Ab initio study of adsorption and diffusion of lithium on transition metal dichalcogenide monolayers

Xiaoli Sun and Zhiguo Wang*

Full Research Paper

Address:
School of Physical Electronics, University of Electronic Science and Technology of China, Chengdu, 610054, P.R. China

Email:
Zhiguo Wang* - zgwang@uestc.edu.cn

* Corresponding author

Keywords:
anode materials; lithium adsorption; lithium diffusion; lithium ion batteries; transition metal dichalcogenide

Beilstein J. Nanotechnol. 2017, 8, 2711–2718.
doi:10.3762/bjnano.8.270

Received: 02 July 2017
Accepted: 19 November 2017
Published: 15 December 2017

Associate Editor: P. Leiderer

© 2017 Sun and Wang; licensee Beilstein-Institut.
License and terms: see end of document.

Abstract

Using first principles calculations, we studied the stability and electronic properties of transition metal dichalcogenide monolayers of the type MX₂ (M = Ti, Zr, Hf, V, Nb, Ta, Mo, Cr, W; X = S, Se, Te). The adsorption and diffusion of lithium on the stable MX₂ phase was also investigated for potential application as an anode for lithium ion batteries. Some of these compounds were found to be stable in the 2H phase and some are in the 1T or 1T' phase, but only a few of them were stable in both 2H/1T or 2H/1T' phases. The results show that lithium is energetically favourable for adsorption on MX₂ monolayers, which can be semiconductors with a narrow bandgap and metallic materials. Lithium cannot be adsorbed onto 2H-WS₂ and 2H-WSe₂, which have large bandgaps of 1.66 and 1.96 eV, respectively. The diffusion energy barrier is in the range between 0.17 and 0.64 eV for lithium on MX₂ monolayers, while for most of the materials it was found to be around 0.25 eV. Therefore, this work illustrated that most of the MX₂ monolayers explored in this work can be used as promising anode materials for lithium ion batteries.

Introduction

Lithium ion batteries (LIBs) have been widely used in portable electronic devices as power supplies, which have potential use in electrical vehicles (EVs) and smart grids. However, the energy and power density of current LIBs cannot satisfy the high demand of EVs. The development of new electrode materials is essential for improvement of the energy density. An ideal electrode material for LIBs should have good electronic conductivity, a lower Li diffusion energy barrier, as well as high energy and power densities. By reducing the bulk electrode materials to low-dimensional materials, a higher energy capacity and higher charge/discharge rate can be obtained as the low-dimensional materials have higher exposure to the electrolyte [1]. Two-dimensional materials, such as Co₂O₄, NiO, phosphorene, SnS and V₂O₅ all exhibit an excellent capacity retention, rate performance, lower energy barrier and long cycling life compared to their bulk counterparts used as electrode materials for LIBs [2-8].

Two-dimensional transition metal dichalcogenides, MX₂ (where M and X correspond to transition metal and chalcogen atoms,
MX₂ monolayers have three types of crystalline structures, hexagonal structure (2H), octahedral structure (1T) and distorted octahedral structure (1T') [23-25]. The structures depend on the arrangements of the M and X atoms. Phase transformation between the different phases occurs during the synthesis process and lithium/sodium intercalation [26-28]. Sun et al. [29] have studied the effect of electron doping on the stability of 2H- and 1T'-MoS₂, and showed that electron doping can stabilize the crystalline structure of 1T'-MoS₂. The crystalline structure can also affect the energy conversion efficiency, for example in the hydrogen evolution reaction (HER). The basal plane of 2H-MoS₂ is inert [30], whereas that of 1T'-MoS₂ is catalytically active for HER [31]. Until now, there is no systematic study on the family of transition metal dichalcogenide monolayers used as anode for LIBs.

In this work, we studied the stability of MX₂ monolayers, and the adsorption and diffusion of Li on the stable MX₂ monolayers (M = Ti, Zr, Hf, V, Nb, Ta, Mo, Cr, W; X = S, Se, Te). These results are helpful for the design of two-dimensional transition metal dichalcogenide based electrodes for LIBs.

