Theoretical investigation of Ti\(_2\)B monolayer as powerful anode material for Li/Na batteries with high storage capacity

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**ARTICLE INFO**

Keywords:
- Monolayer Ti\(_2\)B
- Lithium-ion battery
- Sodium-ion battery
- Magnetism

**ABSTRACT**

Based on the theoretic analysis of Ti\(_2\)B monolayer by first-principles calculations, we find that the Ti\(_2\)B monolayer is one of the promising candidates for lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs) electrode materials. In comparison with other materials, Ti\(_2\)B monolayer exhibits relatively high capacity (503.1 mA h g\(^{-1}\)) and low diffusion barriers (17.2–23.5 meV). During the ion insertion/retraction, extremely high structure stability is indicated by the nearly invisible volumetric variation, and steady metallic character is manifested by the abundant electrons near the Fermi level. In the ground state of ferromagnetism, the magnetic effects are revealed on the thermal stability, charge transfer, ions diffusion, operating voltage and storage capacity.

1. Introduction

Safety and powerful battery devices are important for energy storage systems [1]. LIBs have attracted wide attention because of outstanding reversible capacity, high energy density and long lifetime [2–4]. However, the relatively low capacity of LIBs and the shortage of Li resources limit the further development of LIBs [1,5,6]. To meet the requirements of electric vehicles and portable electronic products, tremendous efforts have been devoted in enhancing the efficiency of LIBs and developing other metal-ion batteries [1,7]. SIBs with high electrochemical performance are recognized as the most promising alternative to LIBs [6,8–11].

The electrodes play important roles in the battery, and their properties have direct relationships with the type of materials [12]. As LIBs anodes, graphite has got a great success in commercialization, but further applications are limited because of the low capacity (theoretical capacity 372 mA h g\(^{-1}\), and experimental capacity 330 mA h g\(^{-1}\)) and high diffusion barrier (0.32 eV) [13]. Another kind of electrode is the multi-element composite oxide glass, such as SnO [14]. Unfortunately, the development of dendrite during the charge/discharge processes restricts the lifetime. Two-dimensional (2D) electrodes have got extra attention, such as transition-metal carbides, carbonitrides and nitrides (MXenes) [15–17], transition-metal boride (MBene) [18,19], transition-metal dichalcogenides (TMDs) and transition metal oxides (TMOs) [20]. 2D materials have been regarded as promising alternatives to commercial graphite because these materials possess large surface areas [16,18], excellent chemical stability and electronic conductivity [15,21]. Furthermore, the charge/discharge performance is enhanced by the fast ions exchange in these 2D materials [14,22].

Numerous MXenes have been reported and predicted as 2D materials, such as Ti\(_3\)C\(_2\) [23], Ti\(_2\)C [24], Ti\(_2\)B\(_2\) [25], Mn\(_2\)C [26], Mo\(_2\)C [27], Ni\(_2\)C [28] et al. [29–31]. Some of them have been synthesized in experiments [29,31–33]. Many MXenes have been investigated and shown good performance as electrode materials. 2D Ti\(_2\)B\(_2\) has been predicted to have high Li/Na storage capacities (456/342 mA h g\(^{-1}\)) and ultralow diffusion barriers (0.017/0.008 eV) [25]. Ti\(_2\)B monolayer has been forecasted and it’s ground state is ferromagnetic (FM) state [34], but the electrochemical properties and applications have not been explored.

This work focuses on the performance of Ti\(_2\)B electrode in the ground state of FM, and systematically analyzes the stability, Li/Na storage capacity, diffusion of ions in Ti\(_2\)B monolayer by DFT calculation. Our calculations reveal that Ti\(_2\)B is a potential anode material for LIBs and SIBs, with high storage capacity and low diffusion barrier. In
addition, the ferromagnetism in the ground state shows a no-ignorable influence on the charge/discharge and ions storage performance according to our calculation.

