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Theoretical investigation of strain-engineered WSe_2 monolayers as anode material for Li-ion batteries

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ABSTRACT

It poses a great challenge to design anode materials with large capacity, excellent cyclic stability and high rate performance. In this paper, through first principle calculations, we computed electronic properties of monolayer WSe_2 with and without strain effects. Our results show that the electronic band gap decreases with strain percent. At 0% tensile strain the value of the band gap is 1.4 eV while at 10% tensile strain the band gap decreases to 0.7 eV. Therefore, the strain effect enhances the electronic conductivity and leads to an increase in the charge carrier transport. In addition, our predictions show that the adsorption energy increases with the strain. Finally, we computed the diffusion barrier for the migration of Li on the surface of a strain engineered WSe_2 monolayer. The lower barrier energy (0.24 eV) reveals that Li can easily overcome this barrier. Our results show that the strain-engineered WSe_2 monolayers are promising anode material for Li-ion battery.

1. Introduction

There is a great need to improve rechargeable ion batteries with high power and energy densities due to the rapid developments of electrical vehicles and electronic devices [1–3]. To meet the ever-increasing demands in storage systems, Li-ion batteries (LIBs) plays a crucial role in energy consumer devices due to their environmental friendliness, high energy density and compact size [4–6]. The goal is to obtain electrode materials with low diffusion barrier, high capacity and large value of conductivity [7]. Compared to cathode materials, there is lacks of systematic studies on anode materials. Experimental approaches examined that lowering the dimensionality of the ordinary anode materials, the capacity increases. Now a days, 2D graphene is the main focus of researchers as anode material due to its low cost, high columbic efficiency and excellent cycling durability [8–10]. On the other hand, the relatively low storage capacity (372 mA hg^{-1}) limits their further applications [11]. In recent years, two dimensional (2D) transition metal dichalcogenide (TMDs) have implemented alarming attention because of their outstanding optoelectronic, chemical and electronic properties [12–15]. The general chemical formula of 2D layered materials is MX_2, where M represents Mo, W, Ti and V elements etc. while X is any chalcogen such as; S, Se, and Te. Compared to their promising applications in electronics and optoelectronics, 2D TMDs are showing enormous interest in energy storage systems (LIBs and super-capacitors) due to their layered structure and large surface area [7,16–18]. These materials have diverse electronic morphologies and display extraordinary electrochemical performances for the intercalation and diffusion of Li ion for LIBs applications [19–21]. Experimentally, Chen et al. synthesized nanocrystalline mesoporous WSe_2 as anode material for LIB and investigated that it deliver a higher reversible capacity of 530 mA hg^{-1} and exhibited stable cyclic performance [22].

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Similarly, Yang et al. prepared WSe_2 nanoplates as anode materials for Li and Na-ion batteries. These anodes reveal ultrahigh cyclic stability and strong reversible capacity [23]. To improve the efficiency of WSe_2 as an anode material for LIBs applications we need to use some theoretical predictions. Therefore, to improve the performance of LIBs, appropriate efforts have been implemented to tune the electronic structure via doping, decorating/coating or designing hybrid composites. Since the advancement of LIBs acquires an effective technique to control its structural properties and assembled a promising anode material [24]. Tuning the electronic morphology is one of the best approache to apply strain effects on TMDs for energy storage purposes. This is because it modulates the band gap, and thus affects the mobility of electrons and also enhances adsorption rate [25,26]. Very recently, Hao et al. predicted strain engineered 2D MoS_2 monolayer for better functioning LIBs and NABs. According to their findings, the applied tensile strain reduces the band gap which strongly affects the electronic properties. Also Li was adsorbed on the surface of monolayer MoS_2 by strain effect which was unable without strain [27]. Similar to MoS_2, monolayer WSe_2 has layered structure, super low thermal conductivity and has been explored for hydrogen evolution reactions and photovoltaic solar cells applications [28]. Because of the structural symmetry to MoS_2, strain engineered WSe_2 (Se–W–Se) is expected to be the favourable anode material for LIB.

