CoB6 Monolayer: A Robust Two-dimensional Ferromagnet

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CoB₆ monolayer: A robust two-dimensional ferromagnet

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Two-dimensional (2D) magnetic materials are essential to developing high-performance spintronic devices. Recent experimental discoveries of several atomic thin 2D ferromagnetic materials have stimulated great interest in further exploring this fascinating class of materials. Here, combining an advanced crystal structure search method and extensive first-principles energetic and dynamic calculations, we have identified a planar CoB₆ monolayer as a stable 2D ferromagnet. We show that the ferromagnetic ground state of the CoB₆ monolayer remains robust in the ambient environment, and the magnetic stability and moment can be remarkably enhanced and tuned by external strain. Moreover, we propose feasible synthesis routes for the newly predicted CoB₆ monolayer, either by Co atom adsorption on the recently proposed δ₁ boron sheet or by direct chemical growth. The present results establish a fundamental material and physics basis for synthesis and characterization of the CoB₆ monolayer among the emerging 2D ferromagnetic materials.

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I. INTRODUCTION

Spintronics utilizes electron spin instead of charge for information storage, transport, and processing, and it holds great promise for next-generation high-performance devices with superior characteristics such as high processing speed and low power consumption. Research and development in the materials physics fields related to spintronics have attracted intensive attention in recent decades [1]. Practical materials for spintronic applications should possess strong structural and magnetic stability, high Curie temperature, high spin polarization ratio, and feasibility for experimental fabrication. Recent studies have predicted a number of nanoscale ferromagnetic materials, such as the Fe₂Si sheet [2], MXene [3], strained NbS₂ and NbSe₂ [4], and defective or partially hydrogenated graphene [5–7]; however, ferromagnetic materials that meet the criteria for practical device implementation have been difficult to obtain due to challenges in material synthesis and stability. For example, although graphene is the most prominently predicted 2D magnetic material when vacancies or zigzag edges are present, it is rarely observed in experiment due to electron delocalization and other issues. Recent experimental progress has led to a breakthrough in the synthesis of truly 2D magnets, realized in pristine Cr₂Ge₂Te₆ [8], CrI₃ [9,10], and VSe₂ [11] atomic thin layers. The control of the transition temperatures between ferromagnetic and paramagnetic states has been achieved under small fields. More interestingly, the magnetism of a 2D CrI₃ layer has been shown to be controllable by electrostatic doping and external electric fields [12,13]. These experimental advances demonstrate the feasibility of the long-sought truly 2D magnets, thereby opening an exciting area of research for exploring additional 2D magnetic materials that exhibit similar or improved material characteristics, such as enhanced structural stability and magnetic transition temperature, that are crucial to device applications.

Boron nanostructures are a promising candidate materials for spintronic applications since they are highly susceptible to metal doping due to the electron deficiency of boron atoms. Boron rings containing central transition-metal atoms that form planar hexa-, hepta-, octa-, and higher coordination with the surrounding boron atoms, such as FeB₆, FeB₇, CoB₆, RuB₆, RhB₆, IrB₆, and VB₆ clusters [14–17], have been revealed by theoretical and experimental investigations. The transition-metal atoms not only can stabilize boron clusters via electron compensation, but also may induce magnetic order in the system. Based on experimentally revealed hypercoordinated planar boron clusters, corresponding 2D layered materials have been theoretically proposed, and their magnetic ground states have been predicted in the planar hypercoordinated 2D iron boride FeBₓ (x = 2–10) alloys [18] and MnBₓ (x = 1, 2, 3, 6) layers [19,20]. However, although cobalt has been shown to form hypercoordination with boron frameworks, as demonstrated by recently synthesized planar CoBₓ⁻, CoB₁², CoB₁⁶, and CoB₁₈ clusters [21,22], hypercoordinated Co-B 2D layers have not been realized. Questions remain on whether such 2D layers can exist or if the Co atoms can induce magnetic orders. Another motivation for the study of embedding transition-metal atoms into 2D boron sheets is that some of these sheets have been experimentally synthesized on Ag substrates [23,24]. It is expected that the electronic and mechanical properties of the boron sheets can be modulated, as demonstrated in MgB₂ [25], BeB₂ [26], and TiB₂ [27].
In this work, we explore cobalt decorated boron sheets using an advanced structure search method combined with first-principles energetic and dynamic calculations. Our results identify a stable 2D CoB$_6$ monolayer that exhibits strong intrinsic ferromagnetism with high stability and an intriguing electronic structure that hosts Dirac cone structures with linear dispersions. The identified planar structure and the associated magnetic order remain robust against the adsorption of common molecules present in the ambient environment, and an externally applied tensile strain is able to effectively tune and enhance the ferromagnetic stability and moment. We propose two feasible approaches for synthesizing the predicted CoB$_6$ monolayer, namely by Co adsorption on the reportedly proposed $\delta_4$ boron framework, or by direct chemical growth, which is supported by our extensive calculations on the stability of planar Co$_4$B$_8^+$ molecular clusters. The high structural and ferromagnetic stabilities of the CoB$_6$ monolayer, together with the strain tunable and enhanced magnetism and highly feasible experimental synthesis, are expected to stimulate efforts to further study and develop this fascinating 2D ferromagnetic material. The present findings lay a strong physics foundation for additional pertinent researches.

