Structural Properties and Phase Transition of Na Adsorption on Monolayer MoS$_2$

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Abstract

First-principles calculations are performed to investigate the structural stability of Na adsorption on 1H and 1T phases of monolayer MoS$_2$. Our results demonstrate that it is likely to make the stability of distorted 1T phase of MoS$_2$ over the 1H phase through adsorption of Na atoms. The type of distortion depends on the concentration of adsorbed Na atoms and changes from zigzag-like to diamond-like with the increasing of adsorbed Na atom concentrations. Our calculations show that the phase transition from 1H-MoS$_2$ to 1T-MoS$_2$ can be obtained by Na adsorption. We also calculate the electrochemical properties of Na adsorption on MoS$_2$ monolayer. These results indicate that MoS$_2$ is one of potential negative electrodes for Na-ion batteries.

Keywords: First-principles, MoS$_2$, Structural stability, Phase transition

Background

In recent years, the study of transition-metal dichalcogenides (TMDs) has been a topic of current interest due to their layered structure [1, 2]. TMDs exhibit a broad range of properties, which are advantageous for a wide range of applications as high-performance functional nanomaterials [3]. Among them, molybdenum disulfide (MoS$_2$) has attracted considerable attention because of its important role in ultrasensitive photodetectors, flexible electronic device, lithium ion battery, field effect transistors, and sodium-ion batteries [4–7]. These applications show high figure of merit in microelectronics, thermoelectrics, and optoelectronics.

Bulk MoS$_2$ crystal is an indirect-gap semiconductor, which is built up of atomic layers stacking by weak van der Waals force. It is possible to exfoliate MoS$_2$ monolayer from the bulk, owing to the weak van der Waals interaction between these layers [8, 9]. The typical monolayers of TMDs come in two varieties, called H and T phase with trigonal or octahedral prismatic coordination, respectively [10]. Consequently, MoS$_2$ monolayers come in two phases, called 1H-MoS$_2$ and 1T-MoS$_2$ [11]. The 1H-MoS$_2$ phase has the space group of P6/mmc and is semiconducting with a direct band gap [12]. The 1T-MoS$_2$ phase is metallic and metastable relative to the 1H-MoS$_2$ phase [13]. However, stable 1T-MoS$_2$ phase can be realized by doping of MoS$_2$ with Re atoms [14] and be stabilized by adsorption of Li atoms [15].

Previous studies demonstrated the phase transition between 1H-MoS$_2$ and 1T-MoS$_2$ in the early lithiation process [16–20]. The charge transfer induced by the adatoms leads to turn 1T-MoS$_2$ phase into a stable MoS$_2$ phase. The phase transition is the main issue for application in Li-ion batteries [20, 21] and Na-ion batteries [22, 23]. A large amount of experimental and theoretical works on the application of MoS$_2$ in Li-ion batteries has emerged in the past years [16–21]. Kan et al. [16] studied possible pathways of structural phase transition between 1H-MoS$_2$ and 1T-MoS$_2$ by increasing lithium adsorption concentration constantly. Esfahani et al. [18] calculated the H-T transition by adsorption of Li atoms on both sides of the MoS$_2$ monolayer. Mortazavi et al. [22] investigated phase transition between 2H-MoS$_2$ and 1T-MoS$_2$ upon Na intercalation. Li-ion batteries are prime energy storage systems at present in amounts of devices used in our daily lives such as smartphones and laptops. Na-ion batteries are excellent alternatives to Li-ion batteries because of their lower cost and the greater availability. However,
to our knowledge, there are few theoretical calculations on Na adsorption on monolayer MoS$_2$.

In this work, we perform a comprehensive first-principles study of the electronic structure, adsorption energies, phase transitions, and electrochemical properties for Na-adsorption compounds. All reasonable structure phases of MoS$_2$ monolayer are introduced. Our results suggest that it is easily to turn to be octahedral phases by Na-adsorption for 1T-MoS$_2$ such as ZT-MoS$_2$ with zigzag Mo-Mo chains and DT-MoS$_2$ in rhombus-shape with Mo-Mo chains. Furthermore, Na adsorption on the MoS$_2$ surface can lead to a structural phase transformation from 1H-MoS$_2$ to an octahedral coordinated MoS$_2$. Average operating voltages by Na adsorption are calculated. This will be helpful to understand the basic processes involved in monolayer MoS$_2$ applied in Na-ion batteries.