Results and Discussion

We systematically investigated the phase stability, Li adsorption and diffusion on MX₂ monolayers (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W; X = S, Se, Te). The combination of these elements have twenty seven possible binary compound materials. Three phases, including 2H, 1T and 1T' structures, were all considered for each of the binary monolayers. All the three structures can be viewed as a positively charged, two-dimensional M atoms, lattice-sandwiched by two hexagonal lattices of negatively charged X atoms. Each M atom is surrounded by six nearest X atoms, and each X atom is connected to three nearest M atoms with ionic M–X bonds. The side and cross-views of the ball and stick models of the MX₂ monolayer are shown in Figure 1. The M atoms are located at the lattice positions of a hexagonal close-packed structure with a trigonal symmetry in the 2H-MX₂ phase (Figure 1a), whereas M atoms are located at

![Figure 1: Top and side views of ball and stick models of a MX₂ monolayer in (a) 2H, (b) 1T and (c) 1T' phase. The M atoms have octahedral and trigonal prismatic coordination in the 1T/1T' and 2H phase, respectively.](image)
the octahedral/disordered octahedral centre of six S atoms in the 1T/1T’ phase (Figure 1b,c). Some compounds are not stable in the 1T phase, which will be relaxed to the 1T phase after relaxation.

The energy related to the 2H phase per formula unit (f.u.), \( E = E_{1T/1T'} - E_{2H} \), is listed in Table 1. A negative value indicates that the 1T/1T’ phase is more stable than the 2H phase. It can be seen from the table that some of these compounds can be stable in the 2H phase, and some in the 1T or 1T’ phase. Only a few of them are stable both in 2H/1T or 2H/1T’ phases. The 2H phase is the minimum energy configuration for monolayers of NbS\(_2\) and TaS\(_2\), which agrees with previously reported results [32,33]. The energy of the 1T phase is smaller than the 2H phase for TiX\(_2\), VX\(_2\), VX\(_2\), ZrX\(_2\), and HfX\(_2\). 1T-VS\(_2\) monolayers are 0.02 eV/f.u. larger than the 2H phase, which indicates that the 1T phase is the energetically favourable one for these compounds, and VS\(_2\) monolayers maybe be stable both in the 2H/1T phase. The results agree with other calculations that imply that the 1T phase is more stable than 2H in TiX\(_2\) [32-34], CrS\(_2\) [35], ZrS\(_2\) [32,33] and HfS\(_2\) [33]. The 2H phase is the stable structure for MoS\(_2\), MoSe\(_2\), WS\(_2\) and WSe\(_2\) monolayers, which has also been predicted by other simulations [36-40]. 1T-VTe\(_2\), 1T-MoTe\(_2\) and 1T'-WTe\(_2\) are the energetically favourable phases. It is also can be seen from Table 1 that 1T-MoTe\(_2\) is 0.06 eV/f.u. more energetically favourable than the 1T phase, which agrees with other simulations [36,39,40]. The energy difference between 2H-WTe\(_2\) and 1T'-WTe\(_2\) is 0.07 eV/f.u., which indicates MoTe\(_2\) and WTe\(_2\) maybe exist in two phases.

The calculated lattice constants and bond length of the M–X bond in the stable phase is listed in Table 2 along with available values from other simulations. The values obtained in the present work agree well with other simulation results. It can be seen from Table 2 that lattice constants and bond lengths increase for the all the MX\(_2\) monolayers as the element X changes from S to Te in group VI for a given element M. The variation can be explained by the increasing atomic radius of elements X from S to Te.