II. COMPUTATIONAL METHODS

Our structure prediction for Co$_x$B$_y$ ($x, y = 1–6$) monolayer is based on a global minimum search of the free energy surfaces by the CALYPSO method [28–30]. The significant feature of this method is its capability of predicting both the ground-state and metastable structures with only the knowledge of the given chemical composition. Its validity has been confirmed by successful predictions of a diverse variety of materials [31–41]. The evolutionary variable cell structure prediction is performed, with each generation containing 30 structures, among which 60% are generated by particle-swarm optimization (PSO) while the others are new and generated randomly. We followed 50 generations to achieve the converged structure. The candidate structures of each composition are fully relaxed until their energy and force are converged to $10^{-6}$ eV and 0.001 eV/Å, respectively, by using the Vienna Ab initio Simulation Package (VASP) code [42]. The projector-augmented wave (PAW) [43] approach is adopted to represent the ion-electron interaction. The generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerhof (PBE) [44] functional has been employed with an energy cutoff of 500 eV for the plane-wave expansion. To check the influence of the correlation effect introduced by the Co 3$d$ electrons, we performed PBE+$U$ calculations ($U = 3.5$ or 6.0 eV), and also used the screened hybrid Heyd-Scuseria-Ernzerhof (HSE06) [45,46] functional to determine the electronic band structure. A vacuum space of at least 15 Å has been introduced to avoid the interaction between periodic images. A Monkhorst-Pack $k$-point mesh of $13 \times 5 \times 1$ is used for the sampling of the Brillouin zone during the geometry optimization. A phonon dispersion analysis is performed using the PHONOPY code [47] to examine the dynamical stability of the CoB$_6$ monolayer. Thermal stability of the predicted CoB$_6$ 2D structure has been checked using ab initio molecular dynamics (AIMD) simulations, and the Nosé-Hoover method [48] was used based on the PAW method and PBE functional. The diffusion energy of the Co atoms on the $\delta_4$ boron sheet is calculated by using the climbing-image nudged elastic band (CI-NEB) method [49].

III. RESULTS AND DISCUSSION

A. Geometric structure of the CoB$_6$ monolayer

We examined over 1000 Co$_x$B$_y$ ($x, y = 1–6$) structures based on the PSO structure search; all these structures were fully relaxed using the VASP code [42], and their dynamical stabilities were then checked by phonon calculations. This extensive and systematic process identifies the global ground-state CoB$_6$ monolayer shown in Fig. 1(a). In this fully optimized structure, the CoB$_6$ sheet is completely planar with a single atomic layer thickness, and the relaxed lattice constants are $a = 2.904$ Å, $b = 7.694$ Å. Each Co atom coordinates with six surrounding B atoms and the optimized Co-B bond lengths range from 2.022 to 2.118 Å. From these structural characteristics, the CoB$_6$ monolayer can be viewed as having Co atoms uniformly embedded in the $\delta_4$ boron sheet [50]. This structure, however, is distinct from the recently

