

Supplementary information: Superconductivity and high hardness in scandium-borides under pressure

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I. STRUCTURE INFORMATION

The crystal structures of all discovered thermodynamically stable and superconducting scandium-borides in our research are listed in Table I. The information of all other thermodynamically stable and superconducting scandium-borides are reference to previous researches [1, 2].

TABLE I: The crystal structures of the discovered thermodynamically stable and superconducting scandium-borides as presented in Fig. 1 of the main text.

Phase	Space Group	Pressure (GPa)	Lattice Parameter	Wyckoff Positions				
				atoms	site	x	y	z
Sc ₈ B	R-3	0	a=8.6373	Sc	18f	0.0240	0.7326	0.6010
			c=9.1605	Sc	6c	0.0000	0.0000	0.1923
				B	3b	0.0000	0.0000	0.5000
ScB	P6 ₃ /mmc	260	a=2.7021	Sc	4f	0.3333	0.6667	0.9181
			c=8.1520	B	2b	0.0000	0.0000	0.2500
				B	2c	0.3333	0.6667	0.2500
ScB ₄	C2/m	0	a=8.7558	Sc	4i	0.0690	0.5000	0.7955
			b=3.0240	B	4i	0.1069	0.0000	0.0938
			c=7.2172	B	4i	0.1170	0.0000	0.5371
			β=119.67	B	4i	0.2123	0.5000	0.1956
				B	4i	0.2333	0.0000	0.3842
ScB ₆	P4/mmm	90	a=2.8386	Sc	1d	0.5000	0.5000	0.5000
			c=5.2039	B	4i	0.0000	0.5000	0.1547
				B	2g	0.0000	0.0000	0.3304
ScB ₆	I4/mmm	90	a=2.8373	Sc	2a	0.0000	0.0000	0.0000
			c=10.4185	B	8g	0.0000	0.5000	0.1727
				B	4e	0.0000	0.0000	0.4155
ScB ₇	Cmcm	90	a=2.7406	Sc	4c	0.0000	0.3312	0.7500
			b=8.2914	B	8f	0.0000	0.0466	0.6475
			c=8.2110	B	8f	0.0000	0.1176	0.0386
				B	4c	0.0000	0.3213	0.0584
ScB ₁₄	Pm-3	0	a=4.7611	Sc	1a	0.0000	0.0000	0.0000
				B	8i	0.3051	0.3051	0.3051
				B	6g	0.0000	0.1766	0.5000

II. EL-PH CALCULATIONS

	kmesh	qmesh
Sc_8B (R-3)	$9 \times 9 \times 9$	$3 \times 3 \times 3$
ScB_4 (C2/m)	$16 \times 16 \times 8$	$4 \times 4 \times 2$
ScB_4 (I4/mmm)	$18 \times 18 \times 9$	$6 \times 6 \times 3$
ScB_6 (P4/mmm)	$18 \times 18 \times 9$	$6 \times 6 \times 3$
ScB_6 (I4/mmm)	$12 \times 12 \times 12$	$4 \times 4 \times 4$
ScB_{14} (Pm-3)	$12 \times 12 \times 12$	$4 \times 4 \times 4$

TABLE II: The adopted k-points and q-points in calculations of all discovered superconductors.

III. FORMATION ENTHALPY OF SCB₄

In order to determine the thermodynamically stable phase of ScB₄ stoichiometry at low and medium pressures, we have calculated the formation enthalpy of three structures, ScB₄ (C2/m), ScB₄ (Pnma) and ScB₄ (I4/mmm), with high precision. As shown in Fig.1, ScB₄ (C2/m) has the lowest formation enthalpy in pressure range of 48-124 GPa.

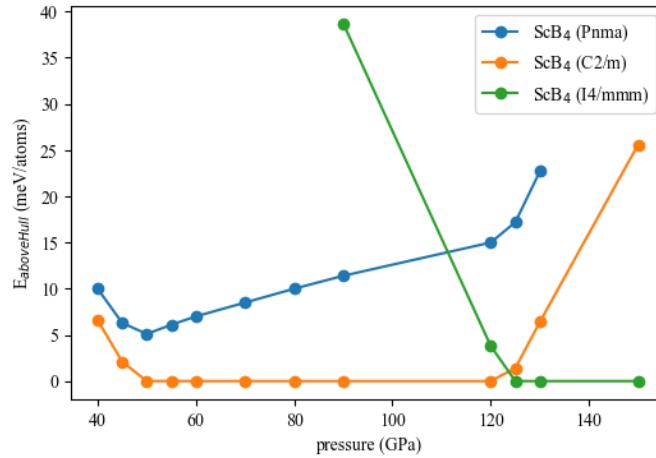


FIG. 1: Formation enthalpy above the convex hull of ScB₄ (C2/m), ScB₄ (Pnma) and ScB₄ (I4/mmm) as a function of pressure. The zero energy points locate at the convex hull.