The band structures of MX\(_2\) monolayers in the stable phase are shown in Figure 2. The MX\(_2\) monolayers can be semiconducting with a direct and indirect bandgap or metallic materials. The electronic conductive behaviour of these compounds are shown in Table 2. The 2H phase shows a semiconducting behaviour, such as 2H-WX\(_2\), 2H-NbX\(_2\), 2H-TaX\(_2\) and 2H-MoX\(_2\). The 1T phase can be metallic or semiconducting, such as in 1T-VX\(_2\) (X = S, Se), and 1T-CrX\(_2\) shows metallic behaviour, while 1T-TiX\(_2\), 1T-ZrX\(_2\) and 1T-HfX\(_2\) show semiconducting and metallic behaviour with X = S/Se and X = Te, respectively. 1T'-VTe\(_2\) and 1T'-MoTe\(_2\) show metallic behaviour and 1T'-WTe\(_2\) has a narrow bandgap of 0.50 eV. The obtained bandgap values are close to those previously reported for TiS\(_2\) [32], CrTe\(_2\) [40], TiX\(_2\) [32,33,47], MoX\(_2\) [33,40,47,50-55], HfX\(_2\) [33,47] and WX\(_2\) [33,40,47,50-55,58]. The metallic MX\(_2\) monolayers have good electrical conductivity, which may make them good anode materials.

As shown in Figure 3a and Figure 3b, there are two stable adsorption sites, that is, the hollow site (H) and the top position above the M atom (T) for Li to be adsorbed on the 2H- and 1T-MX\(_2\) monolayers [18]. Four adsorption sites (T1, T2, H1, and H2) are considered for Li adsorption onto the 1T-MX\(_2\) monolayer, as shown in Figure 3c. To analyse the stability of Li adsorbed on the MX\(_2\) monolayers, the adsorption energy, \( E_{ad}(Li) \), is calculated using Equation 1:

\[
E_{ad}(Li) = E_{MX2+Li} - E_{MX2} - E_{Li},
\]

where \( E_{MX2+Li} \) and \( E_{MX2} \) are the total energy of the MX\(_2\) monolayer with and without Li adsorption, respectively. \( E_{Li} \) is the energy of a Li atom in bulk material. The calculated adsorp-

| M     | 2H  | 1T  | 1T' | 2H  | Se  | 1T  | 1T' | 2H  | 1T  | 1T' |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Ti    | 0.00| -0.44| -   | 0.00| -0.33| -   | 0.00| -0.26| -   |
| V     | 0.00| 0.02| -   | 0.00| -0.16| -   | 0.00| -0.06| -0.15|
| Cr    | 0.00| -0.45| -   | 0.00| -0.16| -   | 0.00| -0.17| -   |
| Zr    | 0.00| -0.54| -   | 0.00| -0.40| -   | 0.00| -0.26| -   |
| Nb    | 0.00| 0.21| -   | 0.00| 0.22 | -   | 0.00| 0.15 | 0.10 |
| Mo    | 0.00| 0.68| 0.60| 0.00| 0.35 | 0.29| 0.00| -0.20| -0.26|
| Hf    | 0.00| -0.62| -   | 0.00| -0.50| -   | 0.00| -0.35| -   |
| Ta    | 0.00| 0.18| -   | 0.00| 0.23 | 0.21| 0.00| 0.15 | 0.54 |
| W     | 0.00| 0.91| 0.61| 0.00| 0.81 | 0.35| 0.00| 0.61 | -0.07|
Table 2: Lattice constants ($a$, $b$) and the bond length of the M–X bond ($d_{MX}$) in the stable phase as calculated in this work as compared to other values found in the literature from other simulations. The electronic conducting behaviour (ECB) of these compounds is also shown.