Herein, we introduce the adsorption and diffusion of Li on the surface of strain-engineered WSe_2 monolayer for LIB. Our simulation shows that adsorption and diffusion increases with the increase of strain effects. Also the electronic band gap reduces due to strain and hence conductivity of the anode upsurges. Thus strain engineered WSe_2 is considered to be the promising anode material for LIBs.

2. Computational details

Using density functional theory (DFT), all calculations were carried out as implemented in the Vienna ab-initio Simulation Package (VASP) [29]. The electron-ion interaction and exchange-correlation energy were calculated with the projector augmented plane wave (PAW) and Perdew-Burke-Ernzerhof (PBE), respectively [30,31]. The cutoff energy was chosen to be 500 eV for the plane wave expansion of monolayer WSe_2. A supercell $4 \times 4 \times 1$ of WSe_2 monolayer was considered for adsorption and diffusion of Li with and without strain effects. To sample the K points in the Brillion zone, the Monkhorst–pack method is followed. The nudged elastic band (NEB) technique was employed to find the energy barrier and minimum energy path for the diffusion of Li ion on the surface of WSe_2 [32].

3. Adsorption of Li on WSe_2 monolayer

Similar to other transition metal dichalcogenides (MoS_2, WS_2, $NbSe_2$ and $MoSe_2$ etc.), WSe_2 monolayer also exists in the hexagonal structure [12,25]. Generally, WSe_2 crystallizes in two phases i.e. trigonal (1T) and hexagonal (2H) under normal conditions of temperature and pressure. Monolayer WSe_2 is more stable energetically in 2H phase and this is the reason we consider 2H–WSe_2 monolayer structure. Our optimized 2H structure (WSe_2 monolayer) has lattice constants ($a = b = 3.3$ Å) which are consistent with the previous reports [33]. The top and side views are shown in Fig. 1(a and b).

It is essential for anode material to compel Li with greater adsorption energy for LIBs. To investigate this, we computed the adsorption energy given by:

$$E_{ads} = E_{LiWSe_2} - E_{WSe_2} - E_{Li}) \quad (1)$$

Where, E_{LiWSe_2} is the net energy of Li adsorbed on WSe_2 surface, E_{WSe_2} is the energy of pristine WSe_2 monolayer and E_{Li} is the energy of bulk Li. Based on this definition, the more favourable exothermic reaction will occur between WSe_2 monolayer and Li for negative value of E_{ads}.

Our calculated adsorption energy gives positive value for both T (Li adsorbed on the top of W is called T site) and H (Li adsorbed on the top of Se is given the name H site), which means Li cannot be adsorbed on the surface of WSe_2 monolayer at a higher concentrations. To avoid this problem, we apply tensile strain (varying from 0% to 10%) in monolayer WSe_2, and study the effects of Li adsorption on top (T) and hollow (H) sites. We can see from Fig. 2 (c) that the adsorption energy becomes negative when 10% of the tensile strain was applied, suggesting that Li intercalation is possible which could be beneficial for batteries applications. Thus an applied tensile strain (10%) is an excellent approach to enhance Li adsorption [7,27]. Table 1 depicts the geometric parameters of strain engineered WSe_2 monolayer.

4. Effect of adsorbing contents and open circuit voltage

Adsorption energies of Li adsorbed on T- and H-sites of monolayer WSe_2 (4×4) supercell are -2.036 eV and -1.874 eV, respectively with 10% strain. We also computed adsorption energies for different concentrations of Li on T-sites by applying 10% of tensile strain. To determine whether WSe_2 monolayer is efficient for LIBs, we computed adsorption energies for different configurations with stoichiometry of Li_xWSe_2 ($x = 0.0625$, 0.11, 0.25, 0.5, and 1) as shown in Fig. 3 which display decease in adsorption energy with increasing Li contents (x). This is because of repulsive

