First-principles investigations to evaluate Mo$_2$B monolayers as promising two-dimensional anode materials for Mg-ion batteries

Tiantian Mei, Jianbao Wu*, Shuhan Lu, Bingqian Wang, Xinxin Zhao, LiLi Wang and ZhiXiang Yin

School of Mathematics, Physics and Statistics, Shanghai University of Engineering Science, 333 Longteng Road, Shanghai 201620, People's Republic of China

* Author to whom any correspondence should be addressed.

E-mail: wujianbao@sues.edu.cn

Keywords: Mo$_2$B monolayer, Mg-ion batteries, DFT

Abstract
Magnesium-ion batteries have the potential to replace the current commercial Li-ion batteries due to their eco-friendliness and cost-effectiveness. However, because of the strong polarization of Mg ions, conventional electrode materials find it difficult to capture Mg ions. In order to find an excellent anode material for Mg-ion batteries, we used density functional theory to evaluate the applicability of T-type and H-type Mo$_2$B monolayers as electrode materials for Mg-ion batteries. The simulation results show that the adsorption energies of T-type and H-type Mo$_2$B monolayers for Mg atoms are $-1.08$ eV and $-0.78$ eV ($-2.16$ eV and $-2.14$ eV with the solvent effect), respectively, which are sufficient to ensure the stability of the procession of magnetization. In addition, the ultra-low diffusion barriers (0.057 eV/0.110 eV) of Mg atoms on their surfaces show a good charge and discharge rate. The theoretical specific capacity (529 mA h g$^{-1}$) and the theoretical voltages (0.65 V/0.40 V) indicate that T-type and H-type Mo$_2$B monolayers are promising anode materials for Mg-ion batteries.

1. Introduction
With the continuous development of portable electronic devices and electric and hybrid vehicles the development of electrochemical energy storage equipment with a high energy density and low cost is urgently required [1–3]. At present, Li-ion batteries are the most widely studied ion batteries, and they also occupy a dominant position in the global renewable energy product market [4, 5]. However, the large-scale energy storage application of Li-ion batteries is limited by the small natural reserves of Li, high production costs and safety problems [6, 7]. Therefore, in order to meet the demands of large-scale electronic equipment for energy storage and a green environment the development of new battery systems is vital [6, 8, 9].

Rechargeable Mg-ion batteries are regarded as a potential alternative to Li-ion batteries due to their low cost and eco-friendliness [10–13]. Magnesium can reach a theoretical specific capacity of 2205 mA h g$^{-1}$ and a volume capacity of up to 3833 mA h cm$^{-3}$, almost twice that of Li (2062 mA h cm$^{-3}$). The reserves of Mg in the earth's crust (2.9%) are much higher than those of Li (0.002%), eliminating the risk of resource depletion and providing cheaper products [7, 14, 15]. Most importantly, compared with Li, Na and K anodes, Mg anodes form a smooth and uniform deposition layer during the electrodeposition process, thereby avoiding the formation and growth of dendrites, making the battery safer [16, 17]. However, due to the strong polarization of Mg ions, it is difficult for Mg to be adsorbed by conventional electrode materials such as Li and Na. Therefore, the development and exploration of electrode materials suitable for Mg-ion batteries are key to promoting the development of Mg-ion batteries and improving their practical applications [2, 18, 19].