![FIG. 1. (a) Top and side views of the CoB$_6$ monolayer. The blue and green spheres represent Co and B atoms, respectively. (b) Calculated phonon dispersion of the CoB$_6$ monolayer. (c) Snapshots of the CoB$_6$ monolayer at 500 K at the end of 1.5 ps of AIMD simulations. (d) The chemical bonding picture of the Co$_4$B$_8^+$ molecule obtained using the AdNDP method. Here ON denotes the occupation number.](image-url)
proposed FeB₆ layered structure where Fe atoms occupy the
hexagonal centers of the graphene-like boron sheet [51] or the
MnB₆ layered structure where Mn atoms are sandwiched
between two boron layers [20].

B. Thermodynamic, kinetic, and thermal
stability of the CoB₆ monolayer

To further evaluate the energetics of the CoB₆ monolayer, we first assess its cohesive energy \( E_{\text{coh}} = (E_{\text{Co}} + 6E_B - E_{\text{CoB₆}})/7 \), where \( E_{\text{Co}}, E_B \), and \( E_{\text{CoB₆}} \) are the total energies
of an isolated Co atom, an isolated B atom, and one unit
cell of the CoB₆ monolayer, respectively. The calculated \( E_{\text{coh}} \)
of the monolayer CoB₆ is 5.84 eV/atom, which is higher
than those of Be₂C (4.86 eV/atom) [52] and FeB₆ (5.56–5.79
eV/atom) [51] at the same computational level. Although
the stability of these materials cannot be directly compared by
their cohesive energies due to differences in the nature of the
bonding configurations in different materials, this result still
serves as a good indication that the CoB₆ monolayer is a
strongly bonded 2D network. Dynamical stability of the CoB₆
monolayer is confirmed by calculating its phonon dispersion.
Results in Fig. 1(b) show no imaginary frequency in the entire
first Brillouin zone. It is noted that the highest frequency of
this CoB₆ monolayer reaches up to 39.05 THz (\( \approx 1303 \text{ cm}^{-1} \)), which is much higher than the highest frequencies of Cu₂Si
(420 cm⁻¹) [53], MoS₂ sheet (473 cm⁻¹) [54], or TiC mono-
layer (810 cm⁻¹) [55], indicating the strong Co-B and B-B
chemical bonding in this predicted CoB₆ sheet. We further
verified the thermal stability of the CoB₆ monolayer by per-
foming AIMD simulations at 500 K using a \( 5 \times 3 \) supercell.
Snapshots taken at the end of a 1.5 ps simulation period [see
Fig. 1(c)] with a time step of 1 fs show that the framework of
the planar sheet is generally well preserved. These systematic
tests show that the predicted CoB₆ monolayer is energetically,
dynamically, and thermally stable.

C. Stabilization mechanism

To better understand the nature of the bonding in the
CoB₆ monolayer, we first check the electron redistribution.
A Bader charge analysis confirms that each Co atom donates
0.38e to B atoms (see Table S1 of the Supplemental Material
[56] for more details), which indicates that Co atoms are
ionized, thus helping to stabilize the boron-sheet framework.
We also examine its molecular building block to understand
the structural stability of the predicted CoB₆ monolayer. We
used the CALYPSO code to search and screen a large number of
Co₄B₆ clusters, and we identified a minimum-energy Co₄B₆⁺
cluster (Fig. S1 [56]), which possesses a planar structure with
\( D_{\text{2h}} \) symmetry and can serve as a precursor for the 2D
CoB₆ monolayer. From the natural electron configurations
and a Wiberg bond index analysis, we find strong covalent
interactions between the Co and B atoms and covalent
characteristics of the B₆ framework (Figs. S2 and S3, Table
S2 [56]) in this cluster. An adaptive natural density parti-
tioning (AdNDP) analysis reveals the coexistence of 2c-2e
(2 center–2 electron), 3c-2e, and 4c-2e \( \sigma \)-bond (Fig. 1(d) and
Figs. S2 [56]) bonding configurations, which help to stabilize
the planar Co₄B₆⁺ cluster as well as the CoB₆ monolayer,
similar to the situation in \( \alpha \)-boron sheets [57].