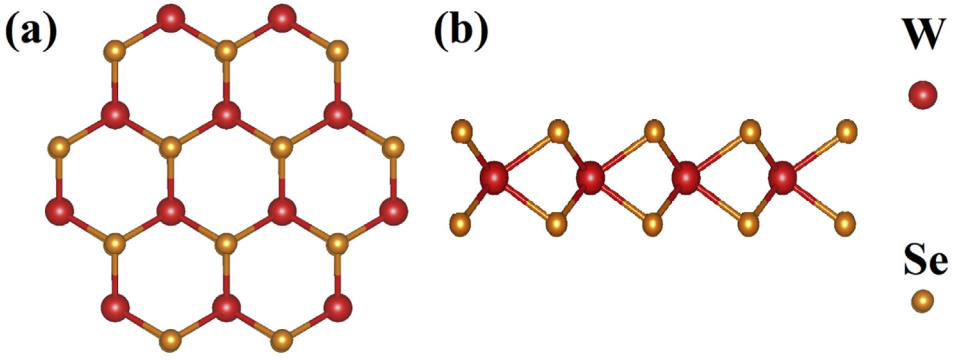

Fig. 1. (a) Top view and side view (b) of the optimized strain engineered single layer WSe_2. Yellowish are the Se atoms while red represent W atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

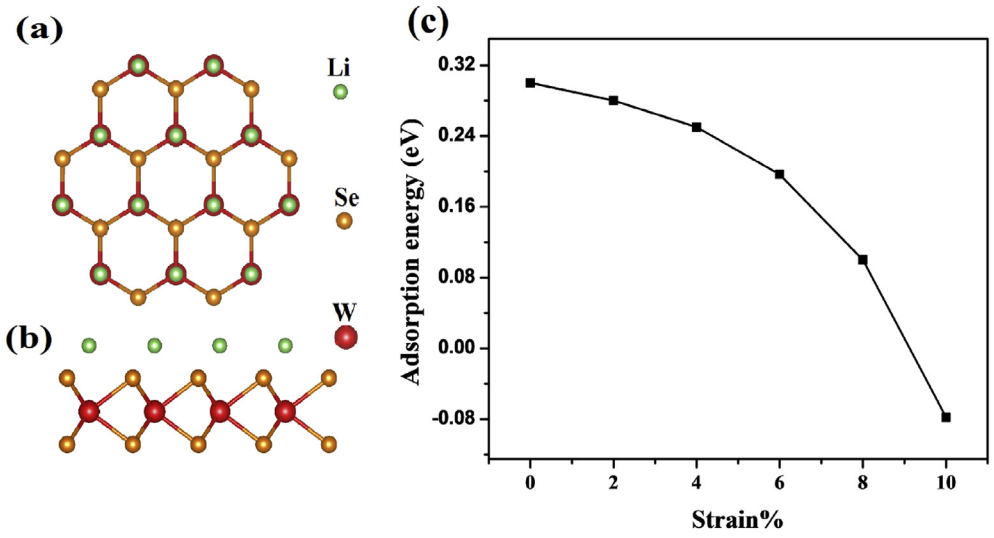

Fig. 2. Top view of the adsorption of Li-ion (green atoms) on the monolayer WSe_2 (a 4 × 4 supercell) (a), while (b) shows the side view. Variation of adsorption energy with strain percent has shown in (c). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Structural parameters (distance between W, Se, Li), adsorption energy, diffusion barrier and average open circuit voltage of Li on WSe_2 monolayer.

Parameters	Computed Values
Adsorption energy (E_{ads})-H-site	-1.874
Adsorption energy (E_{ads})-T-site	−2.036 eV
Bond length of W and Se ($d_{W\text{-}Se}$)	2.5 Å
Distance between Li and Se ($d_{Li\text{-}Se}$)	2.7 Å
Distance between Li and W ($d_{Li\text{-}W}$)	3.5 Å
Lattice constants (a, b)	a = b = 3.3 Å
Diffusion barrier	0.24 eV
Average Open Circuit Voltage	0.67 V

interactions which in results decrease the distance between Li cations [13,34]. Also Fig. 3 shows that WSe_2 monolayer can provide adsorption energy of −0.077 (at x = 1), suggesting that Li atom can be intercalated easily at such a higher concentration.