In recent years, two-dimensional materials have attracted more and more attention due to their wide application prospects, including in electronic devices and energy storage technologies. Previous theoretical
and experimental studies have proved that two-dimensional materials can be used as negative electrodes for Li-ion batteries because of their high specific surface area, low diffusion barriers and abundant adsorption sites [20–23]. Recently, a new type of two-dimensional transition metal boride (MBene; M can be a transition metal element such as V, Cr, Mo and B represents boron) has been widely studied in the field of batteries. The material was first discovered and named by Guo and colleagues in 2017 [24]. They found that in theory MBene can be obtained by selectively etching the A layer in MAB (M2AlB2), and calculated that two-dimensional Mo2B2 and Fe2B2 are suitable anode materials for Li-ion batteries with a small diffusion energy barrier (0.24 eV/0.27 eV) and high storage capacity (444 mAh g−1/665 mAh g−1) [24]. Subsequently, Zhang et al reported for the first time that a dilute HCl solution can selectively etch the Al layer in Cr2AlB2 to form Cr2B2 [25]. Alameda et al also found that Mo2AlB2 can react with NaOH at room temperature to cause Al deintercalation [26]. These works show that MBene is not only a theoretical possibility but can also be synthesized experimentally. Recently, Wang et al studied the possibility of two-dimensional Mo2B with a hexagonal structure as the negative electrode material for Li-ion or Na-ion batteries. The results for adsorption energies, diffusion energy barriers and open circuit voltages show that it is a promising negative electrode material for Li-ion (Na-ion) batteries. The diffusion energy barrier is only 0.073 eV (0.069 eV), and the open circuit voltage ranges from 0.62 V to 1.15 V (0.42–1.41 V) [27]. Yuan et al found through calculation that Zr2B2 is a suitable anode material for Li-ion batteries, and its adsorption energy for Li is 0.628 eV, which is sufficient to ensure the stability of the lithiation process. In addition, the minimal diffusion energy barrier (0.017 eV) for Li atoms on monolayer Zr2B2 shows excellent charge and discharge rates. The theoretical capacity of 526 mA h g−1 is also greater than that of commercial graphite electrodes [28]. Bo et al [29] discovered two new Mo2B2 monolayers by crystal structure prediction, and studied their stability, electronic structures and performance as negative electrode energy storage materials using first-principles methods. The calculated phonon spectra and electronic structures show that the two structures have good stability and conductivity, with a storage capacity of 251 mAh g−1 (251 mAh g−1) and a diffusion energy barrier of 0.029 eV (0.023 eV) [29]. Li et al also discovered a new material (TiB3) through crystal structure prediction combined with first-principles density functional theory (DFT). The theoretical capacities of this material for Li and Na are as high as 1335.04 mAh g−1 and 567.52 mAh g−1, respectively. In addition, the ultra-low barrier energy (only 0.038 eV) and suitable open-circuit voltage indicate excellent charging and discharging capabilities. These results indicate that a TiB3 monolayer is an excellent anode material for Li-ion and Na-ion batteries [30].

Considering the scarcity of anode materials for Mg-ion batteries, after learning about the excellent performance of MBene as an anode material for Li-ion and Na-ion batteries, we decided to calculate the possibility of using H-type and T-type Mo2B as anode materials for Mg-ion batteries. The results for adsorption energies, diffusion barriers, theoretical capacities and theoretical voltages show that these two kinds of Mo2B are suitable anode materials for Mg-ion batteries. Previously, Zha et al made a detailed study of these two Mo2B structures, and their results showed that these two structures are stable and have excellent mechanical, electronic and thermal properties. It is therefore theoretically feasible to use them as anode materials for Mg-ion batteries [31].

2. Computational methods

During battery simulation, the related energy calculations and structural optimizations were carried out using the Vienna ab initio Simulation Package [32]. The exchange–correlation energy of the electrons was described within the generalized gradient approximation framework using the Perdew–Burke–Ernzerhof functional [33]. The interaction between electrons and ions was described using the projector augmented wave method with plane waves up to a cutoff energy of 500 eV [34]. A 4 × 4 × 1 supercell of Mo2B monolayers was employed to model the adsorption of Mg atoms, and the VASP/SOL model [35–37] was used to simulate the adsorption in a solvent with a dielectric constant of 7.09. Brillouin zone integration was performed using a 3 × 3 × 1 k-point grid. All geometric structures were fully relaxed and optimized until the force on the atoms was less than 0.01 eV Å−1, and the convergence criterion for electron self-consistency was set to 10−5 eV. To avoid interlayer interactions resulting from the periodic boundary conditions, a vacuum space layer of 20 Å was set. The van der Waals (vdW) correction DFT–D3 proposed by Grimme was chosen to describe the long vDW interaction for the adsorption of Mg atoms [38]. We used the climbing image nudged elastic band method to determine the energy barriers and minimum energy paths of Mg atom diffusion [39]. The ab initio molecular dynamics (AIMD) simulation was used to study the thermal stability of a 4 × 4 × 1 monolayer Mo2B supercell filled with Mg atoms at 300 K. The AIMD simulation used the NVT ensemble with a duration of 5 ps and a step size of 1 fs.
3. Results and discussions

