

Designing a sensor based on a π -conjugated 6-membered boron ring and its properties

Zihan Zhang ¹, Rajeev Ahuja ^{1,2} and Wei Luo ^{1,*}

¹Condensed Matter Theory Group, Materials Theory Division, Department of Physics and Astronomy,
Uppsala University, Box 516, 75120 Uppsala, Sweden

²Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab 140001, India



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Planar π -conjugated borides not only attract fundamental interests in bonding chemistry, but also offers wide-ranging applications in catalysis, bioimaging, and biosensing. To stabilize π -conjugated B_6 rings without out-of-plane bonding, we propose a design strategy that involves inserting low-compressible CN_3 triangles into tessellation of B_6 rings to create planar borides. Based on this concept, we designed the planar hypercoordinate boride $ScCN_3B_6$, which features the planar structure and represents a theoretically predicted π -conjugated B_6 ring. The molecular dynamics simulations suggested that B_6 rings in $ScCN_3B_6$ remain intact at a high temperature of 1500 K. The metal adsorption energy of B_6 rings in $ScCN_3B_6$ is comparable to borophene, and superior to that of graphene and two-dimensional hexagonal boron nitride. As a result, the designed $ScCN_3B_6$ demonstrates both high stability and chemical activity attributed to CN_3 triangles and B_6 rings, respectively. Consequently, the designed $ScCN_3B_6$ could serve as a potential sensor of for biomolecules. Moreover, the planar ninefold hypercoordinate Sc weakly bonds to the N_3B_6 wheel, drives a flat band of the dz^2 orbital, suggesting that flat band can be generated by splitting of dz^2 orbital in planar hypercoordinate crystal field.

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I. INTRODUCTION

Two-dimensional (2D) materials, such as graphene [1], hexagonal boron nitride [2], and borophene [3], offer a rich platform for exploring low-dimensional physics [4] and various application. However, the high formation energy of 2D materials restricted its utilization for practical use. The sp^2 hybridization is one of the potential approaches to mitigate cohesive energy via conjugated π bonds and facilitates the formation of planar structures, such as 2D carbon allotropes [5]. As a neighboring element of carbon, boron only has 1 p electron, making it challenging to form fully- and quasiplanarized boron-embedded polycyclic π -electron systems [6]. Boron, due to its unoccupied p orbital, generally favors the formation of bulk material rather than forming sp^2 planar structures. The planar 6-membered ring is the representative structure of π -conjugated systems, but boron struggles to form such rings without out-of-plane bonding to metal. The bonding theory of 6-membered ring B_6 in borophene is based on σ -bond resonance differing from traditional π -conjugated systems [7]. Therefore, stabilizing planar boron polycyclic π -conjugated systems remains challenging [6]. The planar hexagonal B_6 ring has been a long-sought goal in boron chemistry due to its

high chemical activity and potential applications in catalyst [8] and sensing [9]. Recently, the focus has been shifted to borides, which could stabilize planar hexagonal B_6 ring. The 6-membered B_6H_6 rings bonded with Ti have been experimentally realized within a $[B_6H_{12}]$ borate [10]. Additionally, the 6-membered B_6 ring can be embedded in crystalline materials like MBene [11] and MgB_2 material families, where they form strong bonds with the metal.

Because boron with π bonding exhibits electron-accepting properties, π -conjugated borides are not only ideal biosensors for detecting the smallest unit of protein, amine $R-NH_3$ [6], but also exhibit complex structural transformation upon metal doping, such as planar hypercoordinated structure [12]. TaB_{10} and NbB_{10}^- anions have been produced by laser vaporization [13], while 2D materials such as ScB_{12} and SrB_8 have been predicted to exhibit planar 12-fold coordination [14,15]. The diverse planar coordination possibilities in 2D metal borides provide a fertile playground for designing catalyst, sensor, and magnetic materials [16–18].

Two-dimensional materials are not only considered as ideal classical biosensors, but also exhibit significant potential in quantum sensing. Landau quantized energy levels of 2D materials are highly sensitive to external magnetic fields, leading to periodic change in transport properties, an effect known as quantum oscillation. Flat-band systems, typical platforms for observing intraband oscillations [19], make the realization of flat band a central focus in condensed matter physics. Two-dimensional kagome lattices have been identified as the feature of crystal structures with flat band [20], and twisted 2D material superlattices have the potential to generate flat band via continuously tunable chemical potential of electrons [21]. Notably, the transition metal with planar hypercoordination,

*Contact author: wei.luo@physics.uu.se

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such as ScB_{12} [14] and $\text{WB}_{12}(\text{NCCN})_3$ [16], generally exhibit flat band above the Fermi level. Moreover, many 2D materials also exhibit topological phonons such as phononic nodal rings in graphene [22].