Open circuit voltage (OCV) is a key factor to enhance the performance of a battery. Theoretically, the approximation of net voltage of metal ion concentrations give the calculation of OCV of the electrode material. The anode of the cell with low OCV leads to achieve a greater net cell voltage. During the charge/discharge process of LIB, the common half-cell reversible reaction at anode is given by:

$$WSe_2 + xLi^+ + xe^- \rightleftarrows Li_xWSe_2 \quad (2)$$

The electrons produced during this reaction move through the outer circuit of the battery while positive ions move between the electrodes and electrolyte. The OCV for Li adsorption on monolayer WSe_2 can be workout as given below:

$$OCV = \left[E_{Li_{x1}}WSe_2 - E_{Li_{x2}}WSe_2 + (x_2 - x_1)\,E_{Li}\right]/(x_2 - x_1)e \quad (3)$$

Where $E_{Li_{x1}}WSe_2$ is the energy of Li_{x1} WSe_2, $E_{Li_{x2}}WSe_2$ is the energy of $Li_{x2}WSe_2$ and E_{Li} is the energy of bulk Li. Fig. 4 reveals that open circuit voltage decreases with increasing Li concentrations. Our computed average open circuit voltage is 0.67 V which is lower than the previously reported WS_2 and WSe_2 and SnS, close to those of commercial anode materials (i.e. 0.11 V for graphite and 1.5–1.8 V for TiO_2) [35–38]. Thus, the appropriate average OCV yields

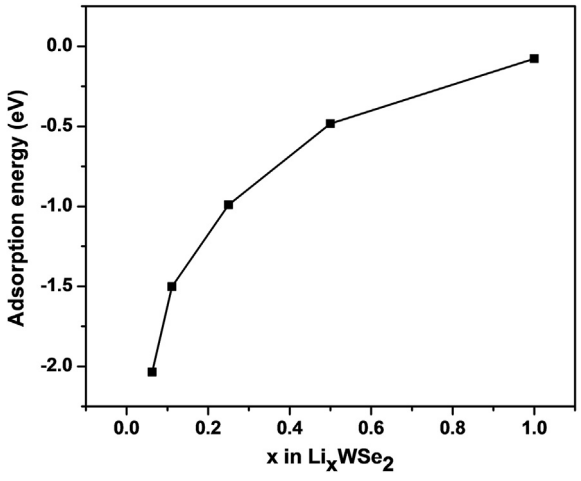

Fig. 3. Variation of adsorption energy with Li concentrations on the surface of WSe_2 monolayer.

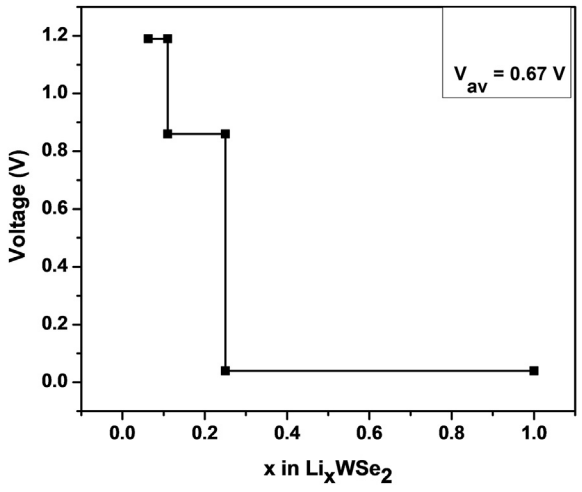

Fig. 4. Open circuit voltage (V_{oc}) with increasing Li contents (x).

