

Supplementary Information for the paper entitled “Pressure
induced evolution of structures and Promising Superconductivity of
ScB₆”

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Table S1 The crystal structural information of ScB₆ under pressure

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phase	Lattice constants (Å)	Atom	Atomic	Positions	
P2 ₁ /m 0GPa	a =5.740	Sc (2e)	0.278	0.25	0.883
	b =4.488	B (4f)	0.291	0.545	0.341
	c =5.004	B (4f)	0.016	0.449	0.663
	$\alpha=\gamma=90^\circ$	B (2e)	0.791	0.25	0.307
	$\beta=65.1^\circ$	B (2e)	0.505	0.25	0.264
C2/m 500GPa	a =7.086	Sc (4i)	0.179	0	0.716
	b =2.392	B (4i)	0.042	0	0.173
	c =7.591	B (4i)	0.348	0	0.057
	$\alpha=\gamma=90^\circ$	B (4i)	0.867	0	0.954
	$\beta=121.8^\circ$	B (4i)	0.037	0.5	0.273
		B (4i)	0.666	0.5	0.411
		B (4i)	0.912	0.5	0.519
Cmcm 800GPa	a =2.249	Sc (4c)	0.5	0.095	0.75
	b =9.672	B (8f)	0	0.203	0.056
	c =4.296	B (8f)	0	0.944	0.912
	$\alpha=\beta=\gamma=90^\circ$	B (4c)	0	0.249	0.75
		B (4c)	0.5	0.107	0.25

Table S2 The calculated bulk modulus B (GPa), shear modulus G (GPa), Young's modulus Y (GPa), B/G ,

Poisson's ratio ν , and hardness H_V (GPa) of three phases of ScB_6 in comparison with available theoretical and experimental results.

structure	work	B	G	Y	G/B	ν	H_V
$\text{P2}_1/\text{m-ScB}_6$	this work	174	126	303	0.722	0.209	20.2
C2/m-ScB_6	this work	220	156	379	0.707	0.214	16.2
Cmcm-ScB_6	this work	205	164	388	0.797	0.185	27.3
C2/m-ScB_3	Ref 25	199	189	430	0.948	0.139	37.1
P6/mmm-ScB_2	Ref 23	191	194	435	1.017	0.12	41.4
P6/mmm-ScB_2	Ref 43	198.9	201.4	451.8	1.013	0.121	42.1
P6/mmm-ScB_2	Exp 43						17.46
Fm-3m-ScB_{12}	Ref 23	219	194	450	0.887	0.157	34.4
R-3m-ScB	Ref 23	109	74	181	0.678	0.224	12.7
$\alpha\text{-BeB}_6$	Ref 12	222	227	508	1.02	0.12	46.0

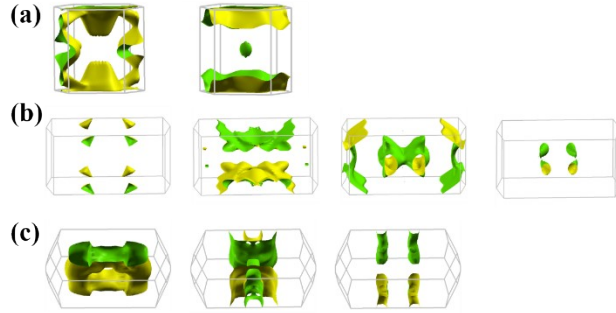


Fig.S1 The Fermi surface (a) $P2_1/m$ at 0GPa (b) $C2/m$ at 500GPa (c) $Cmcm$ at 800GPa.

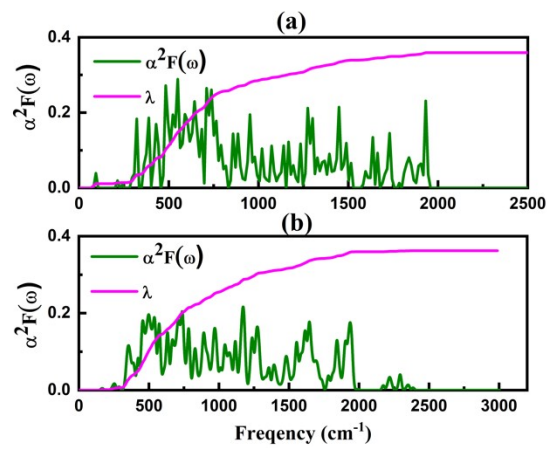


Fig.S2 The Eliashberg EPC spectral function $\alpha^2F(\omega)$, and the cumulative EPC integral $\lambda(\omega)$ of $C2/m$ - and $Cmcm$ - ScB_6 at 500GPa and 800GPa, respectively.