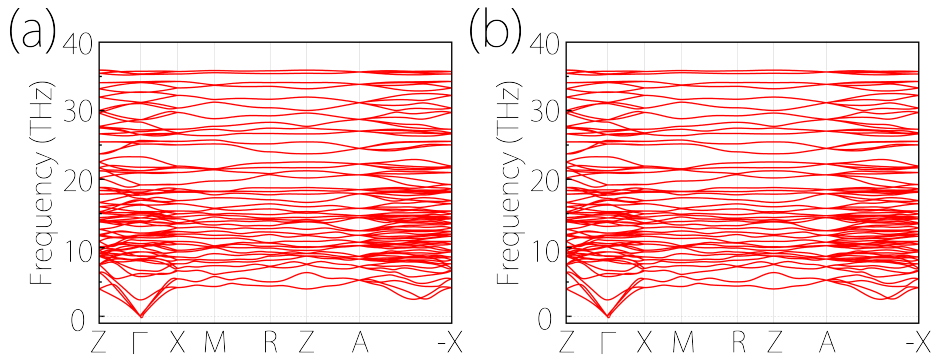
Supplementary Information of "Single-pair charge-2 Weyl–Dirac composite semimetals"

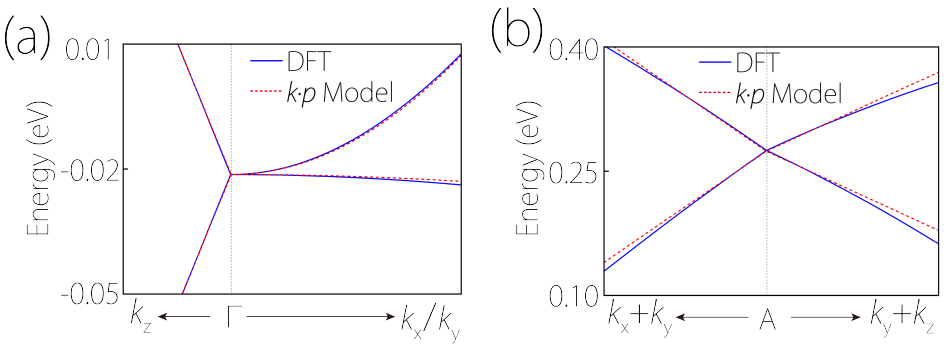
Hui-Jing Zheng*, Ke-Xin Pang*, Yun-Yun Bai, Yanfeng Ge, and Yan Gao†

State Key Laboratory of Metastable Materials Science and Technology & Hebei Key Laboratory of Microstructural Material Physics, School of Science, Yanshan University, Qinhuangdao 066004, China

*These authors contributed equally to this work.
†Corresponding authors: yangao9419@ysu.edu.cn



Supplementary Figure S1 | Dynamical stability of the two chiral boron allotropes *l*-SDHBN-B_{28} and *r*-SDHBN-B_{28}. Phonon spectrum of **a**, *l*-SDHBN-B_{28} and **b**, *r*-SDHBN-B_{28} calculated along the entire high-symmetry paths in the BZ.



Supplementary Figure S2 | The DFT versus the $\boldsymbol{k\cdot p}$ effective Hamiltonian band structures for SDHBN-B_{28}. a, Band dispersion along k_z and k_x/ k_y at Γ from DFT calculations (blue solid lines) and $\boldsymbol{k\cdot p}$ model fitting (red dashed lines). Parameters for the $\boldsymbol{k\cdot p}$ effective Hamiltonian: $\epsilon_0 = -0.02$ eV, $m = -2.41$ eV·Å, $\epsilon_1 = 4.33$ eV·Å^2, $\epsilon_2 = 0.20$ eV·Å^2, $\alpha = 2.43$ eV·Å^2, $\beta = 4.03i$ eV·Å^2. **b**, Band dispersion along k_x+k_y and k_y+k_z at A from DFT calculations (blue solid lines) and $\boldsymbol{k\cdot p}$ model fitting (red dashed lines). Parameters for the $\boldsymbol{k\cdot p}$ effective Hamiltonian: $\alpha = 0.27$ eV, $\beta = 0.20$ eV·Å, $\gamma = 1.78$ eV·Å.