**Methods**

Our calculations are carried out by using the Vienna Ab-initio Simulation Package (VASP) package [24], which is based on density functional theory (DFT) and plane-wave pseudopotential method. The electron exchange-correlation energy is described in the Perdew-Burke-Ernzerhof (PBE) form for the generalized gradient approximation (GGA) [25]. The cut-off energy is set to be 600 eV for the plane-wave expansion of the wave functions. The Brillouin zone integration is represented by the Monkhorst-Pack $k$-point scheme with $9 \times 9 \times 1$ and $5 \times 5 \times 1$ grid meshes for the $(1 \times 1)$ unit cell and $(4 \times 4)$ supercell, respectively. The criterion of convergence of energy is chosen as $10^{-5}$ eV between two ionic steps, and the maximum force allowed on each atom is 0.01 eV/Å. The vacuum space along the $z$ direction is taken to be more than 15 Å for the both 1H-MoS$_2$ and 1T-MoS$_2$.

The geometry structures are shown in Fig. 1. A $(4 \times 4)$ supercell of MoS$_2$ monolayer consisting of 48 atoms, which contains 16 Mo and 32 S, is made up of the primitive cell of MoS$_2$. 1H-MoS$_2$ has single S-Mo-S layer, where the Mo site in a trigonal prism coordination as shown in Fig. 1a. 1T-MoS$_2$ has asymmetric sulphur atoms sites, where the Mo site in octahedral coordination as shown in Fig. 1b.

**Results and Discussion**

**Structural Properties**

To obtain a clear insight into the 1H to 1T phase transition, we first calculate electronic structures of both the trigonal prismatic phase (1H-MoS$_2$) and octahedral prismatic phase (1T-MoS$_2$) by using $(1 \times 1)$ unit cell. Our results show that the optimized lattice parameters $a_0 = 3.166$ Å for both the pristine 1H-MoS$_2$ and the pristine 1T-MoS$_2$ as shown in Table 1.

Electronic structure provides a clear insight into the difference of band structure between 1H-MoS$_2$ and 1T-MoS$_2$. The two phases show completely different electronic structures. Figure 2 shows the band structures of 1H-MoS$_2$ and 1T-MoS$_2$ without spin-orbit coupling. 1H-MoS$_2$ is a direct semiconductor with both conduction band minimum (CBM) and valence band maximum (VBM) located at the $K$ point. The band gap obtained from GGA-PBE calculations is 1.71 eV. However, the electronic structure calculation of the 1T structure shows that this polytype is indeed metallic in Fig. 2b. We also calculate the energy difference between 1H-MoS$_2$ and undistorted 1T-MoS$_2$ unit cell, which shows that the optimized 1H-MoS$_2$ is more stable than the 1T-MoS$_2$ by 0.84 eV. In normal conditions, although both polytypes of monolayer MoS$_2$ have the same element constitution, 1H-MoS$_2$ is more stable than 1T-MoS$_2$. Besides, the equilibrium lattice constant of 1H-MoS$_2$ is close to that of 1T-MoS$_2$ according to Table 1.

**Adsorption Energies and Stability Analysis**

In order to investigate the stability of the two structural phases with Na adsorption, the most stable configuration of an isolated Na atom adsorbed on $(4 \times 4)$ cell for the both structure phases is determined at first. Three different types of adsorption sites are introduced to
determine the most stable position [26], including “t” site (top site directly above a Mo atom), t’ site (top site directly above an S atom), and “h” site (hollow site above the center of hexagons), respectively. Na atoms adsorbed at other positions can eventually relax into one of the three listed adsorption sites [27]. Considering the monolayer hexagonal lattice structure of MoS$_2$ monolayer, it is reasonable to expect the relaxation of foreign atoms on one of these adsorption sites. There is little change for the adsorption geometry of 1H-MoS$_2$ after relaxation. However, the optimized 1T-MoS$_2$ supercell will transform into the distorted 1T phase due to its instability, such as ZT-MoS$_2$ with zigzag Mo-Mo chains. Further, to investigate the relative stabilities of the systems, we defined the adsorption energy as follows:

$$E_a = (E_{X-MoS_2} + E_{Na}) - E_{total}$$

where $X = 1H$, distorted 1T, $E_{X-MoS_2}$ represents the total energy of 1H-MoS$_2$ and distorted 1T-MoS$_2$ system, $E_{total}$ represents the total energy of the adsorption system, and $E_{Na}$ represents the total energy of bulk sodium. The electron configurations of adatom adsorption energies ($E_a$) and structural properties for single adatom-adsorbed MoS$_2$ obtained from our calculations are listed in Table 2. Our calculated results show that the adsorption energy is different for different sites. In all adsorption sites, the site with the largest adsorption energy (minimum total energy) is referred to as the favored one. Comparing the possible sites of h, t, and t’, we found that Na atom prefer to reside on t site for the both structures.

