Adsorption and Diffusion of Magnesium on Nitrogen Doped Mo2C Monolayer

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Research Article

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Abstract

The Mg adsorption and diffusion behaviors on nitrogen doped (N-doped) Mo$_2$C monolayer have been systematically investigated by the first principles based on density functional theory (DFT). The adsorption energies of Mg on pristine Mo$_2$C and Mo$_2$C$_{1-x}N_x$ ($x = 0.0625, 0.125, 0.1875$ and $0.25$) have been studied. The adsorption energies of Mg on N-doped Mo$_2$C are lower than that of pristine Mo$_2$C. Especially, the adsorption energies of Mg are $-1.639$ eV and $-1.625$ eV on T$_{C1}$ and H$_2$ sites for Mo$_2$C$_{0.875}N_{0.125}$, which have decreased by $16.49\%$ and $18.43\%$. Furthermore, the Mg diffuses along H$_3$-B-H$_4$ and H-B-H with the barriers of $0.021$ eV and $0.028$ eV, which indicate that Mo$_2$C$_{0.875}N_{0.125}$ exhibits fast diffusion properties. Additionally, the partial density of states (PDOS) reveals the interaction between Mg and Mo$_2$C$_{0.875}N_{0.125}$. The PDOS results indicate that nitrogen doping causes the PDOS peaks transfer to a lower energy level, which is benefit for the bonding between Mg and MoC$_{0.875}N_{0.125}$. These results suggest that the adsorption and diffusion behaviors of Mg are enhanced by nitrogen doping.

1 Introduction

Lithium ions batteries (LIBs) are widely used to in phones, laptops, digital cameras, and other portable devices [1–3]. However, safety, high costs and resource shortages have restricted the development of lithium batteries [4, 5]. With the development of the intelligent electronic applications such as new energy vehicles, energy storage plant and artificial satellite, which require high battery storage and stable cycle capacity. MIBs have been considered as the potential alternatives to LIBs, due to the natural abundance, low cost, safety and high volumetric energy density (3832 mAh cm$^{-3}$) [6, 7]. However, it is well-known that the performance of rechargeable batteries depends on their anode or cathode materials. Hence, a great deal of efforts has been carried out to search for novel anode materials for MIBs.

As larger surface area and excellent electrochemistry, extensive investigations have been focused on exploring 2-dimensional materials as anodes for MIBs [8]. For example, Sibari et. Al have demonstrated that phosphorene is a good anode material for MIBs with a high capacity of $315.52$ mAh.g$^{-1}$ and diffusion barriers value of $0.05$ eV along the zigzag direction [9]. The monolayer black P as anode for MIBs has also been researched by Jin et. Al based on first-principles, which exhibits excellent properties, such as large adsorption energies of Mg (-1.09 eV on H adsorption sites) and low diffusion barriers of $0.08$ eV along the zigzag directions [5]. Li et al. have found that the g-Mg$_3$N$_2$ is a promising anode material for MIBs with high capacities storage (531 mAh g$^{-1}$) [10].

Recently, a new family of two-dimensional materials, Mxenes, such as WS$_2$, Sr$_2$C, TiS$_2$, has attracted extensive attention in the application of anode materials due to good conductivity, high reversible capacity and high power density [8, 11–14]. Mo$_2$C, a representative of two-dimensional Mxenes materials, has superconductivity and low diffusion barriers as anode materials [15–18]. In addition, Xu et. Al have succeeded in synthesizing the large-area high-quality 2D α-Mo$_2$C [16]. Fan et. Al have reported that Mo$_2$C monolayer is a potential anode material for MIBs [19].
However, the development of two-dimensional materials is restricted by the high diffusion barriers and the low cycling stability [9, 20]. Doping metal elemental, such as Cr [21], Ru [22], Zn [23], Sr [24], and nonmetal elemental, such as C [25], N [26], B [27] are typical strategies to enhance the properties of electrode materials [28]. Moreover, nitrogen doping is an effective way to enhance metal-semiconductor transition and electronic conductivity due to strong electronegativity and similar atomic radius to carbon [29–31]. Daula et. Al indicate that Si$_2$BN as anode materials exhibits excellent theoretical capacity of 647.896 mAh g$^{-1}$ and low migration energy barriers between 0.08 eV and 0.35 eV for MIBs by calculations [30]. Zhang et. Al have reported that the incorporation of nitrogen into graphene like C$_2$N exhibits high theoretical capacities of 588.4 mAh g$^{-1}$ as anode for MIBs [4]. In present work, the first principle calculations are implemented to investigate the adsorption and diffusion behaviors of Mg on the N-doped Mo$_2$C with different nitrogen doping concentrations.