2. Calculation methods

All the calculations in this work are based on density functional theory (DFT) utilizing the Perdew-Burke-Ernzerhof (PBE) formalism of the generalized gradient approximation (GGA) [35] in the Vienna Ab initio Simulation Package (VASP) [36,37]. Pseudo-potentials with valence electrons contain d\(^{2}\)s\(^{1}\) for Ti atoms and s\(^{2}\)p\(^{1}\) for B atoms. The Brillouin zone is sampled using a Monkhorst-Pack k-mesh [38], 21 \(	imes\) 21 \(	imes\) 1k-mesh is used for the primary cell, 7 \(	imes\) 7 \(	imes\) 1 and 14 \(	imes\) 14 \(	imes\) 1-\(\times\) 1-meshes are used in the calculation of 3 \(	imes\) 3 \(	imes\) 1 and 2 \(	imes\) 2 \(	imes\) 1 supercells, respectively. The cut-off energy is set to 570 eV. The Hellmann-Feynman force [39] is less than 0.02 eV during the ionic relaxation loop. The energy convergence criterion of the electronic self-consistency is set to 10\(^{-7}\) eV. To eliminate potential interactions among layers, the vacuum layer with the thickness of 20 Å is applied. Furthermore, DFT-D2 method [40,41] is used to test the effect of long-range van der Waals interaction. The method is commonly used in calculating monolayer structures [26,42–44]. The comparison is also performed between DFT-D2 and DFT-D3 methods. It shows almost invisible difference in band structures, as shown in Fig. S2. 3 \(	imes\) 3 \(	imes\) 1 supercell is used to study the adsorption and diffusion process, and 2 \(	imes\) 2 \(	imes\) 1 supercell is used for the phonon dispersion and capacity calculations. Phonon dispersion curves are calculated by using PHONOPY package [45]. Bader charge methods are used to analyze the charge transfer between Ti and B, Li/Na and the Ti\(_2\)B monolayer. The climbing image nudged elastic band (CI-NEB) method [46] is employed to investigate the diffusibility of Li/Na ions. A Hose-Hoover thermostat (NVT) ensemble and 1 fs time step are adopted during the calculation of ab initio molecular dynamics (AIMD) [47] simulation in 200 K, 300 K, 600 K and 900 K.

The adsorption energy of Li and Na atoms on the Ti\(_2\)B monolayer is defined as:

\[ E = (E_{TBBM} - E_{TB} - nE_{M})/n \]  

where \(E_{TBBM}\) represents the total energy of Li/Na ions inserted into Ti\(_2\)B, and \(E_{TB}\) stands for the total energy of Ti\(_2\)B. \(E_{M}\) is the energy per atom of Li/Na in bulk metal.

The average adsorption energy for multilayer adsorption on the Ti\(_2\)B monolayer is defined as:

\[ E = (E_{TBBM} - E_{TBM,n} - nE_{B})/m \]  

where \(E_{TBBM}\) and \(E_{TBM,n}\) represent the total energy of Ti\(_2\)B with n and (n-1) adsorption layers, respectively. \(E_{B}\) is the energy per atom of Li/Na in bulk metal. m is the number of adsorbed atoms on each layer.

The formation energy for every concentration of Li/Na on Ti\(_2\)B monolayer is calculated according to the formulation:

\[ H = (E_{M,TLB} - E_{TB} - nE_{M})/(n + 1) \]  

where the \(E_{M,TLB}\) denotes the energy of Ti\(_2\)B after Li/Na atoms inserted. \(E_{TLB}\) corresponds to the energy of Ti\(_2\)B. \(E_{M}\) means the energy of Li/Na bulk.

For each concentration of Li/Na ions in Ti\(_2\)B supercell, average electrode potentials are calculated according:

\[ V = (E_{TB} - E_{TBM} + nF)/en \]  

where \(E_{TB}\) and \(E_{TBM}\) represent the total energy of Ti\(_2\)B monolayer before and after adsorbing Li/Na ions. \(E_{M}\) corresponds to the average energy of Li/Na in bulk structure.