Table SI. Structural parameters and topological characteristics of representative boron allotropes. Listed are the space groups, lattice parameters (Å), lattice angles (°), Wyckoff positions, bond lengths (Å), densities (g/cm^3), bulk moduluses (GPa), total energies E_{tot} (eV per B atom) for *l*-SDHBN-B_{28}, *r*-SDHBN-B_{28}, H-boron, Ort-B_{32}, and 3D α' boron. The corresponding topological phases are also indicated, including nodal-line semimetal (NLSM) states and charge-2 Weyl and Dirac nodes (C-2 WP and C-2 DP), which denote Weyl and Dirac points carrying a topological charge of $|C| = 2$, respectively.

Structures		Space groups	Lattice parameters(Å)			Angles(◦)			Wyckoff position			Bond lengths (Å)	Densities (g/cm^3)	Bulk moduluses (GPa)	E_{tot} (eV/B)	Properties
			a	*b*	*c*	*α*	*β*	*γ*	*x*	*y*	*z*					
l-SDHBN-B_{28}	B1(8b)	$P4_32_12$	6.66	6.66	6.00	90	90	90	0.7246	0.4705	1.4018	1.66-1.99	1.89	168.66	-6.26	C-2 WP C-2 DP
	B2(8b)								0.9932	0.1019	1.3884					
	B3(8b)								0.1043	0.4616	1.0904					
	B4(4*a*)								0.7623	0.2378	1.2500					
r-SDHBN-B_{28}	B1(8b)	$P4_12_12$	6.66	6.66	6.00	90	90	90	0.2754	0.5295	0.0982	1.66-1.99	1.89	168.65	-6.26	C-2 WP C-2 DP
	B2(8b)								0.0069	0.8981	0.1116					
	B3(8b)								0.8957	0.5384	0.4096					
	B4(4*a*)								0.2378	0.7623	0.2500					
H-boron	B1(12*k*)	$P6_3/mmc$	6.06	6.06	9.91	90	90	120	0.5727	0.4273	0.5277	1.62-1.71	0.91	70.83	-5.84	NLSM
	B2(4*f*)								0.3333	0.6667	0.3319					
Ort-B_{32}	B1(16*h*)	*Cmcm*	6.61	8.09	4.95	90	90	90	-0.6230	-0.2970	1.4600	1.63-2.09	2.17	193.76	-6.29	NLSM
	B2(8*f*)								-0.5000	0.0870	0.5860					
	B3(8*g*)								-0.2690	-0.1530	1.2500					
3D α′ boron	B1(16*h*)	Cmcm	7.73	8.23	5.07	90	90	90	0.1696	0.7072	0.0837	1.66-1.85	1.78	166.86	-6.36	NLSM
	B2(8g)								0.1778	0.3063	0.2500					
	B3(8f)								-0.0000	0.5992	0.9325					

Table SII. Elastic constants and corresponding stability criteria for *l*-SDHBN-B_{28} and *r*-SDHBN-B_{28}.

Structures	Elasticity constants						Stability criteria
	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	
l-SDHBN-B_{28}	303.475	100.345	103.458	296.467	165.259	178.657	$C_{11} > \|C_{12}\|$; $2C_{13}^2 < C_{33}(C_{11} + C_{12})$; $C_{44} > 0$; $C_{66} > 0$
r-SDHBN-B_{28}	303.463	100.331	103.452	296.437	165.255	178.648	

Table SIII. Energies, coordinates, topological charges, and multiplicities of the C-2 WP and C-2 DP in *l*-SDHBN-B_{28} and *r*-SDHBN-B_{28}.