IV. BADER CHARGES

TABLE III: The atomic net charges from Bader charge analysis in ScB₄ (C2/m) at the ambient pressure.

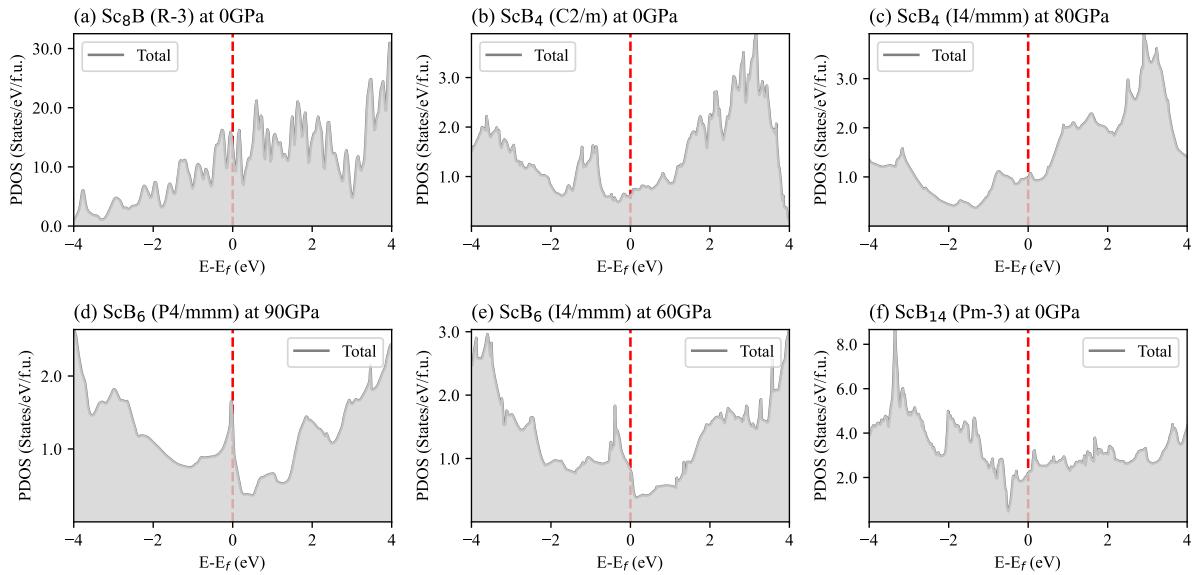
Atom	site	X	Y	Z	Charge (e)
Sc	4i	0.06897	0.5	0.79546	+1.46
B	4i	0.10686	0	0.09382	-0.55
B	4i	0.11696	0	0.53711	-0.50
B	4i	0.21233	0.5	0.19557	-0.51
B	4i	0.2333	0	0.38422	+0.09

TABLE IV: The atomic net charges from Bader charge analysis in ScB_{14} (Pm-3) at the ambient pressure.

Atom	site	X	Y	Z	Charge (e)
Sc	1a	0	0	0	+1.48
B	8i	0.3051	0.3051	0.3051	-0.12
B	6g	0	0.17663	0.5	-0.09

V. ELECTRONIC STRUCTURE

The total DOS, the bandstructures and the Fermi surfaces of all discovered superconducting scandium-borides at their lowest dynamically stable pressures are shown in Fig. 2, Fig. 3 and Fig. 4, respectively. The total DOS of insulating ScB_{15} (P4₁) at the ambient pressure is shown in Fig. 5.

FIG. 2: The total electronic DOS of (a) Sc_8B (R-3), (b) ScB_4 (C2/m), (c) ScB_4 (I4/mmm), (d) ScB_6 (P4/mmm), (e) ScB_6 (I4/mmm) and (f) ScB_{14} (Pm-3), at their lowest dynamically stable pressures.