Recently, a method has been proposed to preserve volatiles using capsules of ultrahard and incompressible materials, such as diamond [23]. Due to the extreme strength of ultrahard and incompressible bonds, the diamond capsules can generate equivalent pressure up to 22 GPa. In this study, we draw the concept of preserving ultrahard and incompressible materials within capsules to stabilize 6-membered ring. We propose a strategy to stabilize planar boride with π -conjugated 6-membered B_6 rings without out-of-plane bonding by inserting low-compressible planar units into tessellation of 6-membered B_6 rings. As a case in point, we utilize CN_3 triangle from carbon nitride, one of the most incompressible materials [24]. The resulting tessellation exhibits 5-membered, 6-membered, and 9-membered rings. To further stabilize the 6-membered B_6 ring, we have added metal atom at the center of nonagon with planar ninefold coordination. Therefore, the 2D material ScCN_3B_6 has been designed with ninefold-coordinated Sc and B_6 rings without out-of-plane bonding. Furthermore, the stability of designed ScCN_3B_6 has been evaluated at finite temperatures via *ab initio* calculations of enthalpy difference and molecular dynamics simulations at high thermal temperatures over 1500 K. The properties of 6-membered B_6 ring have also been analyzed without out-of-plane bonding and nonacoordinate Sc, along with its possible applications in classical and quantum sensing. In addition, the adsorption energy of 6-membered B_6 ring in 2D material ScCN_3B_6 to metal is comparable to borophene and significantly higher than that of graphene and h-BN. For Au atom, the adsorption energies of ScCN_3B_6 , β_{12} -borophene, graphene, and h-BN are -2.71 , -2.72 , -0.35 , and -0.41 eV, respectively. Additionally, the planar hypercoordinated ScCN_3B_6 also results in flat band at 1 eV above Fermi level.

II. METHOD

Details of calculations based on density functional theory

First-principles calculations, including structure optimizations, molecular dynamics simulations, electronic structures, and mechanical strength, were conducted by using the Vienna *Ab initio* Simulation Package (vasp 6) [25]. The exchange-correlation functional was specified as the generalized gradient approximation [26] parametrized by Perdew, Burke, and Ernzerhof [27]. And, pseudopotential for the electron-ion interactions was described by the projector augmented plane-wave approximation [28], where valence electrons $1s^1$, $2s^2 2p^1$, $2s^2 2p^3$, $2s^2 2p^2$, and $3p^6 4s^2 3d^1$ were considered for elements H, B, N, C, and Sc, respectively. The plane-wave cutoff energy was set to 600 eV, and the Monkhorst-Pack k -spacing value was selected as $0.03 2\pi/\text{\AA}$ (k -point grid is $9 \times 9 \times 1$). For density of states calculation, the Monkhorst-Pack k -spacing value was further increased to $0.01 2\pi/\text{\AA}$ (k -point grid is $27 \times 27 \times 1$). To mimic 2D crystal, a large vacuum thickness of $15 \text{\AA}$ along the out-of-plane direction was built in the periodic cell. The crystal

orbital Hamilton populations (COHPs) were calculated using LOBSTER [29]. And, the van der Waals effects were considered by the density-functional theory DFT-D3 method [30]. The dynamic stability was investigated by phonon calculations with $4 \times 4 \times 1$ supercell via the finite-displacement method, which was conducted by using phonopy code [31]. *Ab initio* molecular dynamics simulations based on a $3 \times 3 \times 1$ supercell were carried out to further confirm dynamic stability at temperature 1500 K, where Nosé-Hoover chain thermostat was used to examine temperature with a total simulation time of 20 ps (time step of 1 fs).

Electron-phonon coupling (EPC) matrix elements were calculated for superconducting critical temperature using density-functional perturbation theory as implemented in the quantum espresso package [32]. Optimized norm-conserving Vanderbilt pseudopotentials [33] were used with a 100-Ry kinetic energy cutoff and a 1000-Ry charge-density cutoff. A $12 \times 12 \times 1k$ -point grid was used for Brillouin-zone integration in electronic calculations, and EPC matrix elements were calculated in a $6 \times 6 \times 1q$ -point grid. The number of double-delta smearing values used was 10 and smearing value was varied from 0.005 to 0.05 Ry. Electronic smearing in self-consistent calculation adopts Methfessel-Paxton first-order spreading with the smearing width of 0.045 Ry.

The adsorption energy of metals on the 6-membered rings of ScCN_3B_6 , β_{12} -borophene, graphene, and h-BN was calculated as follows:

$$\Delta E_{\text{ads}} = E(2D \text{ material} + \text{atom}) - E(2D \text{ material}) - E(\text{atom}).$$

Calculated structure of 2D materials ScCN_3B_6 , β_{12} -borophene, graphene, and h-BN are $2 \times 2 \times 1$, $4 \times 2 \times 1$, $4 \times 4 \times 1$, and $4 \times 4 \times 1$ supercell, respectively. The plane-wave cutoff energy was set to 600 eV, and the Monkhorst-Pack k -spacing value was selected as $0.03 2\pi/\text{\AA}$.