D. Magnetic and electronic properties

It is expected that the partially filled Co 3d shell should lead to a magnetically ordered state in the CoB₆ monolayer structure. To explore this scenario, we first calculated the mag-
etic anisotropy energy (MAE) to determine the easy axis of possible ferromagnetic states. Within the PBE functional with the inclusion of the spin-orbit coupling (SOC), it is found that the easy axis initially placed in the basal plane ([i.e., the (100)
or (010) plane] would automatically switch to align in the c, or
(001), direction during self-consistent calculations, indicating
that the easy axis has a strong preferential orientation along
the out-of-plane direction. We then determined the preferred
coupling of magnetic orders by comparing the total energies
using a \( 2 \times 1 \) supercell for three different magnetic configu-
rations: ferromagnetic (FM) state, antiferromagnetic (AFM)
state, and nonmagnetic (NM) state. Calculated results show
that the FM configuration lies 77 and 114 meV lower in energy
than the AFM and NM configurations, respectively, indicating
that monolayer CoB₆ has a FM ground state. The occurrence
of FM ground states can be also understood in terms of the
Stoner criterion, which is described as \( N(E_F)I > 1 \), where
\( N(E_F) \) denotes the DOS at the Fermi level of the NM structure
and \( I \) is the exchange integral. According to our calculated
DOS and band structure in NM states (see Fig. S4 [56]),
localized and high peaks of DOS near the Fermi level, which
are mainly contributed by Co 3d electrons, can be observed.
The broad density of the sharp peak around the Fermi level
indicates the extreme instability of NM states, leading to the
spin splitting. Thus the magnetic moments on the Co sites
are formed. Meanwhile the calculations for possible Fermi
surface nesting indicate FM is stable (Fig. S5) [56]. Spin-
polarized electronic calculations indicate that the magnitude
of the magnetic moment is 0.94\( \mu_B \) per formula unit, and
the spin unpaired electrons are mainly localized on the Co atoms
[see Fig. 2(a)]. The on-site Coulomb interactions among the
Co 3d electrons play a significant role in determining the
electronic properties. Our PBE\(+U \) calculations show that the
FM state is further stabilized and lower in energy by 328 and
344 meV than the AFM state (for more details see Table S3
[56]), with enhanced magnetic moments of 1.377\( \mu_B \) and
1.382\( \mu_B \) per Co atom, respectively, at the \( U \) values of 3.5 and
6.0 eV. It is seen that while the correlation effects influence
the magnetic moment and stability, their main influence is to
enhance the FM ground state.

We also calculated the spin-resolved density of states (DOS)
and the corresponding electronic band structures. The states
at the Fermi level [Fig. 2(c)] are predominantly con-
tributed by the Co 3d electrons, and this result is consistent with
the spin-polarized electron distribution shown in Fig. 2(a).
The spin-polarized band structures [see Figs. 2(b) and 2(d)]
also reveal considerable asymmetric spin states near the Fermi
level. The spin-down channel is metallic while the spin-up channel possesses two Dirac cones [Fig. 2(d)] with linear dis-
persions in the vicinity. Both of these Dirac cones are located
near the Fermi level with slight gap openings. The energy
bands near the two Dirac points exhibit linear dispersions
along the $X-S$ and $Y-\Gamma$ directions, and the associated Fermi velocities are in the range of $(4.25-9.20) \times 10^5$ m/s, which are on the same order compared with graphene \[58\]. These Dirac cones persist in the electronic band structures produced by the HSE calculations (Fig. S6 \[56\]) and PBE+U calculations although they are shifted downwards to the valance band area, and an additional quadratic band is at the same level (Fig. S7 \[56\]).