3.1. Structures and electronic properties of Mg atom adsorption on Mo$_2$B

The optimized geometric structures of T-type and H-type Mo$_2$B are shown in figure 1. Figures 1(a) and (b) show the top and side views of T-type Mo$_2$B. The structure of T-type Mo$_2$B can be viewed as bilayer Mo atomic layers intercalated by a B layer forming an edge-shared Mo$_6$B octahedral structure. It is similar to the previously reported Mo$_2$C \[40\]. The optimized lattice constants $a$ and $b$ are both 3.093 Å, the Mo–B bond length is 2.112 Å and the Mo–Mo bond length is 2.879 Å, all of which are within the previously reported results \[31\]. Figures 1(c) and (d) show the top and side views of H-type Mo$_2$B. The top view presents a typical graphene-like hexagonal structure. The side view reveals a sandwich structure, with the B layer sandwiched between two Mo layers, and the Mo atoms in the top layer are directly above the Mo atoms of the bottom layer. This structure is similar to the previously reported MoS$_2$ \[41\]. The optimized lattice constants $a$ and $b$ are both 2.869 Å, the Mo–B bond length is 2.189 Å and the Mo–Mo bond length is 2.862 Å, which are also consistent with the previously reported results \[31\].

As is well known, the relatively large adsorption energy plays a fundamental role in anode materials that are suitable for specific ion storage. In order to avoid the interaction between adjacent metal atoms, based on a $4 \times 4$ supercell, the stable adsorption sites of Mg atoms on T-type and H-type Mo$_2$B are studied. The adsorption energy is calculated according to the following formula:

$$E_{ad} = E_{Mg/\text{sub}} - E_{\text{sub}} - E_{Mg}.$$ \hspace{1cm} (1)

In this formula, $E_{Mg/\text{sub}}$ and $E_{\text{sub}}$ represent the total energy of T-type or H-type Mo$_2$B with or without Mg atoms, and $E_{Mg}$ is the energy of a Mg atom in the hexagonal close-packed structure. Here, three possible initial adsorption positions are considered for each structure. For T-type Mo$_2$B, the Mo1 site, the B site and the Mo2 site, respectively, indicate that a Mg atom is located above the lower Mo atom, above the B atom and above the upper Mo atom. These three sites are marked in figure 1(b). For H-type Mo$_2$B, the H site, B site and Mo site, respectively, indicate that a Mg atom is located above the center of the hexagonal ring, above the B atom and above the Mo atom. These three sites are marked in figure 1(c). As can be seen from table 1, a Mg atom is stabilized at the top of the Mo atom at the bottom of T-type Mo$_2$B, and its adsorption energy is 0.09 eV lower than that of a Mg atom at the B site and 0.23 eV lower than that of Mg atom at the Mo2 site. In H-type Mo$_2$B, a Mg atom is stable at the top of its hexagonal center, and its total energy is 0.09 eV and 0.19 eV lower than that of a Mg atom at the B site and Mo site, respectively. Compared with the cohesive energy of Mg atoms in a bulk structure (1.51 eV) \[42\], the adsorption of Mg atoms on the surface of the Mo$_2$B is smaller. Considering the solvation effect, the recalculated adsorption energy of Mg atoms is larger at 2.16 eV and 2.14 eV for T-type and H-type Mo$_2$B, respectively. This is sufficient to overcome the agglomeration effect of Mg atoms.

In order to further understand the adsorption process, we studied the charge transfer of Mg atoms adsorbed on T-type or H-type Mo$_2$B by Bader charge analysis; the charge transfer values are shown in...
Table 1. Adsorption energies (\(E_{ad}\)) and transfer charges (\(Q_{tr}\)) of a Mg atom on T-type and H-type Mo\(_2\)B.

| Type | Site | \(E_{ad}\) (eV) | \(Q_{tr}\) (Mg) (e) | \(Q_{tr}\) (Mo) (e) |
|------|------|----------------|-------------------|-----------------|
| T    | Mo1  | −1.08          | −0.92             | 0.30 × 3        |
|      | B    | −0.99          | −0.89             | 0.29 × 3        |
|      | Mo2  | −0.85          | −0.77             | 0.65            |
| H    | H    | −0.78          | −0.96             | 0.28 × 3        |
|      | B    | −0.69          | −0.95             | 0.27 × 3        |
|      | Mo   | −0.59          | −0.88             | 0.66            |

Figure 2. (a)–(c) Differential charge density diagrams of a Mg atom adsorbed on the Mo1 site, the B site and the Mo2 site, respectively, of T-type Mo\(_2\)B. (d)–(f) Differential charge density diagrams of a Mg atom adsorbed on the H site, the B site and the Mo site, respectively, of H-type Mo\(_2\)B.