III. RESULTS AND DISCUSSION

The design of 2D borides with B_6 ring without out-of-plane bonding, initially inspired by ultrahard and incompressible capsules [23], relies on strong chemical bonds that promote the formation of hexagonal boron structures. One of the most incompressible materials is carbon nitride, which has been predicted since 1989 [34] and was recently synthesized under high pressure and high temperature [24]. Notably, one of the synthesized forms of carbon nitride exhibits a quasi-planar honeycomb-like structure with 1:1 C:N composition [24], suggesting that the triangle of carbon and nitrogen could be utilized to stabilize B_6 hexagon. Therefore, planar CN_3 triangle has been inserted into tessellation of honeycomb borophene to stabilize B_6 hexagon as shown in Fig. 1(a). The resulting tessellation of CN_3B_6 exhibits pentagon, hexagon, and nonagon. It is observed that in comparison to the similar tessellation of tripentaphenes [35] from acepentallene C_{10}H_6 [36], tessellation of CN_3B_6 lacks 3 electrons per unit cell. As a result, the nonacoordinate metal atom could be located in the center of nonagon to donate electrons. In addition to the valence electrons, the appropriate radius of metal is also necessary to stabilize the planar hypercoordinate structures [37].

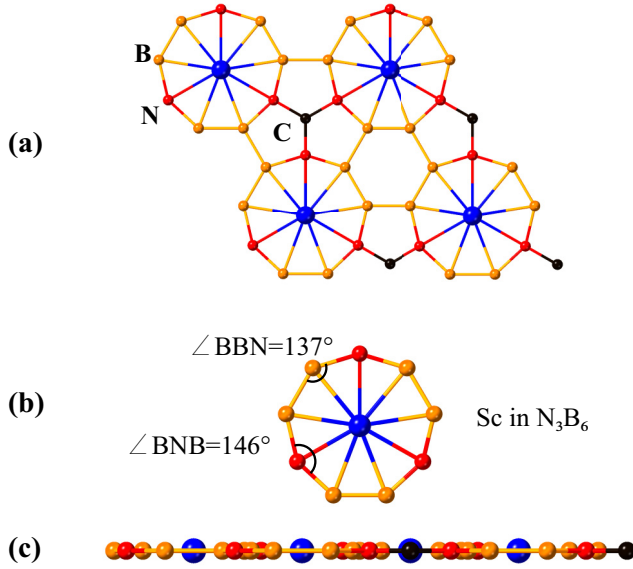


FIG. 1. (a) Structure of planar 9-coordinate material ScCN₃B₆ with space group $P6m2$, in which Sc, C, N, and B atoms are shown in black, red, green, and blue, respectively. (b) The nonacoordinate Sc@N₃B₆ in tessellation of planar nonacoordinate configuration are shown with angles $\angle BNB = 146^\circ$ and $\angle BBN = 137^\circ$, respectively. (c) Planar structure of 9-coordinate material ScCN₃B₆ from the view of x axis.

The planar nonacoordinate Sc has been reported in 2D materials ScB₁₂ [14], implying Sc exhibits both 3 valent electrons and suitable atomic radius for planar nonacoordination. We selected Sc as the nonacoordinate atom as shown in Figs. 1(a) and 1(b), because interior angles of the regular nonagon are 140° , assisting the formation of regular nonacoordinate configuration. After structure optimization, the angles of $\angle BNB$ and $\angle BBN$ in the nonagon of Sc@N₃B₆ are found to be 146° and 137° , respectively, suggesting a great nonacoordinate configuration of Sc@N₃B₆ with angle close to 140° . Therefore, the 2D material ScCN₃B₆ has been designed with nonacoordinate Sc atom stabilizing CN₃ triangle, and 6-membered B₆ ring without out-of-plane bonding as shown in Fig. 1(b), Supplemental Material, Fig. S1 and Table S1 [38]. Moreover, we tried to stabilize CN₃B₆ using Y (radius 1.80 Å) or La (radius 1.87 Å), which have larger atomic radii than that of Sc (radius 1.62 Å). Substituting Y or La will increase the Sc–B/N bond length (~ 2.2 Å) to $\sim 2.4 - 2.5$ and $\sim 2.5 - 2.6$ Å, respectively. In this manner, around 11 and 15% tensile strain will be introduced into the lattice frame. The 12% strain limitation (see Fig. 3 suggests this feasible for Y, while La will exceed this threshold. However, the lattice dynamic is unstable, where out-of-plane optic mode (ZO) is fully imagined in entire symmetry directions as shown in Supplemental Material, Fig. S2 [38].

However, the B–B bond lengths in the 6-membered B₆ ring of ScCN₃B₆ are found to be 1.66 and 1.67 Å, indicating that the bonds are not equal. Therefore, the calculations of partial density of states (PDOS) and crystal orbital Hamilton populations (COHPs) have been performed to clarify the bonding structure of ScCN₃B₆, as shown in Fig. 2. For sp^2