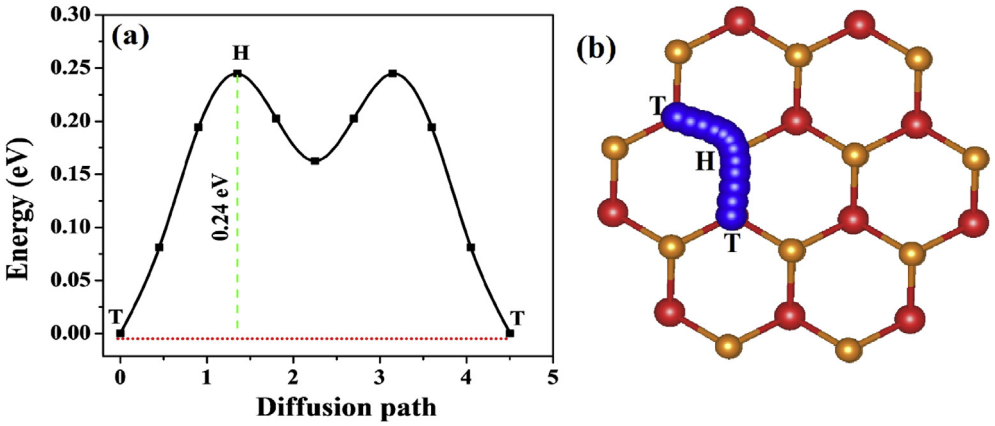

Fig. 5. (a) Shows the diffusion barrier for Li, while (b) represent the corresponding pathways (T-H-T).

substantial usefulness of WSe_2 monolayer to be utilize as LIB anodes. Another important parameter is the specific capacity of an electrode material which is calculated with the formula, $C = xF/m_{WSe_2}$, where x is the concentration of adsorbed Li on WSe_2 monolayer, F is the Faraday constant (which is 26801 mAh mol^{-1}) and m_{WSe_2} is the molar mass of one formula unit WSe_2. A capacity of 77 $mAhg^{-1}$ is achieved when only top T-sites are considered for the adsorption of Li with $x = 1$. If we consider the top and bottom T-sites of monolayers WSe_2 for the adsorption of Li ($x = 2$), a maximum capacity of 144 $mAhg^{-1}$ is expected.

5. Diffusion of Li on WSe_2 surface

It is desirable to diffuse the adsorbed Li with fast kinetics as it is directly linked to the rate capability of a battery [27]. Taking into account Nudged elastic bad (NEB) calculations, the minimum energy path (MEP) for the diffusion of Li was optimized between T- and H-sites [39]. The diffusion trajectory (T–H–T) of Li on the surface of WSe_2 is Zigzag as shown in Fig. 5 (a, b). Next we calculated the diffusion barrier as it determines the charging and discharging processes of LIB. Our calculated barrier for the diffusion of Li on the surface of strain engineered WSe_2 is 0.24 eV as shown in