The specific ion storage capacity is obtained from:

\[ C_{M} = c \times Z \times F/M_{Ti,B} \]  

where \(C_{M}\) is the number of Li/Na ions adsorbed in Ti\(_2\)B surface. \(Z\) refers to the valence number of Li/Na. \(F\) represents the Faraday constant (26801 m Ah mol\(^{-1}\)). \(M_{Ti,B}\) is the molar weight of Ti\(_2\)B.

3. Results and discussions

3.1. Crystal structure

The structure predicted by Ozdemir et al. [34] is used in this work. Ti\(_2\)B possess trigonal symmetry with the space group of P3m1. B atomic layer is sandwiched by two Ti layers. The grey and blue atoms (Fig. 1a) correspond to Ti atoms in the top-layer and bottom-layer, respectively. PBE without spin-orbit coupling (SOC) is used to optimize the lattice parameters. SOC makes no influence on the electronic band structure, as shown in Fig. S3. The SOC effect makes no difference in the electronic properties, and neglectable in the latter simulations. A slightly smaller cell (\(a = b = 3.15\) Å) than the calculated one by Ozdemir et al. [34] is obtained after optimization. After computing the energy of nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic-\(n'e'\) states, the same conclusion is arrived at that FM state is the ground state of Ti\(_2\)B monolayer (Fig. S1) [34]. Ti atoms contain a magnetization of 0.75 µB in the in-plane direction (Fig. 1b), which agrees with the former conclusion [34].

3.2. Electronic structure

Based on the calculations, a clear message is obtained from the total and partial density of state (DOS) in Fig. 2a and b. A large number of electrons near the Fermi level suggest that Ti\(_2\)B possesses metallic electron dispersion. The electrons near the Fermi level make easy interaction between layers and ions. The DOS near the Fermi energy level mostly originates from Ti atoms, exactly 3d orbital of Ti atoms. The great conductivity of Ti\(_2\)B monolayer is almost denoted by Ti-3d electrons. The dynamical and thermal stabilities are investigated by AIMD simulations and phonon dispersion curves. In the phonon dispersion curves, the absence of imaginary modes in the first Brillouin zone demonstrates the dynamically stability, as shown in Fig. S1 (b). After performing AIMD simulations for 10 ps, the thermal stability of Ti\(_2\)B is confirmed by equilibrium values of energy, as shown in Fig. S4.

Fig. 1. Crystal structures of monolayer Ti\(_2\)B from (a) side and (b) top views and the magnetic structure of Ti\(_2\)B. High symmetry adsorption sites of Li/Na on the surface of Ti\(_2\)B (S1, S2, S3, S4) are shown in (b). The green, grey and blue atoms indicate B, Ti-1 and Ti-2, respectively. The S1, S2, S3 and S4 sites represent top sites of Ti-1, Ti-2, B, and the center of three atoms, respectively. The red dotted line in (a) is the surface of Ti-1-B-Ti-2. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
FM-Ti$_2$B is disordered when heated at 600 K, but no obvious structure reconstruction appears in the NM-Ti$_2$B, as shown in Fig. S5. The radius distribution function (RDF) is analyzed to investigate the long-range order of Ti$_2$B monolayer. Peaks appearing from 1 to 6 Å confirm the long-range order, as demonstrated in Fig. 2e, f and S6. The charge transfer between Ti and B atoms is calculated using Bader charge analysis. The amount of charge transfer in NM-Ti$_2$B between Ti and B atoms (0.902 e) is 2.27% bigger than that of FM-Ti$_2$B (0.882 e). According to the electron localization function (ELF) of Ti$_2$B shown in Fig. 3, the ionic bonding features between Ti and B atoms is confirmed. The ELF value of blue areas is nearly 0.5, 0.7, 0, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 2. (a, b) DOS, (c, d) Phonon dispersion curves, (e, f) RDF of Ti$_2$B in FM and NM state, respectively.