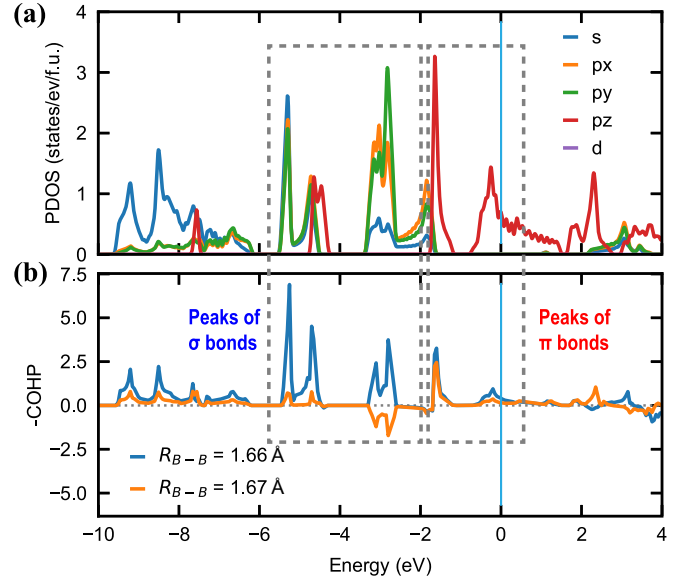


FIG. 2. (a) Projected density of states (PDOS) of boron in ScCN₃B₆. (b) Crystal orbital Hamilton populations (COHPs) of B–B bonds in planar B₆ ring in ScCN₃B₆. The Fermi level was set to 0 eV.

hybridization, σ bonds are primarily formed by s , px , and py orbitals, whereas π bonds are generally contributed by pz orbital. As shown in Fig. 2, the regions of PDOS peaks of s , px and py orbitals are the same, but different from that of pz orbital, exhibiting typical sp^2 hybridization. Below Fermi level, the bands with highest energy are contributed by π bonds (pz orbital), suggesting both B–B bonds exhibits bonding states of π bonds. The occupied bands with the second-highest energy are contributed by σ bonds (s , px , and py orbital),

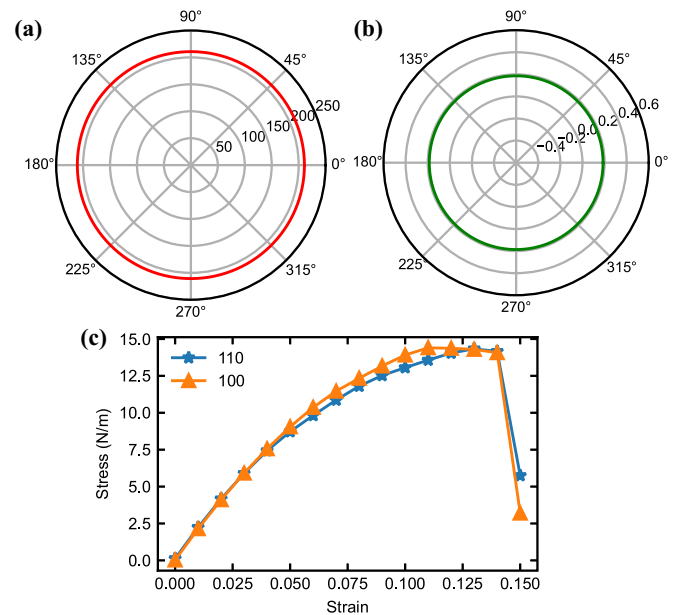


FIG. 3. Mechanical properties planar ScCN₃B₆. (a) Young's modulus and (b) Poisson's ratio of the planar ScCN₃B₆. (c) Stress-strain curves of the planar ScCN₃B₆ along crystal directions $\langle 100 \rangle$ and $\langle 110 \rangle$.

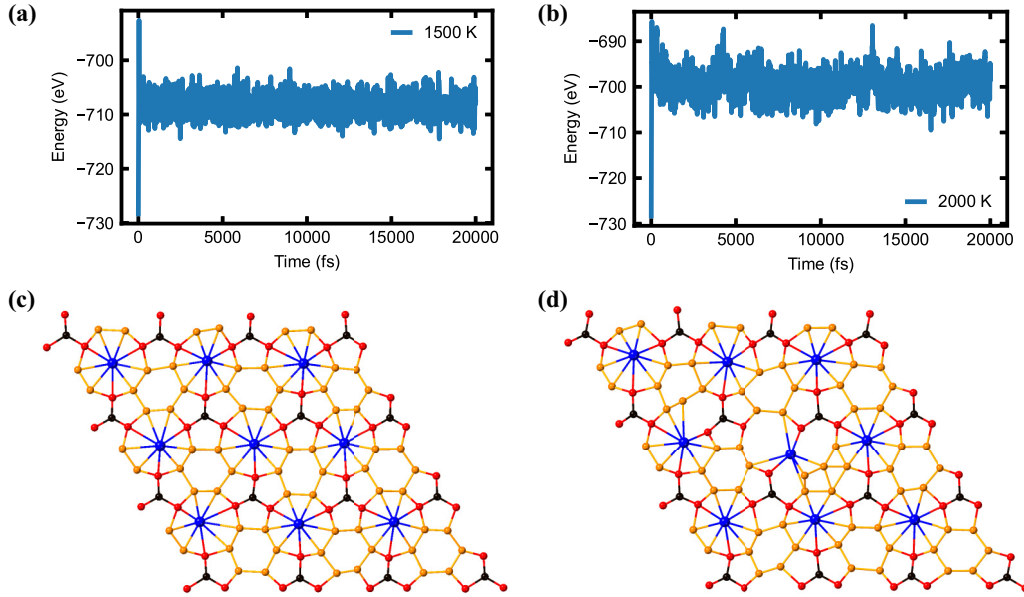


FIG. 4. Energy variations of planar ScCN_3B_6 during MD simulations at (a) 1500 K and (b) 2000 K, with corresponding final structural snapshots at (c) 1500 K and (d) 2000 K.

