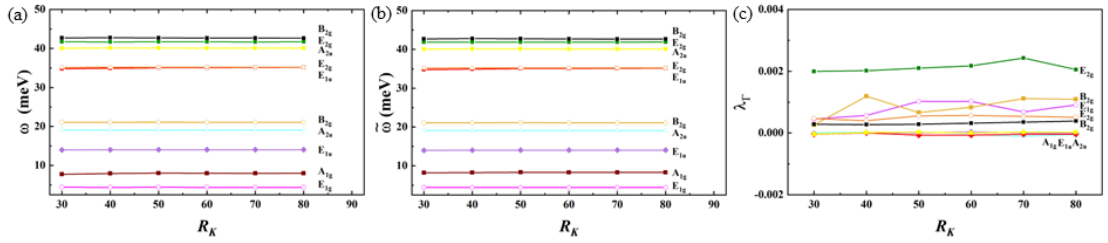

FIG. S10 Zone-center EPC strength calculations for CeBH at 100 GPa.(a) the screened phonon frequencies ω. (b) unscreened phonon frequencies $\tilde{\omega}$. (c) zone-center EPC strength λ. R_k is the reciprocal lattice spacing that determines the k grid density. Each symbol (and color) represents one phonon mode.

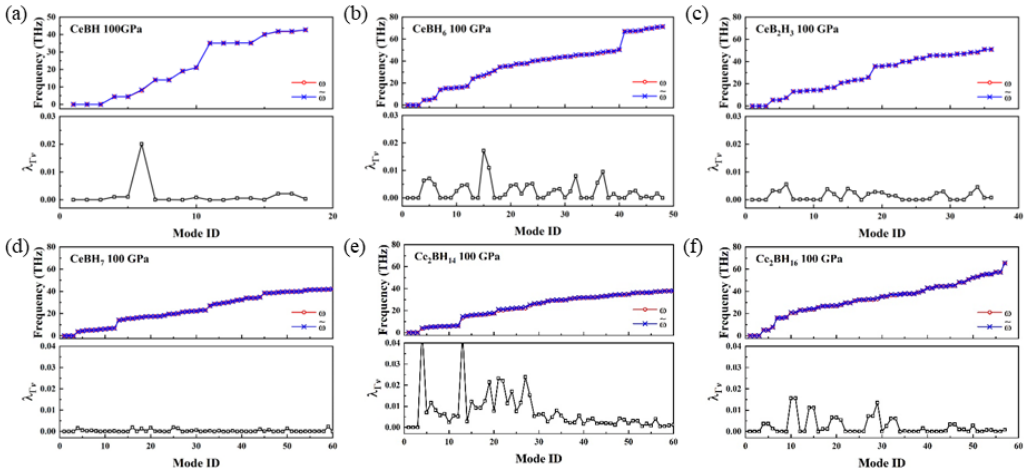

FIG. S11 (a) The screened and unscreened phonon frequencies (top panel) and zone-center EPC strength (bottom panel) of the (a) CeBH, (b) $CeBH_6$, (c) CeB_2H_3, (d) $CeBH_7$,(e) Ce_2BH_{14}-Fdd2-43 and (f) Ce_2BH_{16}-R-3m-166 at 100 GPa.

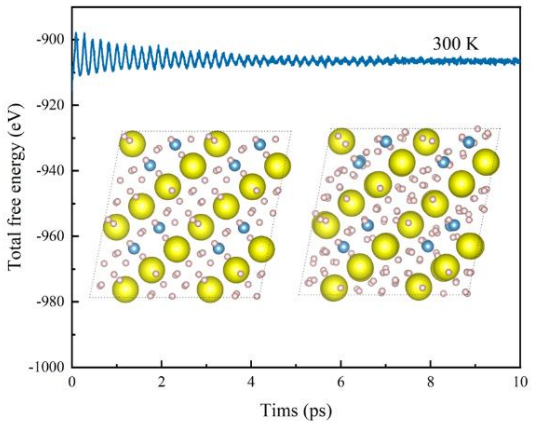

FIG. S11 the total free energy as a function of the ab initio molecular dynamics (AIMD) simulation time at 300 K under 100 GPa. The inset presents the structure snapshots of Ce_2BH_{16} at 0 and 10 ps, respectively.

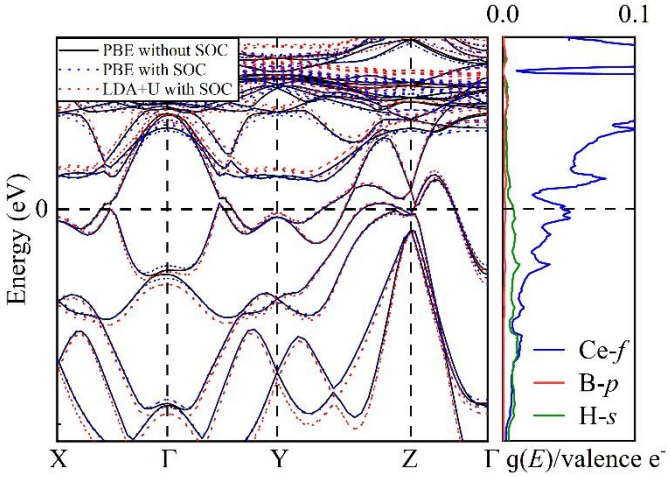

FIG. S12 Energy band of Ce_2BH_{14} at 100 GPa using PBE and LDA+U with/without the inclusion of SOC effect.