2 Computational Methods

All the calculations have been carried out by using SIESTA code by the first-principles [32, 33]. Within SIESTA code, the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof functional (PBE) is widely applied to describe the electron exchange correlation term [34, 35]. Meanwhile, the accuracy of the computed adsorption energies has been improved by the double-basis set [36]. The energy cutoff 150 Ry has been chosen for all calculations. The present calculations are performed with 3×3×1 Brillouin zone k-point sampling. To avoid interactions between periodic permutations, we separate a large vacuum of the monolayer Mo$_2$C by 30 Å. In the present calculations, the 4×4×1 supercell of the sandwich structure including 32 Mo atoms and 16 C atoms has been used to simulate the adsorption and diffusion behaviors of Mg.

3 Results And Discussion

The absorption energies characterize metal ions absorption strength. The negative values of absorption energies indicate the metal ions absorption behaviors are exothermic and spontaneous. The following equation has been used to calculate the adsorption energies $E_{ad}$:

$$E_{ad} = E_{Mo_2C_1-xN_x} - E_{Mo_2C_1} - E_{Mg}$$

Where $x$ is the ratio of the number of N atoms to the number C atoms, $E_{Mo_2C_1-xN_x}$ and $E_{Mo_2C_1}$ represent the total energy of Mo$_2$C$_{1-x}N_x$ with and without Mg absorption, $E_{Mg}$ is the energy of the isolated Mg atom, which has been determined to be -86.461 eV. To investigate the absorption energies of Mg on N-doped Mo$_2$C, four supercells of Mo$_2$C$_{1-x}N_x$ ($x = 0.0625, 0.125, 0.1875$ and $0.25$) have been constructed to accomplish different doping concentrations 6.67%, 14.29%, 23.08% and 33.33%, respectively. Hence, we consider one nitrogen atom, two nitrogen atoms, three nitrogen atoms and four nitrogen atoms to replace the carbon atoms in 4×4×1 supercell.
The four typical adsorption sites on pristine Mo$_2$C have been considered: hollow (H), top (T$_C$ and T$_{Mo}$) and bridge (B) sites as shown in Fig. 1(a). Meanwhile, the adsorption energies of Mg adsorption on H$_1$, H$_2$, H$_3$, H$_4$, T$_{C1}$, T$_{C2}$, T$_{Mo1}$, T$_{Mo2}$ and B$_1$ sites for four N-doped Mo$_2$C structures have been calculated. The adsorption energies of Mg calculated on the same sites for N-doped Mo$_2$C, the Mg adsorption on MoC$_{0.875}$N$_{0.125}$ represents the conformations of N-doped Mo$_2$C as shown in Fig. 1(b), and the results are summarized in Table 1.