E. Effects of strain and environment

The intriguing electronic and magnetic properties of the CoB$_6$ monolayer originate from the B-B and B-Co bonding configurations, which can be tuned by applied strain \[59–62\]. Here we focus on the influence of tensile strains, since compressive strains tend to buckle 2D materials \[63,64\]. Figure 3(a) shows the magnetic moment and Co-Co distance as a function of an external biaxial tensile strain, which causes a significant increase of the magnetic moment, monotonically rising from 1.9 $\mu_B$ to 2.8 $\mu_B$ per supercell at up to 10% strain under the PBE calculations. Meanwhile, the ferromagnetic stabilities of the CoB$_6$ monolayer are also remarkably enhanced, as evidenced by the increased energy differences with other states. As illustrated in Fig. 3(b), $\Delta E_1 (E_{AFM} - E_{FM})$ exhibits a significant increase from 77 to 151 meV and $\Delta E_2 (E_{NM} - E_{FM})$ dramatically increases up to 575 meV at 10% strain, which represents an approximately 400% enhancement. Under an uniaxial tensile strain, similar results were obtained at strains up to 4% (see Fig. S8 \[56\]). The applied strains also affect the spin-polarized electronic band structures, but the Dirac cone structures remain (Figs. S9 and S10 \[56\]).

The strain enhanced ferromagnetic stability can be understood within the Goodenough-Kanamori-Anderson (GKA) rules \[65–67\]. From the bonding structures illustrated in the inset of Fig. 3(a), it is seen that the ferromagnetic coupling strength is governed by two exchange interactions: a short-range direct nearest-neighbor $d$-$d$ exchange ($J_0$) and a superexchange via boron $p$ orbitals ($J_S$) \[68\]. The direct $d$-$d$ exchange originates from the Co $d$ orbitals, and it is in AFM coupling with $J_D < 0$ and is sensitive to the variation of the distance between the adjacent Co atoms. In contrast, since the angle of Co-B-Co (92$^\circ$) is close to 90$^\circ$, the $d$ orbitals on the nearest-neighbor Co atoms overlap with the $p$ orbitals of B atoms and are orthogonal to each other. Consequently, the superexchange mediated by the boron atom is in FM order with $J_S > 0$ according to the GKA rules. The superexchange strength is thus mainly sensitive to the Co-B-Co angle. The different responses of the two exchange parameters lead to a modulation of the magnetic stability under tensile strains, as the overall coupling is determined by $J_D + J_S$. Under biaxial tensile strains, the Co-B-Co angle stays almost unchanged (around 90$^\circ$) although the Co-B bonding distance is increased. As a result, the FM superexchange interaction ($J_S$) is less affected by strains. However, the AFM coupling originating from the direct $d$-$d$ exchange is significantly weakened, with the value of $|J_D|$ decreasing dramatically as the Co-Co distance is appreciably increased, at a rate much faster than that for the Co-B distance. Consequently, the resulting coupling becomes decisively more ferromagnetic under increasing tensile strains.

In practical applications, monolayer CoB$_6$ will likely be in contact with the ambient environment, which may alter the electronic and magnetic properties. Here, we consider the adsorption of common air components O$_2$, CO$_2$, and H$_2$O on the CoB$_6$ monolayer to examine the robustness of its main properties. Several possible adsorption positions of gas molecules on the $2 \times 2$ CoB$_6$ monolayer have been examined, and the most favorable adsorption geometries are shown in Figs. 4(a)–4(c). We find that the O$_2$ molecule is bridged between two Co atoms with an adsorption distance of 1.96 Å, and the CoB$_6$ sheet becomes slightly buckled, indicating the nature of chemisorption [see Fig. 4(a)]. The corresponding DOS in Fig. 4(d) clearly shows that the 2$p$ orbitals of O atoms make strong contributions to the states near the Fermi level. This chemical bonding interaction between O$_2$ and the CoB$_6$ monolayer remarkably modifies the electronic properties (Fig. S9); however, ferromagnetism is well preserved...
and the magnetic moment is actually increased due to the contribution from oxygen (from 0.94μ_B to 1.31μ_B per CoB6 unit), indicating that the oxygen environment is favorable for strong ferromagnetism in the CoB6 monolayer. In contrast, CO2 and H2O are obviously physisorbed on monolayer CoB6 with distances of 3.36 and 2.24 Å, respectively, and the structure of the host is little affected [Figs. 4(b) and 4(c)]. The corresponding DOS from the adsorbed molecules stay far away from the Fermi level [Figs. 4(e) and 4(f)], and the magnetic moment remains nearly the same as in the pristine CoB6 monolayer (Fig. S11 [56]). These results show that the ferromagnetic ground state of the CoB6 monolayer can survive, and even thrive, in the ambient environment.