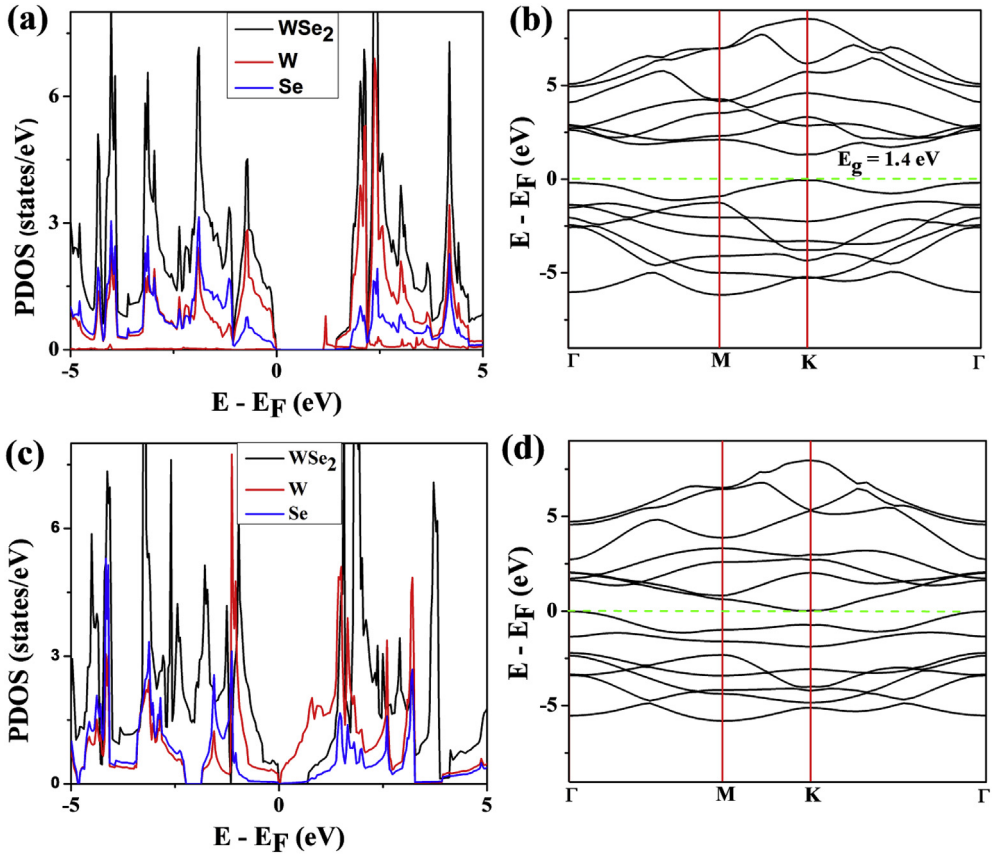

Fig. 6. (a, b, c, d). For 0% and 10% WSe_2 strain the projected (PDOS) and total density of states (TDOS) are shown in (a, c) respectively, while the band structures are shown in (b, d) respectively.