**Phase Transition of 2D MoS$_2$ Monolayer Induced by Na Insertion**

In the previous analysis, we have determined the most stable adsorption site for Na atoms on the surface of MoS$_2$ monolayer, which is top of Mo atom sites. Totally, there are 32 most stable sites for Na atoms on both sides of (4 × 4) MoS$_2$ supercell [28]. In order to investigate systematically Na adsorption on the surface of MoS$_2$ monolayer, we introduce Na atoms on both sides of MoS$_2$ monolayer forming the compound 1H-Na$_x$MoS$_2$ and 1T-Na$_x$MoS$_2$ to induce phase transition, which is a solvent-based exfoliation of MoS$_2$ monolayer and a typical procedure for both the charge/discharge processes in battery.

The geometries of 1H-Na$_x$MoS$_2$ are optimized with adsorption concentration increasing, as shown in Fig. 3. Our results show the variation of energies and structure for 1H-Na$_x$MoS$_2$ with the increasing of Na concentrations. As shown in Fig. 3, Mo-Mo chains appear in 1H-Na$_x$MoS$_2$ when 2–6 Na atoms are added to the system.

| Table 1 Structural parameters of 1H-MoS$_2$ and 1T-MoS$_2$ and band gap |
|---|
| | 1H-MoS$_2$ | 1T-MoS$_2$ |
| a (Å) | Present work | 3.166 | 3.168 |
| References | 3.16 [30]; 3.18 [11] | 3.18 [10] |
| d$_{S-S}$ (Å) | Present work | 3.092 | 3.092 |
| References | 3.089 [30] | – |
| Gap (eV) | Present work | 1.71 | Metal |
| References | 1.71 [30]; 1.67 [11] | Metal |

**Fig. 2** a Band structures of 1H-MoS$_2$. b Band structures of 1T-MoS$_2$.
Triangular Mo-Mo clustering appears in 1H-Na$_x$MoS$_2$ with the increasing of adsorption concentrations. The optimized geometries of 1T-Na$_x$MoS$_2$ with the increasing of adsorption concentrations are shown in Fig. 4a. The substrate structure of 1T-MoS$_2$ directly transits to the ZT-MoS$_2$ after relaxation due to the instability. Some Mo-Mo chains appear in 1T-Na$_x$MoS$_2$ following certain rules. These Mo atoms gradually form a diamond-like chain up to eight Na atoms that are introduced in the system. The system is likely to maintain the diamond chain structure. The geometry configurations of ZT-MoS$_2$ and DT-MoS$_2$ without adsorption are clearly shown in Fig. 4b, c, respectively. The free-standing 1T-MoS$_2$ exhibits metallic property and is metastable. Both ZT-MoS$_2$ and DT-MoS$_2$ belong to distorted octahedral coordinated MoS$_2$.

It is similar to the definition of adsorption energy that the formation energy in different concentrations of Na absorption is calculated using the expression:

$$ E_{f(x)} = E_{(X-Na_xMoS_2)} - E_{(MoS_2)} - nE_{(Na)} $$

(2)

where $X = 1H$, 1T, $E_{(X-Na_xMoS_2)}$ is the total energy of the X-Na$_x$MoS$_2$ compound, $E_{(MoS_2)}$ is the total energy of the same MoS$_2$ polytype, and $E_{(Na)}$ is the total energy of bulk sodium. A negative binding energy indicates an exothermic chemical interaction between Na and MoS$_2$.

Relative formation energy per Na atom of 1T-Na$_x$MoS$_2$ with respect to 1H-Na$_x$MoS$_2$ varies as increasing the Na-adsorption concentration constantly in Fig. 5. The 1H-Na$_x$MoS$_2$ still keeps stability in the low adsorption concentration. However, the 1T-Na$_x$MoS$_2$ becomes more stable than 1H-Na$_x$MoS$_2$ when the adsorption concentration of Na atoms exceeds about 35 %. As the adsorption concentration of Na increases, the 1T-Na$_x$MoS$_2$ will become stable further.