Structures		*E* (eV)	Coordinate (k_1, k_2, k_3)	Charge	Multiplicity
l-SDHBN-B_{28}	WP	-0.020	(0,0,0)	+2	1
	DP	0.274	(0.5, 0.5, 0.5)	-2	1
r-SDHBN-B_{28}	WP	-0.017	(0,0,0)	-2	1
	DP	0.277	(0.5, 0.5, 0.5)	+2	1

Table SIV. All possible magnetic space groups that can host single-pair charge-2 Weyl–Dirac nodes. MSG No. indicates the magnetic space group number. HSP (HSL) refer to the high-symmetry point (high-symmetry line) where the charge-2 Weyl point (WP) and Dirac point (DP) are located. C-2 WP and C-2 DP represent Weyl and Dirac nodes carrying a topological charge of $|C| = 2$, respectively. IRR denotes the irreducible (co)representation of the corresponding little group at the $|C| = 2$ WP or DP.

MSG No.	Generators	HSP/ HSL for C-2 DP (Irreps)	HSP/ HSL for C-2 WP (Irreps)
Type-II MSGs (without SOC)			
92.112	$\{C_{4z}^{+}\|00\frac{1}{4}\}$, $\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$, T	A ($\{R_6,R_7\}$)	Γ (R_5)
96.144	$\{C_{4z}^{+}\|00\frac{3}{4}\}$, $\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$, T	A ($\{R_6,R_7\}$)	Γ (R_5)
Type-III MSGs (without SOC)			
90.98	$\{C_{4z}^{+}\|000\}$, $\{C_{2x}T\|\frac{1}{2}\frac{1}{2}0\}$	MA($\{V_1V_3,V_2V_4\}$)	ΓZ($\{\Lambda_1,\Lambda_3\};\{\Lambda_2,\Lambda_4\}$)
92.114	$\{C_{4z}^{+}\|00\frac{1}{4}\}$, $\{C_{2x}T\|\frac{1}{2}\frac{1}{2}0\}$	MA($\{V_1V_3,V_2V_4\}$)	ΓZ($\{\Lambda_1,\Lambda_3\};\{\Lambda_2,\Lambda_4\}$)
92.115	$\{C_{2a}\|\frac{1}{2}\frac{1}{2}\frac{1}{4}\}$, $\{C_{2b}\|\frac{1}{2}\frac{1}{2}\frac{3}{4}\}$, $\{C_{2x}T\|\frac{1}{2}\frac{1}{2}0\}$	A(T_1T_2)	Γ($\Gamma_2\Gamma_4$)
94.130	$\{C_{4z}^{+}\|00\frac{1}{2}\}$, $\{C_{2x}T\|\frac{1}{2}\frac{1}{2}0\}$	MA($\{V_1V_3,V_2V_4\}$)	ΓZ($\{\Lambda_1,\Lambda_3\};\{\Lambda_2,\Lambda_4\}$)
96.146	$\{C_{4z}^{+}\|00\frac{3}{4}\}$,	MA($\{V_1V_3,V_2V_4\}$)	ΓZ($\{\Lambda_1,\Lambda_3\};\{\Lambda_2,\Lambda_4\}$)