Table 1. The three-dimensional charge density difference diagram is shown in figure 2, which can be obtained from equation (2) as follows:

\[
\Delta \rho = \rho (\text{Mg/sub}) - \rho (\text{sub}) - \rho (\text{Mg}).
\]

In this expression \(\rho (\text{Mg/sub})\) and \(\rho (\text{sub})\) represent the total electron density of monolayer Mo\(_2\)B with or without a Mg atom, respectively. \(\rho (\text{Mg})\) represents the total electron density of a Mg atom. Yellow and blue represent the accumulation and depletion of charge, respectively. It can be seen from figure 2 that the Mg atoms are all charge donors in these six adsorption configurations, and during the adsorption process the Mg atom transfers electrons to Mo\(_2\)B. In addition, it can be seen that electrons tend to accumulate between the Mg atom and adjacent Mo atoms, which leads to the formation of bonds between the Mg atom and Mo atoms. It can also be found from table 1 that the electrons lost by the Mg atom are basically taken by Mo atoms. Since in the four adsorption configurations of the Mo1 site and B site of T-type Mo\(_2\)B and the H site and B site of H-type Mo\(_2\)B, Mg atoms interact with three adjacent Mo atoms, so the corresponding number of transferred electrons in table 1 is also multiplied by 3. To sum up, it can be inferred that the Mg atom mainly interacts with adjacent Mo atoms during adsorption, while B atoms basically do not participate in the reaction. The calculated crystal orbital Hamiltonian population (COHP) also verified this conclusion. Here, we also multiplied the –COHP value of the Mo1 site and B site in T-type Mo\(_2\)B and the H site and B site in H-type Mo\(_2\)B by 3, as shown in figure 3. As can be seen from figure 3, in all adsorption systems, when the energy is negative, only the –COHP value between the Mg atom and the Mo atom is basically higher than 0, while the –COHP value between the Mg atom and the B atom is basically 0, indicating that only Mg and Mo atoms have bond states. In addition, it can be found that for each monolayer Mo\(_2\)B adsorption configuration, the larger the adsorption energy is, the higher the peak value of –COHP is, and the larger the charge transfer...
value. These facts indicate that the larger the adsorption energy is, the stronger the bond state of the Mg and Mo atoms. This strong bond state ensures that the Mg atoms are tightly bound to the Mo$_2$B monolayer.

3.2. Diffusion energy barriers of Mg atoms on Mo$_2$B
Since the migration energy barrier is a key parameter that determines the charge and discharge rates of Mg-ion batteries [43, 44], we have studied the diffusion properties of Mg atoms on the surface of T-type and H-type Mo$_2$B under the premise of determining the stable position for a Mg atom. The diffusion paths of a Mg atom on T-type and H-type Mo$_2$B are shown in figures 4(b) and (c). For each Mo$_2$B monolayer, we investigated two possible migration paths. In T-type Mo$_2$B, path 1 is shown by the purple solid line in figure 4(b). The Mg atom diffuses from the top of the bottom Mo atom to the top of the middle B atom, and then moves to the top of the adjacent bottom Mo atom. Path 2 is shown by the purple dotted line in figure 4(b). The Mg atom diffuses from the top position of the bottom Mo atom to the adjacent top Mo atom position, and then moves to the top of the adjacent bottom Mo atom. The diffusion energy barriers corresponding to path 1 and path 2 are 0.057 eV and 0.254 eV, respectively. In H-type Mo$_2$B, path 1 is shown by the solid green line in figure 4(c). The Mg atom diffuses from the top of the center of the hexagon to the top of the adjacent B atom, and then diffuses to the top position of the center of the adjacent hexagon. Path 2 is shown by the green dashed line in figure 4(c). The Mg atom diffuses from the top of the center of the hexagon to the top of the adjacent Mo atom, and then diffuses to the top of the center of the adjacent hexagon. The diffusion energy barriers of path 1 and path 2 are 0.110 eV and 0.137 eV, respectively. The finally obtained diffusion energy barriers of the two structures are shown in figure 4(a). Obviously, in the diffusion energy barriers of T-type and H-type Mo$_2$B the energy barriers along the solid line are lower than those along the dotted line, indicating that Mg atoms are more inclined to spread across the top of the B atoms. Overall, both show fast charge and discharge rates. The low diffusion energy barriers (0.057 eV/0.110 eV) obtained for Mg atoms on the two Mo$_2$B monolayers are far superior to those of typical electrode materials, such as monolayer VO$_2$ (0.517 eV) [45], borophene (0.97 eV) [46] and monolayer black phosphorus (0.09 eV). Although the value of 0.09 eV is already very small, it is still a bit larger than our minimum energy barrier value of 0.057 eV [47].