|       | Mo$_2$C$_{0.9375}$N$_{0.0625}$ | Mo$_2$C$_{0.875}$N$_{0.125}$ | Mo$_2$C$_{0.8125}$N$_{0.1875}$ | Mo$_2$C$_{0.75}$N$_{0.25}$ | Mo$_2$C |
|-------|-------------------------------|-------------------------------|-------------------------------|---------------------------|---------|
| H$_1$ | -1.420                        | -1.567                        | -1.426                        | -1.437                    | -1.395  |
| H$_2$ | -1.423                        | -1.625                        | -1.424                        | -1.546                    |         |
| H$_3$ | -1.438                        | -1.550                        | -1.422                        | -1.430                    |         |
| H$_4$ | -1.413                        | -1.567                        | -1.409                        | -1.436                    |         |
| T$_{C1}$ | -1.446                       | -1.580                        | -1.483                        | -1.514                    | -1.384  |
| T$_{C2}$ | ---                          | -1.639                        | -1.492                        | -1.505                    |         |
| T$_{Mo1}$ | -1.431                       | -1.517                        | -1.374                        | -1.376                    | -1.363  |
| T$_{Mo2}$ | -1.437                       | -1.595                        | -1.459                        | -1.514                    |         |
| B$_1$ | -1.430                        | -1.552                        | -1.423                        | -1.427                    | -1.361  |

As shown in Table 1, the negative values of absorption energies indicate the Mg adsorption behaviors are spontaneous. The absorption energies of Mg on H, T$_C$, T$_{Mo}$, B sites for pristine Mo$_2$C are $-1.395$ eV, $-1.384$ eV, $-1.363$ eV and $-1.361$ eV, respectively. The absorption energies of Mg on the four considered N-doped Mo$_2$C all have decreased, which suggest that N-doped Mo$_2$C is benefit for Mg adsorption. Especially, the adsorption energies of Mg for Mo$_2$C$_{0.125}$N$_{0.875}$ are about in the region between $-1.64$ and $-1.55$ eV, much lower than that of pristine Mo$_2$C. For example, the adsorption energies of Mg on T$_{C1}$ and H$_2$ sites for Mo$_2$C$_{0.875}$N$_{0.125}$ is $-1.639$ eV and $-1.625$ eV, which has decreased by $16.49\%$ and $18.43\%$. The adsorption energies of Mg for N-doped Mo$_2$C show that the enhancement of Mg adsorption behaviors is attributed to nitrogen doping.

It is well-known that the diffusion barrier is an important feature to evaluate diffusion mobility of metal ions. In order to obtain the effect of nitrogen doping on Mg diffusion behaviors, the diffusion barriers of Mg on pristine Mo$_2$C and Mo$_2$C$_{0.125}$N$_{0.875}$ have been calculated. For pristine Mo$_2$C, the energy barrier of Mg diffusion along H-B-H pathway is about $0.039$ eV. For comparison, three diffusion pathways (H$_4$-B-H$_3$, H$_2$-B-H$_3$, H$_3$-B-H$_2$) for N-doped Mo$_2$C are examined.
H-B-H₃, H-B-H) for Mo₂C₀.₁₂₅N₀.₈₇₅ have been considered. The diffusion pathways are named path1, path2 and path3, respectively, with the corresponding diffusion energy barriers as shown in Fig. 2. It can be seen that the diffusion barriers are only 0.042 eV, 0.021 eV and 0.028 eV along three pathways, respectively, which indicate that the Mg diffusion behaviors can easily occur on Mo₂C₀.₁₂₅N₀.₈₇₅. The diffusion barrier of Mg along path1 is slightly higher than that of pristine Mo₂C, however, the diffusion barriers of Mg along the path2 and path3 is much lower than that on pristine Mo₂C. The results show that nitrogen doping is a positive approach to decrease the diffusion barriers, which is beneficial to the diffusion of Mg on Mo₂C₀.₁₂₅N₀.₈₇₅. The MoC₀.₈₇₅N₀.₁₂₅ shows lower adsorption energies and diffusion barriers of Mg, which indicate MoC₀.₈₇₅N₀.₁₂₅ is a potential anode material for MIBs.