Fig. 3. The electron localization function of (a) NM and (b) FM Ti$_2$B along the surface of Ti-1-B-Ti2. The ELF value of green, yellow and blue areas is nearly 0.5, 0.7, 0, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 4. The adsorption energy after inserting Li and Na ions on the Ti$_2$B monolayer. The charge density difference in Ti$_2$B monolayer after absorbing (b) Li and (c) Na ions. The yellow and blue areas represent sufficient and deficient areas. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
3.3. Battery performance

3.3.1. Ion insertion

In order to know the possibility of 2D Ti₂B as an electrode material, we calculate the adsorption energy of different adsorption sites. The negative adsorption energy indicate that Ti₂B has the ability to storage Li/Na atoms, so further investigations of battery performance are worthwhile. The most favourable adsorption site is evaluated by Eq. (1). According to the symmetry of Ti₂B, four adsorption sites (S1-S4) are taken into consideration. The most favourite adsorption site with the lowest adsorption energy is S3 (B) in Fig. 4a. For the multi-layer configurations, the ions are hardly inserted into this material, so the monolayer configuration is suitable to be made as battery electrode.

3.3.2. Charge transfer

To further analyze the chemical bonding between Li/Na and Ti₂B, the charge transfer is estimated via Bader charge analysis, as shown in Fig. 4b and c. The number of charge transfer between ions and surface is 0.812 e for LIB and 0.581 e for SIB. The chemical bond between Li/Na ions and Ti₂B surface is confirmed by the charge transfer. The radius of Li is smaller than that of Na, so Li naturally sits close to the surface (2.348 Å and 2.750 Å for Li-B Na-B, respectively). The larger charge transfer and smaller distance between Li and Ti₂B surface deduce that the interaction between Li and surface is stronger than that of Na [43]. This strong interaction between Li/Na ions and layer may influence the diffusion process, which will be confirmed in the next part.

3.3.3. Diffusion processes

The diffusion process makes influence on the charge/discharge process [26]. The optimum adsorption site is S3 (B atoms), as shown in Fig. 1b. Under the symmetry of the system, three nearest pathways are considered. After optimization, three diffusion pathways are demonstrated in Fig. 5a. The favourite diffusion pathway with the lowest diffusion barrier is S2-S3-S2, as displayed in Fig. 5b, and the diffusion barrier is 17.2 meV for Na and 23.5 meV for Li. The lower diffusion barrier of Na also confirms the suppose that the strong interaction between Li and surface impedes the ion moving. Even though, both the diffusion barriers (< 0.03 eV) are much lower than those of graphite (> 0.32 eV) [48], graphene (0.53–0.7 eV) [49], and graphdiyne (0.92 eV in-plane, 0.18 eV out-of-plane) [50]. In conclusion, Ti₂B possesses extremely low diffusion barriers, which is a considerable advantage of Ti₂B as an electrode material.

3.3.4. Open circuit voltages

The open-circuit voltage (OCV) is an important property in the charge/discharge process. The adsorption energy of Li/Na atoms is calculated by Eq. (1). The sites of atoms in every concentration are shown in Fig. S8 and 9. The average adsorption energy for second layer adsorption is calculated by Eq. (2). The nearly zero energy indicates weak multilayer adsorption. According to the adsorption energy for each concentration, the enthalpies of formation are finally calculated by Eq. (3). The enthalpy of every concentration located on the hull indicates the thermodynamic stability after adsorption [25], as demonstrated in Fig. S7c and d. The average electrode potentials are analysed by Eq. (4), with the structure located on the hull. As shown in Fig. 5c, LIB possesses stable OVC with only one plateau (0.381 V), while SIB contains four plateaus: Ti₂B → Na₀.5Ti₂B, Na₀.5Ti₂B → Na₁Ti₂B, Na₁Ti₂B → Na₁.25Ti₂B, Na₁.25Ti₂B → Na₂Ti₂B. The range of OCV is 0.455–0.033 V for SIB, within the limits of 0–1 V, which is the operating voltage of anode material [25]. It demonstrates that Ti₂B monolayer is a promising anode material and Ti₂B monolayer suppresses the Li/Na dendrite growth during the charge-discharge processes [51].