3.3. Theoretical storage capacities of Mg atoms on Mo$_2$B and average open-circuit voltages
The insertion process of Mg atoms is simulated by gradually adding Mg atoms to the 2 × 2 T-type and H-type Mo$_2$B supercells, and the energy change in the $n$th step is calculated by formula (3):

$$\Delta E_{ad} = E_{Mg_n/sub} - E_{Mg_{n-1}/sub} - E_{Mg}.$$  (3)
Figure 4. (a) Diffusion energy barriers of a Mg atom on the surfaces of T-type Mo$_2$B and H-type Mo$_2$B. (b), (c) Schematic diagrams of the diffusion paths in T-type and H-type Mo$_2$B, respectively.

$E_{\text{Mg}_n/\text{sub}}$ and $E_{\text{Mg}_{n-1}/\text{sub}}$ represent the total energy of $n$ and $n-1$ Mg atoms adsorbed on T-type or H-type Mo$_2$B, respectively. Each time a Mg atom is placed into a supercell, several adsorption configurations are considered to determine the most stable adsorption configuration. Then the energy change at each step of Mg atom insertion is obtained by formula (3). The final result is shown in figure 5. It can be seen that for T-type and H-type Mo$_2$B, when the Mg atomic number on the $2 \times 2$ supercell is less than 8, the energy difference of each Mg atomic intercalation step is always negative. However, when the ninth Mg atom is introduced into the substrate, the energy difference becomes positive, indicating that the substrate has no adsorption effect on the ninth Mg atom at this time, that is to say, the adsorption has reached saturation. Therefore, the Mg atomic intercalation step will stop at $n = 8$, which corresponds to the stoichiometric ratio of Mg$_8$(Mo$_2$B)$_4$. The maximum theoretical capacity can be calculated by formula (4):

$$C = \frac{xqF}{M}$$

(4)

Here, $q = 2$ represents the valence state of the Mg atom, $x = 8$ is the final product of the Mg atom intercalation state, $F$ is the Faraday constant and $M$ represents the molecular weight of T-type or H-type (Mo$_2$B)$_4$. The average open circuit potential (OCP) can be calculated by the following formula:

$$\text{OCP} = -\frac{E(\text{Mg}_x/\text{sub}) - E(\text{sub}) - xE(\text{Mg})}{qx}.$$ 

(5)

According to the current simulation results, the output capacities of T-type and H-type Mo$_2$B are both 529 mA h g$^{-1}$, and their average voltages are 0.65 and 0.42 V (both between 0 and 1 V), respectively, indicating that they are both suitable for the anode materials of Mg-ion batteries. Although in terms of capacity, T-type or H-type Mo$_2$B has no great advantage as a negative electrode material for Mg-ion
batteries, the capacity is not low compared with the currently reported theoretical capacity of negative electrode materials for Mg-ion batteries. For example, Si$_2$BN previously reported by Panigrah as a negative electrode material for Mg-ion batteries has a theoretical capacity of 647.896 mA h g$^{-1}$ [48]. Fan et al calculated that Mo$_2$C used as a negative electrode material for Mg-ion batteries has a theoretical capacity of 469.79 mA h g$^{-1}$ [49]. Vakili-Nezhaad et al found that the maximum storage capacity of WS$_2$ for Mg is only 360.78 mA h g$^{-1}$ [50], which is much smaller than the theoretical capacity calculated by us.