MSG No.	Generators	HSP/ HSL for C-2 DP (Irreps)	HSP/ HSL for C-2 WP (Irreps)
	$\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$		
96.147	$\{C_{2a}\left\|\frac{1}{2}\frac{1}{2}\frac{3}{4}\right\}$, $\{C_{2b}\left\|\frac{1}{2}\frac{1}{2}\frac{1}{4}\right\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$A(T_1T_2)$	$\Gamma(\Gamma_2\Gamma_4)$
Type-III MSGs (with SOC)			
90.98	$\{C_{4z}^{+}\|000\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$MA(\{V_5V_7,V_6V_8\})$	$\Gamma Z(\{\Lambda_5,\Lambda_7\};\{\Lambda_6,\Lambda_8\})$
92.114	$\{C_{4z}^{+}\left\|00\frac{1}{4}\right\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$MA(\{V_5V_7,V_6V_8\})$	$\Gamma Z(\{\Lambda_5,\Lambda_7\};\{\Lambda_6,\Lambda_8\})$
92.115	$\{C_{2a}\left\|\frac{1}{2}\frac{1}{2}\frac{1}{4}\right\}$, $\{C_{2b}\left\|\frac{1}{2}\frac{1}{2}\frac{3}{4}\right\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$M(Y_5Y_5)$	$Z(Z_2Z_3)$
94.130	$\{C_{4z}^{+}\left\|00\frac{1}{2}\right\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$MA(\{V_5V_7,V_6V_8\})$	$\Gamma Z(\{\Lambda_5,\Lambda_7\};\{\Lambda_6,\Lambda_8\})$
96.146	$\{C_{4z}^{+}\left\|00\frac{3}{4}\right\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$MA(\{V_5V_7,V_6V_8\})$	$\Gamma Z(\{\Lambda_5,\Lambda_7\};\{\Lambda_6,\Lambda_8\})$
96.147	$\{C_{2a}\left\|\frac{1}{2}\frac{1}{2}\frac{3}{4}\right\}$, $\{C_{2b}\left\|\frac{1}{2}\frac{1}{2}\frac{1}{4}\right\}$, $\{C_{2x}T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$M(Y_5Y_5)$	$Z(Z_4Z_5)$
Type-IV MSGs (without SOC)			
91.109	$\{C_{4z}^{+}\left\|00\frac{1}{4}\right\}$, $\{C_{2x}\|000\}$, $\{T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$A(A_1A_2)$	$\Gamma(\Gamma_5)$

MSG No.	Generators	HSP/ HSL for C-2 DP (Irreps)	HSP/ HSL for C-2 WP (Irreps)
91.110	$\{C_{4z}^{+}\left\|00\frac{1}{4}\right\}$, $\{C_{2x}\|000\}$, $\{T\left\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\right\}$	$A(A_1A_2)$	$\Gamma(\Gamma_5)$
92.116	$\{C_{4z}^{+}\left\|00\frac{1}{4}\right\}$, $\{C_{2x}\left\|\frac{1}{2}\frac{1}{2}0\right\}$, $\{T\left\|00\frac{1}{2}\right\}$	$A(A_1A_2)$	$\Gamma(\Gamma_5)$
95.141	$\{C_{4z}^{+}\left\|00\frac{3}{4}\right\}$, $\{C_{2x}\|000\}$, $\{T\left\|\frac{1}{2}\frac{1}{2}0\right\}$	$A(A_1A_2)$	$\Gamma(\Gamma_5)$
95.142	$\{C_{4z}^{+}\left\|00\frac{3}{4}\right\}$, $\{C_{2x}\|000\}$, $\{T\left\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\right\}$	$A(A_1A_2)$	$\Gamma(\Gamma_5)$
96.148	$\{C_{4z}^{+}\left\|00\frac{3}{4}\right\}$, $\{C_{2x}\left\|\frac{1}{2}\frac{1}{2}0\right\}$, $\{T\left\|00\frac{1}{2}\right\}$	$A(A_1A_2)$	$\Gamma(\Gamma_5)$
Type-IV MSGs (with SOC)			
91.110	$\{C_{4z}^{+}\left\|00\frac{1}{4}\right\}$, $\{C_{2x}\|000\}$, $\{T\left\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\right\}$	$M(M_6M_7)$	$Z(Z_7)$
92.116	$\{C_{4z}^{+}\left\|00\frac{1}{4}\right\}$, $\{C_{2x}\left\|\frac{1}{2}\frac{1}{2}0\right\}$, $\{T\left\|00\frac{1}{2}\right\}$	$M(M_6M_7)$	$Z(Z_7)$
95.142	$\{C_{4z}^{+}\left\|00\frac{3}{4}\right\}$, $\{C_{2x}\|000\}$,	$M(M_6M_7)$	$Z(Z_7)$

MSG No.	Generators	HSP/ HSL for C-2 DP (Irreps)	HSP/ HSL for C-2 WP (Irreps)
	$\{T\left\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\right\}$		
96.148	$\{C_{4z}^{+}\left\|00\frac{3}{4}\right\}$, $\{C_{2x}\left\|\frac{1}{2}\frac{1}{2}0\right\}$, $\{T\left\|00\frac{1}{2}\right\}$	$M(M_6M_7)$	$Z(Z_7)$