3.3.5. Theoretical storage capacity

The theoretical storage capacity of the electrode has a direct relationship with the energy density of the battery, and it is important for practical application. After calculated using Eq. (5), the same values of LIBs and LIBs (503.1 mA h g⁻¹) are obtained. What is more important, the capacity of Ti₂B is larger than that of graphite [48]. During the process of ions insertion, with the continuously accumulate of electrons on the Ti₂B surface, the repulsive force coming from the surface electrons increases, which obstructs the further adsorption. The electrostatic force between ad-atoms also confines further adsorption. Although Ti₂B has no multilayer adsorption, the relatively high storage ability makes it a high capacity anode material.

3.3.6. DOS and volume changes

The big volume change of the electrode will weaken the recycling Fig. 5. (a) High symmetry diffusion pathways in FM-Ti₂B monolayer. The blue and grey balls represent Ti atoms in the bottom and top layers. The green atoms represent B. The green, blue and red paths are S3-S2-S3, S3-S1-S3, S3-S4-S3, respectively. (b) The diffusion barriers of Li or Na in each paths. The different coloured lines correspond to the different diffusion paths. (c) OCV as a function of x. (d) The density of states after adsorbing Li and Na on the surface of Ti₂B monolayer. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
and stability of the battery [26]. To study the stability of the electrode, the DOS and volume change are required to be considered after adsorbing ad-atoms on Ti2B. A larger charge density near Fermi level after the insertion of Li/Na atoms means that Ti2B remains wonderful conductivity and stability during the operating time, shown in Fig. 5d. The volume change during the operating time impacts on the cyclability of the battery. The volume variation of Ti2B slab is only $-2.194\%$ and $-2.410\%$ for Li and Na inserted. These constant properties indicate the steady of battery performance during the charge-discharge, which is suitable for the practical applications [43]. The elastic stiffness constants are investigated to test the mechanical properties of Ti2B, as shown in Table 2 in the supplementary information. The elastic constants satisfy the mechanical stability criteria: $C_{11} \times C_{12} - C_{11}^2 > 0$, implying the mechanically stable of Ti2B.

### 3.3.7. Influences of magnetism

Although the magnetism has been taken into consideration during the calculations of battery properties, the effects of magnetism on the battery properties are still unclear.

The battery properties of NM-Ti2B are systematically investigated in this section. The favorite adsorption site is S2 (Ti-2) and the adsorption energy is lower than that of FM-Ti2B. The magnetism prevents the charge transfer between the ions and surface, as shown in Fig. S12. The amount of charge transfer is less than one electron, which is consistent with only one valence electron of Li/Na.

After simulating the diffusion process, the lowest diffusion barriers (11.0 meV for Na and 19.4 meV for Li) in NM state are smaller than those of FM-Ti2B, but the optimum diffusion pathway does not change, as displayed in Fig. 6. After comparing the bonding distance between ions and surface, we find that Li/Na ions sit farther to the surface of NM-Ti2B (2.402 Å for Li and 2.756 Å for Na) than FM-Ti2B. As the bond strength is reflected by the bonding distance [30,43], the short distance between Li/Na ions and FM-Ti2B surface indicate the strong adsorption. So that FM-Ti2B possesses a higher diffusion barrier for Li/Na than NM-Ti2B. The OCV of NM-Ti2B is lower than that of FM-Ti2B. After calculating the capacity of NM-Ti2B (440.2 mA h g$^{-1}$), the outcomes show that magnetism makes no influence on the storage capacity of Li, but enhances the Na storage ability. The DOS and volume also show invisible changes during the ion’s insertion/retraction. The elastic stiffness constants are calculated. The elastic constants satisfy the mechanical stability criteria: $C_{11} \times C_{12} - C_{11}^2 > 0$, implying the mechanically stable of Ti2B during the ion insertion and retraction.