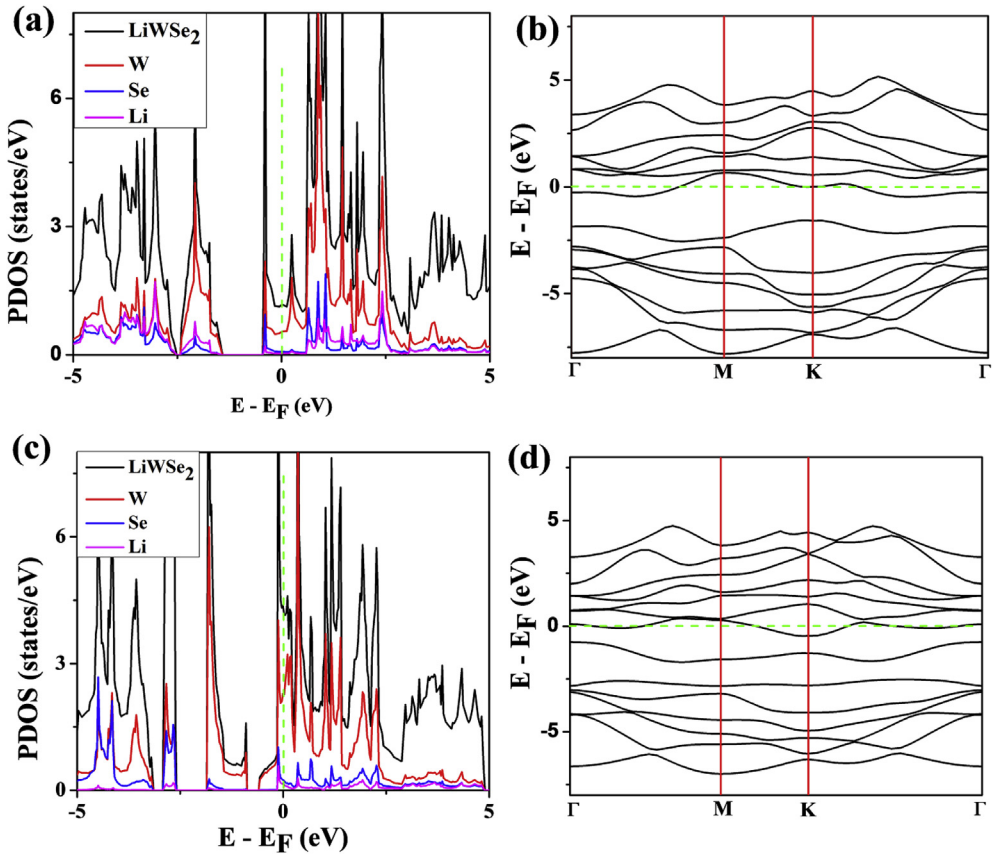

Fig. 7. (a, b, c, d). For 0% and 10% WSe_2 strain the projected (PDOS) and total density of states (TDOS) are shown in (a, c) respectively, while the band structures are shown in (b, d) respectively.

Fig. 5 (a) which is closer to other theoretical reports [35,40–43]. Since the calculated barrier (0.24 eV) is lower than MoS_2 (0.29 eV) and SnS (0. 45 eV). Therefore, Li can diffuse easily on the surface of monolayer WSe_2. Also our calculated diffusion barriers is consistent with the prior WS_2 (0.27 eV) and WSe_2 (0.28 eV) monolayers [38]. Thus, it is concluded that strain-engineered WSe_2 monolayer is an excellent choice as anode material for LIBs.

6. Electronic properties

Generally, the electronic structure is a key aspect to justify the battery's performance [44]. Also it is known that strain effects can alter the electronic properties, and enhance the adsorption rate [27]. Due to this factor, we estimated density of states (DOS) and band structure of pristine WSe_2 monolayer with and without tensile strain. Monolayer WSe_2 reveals semiconducting nature with a direct band gap of 1.4 eV with 0% strain as shown in Fig. 6 (a, b), which is in accordance with the earlier reports [25,26]. The states near the top of valence bands are mainly from the Se_p orbitals, while the states near the bottom of conduction bands are mainly from the contribution of d orbital of W atom (Fig. 6). Our predictions reveal that conduction band minimum (CBM) and valence band maximum (VBM) are located at K-point as shown in Fig. 6. When we applied 10% strain the band gap reduced from 1.4 eV to 0.7 eV as shown in Fig. 6 (c, d) (DOS and band structure). Thus, strain up to 10% in this study strongly affect the monolayer WSe_2, which further enhance the electrochemical performance [4,12].

After the adsorption of Li on WSe_2 monolayer, it is crucial that the material should be metallic for high performance battery applications. So the computed DOS with adsorbed Li on the surface of WSe_2 monolayer indicate that d orbital of W, p orbital of Se and s orbital of Li hybridize well under 10% strain rather than 0% strain as shown in Fig. 7. Thus adsorption of Li leads to enhance the electronic conductivity. Also from DOS and band structure plots as shown in Fig. 7 (c, d), we clearly see that the band gap disappear i.e. the Fermi level shifted to conduction band, showing metallic character, as greatly preferred for LIBs [45–47].

7. Conclusions

To summarize, we examined the monolayer WSe_2 as anode material for LIBs by applying strain effects using density functional theory (DFT) calculations. Our simulations suggest that increasing strain percent (up to 10%), the band gap of WSe_2 monolayer reduces from 1.4 eV to 0.7 eV, and adsorption of Li occurs on WSe_2 surface without any resistance, leading to enhance conductivity and stability. Also the simulated results reveal that the predicted strain engineered WSe_2 monolayer is promising anode material for LIBs with fast charging/discharging rates and low diffusion barrier (0.24 eV). Further, we calculated OCV (0.67 V), which agree well with the prior attempts. Thus, it is concluded that strain-engineered WSe_2 monolayer is an efficient anode material for Li-ion batteries applications.

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