Finally, in order to evaluate the reliability of the capacities obtained above, we performed a 5 ps dynamic simulation on T-type and H-type Mo$_2$B loaded with Mg atoms at 300 K. The simulation results are shown in figure 6, where the inset figures show that the two fully loaded configurations do not undergo bond breakage or atomic structure remodeling after the 5 ps kinetics simulation, and Mg atoms also do not form clusters. In addition, the total energies of the two fully loaded configurations only fluctuate slightly. All these factors indicate that the thermodynamics of the two fully loaded configurations are stable at 300 K, so the maximum capacities obtained above are reliable.
4. Conclusions

The performance of MBene as an anode material for Mg-ion batteries was evaluated by a first-principles method. The simulation results show that both T-type and H-type Mo$_2$B have a strong adsorption effect on Mg atoms. When a Mg atom is adsorbed on both surfaces, it mainly interacts with Mo atoms on the surface, but hardly reacts with B atoms. In addition, the minimum diffusion energy barriers for a Mg atom on T-type and H-type Mo$_2$B structures are only 0.057 eV and 0.110 eV, respectively. According to the current simulation study, when all the most stable adsorption sites are occupied, the Mg atom intercalation process stops. Finally, we calculated that the storage capacities of these two structures for Mg atoms are both 529 mA h g$^{-1}$, and the average voltages are 0.65 V and 0.42 V, respectively. Therefore, in terms of diffusion energy barrier, theoretical capacity and theoretical voltage, T-type and H-type Mo$_2$B are suitable candidates for use as anode materials in Mg-ion batteries. In particular, the minimum diffusion energy of a Mg atom on T-type Mo$_2$B is only 0.057 eV, which is smaller than the diffusion energy barriers of most Mg-ion battery anode materials previously reported. The theory shows that T-type Mo$_2$B, as an excellent anode for Mg-ion batteries, provides more choices for the design of electrode materials of Mg-ion batteries.

Data availability statement

No new data were created or analyzed in this study.

Acknowledgments

J B W was supported by the National Natural Science Foundation of China (No. 11047164), the Shanghai College Foundation for Excellent Young Teachers of China (No. gjd10023) and the Academic Program of Shanghai Municipal Education Commission (Nos. 11XK11 and 2011X34). Z X Y was supported by the National Natural Science Foundation of China (No. 62072296).

Conflict of interest

There are no conflicts to declare.

ORCID iD

Jianbao Wu https://orcid.org/0000-0001-7777-8767

References

[1] Chen K, Song S, Liu F and Xue D 2015 Structural design of graphene for use in electrochemical energy storage devices Chem. Soc. Rev. 44 6230–57
[2] Shah R, Mittal V, Matsil E and Rosenkranz A 2021 Magnesium-ion batteries for electric vehicles: current trends and future perspectives Adv. Mech. Eng. 13 1–9
[3] Zhou H, Wang Y, Li H and He P 2010 The development of a new type of rechargeable batteries based on hybrid electrolytes ChemSusChem 3 1099–19
[4] Wang H W, Fu J Z, Wang C, Wang J Y, Yang A K, Li C C, Sun Q F, Cui Y and Li H Q 2020 A binder-free high silicon content flexible anode for Li-ion batteries Energy Environ. Sci. 13 868–58
[5] Ellis B L, Lee K T and Nazar L F 2010 Positive electrode materials for Li-ion and Li-batteries Chem. Mater. 22 691–714
[6] Mauger A, Armand M, Julien C M and Zaghib K 2017 Challenges and issues facing lithium metal for solid-state rechargeable batteries J. Power Sources 353 333–42
[7] Zhang Y, Geng H, Wei W, Ma J, Chen L and Li C C 2019 Challenges and recent progress in the design of advanced electrode materials for rechargeable Mg batteries Energy Storage Mater. 20 118–38
[8] Wu F, Maier J and Yu Y 2020 Guidelines and trends for next-generation rechargeable lithium and lithium-ion batteries Chem. Soc. Rev. 49 1569–614
[9] Larcher D and Tarascon J M 2015 Towards greener and more sustainable batteries for electrical energy storage Nat. Chem. 7 19–29
[10] Doe R L, Han R, Hwang J, Gmitter A J, Shterenberg I, Yoo H D, Pour N and Aurbach D 2014 Novel, electrolyte solutions comprising fully inorganic salts with high anodic stability for rechargeable magnesium batteries Chem. Commun. 50 243–5
[11] Yoo H D, Shertenberg I, Gofer Y, Gershinsky G, Pour N and Aurbach D 2013 Mg rechargeable batteries: an on-going challenge Energy Environ. Sci. 6 2265–79
[12] Jin W, Wang Z and Fu Y Q 2016 Monolayer black phosphorus as potential anode materials for Mg-ion batteries J. Mater. Sci. 51 7355–60
[13] Hou S Y, Ji X, Gaskell K, Wang P F, Wang L N, Xu J J, Sun R M, Borodin O and Wang C S 2021 Solvation sheath reorganization enables divalent metal batteries with fast interfacial charge transfer kinetics Science 374 172
[14] You C, Wu X, Yuan X, Chen Y, Liu L, Zhu Y, Fu L, Wu Y, Guo Y-G and van Ree T 2020 Advances in rechargeable Mg batteries J. Mater. Chem. A 8 25601–25
[15] Huang Z D, Maese T, Orikasa Y, Mori T, Minato T, Tassel C, Kobayashi Y, Kageyama H and Uchimoto Y 2014 MgFePO$_4$F as a feasible cathode material for magnesium batteries J. Mater. Chem. A 2 11578–82
Ding M S, Diemant T, Behm R J, Passerini S and Giffin G A 2018 Dendrite growth in Mg metal cells containing Mg(TFSI)$_2$/glyme electrolytes J. Electrochem. Soc. 165 A1983–90