In conclusion, magnetism makes a non-ignorable influence on battery performance, such as storage ability and charge/discharge process which is important for the operation of the battery. Magnetism is considered during the calculation of battery properties. Further analysis should be made in experiments to investigate the effect on the performance and this is beyond the scope of our article.

### 3.4. Comparisons with other materials

Countless efforts have been made to explore the 2D anode materials and many materials have been reported. Excellent charge-discharge and storage capacity of batteries are two important aspects to fulfill the demands of electricity consumers. Clear comparisons with other reported materials are made in this section. For the storage capacity, different rules are used in these materials. Only first layer adsorption is considered in some studies, such as VS$_2$ [52], Ta$_2$N [53], Ti$_2$N [53], V$_2$N [53], V$_2$Na [53]. Most of studies considered the second layer adsorption, such as Ga$_2$N [54], Mo$_2$C [27], V$_2$C [43], Ti$_2$B$_2$ [25]. In our calculation of Ti2B, the seconded layer adsorption is also introduced. The ability of Ti2B as LIBs electrode is compared with other materials in Fig. 7a. Ti$_2$B has relatively high capacity and low diffusion barrier than other materials, such as Graphite [48] and MoS$_2$ [31], and TiS$_2$ [55], et al [23,24,52,56–58]. Ti$_2$B is a potential electrode material with lower diffusion barriers and higher capacities than these materials, but materials such as hydrogenated borophene [59], graphyne [60], C$_2$N$_{14}$ [61] possess enormous storage capacity than Ti$_2$B, nevertheless. The low diffusion barriers guarantee the fast ions transportation is the merit of Ti$_2$B when compare with these high capacity materials. Ti$_2$B possesses lower diffusion barrier but smaller capacity than silicon [57]. Even Ti$_2$B possess low capacity than Si but it has few volume changes

![High symmetry diffusion pathways in NM-Ti$_2$B monolayer without magnetism.](image)
makes Ti$_2$B more suitable to become LIBs electrode.

In comparison with other SIB materials, as shown in Fig. 7b. Ti$_2$B possesses higher diffusion barriers than Ti$_2$B$_2$ [25], Tetr-Mo$_2$B$_2$ [62], Tri-Mo$_2$B$_2$ [62], Nb$_2$C [63], and Sr$_2$N [58], but Ti$_2$B provides relatively high capacity than these materials. Ti$_2$B has higher capacity and lower barrier than Ti$_2$S [58], and MoS$_2$ [31], etc [10,55,58,63,64]. Even if the capacities of Ti$_2$B are lower than those of Ca$_2$N [54], hydrogenated borophene [59], C$_{24}$N$_{14}$ [61], V$_2$C$_2$ [43], graphene [60], α-PC [66] and ZnP [22], but the diffusion barriers of these materials are relative higher than that of Ti$_2$B. In brief, high capacity and low diffusion barrier demonstrate that Ti$_2$B is worth developing as LIB and SIB electrode materials.

4. Conclusions

In conclusion, the potential application of 2D Ti$_2$B as an anode material of LIB and SIB is elaborated by DFT calculations. The favourable adsorption site and diffusion pathway for ions with low diffusion barriers are explored. The easy charge/discharge process is suggested by the low diffusion barrier (< 23.5 meV) of Li/Na. Furthermore, the considerable capacity of Ti$_2$B makes the application in the energy storage systems possible. The almost invisible variations of DOS and volume during the charge/discharge process are suitable for the stability of battery operation. All these aspects make 2D Ti$_2$B a promising anode material for LIBs and SIBs. The influences of magnetism on the theoretic calculations of battery performance are demonstrated in this research. Further research should be made in experiments to explore the FM-Ti$_2$B as a promising electrode material.

CRediT authorship contribution statement


Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This research was supported by the National Natural Science Foundation of China (Grant No. 11675195 & 11675255 & U1932220), the National Key R&D Program of China (2016YFA0401503& 2017YFA0403700), and Key Research Program of Frontier Sciences, CAS, Grant No. 292016YQYXJ0135.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apsusc.2020.148048.

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