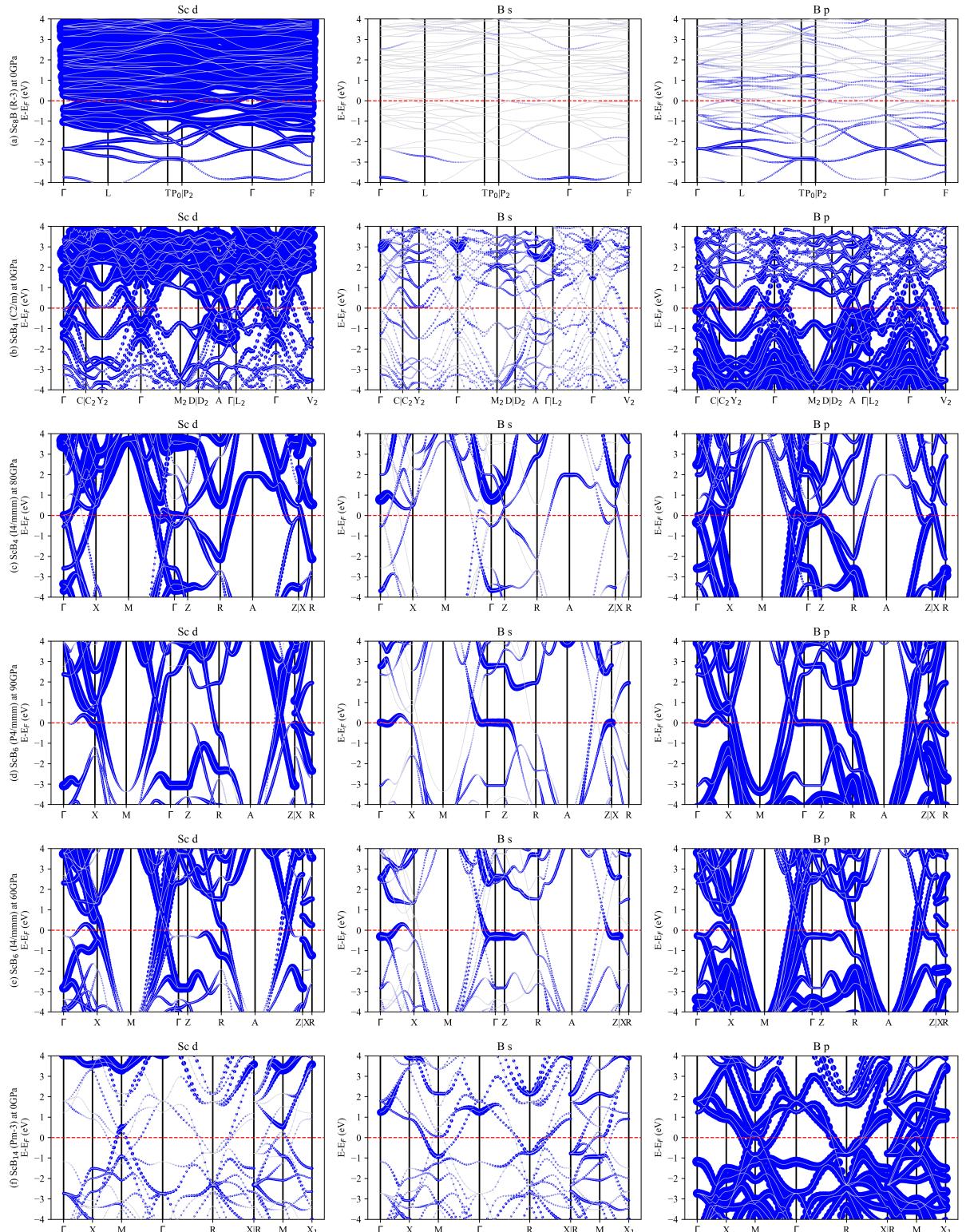


FIG. 3: Projected band structure of superconducting scandium-borides (a) Sc_8B (R-3), (b) ScB_4 ($\text{C}2/\text{m}$), (c) ScB_4 ($\text{I}4/\text{mmm}$), (d) ScB_6 ($\text{P}4/\text{mmm}$), (e) ScB_6 ($\text{I}4/\text{mmm}$) and (f) ScB_{14} ($\text{P}m-3$), at their lowest dynamically stable pressures.