| MX$_2$  | $a/b$ (Å) | $d_{MX}$ (Å) | $a$ (Å) [Ref.] | $d_{MX}$ (Å) [Ref.] | ECB   |
|---------|-----------|--------------|----------------|---------------------|-------|
| 1T-TiS$_2$ | 3.40      | 2.42         | 3.39 [33]      | 2.39 [41]           | 0.59  |
| 1T-TiSe$_2$ | 3.56      | 2.57         | 3.53 [33]      | 2.51 [41]           | 0.29  |
| 1T-TiTe$_2$ | 3.72      | 2.77         | 3.74 [33]      | 2.73 [41]           | metal |
| 2H-VS$_2$  | 3.19      | 2.39         | 3.17 [42-44]   | 2.36 [42-44]        | 0.58  |
| 1T-VS$_2$  | 3.25      | 2.38         | 3.18 [43,45]   | 2.35 [43,44,46]     | metal |
| 1T-VSe$_2$ | 3.37      | 2.55         | 3.24 [41]      | 2.49 [46]           | metal |
| 1T'-VTe$_2$ | 3.80/7.60 | 2.71/2.76/2.79/2.81 | –             | –                   | metal |
| 1T-CrS$_2$ | 3.33      | 2.41         | –              | –                   | metal |
| 1T-CrSe$_2$ | 3.47      | 2.56         | –              | –                   | metal |
| 1T-CrTe$_2$ | 3.67      | 2.81         | –              | –                   | metal |
| 1T-ZrS$_2$ | 3.57      | 2.55         | 3.68 [33,47]   | –                   | metal |
| 1T-ZrSe$_2$ | 3.70      | 2.68         | 3.79 [47]      | –                   | metal |
| 1T-ZrTe$_2$ | 3.89      | 2.90         | 3.98 [33]      | –                   | metal |
| 2H-NbS$_2$ | 3.35      | 2.50         | 3.36 [48]      | 2.49 [48]           | 1.22  |
| 2H-NbSe$_2$ | 3.49      | 2.64         | 3.48 [48]      | 2.62 [48]           | 1.00  |
| 2H-NbTe$_2$ | 3.71      | 2.83         | 3.70 [48]      | 2.82 [48]           | 0.78  |
| 2H-MoS$_2$  | 3.17      | 2.42         | 3.18 [47,49]   | 2.42 [48]           | 1.71  |
| 2H-MoSe$_2$ | 3.32      | 2.55         | 3.32 [47]      | 2.55 [48]           | 1.41  |
| 1T-MoTe$_2$ | 3.84      | 2.81         | –              | –                   | metal |
| 1T'-MoTe$_2$ | 3.89/6.98 | 2.53/2.60/2.61 | –              | –                   | 0.12  |
| 1T-HfS$_2$ | 3.57      | 2.54         | 3.64 [33]      | –                   | 1.09  |
| 1T-HfSe$_2$ | 3.69      | 2.67         | 3.76 [33]      | –                   | 0.50  |
| 1T-HfTe$_2$ | 3.88      | 2.87         | 3.97 [33]      | –                   | metal |
| 2H-TaS$_2$  | 3.35      | 2.50         | 3.34 [48]      | 2.48 [48]           | 0.20  |
| 2H-TaSe$_2$ | 3.47      | 2.63         | 3.48 [48]      | 2.62 [48]           | 0.46  |
| 2H-TaTe$_2$ | 3.69      | 2.82         | 3.76 [48]      | 2.82 [48]           | 0.37  |
| 2H-WS$_2$  | 3.18      | 2.44         | 3.18 [49]      | 2.42 [48]           | 1.96  |
| 2H-WSe$_2$ | 3.32      | 2.57         | 3.32 [47,48]   | 2.55 [48]           | 1.66  |
| 2H-WTe$_2$ | 3.56      | 2.76         | –              | –                   | 1.22  |
| 1T'-WTe$_2$ | 3.49/6.98 | 2.74/2.75/2.78/2.81 | –              | –                   | 0.38  |