Table. S1 Structural information of Ce-B and Ce-B-H.compounds

Space group pressure	lattice parameter (Å，°)	atomic coordinate	x	y	z	sites
CeB $R\bar{3}m$	*a*=b=2.639	Ce1	0.000	0.000	0.103	6*c*
	c=17.071	B1	0.000	0.000	0.331	6*c*
200 GPa	α=β= 90					
	γ=120					
CeB_2 *P*6/*mmm*	*a*=b=2.791	Ce1	0.000	0.000	0.000	3a
	c=3.855	B1	0.667	0.333	0.500	6c
100 GPa	α=β=90					18h
	γ=120					
Ce_2B_3 $R\bar{3}m$	*a*=b=2.810	Ce1	0.667	0.333	0.472	4i
	c=40.614	Ce2	0.333	0.667	0.620	4i
100 GPa	α=β=90	B1	0.667	0.333	0.667	4i
	γ=120	B2	0.000	0.000	0.428	2a
		B3	0.667	0.333	0.572	
Ce_2B_5 *C*2/*m*	*a*=8.725	Ce1	-0.698	0.000	0.739	6c
	b=2.630	B1	-0.043	0.000	0.365	6c
200 GPa	*c*=4.24	B2	-0.426	0.000	0.816	6c
	α=90	B3	0.000	0.000	0.000	6c
	β=79.258					6c
	γ=90					
CeB_5 *P*4/*mmm*	*a*=b=3.864	Ce1	0.000	0.000	0.000	1a
	c= 2.765	B1	0.500	0.500	0.000	2d
100 GPa	α=β=γ=90	B2	0.201	0.500	0.500	
CeB_8 $R\bar{3}m$	*a*=b=4.492	Ce1	0.000	0.000	0.000	3a
	c=8.221	B1	0.000	0.000	0.281	6c
200GPa		B2	-0.276	-0.138	0.429	18h
CeBH *P*6/*mmm*	*a*=b=2.822	Ce1	0.000	0.000	0.000	2e
	c= 6.545	B1	0.333	0.667	0.500	2d
100 GPa	α=β=90	H1	0.333	0.667	0.000	2c
	γ=120					
$CeBH_6$ *C*2/*c*	*a*=7.352	Ce1	-1.500	0.462	-0.750	4e
	b=3.623	B1	-1.000	0.541	-0.250	4e
100 GPa	*c*=5.267	H1	-0.474	0.176	-0.110	8f
	α=γ=90	H2	-1.030	0.320	-0.795	8f
	β=138.135	H3	-0.701	0.411	-0.104	8f
$CeBH_7$ *Pnma*	*a*=7.352	Ce1	1.398	0.250	0.732	4c
	b=3.623	B1	0.648	0.750	0.784	4c
100 GPa	*c*=5.267	H1	1.327	0.519	0.059	8d
	α=β=γ=90	H2	0.859	0.519	0.117	8d
		H3	1.440	0.750	0.562	4c
		H4	0.985	0.750	0.611	4c
		H5	1.311	0.750	0.785	4c

CeB_2H_3 *C*2/*c*	*a*=b=4.284	Ce1	-0.500	0.122	0.250	4e
	c= 9.435	B1	-0.803	0.616	0.042	8f
100 GPa	α=γ=90	H1	-0.929	0.102	-0.052	8f
	β=132.742	H2	-1.000	0.126	-0.250	4e
Ce_2BH_{14} *Fdd2*	*a*=7.2002	Ce1	-0.750	-0.750	-0.752	8a
	b=7.1316	Ce2	-0.750	-0.750	-0.237	8a
100 GPa	*c*=10.2105	B1	-0.750	-0.750	-0.494	8a
	α=β=γ=90	H1	-0.516	-0.762	-0.371	16b
		H2	-0.871	-0.507	-0.683	16b
		H3	-0.750	-0.616	-0.930	16b
		H4	-0.744	-0.381	-0.555	16b
		H5	-0.750	-0.886	-0.424	16b
		H6	-1.115	-0.750	-0.561	16b
		H7	-0.617	-0.750	-0.567	16b
Ce_2BH_{16} $R\bar{3}m$	*a*=b=3.685	Ce1	0.000	0.000	0.253	6c
	c=17.347	B1	0.000	0.000	0.500	3b
100 GPa	α=β=90	H1	0.000	0.000	0.625	6c
	γ=120	H2	0.181	-0.181	0.535	18h
		H3	-0.170	0.170	0.358	18h
		H4	0.000	0.000	0.067	6c