where the $-\text{COHP}$ value of long B–B bond is much lower than that of short B–B bond, and the σ bonds at 3 eV are contributed by antibonding π^* orbital. Therefore, σ bonds of long B–B bond is much weaker than that of short B–B bond. As a result, all the boron atoms in planar 6-membered B_6 -ring atom are bonding to each other through σ bonds, and provide a p_z orbital perpendicular to the plane of the B_6 ring that facilitates the formation of delocalized π bonds, creating a typical π -conjugated system. Notably, the π bonds near Fermi level consist of half-occupied bonding states of π orbital, suggesting that electron transition to the B_6 ring will first occupy these bonding states, thereby lowering the energy of the system. Consequently, the B_6 ring of ScCN_3B_6 serves as a promising electron acceptor. The B_6 ring of ScCN_3B_6 , representing a realization of π -conjugated B_6 ring without out-of-plane bonding, has the potential to capture and sense objects that transfer electron to B_6 ring without out-of-plane bonding.

Furthermore, the mechanical and dynamic stability has been addressed via elastic constants and molecular dynamics simulations. The calculated elastic constants C_{11} , C_{12} , and C_{66} are 218.3, 40.7, 218.3, and 88.8 N/m, respectively. As an isotropic hexagonal-lattice system with space group $P-6m2$, elastic constant C_{22} of ScCN_3B_6 is the same as C_{11} [39]. The elastic constants C_{ij} satisfy Born-Huang criteria [40] for mechanical stability of 2D hexagonal symmetry: $C_{66} = \frac{C_{11}-C_{12}}{2} > 0$ and $C_{11} > |C_{12}|$, suggesting a static stability of 2D structures. As shown in Fig. 3, the Young modulus and Poisson ratio of planar ScCN_3B_6 from elastic constants are isotropic, with values of 210.7 N/m and 0.186, respectively. The calculated Young modulus of planar ScCN_3B_6 is high in comparison to the reported 2D transition-metal material such as MBenes [11] and transition-metal dichalcogenides [41], suggesting that the planar ScCN_3B_6 exhibits excellent mechanical stability. Moreover, the stress-strain curves of planar ScCN_3B_6 along crystal directions $\langle 100 \rangle$ and $\langle 110 \rangle$ show

obvious brittle-fracture characteristics; as shown in Fig. 3(c), rupture occurs with less prior noticeable change in the rate of elongation. The intrinsic strength is defined as the highest stress point along the stress-strain curve, serving as a measure of the mechanical performance of planar structures. The intrinsic strength of planar ScCN_3B_6 is found to be 14 N/m.

The polygon intactness of the designed 9-coordinate configuration has also been examined at high temperatures through molecular dynamics (MD) simulations at temperature 1500 and 2000 K as shown in Fig. 4. The structural snapshots exhibited intact 5-membered, 6-membered, and 9-membered B_6 -ring configuration at 1500 K with ripples caused by temperature, suggesting good thermal stability for planar 6-membered B_6 ring and 9-coordinate configuration of ScCN_3B_6 . When temperature is further increased to 2000 K, the strong N–B bonds break, causing the planar π -conjugated 6-membered B_6 ring to transform into a B_3 triangle. However, the CN_3 triangle remains intact at 2000 K, keeping the CN_3 sublattice in ScCN_3B_6 almost unchanged with total energy remaining stable. As a result, the emergence of B_3 triangle, a signal of $3c-2e$ bond [7], does not increase the total energy, suggesting the excellent thermal stability of triangle- CN_3 -stabilized 6-membered B_6 ring without out-of-plane bonding.

We have also explored the vibration of bonds in ScCN_3B_6 to further clarify the origin of stability via phonon dispersion. As shown in Fig. 5, ScCN_3B_6 possesses dynamic stability with positive phonon dispersions. Due to the hypercoordination state of Sc, Sc is weakly bonding to the atoms in the wheel of N_3B_6 . The weak bonding typically suggests low vibrational frequency. Therefore, the lowest optical out-of-plane mode (ZO) is contributed by the out-of-plane motions of Sc, whereas the C–N bonds are remarkably strong, which implies that the compression and stretching of these chemical bonds contribute to the highest in-plane mode (TO) at high frequency. Metallic σ band is one of the reasons for high-temperature superconductivity of boride [42], and

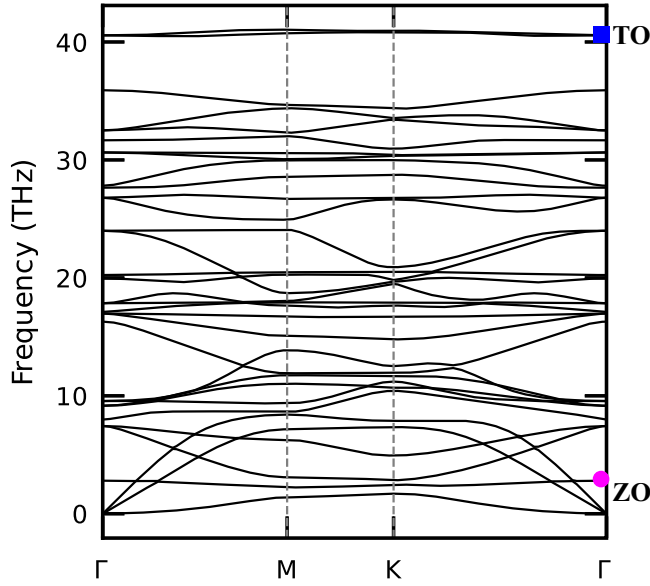


FIG. 5. Phonon dispersion of ScCN_3B_6 and typical vibration modes including the out-of-plane optical mode (ZO) and the highest transverse optical (TO). The ZO and TO modes at gamma point are shown in pink circles and blue squares, respectively.