The adsorption energy of Li on the stable phase of the MX$_2$ monolayers is shown in Figure 4. The adsorption energy has positive values for Li adsorbed on 2H-WS$_2$ and 2H-WSe$_2$, which indicates that Li cannot be adsorbed on these two compounds and they are not ideal anodes for LIBs. The other compounds have negative values of adsorption energy. The adsorption energy of Li on 2H-MoS$_2$ is $-0.05$ and $-0.25$ eV for H and T sites, respectively. The materials will have a large energy storage capacity if they have a large exothermic reaction energy with Li [19]. Previous studies have shown that the 2H-MoS$_2$ monolayer is a good anode material for LIBs [26-28]. The absolute value of the adsorption energy for Li adsorbed on other compounds is larger than that of 2H-MoS$_2$, so other MX$_2$ compounds are also good anode candidates for LIBs. The adsorption energy as a function of the bandgap of the MX$_2$ monolayer is show in Figure 4. It can also be seen from the figure that MX$_2$ is a semiconducting material with a narrow bandgap, and for metallic materials, the adsorption energy has larger negative values. The materials with a large bandgap have smaller adsorption energy, even those with positive values. For example, the bandgap energies are 1.96, 1.71, 0.78, 0.58 and 0.29 eV and the adsorption energies for Li adsorbed at H/T sites are 0.37/0.24, $-0.05/-0.25$, etc.
Figure 2: Band structures of MX$_2$ monolayers in the stable phase. Fermi energy level is set to be 0.

$-0.51/-0.65, -1.79/1.87$ and $-2.08/2.07$ eV on 2H-WS$_2$, 2H-MoS$_2$, 2H-NbTe$_2$, 2H-VS$_2$ and 1T-TiSe$_2$ monolayers, respectively.

The diffusion of Li on the MX$_2$ monolayers is through the T→H→T and T1→H1→T2→H2→T1 paths for the 2H/1T and 1T' phases, respectively [59], as shown in Figure 3a–c. The typical diffusion energy profiles are shown in Figure 3d, Figure 3e and Figure 3f for Li on 2H-MoS$_2$, 1T-TiS$_2$, and 1T'-MoTe$_2$ monolayers, respectively. The constrained method was used to evaluate the diffusion behaviour of Li on MX$_2$ monolayers – this method is more simple and intuitive compared to the nudged elastic band method and dimer method [60]. The diffusion energy barriers are 0.29, 0.25 and 0.28 eV for Li on 2H-MoS$_2$, 1T-TiS$_2$, and 1T'-MoTe$_2$ monolayers, respectively. These values are reasonable for use as anodes for LIBs. The Li diffusion energy barrier on a MX$_2$ monolayer is shown in Figure 4. Our calculated values agree well with those reported by other researchers. The diffusion energy barrier of Li on 2H-MoS$_2$ monolayer is 0.29 eV, which is consistent with the previously reported value of 0.25 eV [18,42].

A good anode material should have a high electron and Li mobility and a large exothermic reaction energy with lithium. High electronic and ion mobility determine the rate capability and cycling performance, and a large exothermic reaction energy indicates the anode materials have a large energy storage capacity. The diffusion energy barrier is in the range between 0.17 and 0.63 eV, and most are around 0.25 eV, which indicates that all the MX$_2$ monolayers have a reasonable diffusion energy barrier for lithium. The metallic MX$_2$ monolayers and those with small bandgaps have a large adsorption energy for Li, which indicates that they are good anode materials for LIBs with high electronic and ion mobility and large energy storage capacity.

Conclusion

Using density functional theory (DFT) simulations, the stability and electronic properties of MX$_2$ monolayers were investigated. TiX$_2$, VSe$_2$, CrX$_2$, ZrX$_2$ and HfX$_2$ are energetically favourable
in the 1T phase, and 1T-VS$_2$ can be stable both in the 2H/1T phase. The 2H phase is the stable structure for MoS$_2$, MoSe$_2$, WS$_2$ and WSe$_2$. The 1T' phase is the most energetically favourable for VTe$_2$, MoTe$_2$ and WTe$_2$. The 2H phase shows a semiconducting behaviour, for example, 2H-WX$_2$, 2H-NbX$_2$, 2H-TaX$_2$ and 2H-MoX$_2$. The 1T phase can be metallic or semiconducting, for example 1T-CrX$_2$ shows a metallic behaviour while 1T-TiX$_2$, 1T-ZrX$_2$ and 1T-HfX$_2$ show semiconducting and metallic behaviour with X = S/Se and X = Te, respectively. 1T'-VTe$_2$ and 1T'-MoTe$_2$ show metallic behaviour and 1T'-
1. Tianjin, and the calculations were performed on TianHe-1(A).