Davidson R et al 2018 Formation of magnesium dendrites during electrodeposition ACS Energy Lett. 4 375–6

Kong L, Yan C, Huang J Q, Zhao M-Q, Titirici M-M, Xiang R and Zhang Q 2018 A review of advanced energy materials for magnesium-sulfur batteries Energy Environ. Mater. 1 100–12

Zhao-Karger Z and Fichtner M 2018 Beyond intercalation chemistry for rechargeable Mg batteries: a short review and perspective Front. Chem. 6 656

Wang X, Luo Y, Yan T, Cao W and Zhang M 2017 Strain enhanced lithium adsorption and diffusion on silicene Phys. Chem. Chem. Phys. 19 6563–8

Liu F, Zhou J, Wang S, Wang B, Shen C, Wang L, Hu Q, Huang Q and Zhou A 2017 Preparation of high-purity V$_2$C MXene and electrochemical properties as Li-ion batteries J. Electrochem. Soc. 164 A709–13

Jena N K, Araujo R B, Shukla V and Ahuja R 2018 Borophane as a benchmate of graphene: a potential 2D material for anode of Li and Na-ion batteries ACS Appl. Mater. Interfaces 9 16148–58

Xie Y, D’All’Agnese Y, Naguib M, Gogotsi Y, Barsoum M W, Zhuang H L L and Kent P R C 2014 Prediction and characterization of MXene nanosheet anodes for non-lithium-ion batteries ACS Nano 8 9606–15

Guo Z, Zhou J and Sun Z 2017 Two-dimensional transition metal borides for Li-ion batteries and electrocatalysis J. Mater. Chem. A 5 23530–5

Zhang H M, Xiang H M, Dai F Z, Zhang Z L and Zhou Y C 2018 First demonstration of possible two-dimensional MBene CrB derived from MAB phase Cr$_2$AlB$_2$ J. Mater. Sci. Technol. 34 2022–6

Alamedia I T, Moradifar P, Metzger Z P, Alem N and Schak R E 2018 Topochemical deintercalation of Al from MoAlB: stepwise etching pathway, layered intergrowth structures, and two-dimensional MBene J. Am. Chem. Soc. 140 8833–40

Wang Z, Fan S W, Piao H G and Lu Z S 2021 Monolayer Mo$_2$B$_2$: a non-magnetic metal and potential application as anode material for ion batteries and catalyst for hydrogen evolution Appl. Surf. Sci. 538 148026

Yuan G, Bo T, Q X, Liu P F, Huang Z and Wang B T 2019 Monolayer Zr$_2$B$_2$: a promising two-dimensional anode material for Li-ion batteries Appl. Surf. Sci. 480 448–53

Bo T, Liu P F, Zhang J, Wang F and Wang B T 2019 Tetragonal and trigonal Mo$_3$B$_2$: monolayers: two new low-dimensional materials for Li-ion and Na-ion batteries Phys. Chem. Chem. Phys. 21 5178–88