there is no σ band (s , px , and py orbital) at Fermi level of ScCN_3B_6 . It is interesting to clarify the properties of superconducting borides without σ band at Fermi level. Thus, we further explore the electron-phonon coupling and superconductivity of ScCN_3B_6 , with the predicted superconducting critical temperature T_c , electron-phonon coupling coefficient λ , and logarithmic average frequency $\omega_{\log}$ being 0.1 K, 0.27, and 552.9 K, respectively. Unlike other borides, the T_c of π -conjugated ScCN_3B_6 is remarkably low due to its low electron-phonon coupling coefficient (λ), as predicted by the theory of metallic σ band. However, weak electron-phonon coupling might suggest weak scattering of electrons by phonons and excellent electrical conductivity.

After examining the stability and bonding of π -conjugated B_6 rings, we explored the electronic properties of hypercoordinate Sc in ScCN_3B_6 as shown in Fig. 6. Notably, the flat band, which has been contributed by d_{z^2} orbital of Sc, emerges at 1 eV above Fermi level and drives a large density

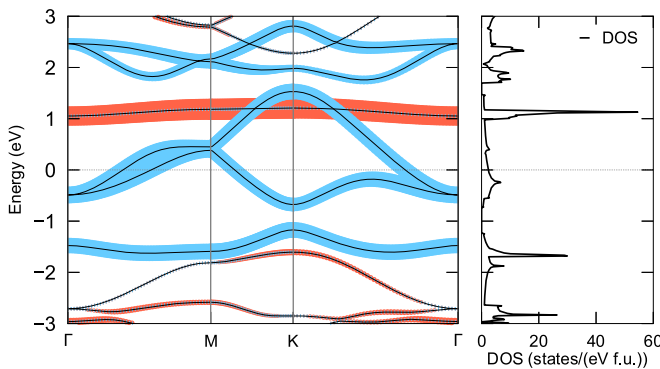


FIG. 6. Band structure with contribution of bands and total density of states (DOS) of ScCN_3B_6 , where the orange and blue circles denote the PDOS of d_{z^2} orbital of Sc and p_z orbital of B, respectively.

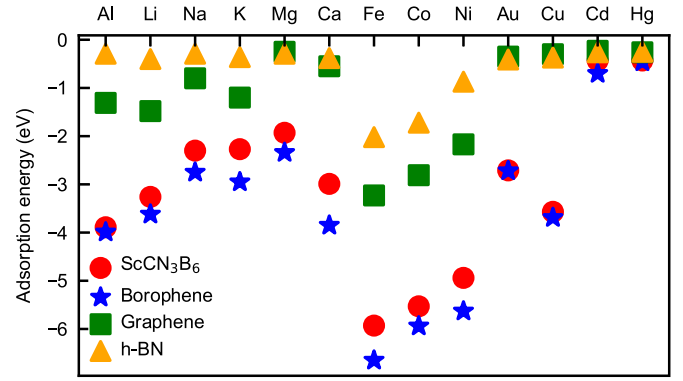


FIG. 7. Adsorption energy of metals on the 6-membered rings of ScCN_3B_6 , β_{12} -borophene, graphene, and h-BN.

of states, while the other planar hypercoordinate 2D materials also exhibit flat band such as 2D materials SrB_8 [15] and $\text{WB}_{12}(\text{NCCN})_3$ [16]. Due to hypercoordination, central atoms form weak bond with neighboring atoms in the wheels, making them relatively isolated, and it is possible to realize the flat energy level of isolated atoms in band structures of central atoms. Therefore, planar hypercoordinate materials represent a potential family with flat band. Shifting this flat band to Fermi level is a challenging and important avenue for future research, with doping potentially facilitating this task. In ScCN_3B_6 , flat band lies above the Fermi level due to empty d_{z^2} orbital of Sc. It is suggested that incorporating a transition metal with more d electrons into ScCN_3B_6 could bring the flat band closer to the Fermi level.

The adsorption ability of planar B_6 ring in ScCN_3B_6 has been compared with typical 6-membered rings from β_{12} -borophene, graphene, and h-BN as shown in Table I and Fig. 7. The considered metals are from s -, p -, and d -block metals. The adsorption energy of ScCN_3B_6 is much larger than those of graphene and h-BN, as the bonding orbitals of π bonds in ScCN_3B_6 are electron deficient as shown in Fig. 2, whereas the bonding orbitals of graphene and h-BN are fully occupied. Additionally, β_{12} -borophene features $3c-2e$ bonds with σ -bond resonance, which also lack electrons. Therefore, the adsorption energy of ScCN_3B_6 is comparable with β_{12} -borophene. However, since the boron orbitals in ScCN_3B_6 are already partially occupied by electrons from Sc, the adsorption ability of planar B_6 ring in ScCN_3B_6 is slightly lower than that of β_{12} -borophene.

