Interfacial electronic states and self-formed p–n junctions in hydrogenated MoS2/SiC heterostructure†

Qinglong Fang, Xumei Zhao, Yuhong Huang, Kewei Xu, Tai Min, Paul K. Chu* and Fei Ma*

It is difficult to generate p–n junctions in atomically thin transition metal dichalcogenides (TMDs) because of the great challenge of selective doping. First-principles calculations demonstrate that the electronic states in monolayer MoS2 could be substantially tuned through contact with hydrogenated SiC sheets, as a result of interface-induced electronic doping. Specifically, monolayer MoS2 exhibits metallic characteristics when put in contact with the Si termination of SiC–H (MoS2/SiC–H), but exhibits ambipolar type polarization when in contact with the C termination of CSi–H (MoS2/CSi–H). Furthermore, monolayer MoS2 can be switched from p-type on H–Si terminations (MoS2/H–SiC and MoS2/H–SiC–H) to n-type on H–C terminations (MoS2/H–CSi and MoS2/H–CSi–H). Accordingly, p–n junctions can be generated in bilayer MoS2 if a fully hydrogenated monolayer SiC is inserted between the layers. In addition, the staggered band alignment of the top and bottom monolayers of MoS2 leads to considerable rectification of current. The results are helpful for the design of TMD based nanoelectronic devices.

1. Introduction

Two-dimensional (2D) crystals exhibit new physics and potential applications in novel devices. Up to now, a great number of 2D materials, such as molybdenum disulfide (MoS2), boron nitride (BN), silicon carbide (SiC), and black phosphorous, have been successfully fabricated, which has greatly stimulated research interest in academic society. Compared to its bulk counterpart, monolayer MoS2 is a direct-band-gap semiconductor with a bandgap of 1.8 eV, high carrier mobility and high on/off ratio. Moreover, it is abundant in nature and could be fabricated at a large scale. Thus, a wide variety of MoS2 have been used as active materials to fabricate atomically thin field-effect transistors (FETs), integrated circuits, light-emitting diodes, solar cells, and photodiodes.

The p–n diodes represent the most fundamental building blocks for applications. Commonly, MoS2 exhibits n-doping owing to sulfur vacancies, and the lack of p-type doping limits its applications in electronic devices. Compared to traditional semiconductors, it is particularly difficult to generate p–n diodes in atomically thin MoS2 due to the challenges of selective doping. However, nearly all the atoms in monolayer MoS2 can “feel” the surface and interface, and the fundamental physics should be strongly sensitive to the surface and interface configuration. For example, an atomically thin p–n junction is generated in bilayer MoS2/WSe2 heterostructures fabricated by chemical vapor deposition (CVD). The different work function and band gap between these two monolayers lead to an atomically sharp heterointerface with type-II band alignment, but with a lower photovoltage. Interestingly, it was predicted that an asymmetrical functionalization might be induced in graphene by adsorption of H and F and, consequently, monolayer MoS2 can be switched from n- to p-type or vice versa. The hydrogenation sites and stacking patterns are crucial for modulating the physical properties of monolayer MoS2/AlN. Hence, it is fundamentally important to exploit suitable contact materials so that the interfacial electronic states and the physical properties of monolayer MoS2 could be well controlled.

Silicon carbide (SiC) is an important substrate for the fabrication of electronic devices adopted in extreme conditions. Monolayer SiC is a nonmagnetic semiconductor with a band
gap of 2.53 eV, high stability and large in-plane stiffness.\textsuperscript{10,30} Rajan et al.\textsuperscript{31} illustrated the direct growth of high-quality few-layer MoS\textsubscript{2} on SiC by a solvothermal reaction, and they found that the heterostructures exhibit rectification characteristics. Gou et al.\textsuperscript{32} fabricated a flower-like MoS\textsubscript{2}/SiC hybrid structure by a solvothermal reaction and the hybrid structure exhibits enhanced hydrogen evolution properties. Hydrogenation is an effective approach for changing the electronic states.\textsuperscript{33–35} The lattice constants of monolayer SiC and hydrogenated SiC are 3.10 Å and 3.13 Å, respectively. Since Si and C terminations on SiC exhibit different bonding states with H atoms,\textsuperscript{36} monolayer MoS\textsubscript{2} on hydrogenated SiC with Si and C terminations should possess distinct interfacial electronic states and physical properties. In this paper, first-principles calculations are done to study the influences of hydrogenation on the interfacial electronic states of MoS\textsubscript{2}/SiC. It was found that the electronic states of monolayer MoS\textsubscript{2} depend on the surface termination of SiC after hydrogenation, which might be changed from n-type to p-type or even to metal. Furthermore, a p–n junction could be generated if the fully hydrogenated monolayer SiC is sandwiched between two monolayer MoS\textsubscript{2}. The results are helpful in the design and fabrication of TMD-based new-concept devices.