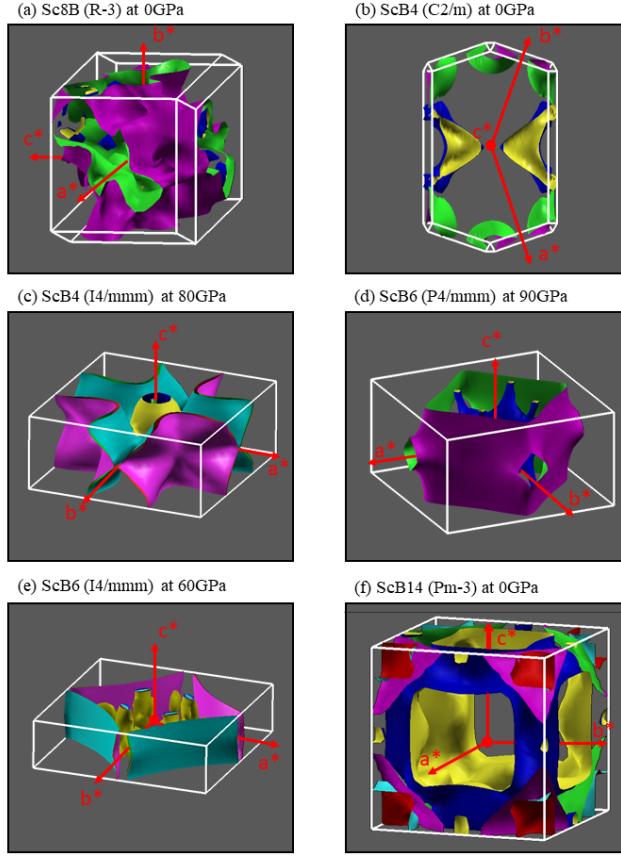


FIG. 4: Fermi surface of superconducting scandium-borides (a) Sc₈B (R-3), (b) ScB₄ (C2/m), (c) ScB₄(I4/mmm), (d) ScB₆ (P4/mmm), (e) ScB₆ (I4/mmm) and (f) ScB₁₄ (Pm-3), at their lowest dynamically stable pressures.

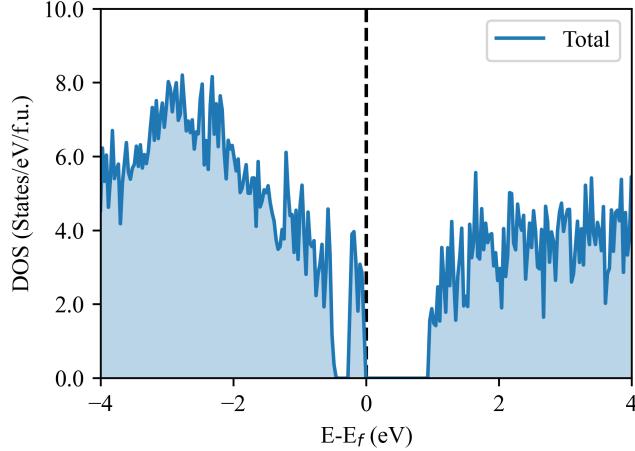


FIG. 5: The total DOS of ScB₁₅ (P4₁) at the ambient pressure.

VI. HARDNESS

The mechanical properties of the three superconducting scandium-borides, Sc_8B (R-3m), ScB_4 (C2/m) and ScB_{14} (P-3m), are calculated at the ambient pressure as shown in the following table. All data meet the stability criteria for the corresponding lattice type.[3]

TABLE V: The calculated elastic constants C_{ij} (GPa) of superconducting scandium-borides, Sc_8B (R-3m), ScB_4 (C2/m) and ScB_{14} (P-3m), at the ambient pressure.

Sc_8B (R-3m)						
113.835	33.795	40.191	-6.826	1.637	0	
33.795	113.835	40.191	6.826	-1.637	0	
40.191	40.191	98.979	0	0	0	
-6.826	6.826	0	32.422	0	-1.637	
1.637	-1.637	0	0	32.422	-6.826	
0	0	0	-1.637	-6.826	40.02	
ScB_4 (C2/m)						
476.484	77.154	77.231	0	20.509	0	
77.154	527.696	62.026	0	-6.383	0	
77.231	62.026	431.766	0	27.511	0	
0	0	0	47.155	0	13.855	
20.509	-6.383	27.511	0	180.515	0	
0	0	0	13.855	0	199.496	
ScB_{14} (P-3m)						
365.786	175.148	175.148	0	0	0	
175.148	365.786	175.148	0	0	0	
175.148	175.148	365.786	0	0	0	
0	0	0	137.257	0	0	
0	0	0	0	137.257	0	
0	0	0	0	0	137.257	
ScB_{15} (P4 ₁)						
462.079	92.563	61.453	0	0	2.021	
92.563	462.079	61.453	0	0	-2.021	
61.453	61.453	478.950	0	0	0	
0	0	0	201.404	0	0	
0	0	0	0	201.404	0	
2.021	-2.021	0	0	0	205.098	

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- [2] B.-H. Chu and Y. Zhao, Chinese Physics B **30**, 076107 (2021), URL <https://dx.doi.org/10.1088/1674-1056/abe116>.
- [3] F. Mouhat and F. m. c.-X. Coudert, Phys. Rev. B **90**, 224104 (2014), URL <https://link.aps.org/doi/10.1103/PhysRevB.90.224104>.