We further explore the potential of quantum sensing, considering the isolation effect caused by the hypercoordinate Sc in ScCN_3B_6 . For the vibration mode of ScCN_3B_6 , both the lowest and second-lowest optical mode exhibit remarkably low frequencies, and cross the acoustic modes. We found 6 phononic nodal rings as shown in Figs. 8(a)–8(d). Similar to graphene, out-of-plane optical vibrational modes (ZO modes) of ScCN_3B_6 exhibit lower frequency than the frequency of in-plane acoustic modes (LA and TA modes) along M - K high-symmetry path [edge of the first Brillouin zone of ScCN_3B_6) in Q space, as shown in Fig. 8(e)]. Therefore, there are 6 crossings of ZO modes and in-plane acoustic modes along any paths from Γ point to edge of the first Brillouin zone, suggesting that crossings form phononic nodal ring around Γ point [22]. The concept of topological phonon is from topological

TABLE I. Adsorption energy of metals on the 6-membered rings of ScCN_3B_6 , β_{12} -borophene, graphene, and h-BN. The unit of adsorption energy is eV.

2D Materials	Adsorption energy of metals on 2D materials (eV)												
	Al	Li	Na	K	Mg	Ca	Fe	Co	Ni	Au	Cu	Cd	Hg
ScCN_3B_6	-3.89	-3.26	-2.30	-2.27	-1.93	-2.99	-5.93	-5.53	-4.94	-2.71	-3.57	-0.43	-0.43
β_{12} -borophene	-3.99	-3.62	-2.75	-2.95	-2.34	-3.85	-6.65	-5.94	-5.63	-2.72	-3.69	-0.70	-0.46
Graphene	-1.31	-1.48	-0.80	-1.20	-0.25	-0.55	-3.23	-2.81	-2.17	-0.35	-0.30	-0.23	-0.26
h-BN	-0.29	-0.4	-0.29	-0.36	-0.29	-0.38	-2.02	-1.72	-0.87	-0.41	-0.37	-0.26	-0.25

electronic states; topological electronic states near Fermi level were used for quantum application, and topological phonon at any frequency could be used, which is the advantage of topological phonon. The vibration modes of Sc are relatively isolated from the wheel of N_3B_6 , and sensitive to electric field or force. Therefore, the vibration modes of Sc with topology could potentially be used in electric field or force sensing. For the electronic states of ScCN_3B_6 , the unoccupied d_{z^2} orbital of Sc is flat. The band structure of electron-doped ScCN_3B_6 has also been calculated. Upon electron doping, a band inversion emerges and makes the flat band steep. Additionally, the system of ScCN_3B_6 becomes occupied below Fermi level and spin polarized after doping with 3 electrons, as shown in Fig. 8. Since the Sc only has 1 d electron, it is different to use the spin properties of Sc. A hypercoordinated transition metal with more d electrons would be a better candidate. $\text{W@B}_{12}(\text{NCCN})_3$ [16] displays similar degenerate d orbital as Sc in ScCN_3B_6 , and the flat band of isolated W is close to Fermi level with intrinsic magnet. The spin states and quantum oscillations driven by flat bands of hypercoordinated metals show promising potential for application in quantum biosensing.

We explore the experimental feasibility for ScCN_3B_6 using calculated enthalpy difference in reactions (1)–(4):

$$\begin{aligned}\Delta E_1 &= E(\text{ScCN}_3\text{B}_6) - E(\text{Sc, atom}) - E(\text{N}_2, \text{ gas}) \\ &\quad - E(\text{B, borophene}) - E(\text{C, graphene}) \\ &= -0.694 \text{ eV/atom},\end{aligned}\quad (1)$$

$$\begin{aligned}\Delta E_2 &= E(\text{ScCN}_3\text{B}_6) - E(\text{Sc, hcp}) - E(\text{N}_2, \text{ gas}) \\ &\quad - E(\text{B, borophene}) - E(\text{C, graphene}) \\ &= -0.276 \text{ eV/atom},\end{aligned}\quad (2)$$

$$\begin{aligned}\Delta E_3 &= E(\text{ScCN}_3\text{B}_6) - E(\text{Sc, atom}) - E(\text{N}_2, \text{ gas}) \\ &\quad - E(\text{B, } R\bar{3}m) - E(\text{C, graphene}) \\ &= -0.407 \text{ eV/atom},\end{aligned}\quad (3)$$

$$\begin{aligned}\Delta E_4 &= E(\text{ScCN}_3\text{B}_6) - E(\text{Sc, hcp}) - E(\text{N}_2, \text{ gas}) \\ &\quad - E(\text{B, } R\bar{3}m) - E(\text{C, graphene}) \\ &= 0.011 \text{ eV/atom}.\end{aligned}\quad (4)$$