Li R, Wang Y, Xu L, Shen J, Zhao W, Yang Z, Liu R, Shao J L, Guo C and Li X 2020 A boron-exposed TiB$_2$ monolayer with a lower electrostatic-potential surface as a higher-performance anode material for Li and Na-ion batteries Phys. Chem. Chem. Phys. 22 22236–43

Zha X, Xu P, Huang Q, Du S and Zhang R-Q 2020 Mo$_2$B, an MBene member with high electrical and thermal conductivities, and satisfactory performances in lithium ion batteries Nanoscale Adv. 2 347–55

Kresse G and Furthmüller J 1996 Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set Phys. Rev. B 54 11169–86

Perdew J P, Burke K and Ernzerhof M 1996 Generalized gradient approximation made simple Phys. Rev. Lett. 77 3865–8

Blöchl P E 1994 Projector-augmented-wave method Phys. Rev. B 50 17953–79

Cramer C J and Truhlar D G J C R 1999 Implicit solvation models: equilibria, structure, spectra, and dynamics Chem. Rev. 99 2161–200

Zhang Q and Anghirini A 2019 Solvation effects on DFT predictions of ORR activity on metal surfaces Catal. Today 323 35–43

Oguz I C, Vassetti D and Labat F 2021 Assessing the performances of different continuum solvation models for the calculation of hydration energies of molecules, polymers and surfaces: a comparison between the SMD, VASP sol and FDPB models Theor. Chem. Acc. 140 9901–13

Grimes S 2004 Accurate description of van der Waals complexes by density functional theory including empirical corrections J. Comput. Chem. 25 1463–73

Henkelman G, Ueberuag B P and Jönsson H 2000 A climbing image nudged elastic band method for finding saddle points and minimum energy paths J. Chem. Phys. 113 9901–4

Çakır D, Sevik C, Gülsener O and Peeters F M 2016 Mo$_2$C as a high capacity anode material: a first-principles study J. Mater. Chem. A 4 6029–35

Yu D, Yang B, Zhang S, Ruckenstein E and Chen H 2021 Reshaping two-dimensional MoS$_2$ for superior magnesium-ion battery anodes J. Colloid Interface Sci. 597 401–3

Jäckle M and Groß A 2014 Microscopic properties of lithium, sodium, and magnesium battery anode materials related to possible dendrite growth J. Chem. Phys. 141 171401

Jin W, Li Z, Wang Z and Fu Y Q 2016 Mg ion dynamics in anode materials of Sn and Bi for Mg-ion batteries Mater. Chem. Phys. 182 167–72

Lu T, Zhang Z, Chen B, Dong S, Wang C, Du A, Wang L, Ma J and Cui G 2020 A superior electronic conducting tellurium electrode enabled high rate capability rechargeable Mg batteries Mater. Today Energy 17 1025–9

Wang Y, Song N, Song X, Zhang T, Zhang Q and Li M 2018 Metallic V$_2$O$_3$ monolayer as an anode material for Li, Na, K, Mg or Ca ion storage: a first-principle study RSC Adv. 8 10848–54

Mortazavi B, Rahman O, Ahzi S and Rabczuk T 2017 Flat borophene films as anode materials for Mg, Na or Li-ion batteries with ultra high capacities: a first-principles study Appl. Mater. Today 8 60–67

Han X P, Liu C, Sun J, Sendek A D and Yang W S 2018 Density functional theory calculations for evaluation of phosphorene as a possible anode material for magnesium batteries RSC Adv. 8 7196–204

Panigrahi P, Mishra S B, Hussain T, Nanda B R K and Ahuja R 2020 Density functional theory studies of Si$_2$BN nanosheets as anode materials for magnesium-ion batteries ACS Appl. Nano Mater. 3 9055–63

Fan K M, Tang J and Sun Q G 2020 Monolayer Mo$_2$C as anodes for magnesium-ion batteries J. Mol. Model. 26 1–7

Vakili-Nezhad G R, Gujarathi A M, Al Rawahi N and Mohammad M 2019 Performance of WS$_2$ monolayers as a new family of anode materials for metal-ion (Mg, Al and Ca) batteries Mater. Chem. Phys. 230 114–21