**Transition Barrier from 1H Phase to 1T Phase**

The procedure of transition can be viewed as a shift of one S atom layer in the 1H-MoS$_2$ structure to the position h in Fig. 1a. Therefore, the barrier energy of 1H-MoS$_2$ structure to 1T-MoS$_2$ structure transition is able to be calculated by shearing one S layer from the

| Site   | $E_a$ (eV) | $d_{Na-S}$ (Å) | $d_{Mo-Mo}$ (Å) |
|--------|-----------|----------------|-----------------|
| 1H-MoS$_2$ | h        | 2.1            | 2.74            | 2.97            |
|         | t’       | 3.2            | 2.68            | 3.04            |
|         | t        | 1.8            | 2.76            | 3.02            |
| Distorted 1T-MoS$_2$ | h | 2.7 | 2.75 | 2.89 |
|         | t’       | 3.6            | 2.66            | 2.92            |
|         | t        | 2.3            | 2.76            | 2.93            |

Fig. 3 The optimized structures of the most stable 1H-Na$_x$MoS$_2$, triangular Mo-Mo clustering as highlighted in red.
1H structure toward the 1T structure when fixing the Mo atoms, while the other atoms are allowed to relax. Nudged Elastic Band (NEB) method is adopted to calculate the barrier energy from 1H to 1T structure transition as shown in Fig. 6a. Our results show that the barrier of phase transition from 1H to 1T structure is approximately 1.61 eV in the absence of external adatoms. The phase transition involves one of the S atoms moving from one pyramidal position to the other pyramidal position. The relative energy of Na-intercalated 1T-MoS$_2$ is 0.52 eV. Meanwhile, the barrier from 1H-MoS$_2$ to 1T-MoS$_2$ reduces to 0.91 eV when Na atoms are adsorbed completely on one side of MoS$_2$ monolayer. The barrier energy reduces considerably from 1H to 1T structure transition by the Na atom adsorption on MoS$_2$ monolayer. These results suggest that the Na atoms are not only effective to make the 1T-MoS$_2$ energetically favorable but also play an important role in the process of phase transition. According to our theoretical calculation and experimental works, we summarize the pathways for structural phase transition among different structures in Fig. 6b. The detailed process is the following: (1) When Na atoms are adsorbed to 1H-MoS$_2$, the 1H-MoS$_2$ remains stable until the Na concentration reaches 35 %. When more Na atoms are adsorbed on both sides of MoS$_2$ monolayer, the distorted 1T-MoS$_2$ will become more stable. Besides, the structure finally transform to the distorted 1T-MoS$_2$ phase with diamond-like chains. (2) When all of the Na atoms are extracted from the system, the structure will become ZT-MoS$_2$. (3) The ZT-MoS$_2$ will transform back to 1H-MoS$_2$ phase by heating or aging.

**Electrochemical Properties of Na$_x$MoS$_2$**

In order to inspect the suitability of Na$_x$MoS$_2$ compound as an electrode material for Na-ions, we calculate the average adsorption voltage. The electrode
potential between \(Na_{x_1}MoS_2\) and \(Na_{x_2}MoS_2\) (\(x_2 > x_1\)) is calculated as [29]:

\[
\bar{V} = -\frac{G_{x_2} - G_{x_1} - (x_2 - x_1)G_{Na}}{(x_2 - x_1)e}
\]

(3)

where \(G_{x_2}\) and \(G_{x_1}\) are the total energies of \(Na_{x_1}MoS_2\) systems and \(G_{Na}\) is the energy per atom of Na in its bulk state. The electrode potential for 1H-\(Na_{x}MoS_2\) and 1T-\(Na_{x}MoS_2\) as the change of concentration is shown in Fig. 7, respectively. Our results show that the voltage profile for 1H-\(Na_{x}MoS_2\) varies with a decreasing trend in a range of 0~1 V as shown in Fig. 7a, with an average value of 0.72 V. The electrode potential for 1T-\(Na_{x}MoS_2\) varies in a range of 0~3.5 V as shown in Fig. 7b. However, 1T-\(Na_{x}MoS_2\) systems are unstable for concentrations \(x < 0.35\), as shown in Fig. 5. Therefore, the large magnitudes of the potential of 1T-\(Na_{x}MoS_2\) compounds for low concentrations are unlikely to use practically. Our results show that the average potential of 1T-\(Na_{x}MoS_2\) is obtained approximately as 1.28 V. Compared with Li-intercalated MoS\(_2\), the average potential of \(Na_{x}MoS_2\) is much lower because of the weaker binding of Na atoms. Since ideally a good anode should have a low electrode potential, our calculated voltage profile suggests that layered MoS\(_2\) is suitable as an anode for an

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**Fig. 5** Relative formation energy per Na atom of 1T-\(Na_xMoS_2\) with respect to 1H-\(Na_xMoS_2\) as a function of Na concentration

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**Fig. 6**

(a) Evolution of the energy per S atom for 1H to 1T structure transition as a function of the reaction coordinate, for pure and Na-covered MoS\(_2\).