2. Computational details

First-principles calculations based on density functional theory were carried out by using the Vienna \textit{ab initio} simulation package (VASP).\textsuperscript{37,38} The projector augmented wave (PAW) method\textsuperscript{39} was used to describe the electron–ion core interaction, which is more accurate than the ultra-soft pseudo-potentials. Commonly, the Perdew–Burke–Ernzerhof (PBE)\textsuperscript{40} method underestimates the band gap of semiconductors; thus the gap values should be corrected by a hybrid functional, in which the Hartree–Fock exchange is included. So we have checked the reported results by using PBE and HSE06 methods, respectively. As for bulk MoS\textsubscript{2}, the measured band gap is 1.29 eV;\textsuperscript{41} however, Botti et al.\textsuperscript{42} calculated band gaps of 0.87 eV and 1.42 eV by using PBE and HSE06 methods, respectively. As for monolayer MoS\textsubscript{2}, Mak et al.\textsuperscript{6} reported a band gap of 1.90 eV via optical spectroscopy measurement, but Lebègue et al.\textsuperscript{43} and Ataca et al.\textsuperscript{44} reported band gaps of 1.78 eV and 2.23 eV by using PBE and HSE06 methods, respectively. Obviously, the PBE method underestimates the band gap of both bulk and monolayer MoS\textsubscript{2}, while the hybrid functional overestimates the band gap.\textsuperscript{45} Tran et al.\textsuperscript{46} and Singh et al.\textsuperscript{47} found that the PBE and HSE06 methods provide the same variation trend of band gaps for different materials or for one material but under different pressures. So the PBE and HSE06 calculations only influence the specific values of band gaps but have little influence on the variation trend.\textsuperscript{45–47} Since the calculations by the HSE06 method will cost an extremely long computing time, the PBE method underestimates the band gap of both bulk and monolayer MoS\textsubscript{2}, while the hybrid functional overestimates the band gap.\textsuperscript{48} The cutoff energy for the plane-waves was chosen to be 450 eV. The Brillouin-zone integration was performed by using an 11 × 11 × 1 \textit{k}-mesh according to the Monkhorst–Pack scheme, and Gaussian smearing broadening of 0.05 eV was adopted. To avoid artificial interactions between the periodic images of the structures, a vacuum region of at least 15 Å was used. A conjugate-gradient algorithm was employed to relax the ions to the ground states with an energy convergence of 1.0 × 10\textsuperscript{−5} eV and a force convergence of 0.02 eV Å\textsuperscript{−1} on each ion. Visualizations of supercells and structures were made with VESTA software.\textsuperscript{49}

The transport properties were calculated using the Atomistix Toolkit ( ATK) package based on the non-equilibrium Green’s function (NEGF) method combined with DFT calculations.\textsuperscript{50,51} The two-probe configuration was used to simulate the device with Au as the electrodes. The electrodes and the central regions were separately optimized, in which supercell models with a vacuum space of at least 15 Å in thickness were adopted. The single zeta polarized (SZP) basic set was adopted. A force mesh cutoff of 150 Ry was chosen to balance the calculation efficiency and accuracy. The \textit{k}-points of the electrodes and the central region were set to 20 × 20 × 100 and 20 × 20 × 1, respectively, in the Monkhorst–Pack scheme. The transmission coefficient \( T^{k_{i}}(E) \) (where \( k_{i} \) is a reciprocal lattice vector along an in-plane direction) was calculated as follows:

\[
T^{k_{i}}(E) = \text{Tr} \left[ I^{k_{i}}_{L/R}(E) G^{k_{i}}_{L/R}(E) I^{k_{i}}_{L/R}(E) G^{k_{i}}_{L/R}(E) \right],
\]

in which \( G^{k_{i}}(E) \) is the retarded Green’s function and \( I^{k_{i}}_{L/R}(E) = \sum_{\ell_{L/R}} \sum_{k_{L/R}} \delta(E - E_{\ell_{L/R}}) \) represents the level broadening due to left and right electrodes in terms of the self-energies of the electrodes, \( E_{\ell_{L/R}} \). The transmission function at a given energy \( T(E) \) is averaged over different \( k_{i} \) in the irreducible Brillouin zone.