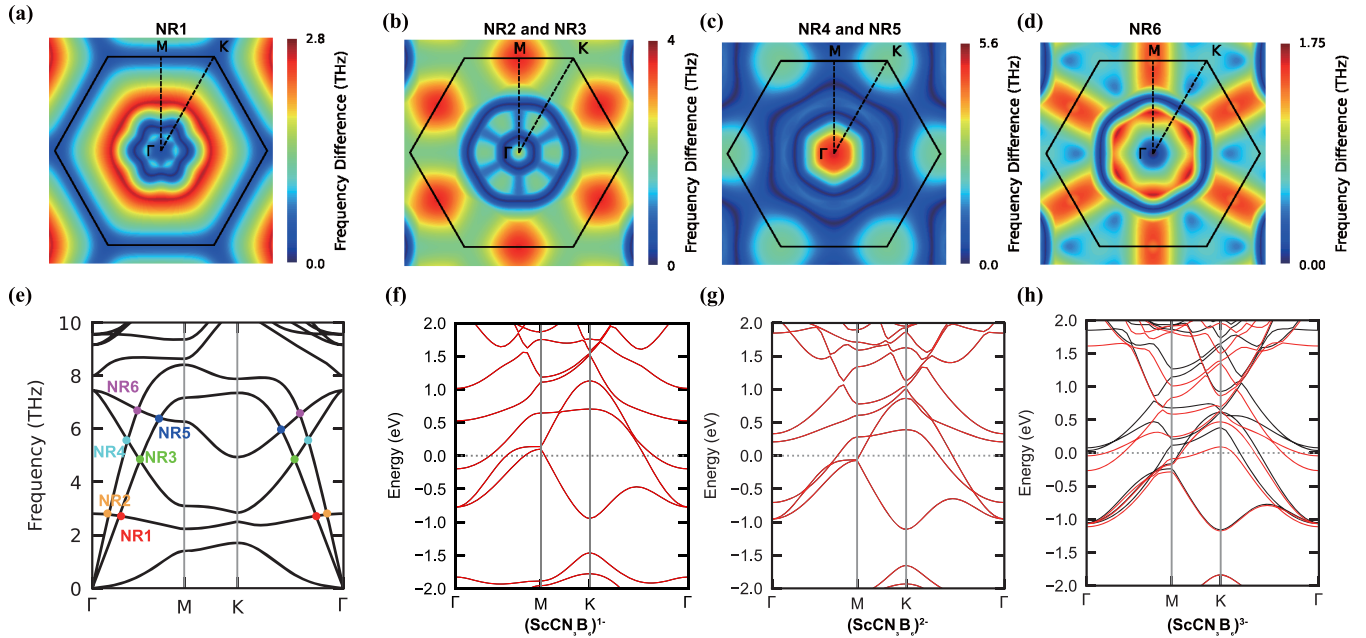


FIG. 8. Frequency difference of (a) nodal ring 1 (NR1); (b) nodal ring 2 (NR2) and nodal ring 3 (NR3); (c) nodal ring 4 (NR4) and nodal ring 5 (NR5); and (d) nodal ring 6 (NR6). (e) Topology of optical and acoustical phonon in ScCN_3B_6 . Band structures with spin polarization of (f) $(\text{ScCN}_3\text{B}_6)^{1-}$, (g) $(\text{ScCN}_3\text{B}_6)^{2-}$, and (h) $(\text{ScCN}_3\text{B}_6)^{3-}$. Spin-up bands are the same as spin-down bands in the electronic structures of $(\text{ScCN}_3\text{B}_6)^{1-}$ and $(\text{ScCN}_3\text{B}_6)^{2-}$. Red and black lines denote spin up and spin down, respectively.

When 2D material borophene is considered as boron-source reactions (1) and (2), large negative value of reaction energy suggests that ScCN_3B_6 is potential product in reactions (1) and (2). Because borophene is metastable, we further consider bulk boron as boron-source reactions (3) and (4). When the atomic phase of Sc was considered as Sc source, the reaction energy for ScCN_3B_6 was -0.407 eV per atom. But, for bulk phase of Sc as Sc source, the reaction energy for ScCN_3B_6 is 0.011 eV per atom. From the results, it is suggested to consider reaction from atomic phase of Sc such as chemical vapor deposition for ScCN_3B_6 .

IV. SUMMARY

In summary, we proposed a possible strategy to stabilize planar B_6 ring using CN_3 triangles without out-of-plane bonding. The planar 2D material ScCN_3B_6 has been designed with planar B_6 ring and planar nonacoordinate Sc. Co doping of CN_3 triangles and Sc into tessellation of B_6 rings stabilizes planar B_6 ring without out-of-plane bonding, marking a realization of planar B_6 ring in a 2D material. The B_6 ring in ScCN_3B_6 demonstrates exceptional metal adsorption capability. Ions with planar hypercoordination are proposed

to generate flat band and topological phonon states. Planar ScCN_3B_6 holds potential as both a classical biosensor utilizing the π bonds of B_6 rings, and a quantum biosensor leveraging Sc tripped in the wheel like N_3B_6 structure. Our design sparks a field that combines planar polycyclic hyper-coordinate materials with biosensing applications.

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DATA AVAILABILITY

Data is provided within the manuscript or supplementary information files, and will be provided upon reasonable request.

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