(b) The pathways of structural phase transition of Na adsorption on monolayer MoS\(_2\).
NIB. When this Na-intercalated MoS$_2$ anode is combined with high-capacity cathode materials such as Na$_3$MnPO$_4$CO$_3$, the Na-ion battery cell can yield a desirable open circuit voltage in the range of 2.5~3.5 V.

Conclusions
In conclusion, we investigated the adsorption energies, phase transition for the adsorption of Na onto MoS$_2$ monolayer, and electrochemical properties of Na$_x$MoS$_2$ by using the first-principles DFT method. The traditional trigonal prismatic 1H-MoS$_2$ phase is stable under normal conditions. However, a comprehensive study of the relative phase stability of MoS$_2$ tells us that the other structural phase transition can be stable by adsorption. Our results show that some triangular Mo-Mo clustering appears in 1H-Na$_x$MoS$_2$ with the increasing of Na-adsorption concentration. On the other hand, some diamond-like Mo-Mo chains appear in 1H-Na$_x$MoS$_2$ when the Na-adsorption concentration is beyond 25%. What is more, the adsorption of Na on MoS$_2$ induces a phase transformation at $x=0.35$ from the 1H to 1T phase. Our calculated results show that the adsorption of Na onto MoS$_2$ monolayer results in a lower energy barrier from 1H-MoS$_2$ to 1T-MoS$_2$. Finally, Na$_x$MoS$_2$ compound is likely to become a battery anode material with a low average electrode potential of 0.72~1.28 V.

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Competing Interests
The authors declare that they have no competing interests.

Authors’ Contributions
HH carried out the calculations and HH and PFL wrote the manuscript. LYW, CFZ, YXS, and SMW helped in the discussions and analysis of the results. PFL and PFG proposed the initial work, supervised the analysis, and revised the manuscript. All authors read and approved the final manuscript.

References
1. Komsa HP, Krasheninnikov AV (2013) Electronic structures and optical properties of realistic transition metal dichalcogenide heterostructures from first principles. Phys Rev B 88(8):085318
2. Pandey M, Vojvodic A, Thygesen KS, Jacobsen KW (2015) Two-dimensional metal dichalcogenides and oxides for hydrogen evolution: a computational screening approach. J Phys Chem Lett 6(9):1577–1585
3. Kang J, Tongay S, Zhou J, Li J, Wu J (2013) Band offsets and heterostructures of two-dimensional semiconductors. Appl Phys Lett 102(1):012111
4. Baugher BW, Churchill HO, Yang Y, Jarillo-Herrero P (2013) Intrinsic electronic transport properties of high-quality monolayer and bilayer MoS$_2$. Nano Lett 13(9):4212–4216
5. Lopez-Sanchez O, Lembitke D, Kayci M, Radenovic A, Kis A (2013) Ultrasensitive photodetectors based on monolayer MoS$_2$. Nat Nanotechnol 8(7):497–501
6. Wang S, Tu J, Yuan Y, Ma R, Jiao S (2016) Sodium modified molybdenum sulfide via molten salt electrolysis as an anode material for high performance sodium-ion batteries. Phys Chem Chem Phys 18(4):3204–3213
7. Yang E, Ji H, Jung Y (2015) Two-dimensional transition metal dichalcogenide monolayers as promising sodium ion battery anodes. J Phys Chem C 119(47):26374–26380
8. Komsa HP, Krasheninnikov AV (2012) Effects of confinement and environment on the electronic structure and exciton binding energy of MoS\textsubscript{2} from first principles. Phys Rev B 86(24):241201

9. Lee C, Li Q, Kalb W, Liu XZ, Berger H, Carpick RW, Hone J (2010) Frictional characteristics of atomically thin sheets. Science 328(5974):76–80