The binding energy (\( E_{b} \)) is defined as \( E_{b} = (E_{\text{h}} - E_{\text{MoS}_{2}} - E_{\text{s}}) / N_{s} \) in which \( E_{\text{h}} \), \( E_{\text{MoS}_{2}} \), and \( E_{\text{s}} \) are the free energies of the heterostructure, free-standing MoS\textsubscript{2} and the SiC nanosheet. \( N_{s} \) is the number of S atoms in the supercell. The system is stable for negative \( E_{b} \), and the smaller the \( E_{b} \) value, the stronger the heterostructure binding. The Mulliken charge distribution, including atomic charge, bond population, and charge transfer in the heterostructures, is analyzed by using a projection of a linear combination of atomic orbitals. To gain further insight into the bonding nature and interlayer interaction, the plane-averaged charge density difference, \( \Delta \rho = \rho_{\text{h}} - \rho_{\text{MoS}_{2}} - \rho_{\text{s}} \), is calculated, in which \( \rho_{\text{h}} \), \( \rho_{\text{MoS}_{2}} \), and \( \rho_{\text{s}} \) are the plane-averaged charge densities of the heterostructure, MoS\textsubscript{2}, and SiC nanosheet.
3. Results and discussion

3.1. Structural stability

An infinite 2D MoS$_2$/SiC heterostructure is constructed by stacking monolayer MoS$_2$ and SiC on each other. The optimized lattice constants of the $4 \times 4 \times 1$ supercells of monolayer MoS$_2$ and SiC are 3.190 Å and 3.096 Å, respectively (Fig. S1, in the ESI†), which show good consistency with the experimental and theoretical results. The optimized Mo–S bond length in the monolayer MoS$_2$ is 2.413 Å, and monolayer SiC as an analog of graphene has a bond length of 1.787 Å, and nearly all the atoms are in the same plane (Table S1, ESI†). A $4 \times 4 \times 1$ supercells of an SiC/MoS$_2$ heterostructure with a lattice mismatch of 1.2% are established, in which the lattice constant of MoS$_2$ is slightly compressed but that of SiC is stretched. It was reported that the direct band gap is maintained and the band gap is reduced from 1.9 eV to 1.6 eV as the lattice constant is increased from 3.119 Å to 3.169 Å for the monolayer MoS$_2$. A strain of at least 1.6% is needed to induce substantial change in the electronic states of MoS$_2$. So the influence of mismatch strain on the electronic states of the MoS$_2$/SiC heterostructure is negligible.

van der Waals heterostructures are typically fabricated by mechanical exfoliation and subsequent attachment, so the orientation cannot be well controlled. For an MoS$_2$/SiC heterostructure, the six most likely stacking configurations are explored, as shown in Fig. S2 (ESI†). The rotation angles of monolayer MoS$_2$ with respect to monolayer SiC are 0°, 60°, 120°, 180°, 240° and 300°. Fig. S3 (ESI†) shows the calculated binding energies, and the heterostructure of configuration $d$ is the most stable with a binding energy of $-144$ meV per S atom. Furthermore, the binding energy is much lower than that of monolayer MoS$_2$ on silicene ($-64$ meV) or on germanene ($-71$ meV). The interlayer separation ($d_0$) in the MoS$_2$/SiC heterostructure of configuration $d$ is 2.928 Å, illustrating physical adsorption between them. Therefore, MoS$_2$ is bonded to monolayer SiC via van der Waals interaction or electronic interaction, but not orbital hybridization. The structural and electronic properties of all the configurations are almost the same. So only configuration $d$, as shown in Fig. 1a, is considered in the following.