F. Feasible synthesis routes

We finally examine and propose two feasible synthesis routes for the predicted CoB6 monolayer. The first is based on the recently proposed boron nanosheet [23,24,69]. From its configurational characteristics, the CoB6 monolayer can be viewed as a combination of Co atoms and the δ4 boron framework [Fig. 5(a)], with the sheet having a vacancy density of η = 1/4 as discussed in a previous report [49]. It is noted that even though the cohesive energy of the δ4 boron sheet is a little higher than an experimentally synthesized β12 and χ3 monolayer [24], it is lower than that of a recently fabricated graphene-like boron sheet [69], thus showing great potential to be obtained in experiment. We propose to synthesize monolayer CoB6 via depositing Co atoms on the δ4 boron sheet. To determine the preferred adsorption position, Co atoms are initially placed on seven possible sites of the boron network [see Fig. 5(a)]. Adsorption energy calculations (E_{ads} = E_{Co} + E_{δ4} − E_{Co-δ4}) show that the most preferred adsorption site for the Co atoms is the hexagon center of the δ4 boron sheet [see inset in Fig. 5(b)]. The embedding of Co atoms significantly expands the lattice constant along the b direction and immerses Co atoms into the boron sheet plane, leading to the atomic thick monolayer CoB6 structure. During the structural relaxation, the total energy linearly decreases without any energy barrier and the lattice along the b direction is automatically expanded by 16% as shown in Fig. 5(d). When Co atoms are initially adsorbed on other positions [1, 2, 3, 5, and 7; see Fig. 5(a)], they are in metastable states, and the associated adsorption energies are much lower. The results of our CI-NEB calculations show that the Co atoms will diffuse to the hollow position after overcoming a reasonably low energy barrier of 0.33 eV [Fig. 5(c)], and the structure will then automatically expand into the CoB6 monolayer [Fig. 5(d)]. These results indicate that the atomic thin CoB6 monolayer can be fabricated by depositing Co.
FIG. 5. (a) The geometry of the $\delta_4$ boron sheet and seven initial positions for Co adsorption. (b) Adsorption energies and the lowest energy configuration of the Co-adsorbed $\delta_4$ boron sheet; a Co atom initially placed at position 6 will automatically relax to position 4, thus positions 5 and 7 are connected by a dashed line. (c) Kinetic energy barrier from position 3 to position 4 from CI-NEB calculations; insets show initial, transition state, and final configurations. (d) The total energy of optimized structures as a function of strain; insets show the initial geometry and the lowest energy configuration.

atoms on the $\delta_4$ boron sheet. Alternatively, it is also possible to fabricate CoB$_6$ monolayer via direct chemical growth, based on our cluster calculations. Since the planar Co$_4$B$_8^+$ cluster is structurally stable, it is expected to be a highly efficient precursor for growing the CoB$_6$ monolayer. However, precise synthesis details such as the optimal pressure and temperature conditions will have to be further explored experimentally.

IV. CONCLUSION

Our extensive structure search in conjunction with first-principles energetic, dynamic, and thermodynamic calculations has uncovered a 2D CoB$_6$ monolayer that exhibits strong intrinsic ferromagnetism. This atomic thin planar ferromagnet hosts a robust ferromagnetic ground state with a large magnetic moment that can be effectively tuned and considerably enhanced by applied tensile strains. The ferromagnetic state remains stable upon the adsorption of common air components O$_2$, CO$_2$, and H$_2$O. Electronic band structure calculations reveal remarkable Dirac cone features with characteristic linear dispersions and high Fermi velocities. Our study introduces an outstanding candidate material into the family of intrinsic 2D ferromagnets, and provides a strong physics foundation for elucidating the structural, electronic, and magnetic properties as well as possible synthesis routes. The present results offer crucial guidelines for realizing and implementing the CoB$_6$ monolayer as a promising component for magnetoelectric devices.

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