This work was carried out at National Supercomputer Center in Research Funds for the Central Universities (ZYGX2016J202). Science Foundation of China (11474047) and the Fundamental monolayers.

**Simulation Details**

All the spin-polarized DFT calculations were performed with SIESTA code [62], in which norm-conserving pseudopotentials and a Perdew–Burke–Ernzerhof functional was used to describe the electron–ion interaction and electron exchange correlation, respectively. Numerical atomic orbits were represented as double zeta basis sets plus polarization, and a cut-off energy of 250 Ry was chosen to calculate the Hamiltonian element. The Monkhorst–Pack scheme with $11 \times 11 \times 1$ $k$-point meshes were used for integration in the irreducible Brillouin zone for the relaxation of the primitive cell. A $2 \times 2 \times 1$ $k$-point mesh was used for the calculation of adsorption and diffusion of Li on a $6 \times 6 \times 1$ supercell. As the electrochemical process involves insertion of Li ions into anode materials with a concurrent flow of electrons to compensate charge balance, and therefore, the neutral state of Li was considered in this work. The atomic positions were relaxed by using a conjugate gradient minimization until the Hellmann–Feynman force is less than 0.02 eV/Å on each atom. A vacuum spacing between the slabs and its image of greater than 20 Å is given to avoid the periodic image interactions. As the radii are different for different elements of X in MX$_2$ monolayers (i.e., the radius increases from S to Te in group VI), the lattice constants and bond length of the monolayers (i.e., the radius increases from S to Te) in MX$_2$ elements, which can affect the adsorption and diffusion of Li on MX$_2$ monolayers, and most of the materials are around 0.25 eV. It is therefore concluded that most of the MX$_2$ monolayers can be used as promising anode materials for lithium ion batteries.

**Acknowledgements**

This work was financially supported by the National Natural Science Foundation of China (11474047) and the Fundamental Research Funds for the Central Universities (ZYGX2016J202). This work was carried out at National Supercomputer Center in Tianjin, and the calculations were performed on TianHe-1(A).