Since each partially hydrogenated SiC has two terminations, there are four types of stacking configurations of MoS$_2$ on partially hydrogenated SiC (Fig. S4a and b, ESI†). For H–SiC, MoS$_2$ can be contacted with the C termination of H–SiC (labeled MoS$_2$/Si–C–H, Fig. 1b) and the H terminated side of H–SiC (labeled MoS$_2$/H–Si–C, Fig. 1c); for SiC–H, MoS$_2$ can be in contact with the Si termination (labeled MoS$_2$/Si–C–H, Fig. 1d) and the H terminated side (labeled MoS$_2$/H–C–Si, Fig. 1e). The Mo–S bond length is the same as that in monolayer MoS$_2$, but the Si–C, Si–H, and C–H bond lengths are slightly lengthened (Table S1, ESI†). As compared to MoS$_2$ on SiC, the $d_0$ value is shortened, especially for the MoS$_2$/Si–H heterostructure, implying enhanced interlayer interaction. As listed in Table 1, the binding energies of MoS$_2$ on H–SiC (MoS$_2$/C–Si–H and MoS$_2$/H–Si–C) are higher than those of MoS$_2$ on Si–C (MoS$_2$/Si–C–H and MoS$_2$/H–C–Si). Moreover, the binding energies of MoS$_2$ on partially hydrogenated SiC are higher than those of MoS$_2$ on SiC by 200–700%; that is, partial hydrogenation enhances the interaction between MoS$_2$ and SiC, and thus improves the structural stability of monolayer MoS$_2$ on SiC.

For MoS$_2$ on fully hydrogenated SiC (labeled H–Si–C–H), there are two kinds of heterostructures, labeled MoS$_2$/H–Si–C–H (Fig. 1f) and MoS$_2$/H–C–Si–H (Fig. 1g). The calculated structural parameters are also summarized in Table 1, and little difference in structural properties and binding energies is in evidence. As compared to monolayer MoS$_2$ on SiC and on partially hydrogenated SiC, the structure of monolayer MoS$_2$ on fully hydrogenated SiC changes little. Although the interlayer separation of MoS$_2$ and fully hydrogenated SiC is reduced, the binding

![Fig. 1](https://example.com/fig1.png)  
Schematic illustration of monolayer MoS$_2$ on an SiC sheet with and without hydrogenation.
energy in MoS₂ on fully hydrogenated SiC is close to that in MoS₂ on SiC.

3.2. Charge transfer and redistribution

The interlayer interaction from MoS₂ is through the charge redistribution in the heterostructure. In order to investigate the electronic properties of MoS₂ on SiC with or without hydrogenation, the planar-averaged charge density difference along the z-direction is calculated, as depicted in Fig. 2. As is well known, the charge redistribution might lead to polarization as well as the formation of an interface dipole. The interface charge depletion is direct evidence of a surface charge repulsion effect. According to Mulliken charge analysis, 0.091 e is transferred from the SiC sublayer to the MoS₂ sublayer and the holes remain in the SiC sublayer (Fig. 2a). This charge redistribution induces a built-in electric field across the heterostructure, and hinders the diffusion of electrons and holes, and finally a balance is established. For MoS₂ on the hydrogenated SiC, the charge transfer from SiC to MoS₂ is not considerable except for the MoS₂/SiC–H heterostructure (Fig. 2b and c). Similar results were found in MoS₂ on decorated AlN nanosheets. For MoS₂ on H–SiC, the charge in the interface is close to the MoS₂ sublayer, but the charge is close to SiC–H for MoS₂ on SiC–H. The maximum Δρ in MoS₂/SiC–H is larger than those of MoS₂/CSI–H, MoS₂/H–SiC, and MoS₂/H–CSI by 300% or so (Fig. 2b), which is consistent with the changes in the interlayer separation and binding energy, as listed in Table 1. Commonly, the stronger the interaction between sublayers, the more charge transfer occurs. The d₀ is only 2.174 Å, which is shorter than that of the Si–S bond (~2.2 Å), resulting in bonding between Si and S atoms. The electronic transfer from SiC–H to MoS₂ (0.097 e) and enhances the bonding between MoS₂ and SiC–H. In addition, the plane-averaged electrostatic potentials of MoS₂ on the SiC nanosheet with or without hydrogenation are calculated and shown in Fig. 3. It can be found that the potential of SiC (8.613 eV) in the MoS₂/SiC heterostructure is deepened (Fig. 3a). The large potential drop of the MoS₂/SiC heterostructure indicates a strong electrostatic field across the interface, which may affect the kinetics of photo-generated carriers. Although the hydrogenated SiC also has a deeper potential than that of MoS₂ in the heterostructure, the potential difference between the hydrogenated SiC and MoS₂ is reduced compared to that between SiC and MoS₂ (Fig. 3b–g).