10. Gordon RA, Yang D, Crotzer ED, Jiang OT, Friendt RF (2002) Structures of exfoliated single layers of WS\textsubscript{6}, MoS\textsubscript{2}, and MoSe\textsubscript{2} in aqueous suspension. Phys Rev B 65(12):125407

11. Fan XL, Yang Y, Xiao P, Lau WM (2010) Frictional characteristics of atomically thin sheets. Science 328(5974):76–80

12. Kadantsev ES, Hayrylak P (2012) Electronic structure of a single MoS\textsubscript{2} monolayer. Solid State Commun 152(10):909–913

13. Calandra M (2013) Chemically exfoliated single-layer MoS\textsubscript{2}: stability, lattice dynamics, and catalytic adsorption from first principles. Phys Rev B 88(24):245428

14. Enyashin AN, Yadgarov L, Houben L, Popov I, Weidenbach M, Tenne R, Seifert G (2011) New route for stabilization of 1T-WS\textsubscript{2} and MoS\textsubscript{2} phases. J Phys Chem C 115(50):24586–24591

15. Wang H, Lu Z, Xu S, Kong D, Cha JJ, Zheng G, Cui Y (2013) Electrochemical tuning of vertically aligned MoS\textsubscript{2} nanofilms and its application in improving hydrogen evolution reaction. Proc Natl Acad Sci USA 110(49):19701–19706

16. Kan M, Wang YJ, Li KW, Zhang SH, Li YW, Kawazoe Y, Jena P (2014) Structures and phase transition of a MoS\textsubscript{2} monolayer. J Phys Chem C 118(3):1515–1522

17. Cheng Y, Nie A, Zhang Q, Gan LY, Shahbazyan-Yassar R, Schwingenschlogl U (2014) Origin of the phase transition in lithiated molybdenum disulfide. ACS Nano 8(11):11447–11453

18. Nasr Esfahani D, Leenaerts O, Sahin H, Partoens B, Peeters FM (2015) Structural transitions in monolayer MoS\textsubscript{2} by lithium adsorption. J Phys Chem C 119(19):10602–10609

19. Pandey M, Botha P, Pati SK (2016) Phase transition of MoS\textsubscript{2} bilayer structures. J Phys Chem C 120(7):3776–3780

20. Du G, Guo Z, Wang S, Zeng R, Chen Z, Liu H (2010) Superior stability and high capacity of restacked molybdenum disulfide as anode material for lithium ion batteries. Chem Commun 46(7):1106–1108

21. Stephenson T, Li Z, Olsen B, Mitlin D (2014) Lithium ion battery applications of molybdenum disulfide (MoS\textsubscript{2}) nanocomposites. Energy Environ Sci 7(1):209–231

22. Mortazavi M, Wang C, Deng J, Shenoy VB, Medhekar NV (2014) Ab initio characterization of layered MoS\textsubscript{2} as anode for sodium-ion batteries. J Power Sources 268:279–286

23. Gao F, Wang L, Zhang Y, Huang Y, Liu K (2015) Atomic-scale probing of the dynamics of sodium transport and intercalation-induced phase transformations in MoS\textsubscript{2}. ACS Nano 9(11):11296–11301

24. Kresse G, Furthmüller J (1996) Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Comput Mater Sci 6(1):15–50

25. Perdew JP, Burke K, Ernzerhof M (1996) Generalized gradient approximation made simple. Phys Rev Lett 77(18):3865

26. Rastogi P, Kumar S, Shovmick S, Agarwal A, Chaubey YS (2014) Doping strategies for monolayer MoS\textsubscript{2} via surface adsorption: a systematic study. J Phys Chem C 118(51):30309–30314

27. Li XD, Fang YM, Wu SQ, Zhu ZZ (2015) Adsorption of alkali, alkaline-earth, simple and 3d transition metal, and nonmetal atoms on monolayer MoS\textsubscript{2}. AIP Adv 5(5):057143

28. Su J, Pei Y, Yang Z, Wang X (2014) Ab initio study of graphene-like monolayer molybdenum disulfide as a promising anode material for rechargeable sodium ion batteries. RSC Adv 4(81):43183–43188

29. Aydinol MK, Kohan AF, Ceder G, Cho K, Joannopoulos J (1997) Ab initio study of lithium intercalation in metal oxides and metal dichalcogenides. Phys Rev B 56(3):1354

30. Lebegue S, Eriksson O (2009) Electronic structure of two-dimensional crystals from ab initio theory. Phys Rev B 79(11):115409

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