**References**

1. Goodenough, J. B.; Kim, Y. Chem. Mater. 2010, 22, 587–603. doi:10.1021/cm901452z
2. Cheng, C.; Zhou, G.; Du, J.; Zhang, H.; Guo, D.; Li, Q.; Wei, W.; Chen, L. New J. Chem. 2014, 38, 2250. doi:10.1039/c3nj01642k
3. Chen, G.; Fu, E.; Zhou, M.; Xu, Y.; Fei, L.; Deng, S.; Chattany, V.; Wang, Y.; Luo, H. J. Alloys Compd. 2013, 578, 349–354. doi:10.1016/j.jallcom.2013.06.042
4. Wang, L.; Dong, Z.; Wang, D.; Zhang, F.; Jin, J. Nano Lett. 2013, 13, 6244–6250. doi:10.1021/nl403715h
5. Vasilyeva, E.; Nasibulin, A.; Tolochko, O.; Rudskoy, A.; Sachdev, A.; Xiao, X. Z. Phys. Chem. 2015, 229, 1429–1437. doi:10.1515/zpch-2015-0573
6. Yao, G.; Huang, C.; Yuan, Y.; Liu, S.; Deng, K.; Kan, E. J. Phys. Chem. C 2015, 119, 6923–6928. doi:10.1021/acs.jpcc.0b02130
7. Kang, J.-G.; Park, J.-G.; Kim, D.-W. Electrochem. Commun. 2010, 12, 307–310. doi:10.1016/j.elecom.2009.12.025
8. Wang, Z.; Su, Q.; Deng, H. Phys. Chem. Phys. 2013, 15, 8705–8709. doi:10.1039/c3cp51167g
9. Radisavljevic, B.; Radenovic, A.; Brivio, J.; Giacometti, V.; Kis, A. Nat. Nanotechnol. 2011, 6, 147–150. doi:10.1038/nnano.2010.279
10. Lee, C.; Yan, H.; Brus, L. E.; Heinz, T. F.; Hone, J.; Ryu, S. ACS Nano 2010, 4, 2695–2700. doi:10.1021/nn1003937
11. Lauritsen, J. V.; Kibsgaard, J.; Helveg, S.; Topsæe, H.; Clausen, B. S.; Lægsgaard, E.; Besenbacher, F. Nat. Nanotechnol. 2007, 2, 53–58. doi:10.1038/nnano.2006.171
12. Liu, K.-K.; Zhang, W. J.; Lee, Y.-H.; Lin, Y.-C.; Chang, M.-T.; Su, C.-Y.; Chang, C.-S.; Li, H.; Shi, Y.; Zhang, H.; Lai, C.-S.; Li, L.-J. Nano Lett. 2012, 13, 1538–1544. doi:10.1021/nl2014361
13. Lee, H. S.; Min, S.-W.; Chang, Y.-G.; Park, M. K.; Nam, T.; Kim, H.; Kim, J. H.; Ryu, S.; Im, S. Nano Lett. 2012, 12, 3695–3700. doi:10.1021/nl301485q
14. Lee, Y.-H.; Zhang, X.-Q.; Zhang, W.; Chang, M.-T.; Lin, C.-T.; Chang, K.-D.; Yu, Y.-C.; Wang, J. T.-W.; Chang, C.-S.; Li, L.-J.; Lin, T.-W. Adv. Mater. 2012, 24, 2320–2325. doi:10.1002/adma.201104798
15. Cai, Y.; Yang, X.; Liang, T.; Dai, L.; Ma, L.; Huang, G.; Chen, W.; Chen, H.; Su, H.; Xu, M. Nanotechnology 2014, 25, 465401. doi:10.1088/0957-4484/25/46/465401
16. Xiao, J.; Choi, D.; Cosimbecu, L.; Koech, P.; Liu, J.; Lemmon, J. P. Chem. Mater. 2010, 22, 4522–4524. doi:10.1021/cm101254j
17. Liu, Y.; Zhao, Y.; Jiao, L.; Chen, J. J. Mater. Chem. A 2014, 2, 1309–1315. doi:10.1039/c4ta01644k
18. Li, Y.; Wu, D.; Zhou, Z.; Cabrera, C. R.; Chen, Z. J. Phys. Chem. Lett. 2012, 3, 2221–2227. doi:10.1021/jl300792n
19. Sun, X.; Wang, Z.; Fu, Y. Q. Sci. Rep. 2015, 5, 18712. doi:10.1038/srep18712
20. Xie, X.; Chen, S.; Sun, B.; Wang, C.; Wang, G. ChemSusChem 2015, 8, 2948–2955. doi:10.1002/cssc.201500149
21. Wang, X.; Li, G.; Seo, M. H.; Hassan, F. M.; Houque, M. A.; Chen, Z. Adv. Energy Mater. 2015, 5, 1501106. doi:10.1002/aenm.201501106
22. Jian, Z.; Zhao, B.; Liu, P.; Li, F.; Zheng, M.; Chen, M.; Shi, Y.; Zhou, H. Chem. Commun. 2014, 50, 1215–1217. doi:10.1039/c3cc47977c
23. Hu, T.; Li, R.; Dong, J. J. Chem. Phys. 2013, 139, 174702. doi:10.1063/1.4827082
24. Song, I.; Park, C.; Choi, H. C. J. RSC Adv. 2015, 5, 7495–7514. doi:10.1039/c4ra11852a
25. Wypych, F.; Schöllhorn, R. J. Chem. Soc., Chem. Commun. 1992, 1386–1388. doi:10.1039/C29920001386
26. Wang, X.; Shen, X.; Wang, Z.; Yu, R.; Chen, L. ACS Nano 2014, 8, 11394–11400. doi:10.1021/nn505501v