To comprehensively understand the interaction between Mg and MoC₀.₈₇₅N₀.₁₂₅, the partial density of states (PDOS) has been calculated. The PDOS reveal the hybridization interaction of Mg and the neighboring C and Mo atoms. The present calculations indicate that the major electron contribution is mainly attributed to the s state of Mg, the p state of C and the d state of Mo, so, the PDOS of Mg-3s, C-2p and Mo-4d states are plotted in Fig. 3. As shown in Fig. 3, the Mg-3s(no), C-2p(no) and Mo-4d(no) states represent the PDOS for Mg adsorption on the pristine Mo₂C. The Fermi level has been depicted by vertical dashed line in Fig. 3. Obviously, it can be seen that the Fermi level locates at the peak of Mg-3s orbits, which suggest that the Mg adsorption on pristine Mo₂C and MoC₀.₈₇₅N₀.₁₂₅ is stable [37]. Additionally, the major electron contribution of Mo₂C and MoC₀.₈₇₅N₀.₁₂₅ is Mo-4d orbits, which is similar to Li, Na and K adsorption on Mo₂C [15, 17]. Furthermore, it is noticed that the C-2p, Mg-3s and Mo-4d states are across the Fermi level, which suggest that the metallic nature has been maintained for MoC₀.₈₇₅N₀.₁₂₅ [38, 39]. The metallicity of MoC₀.₈₇₅N₀.₁₂₅ indicate its good electronic conductivity, which is benefit for Mg diffusion [40]. Interestingly, it is found that nitrogen doping causes the peak of electron orbits transfer to lower energies. This indicate that the bonding between Mg and MoC₀.₈₇₅N₀.₁₂₅ is more stable [41]. It can be concluded that when pristine Mo₂C is doped by nitrogen, the strong interaction between Mg and MoC₀.₈₇₅N₀.₁₂₅ is beneficial to the adsorption and diffusion of Mg.

4 Conclusion

In this paper, the adsorption and diffusion properties of Mg on N-doped Mo₂C have been investigated by first-principles principles. For the adsorption of Mg on the considered N-doped Mo₂C, the adsorption energies of Mg have decreased. Especially, MoC₀.₈₇₅N₀.₁₂₅ exhibits the lowest adsorption energies. For example, the adsorption energies of H₂ and T₂C on MoC₀.₈₇₅N₀.₁₂₅ has decreased by 16.49% and 18.43% compared to that of pristine Mo₂C. Furthermore, the present calculations show that MoC₀.₈₇₅N₀.₁₂₅ can obtain the diffusion barriers of 0.021 eV and 0.028 eV, which are lower than that of Mg on pristine Mo2C. Moreover, the PDOS calculations reveal the strong interaction between Mg and MoC₀.₈₇₅N₀.₁₂₅ due to the presence of N. In summary, N-doped Mo₂C shows lower adsorption energies and diffusion barriers of Mg, which indicate that MoC₀.₈₇₅N₀.₁₂₅ can be regard as a potential candidate anode material for MIBs.
Declarations

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Conflicts of interest/Competing interests The authors declare no competing interests.

Availability of data and material All data generated or analysed during this study are included in this published article.

Code availability N/A

Authors' contributions Jiangfeng Ni: Calculations, writing, and data analysis. Kaimin Fan: Conceiving problem, result analysis, manuscript editing, and supervision. Jing Tang: Result analysis and manuscript editing.

Ethics approval and consent to participate N/A

Consent for publication N/A

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**Figures**

![Figure 1](image)

**Figure 1**

The configurations of Mg absorption on the (a) pristine Mo2C and (b) Mo2C1-xNx.
Figure 2

(a) The three diffusion paths, path1, path2 and path3 and (b) the diffusion barriers of Mg on monolayer MoC0.875N0.125.
Figure 3

The partial density of states (PDOS) of Mg and its nearest neighbor C and Mo atoms, (a) C-2p, (b) Mg-3s (c) Mo-4d for Mo2C and MoC0.875N0.125 monolayer.