### Table 1

<table>
<thead>
<tr>
<th>Configuration</th>
<th>L_{Mo-S} (Å)</th>
<th>L_{Si-C} (Å)</th>
<th>L_{Si-H} (Å)</th>
<th>L_{C-H} (Å)</th>
<th>d₀ (Å)</th>
<th>h (Å)</th>
<th>Eₘ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS₂/SiC</td>
<td>2.401</td>
<td>1.808</td>
<td>2.928</td>
<td>2.975</td>
<td>0.370</td>
<td>~188</td>
<td>−144</td>
</tr>
<tr>
<td>MoS₂/CSI–H</td>
<td>2.408</td>
<td>1.866</td>
<td>1.522</td>
<td>2.356</td>
<td>0.286</td>
<td>~426</td>
<td>−1273</td>
</tr>
<tr>
<td>MoS₂/H–SiC</td>
<td>2.406</td>
<td>1.852</td>
<td>1.534</td>
<td>2.174</td>
<td>0.579</td>
<td>~1273</td>
<td>−153</td>
</tr>
<tr>
<td>MoS₂/SiC–H</td>
<td>2.401</td>
<td>1.911</td>
<td>1.116</td>
<td>1.493</td>
<td>2.924</td>
<td>0.567</td>
<td>−153</td>
</tr>
<tr>
<td>MoS₂/H–CSI–H</td>
<td>2.401</td>
<td>1.911</td>
<td>1.116</td>
<td>1.493</td>
<td>2.245</td>
<td>0.562</td>
<td>−185</td>
</tr>
<tr>
<td>MoS₂/H–CSI–H</td>
<td>2.405</td>
<td>1.905</td>
<td>1.108</td>
<td>1.493</td>
<td>2.245</td>
<td>0.562</td>
<td>−185</td>
</tr>
</tbody>
</table>

### Fig. 2

Averaged charge density difference of MoS₂ on SiC with and without hydrogenation.
in the partially hydrogenated SiC sheet, but not in the MoS$_2$ sublayer for which the spin-up and spin-down channels are almost symmetric. This is confirmed by the magnetic density in Fig. S5 (ESI†). Spin polarization emerges on the C and H atoms (Si atoms) in MoS$_2$/CSi–H and MoS$_2$/H–SiC (MoS$_2$/H–CSi) heterostructures, similar to that of partially hydrogenated SiC sheets (Fig. S4c–f, ESI†). Specifically, as for the MoS$_2$ sublayer in the MoS$_2$/CSi–H heterostructure, the energy difference between the $E_F$ and the VBM is almost equal to that between the CBM and $E_F$ (Fig. 5a), while for the MoS$_2$/H–SiC heterostructure, the electronic structure of the MoS$_2$ sublayer is almost maintained with respect to the isolated monolayer MoS$_2$ (Fig. 5b). For the MoS$_2$/H–CSi heterostructure, the $E_F$ shifts towards the CBM of the MoS$_2$ sublayer, implying that the MoS$_2$ sublayer is changed into an n-type one (Fig. 5d). The MoS$_2$/SiC–H heterostructure
exhibits similar behavior, but the MoS₂ sublayer in the MoS₂/H–SiC heterostructure exhibits a metallic feature (Fig. 5c). As for the MoS₂/H–SiC–H heterostructure, the $E_p$ is slightly above the VBM (0.167 eV) of the MoS₂ sublayer and far away from the CBM (1.529 eV), characteristic of the p-type feature of the MoS₂ sublayer (Fig. 5e). Since MoS₂ is physically absorbed on H–SiC–H, the electronic state of MoS₂ is nearly unperturbed. However, as the dipole of H–SiC–H is rotated by 180° (i.e., MoS₂/H–SiC–H), the $E_p$ is close to the CBM (0.617 eV) of MoS₂, characteristic of the n-type feature of the MoS₂ sublayer (Fig. 5f). The fully hydrogenated SiC can be switched from n- to p-type or vice versa (Fig. 5f). The partially hydrogenated SiC can be switched from n- to p-type by changing the orientation of the intrinsic dipole moment.

To understand the role of the termination surface of SiC, a model of a hydrogenated monolayer SiC sandwiched by two monolayer MoS₂ (MoS₂/H–SiC–H/MoS₂) is built, as shown in Fig. 6a. Although the interlayer distance between the bottom and top MoS₂ on H–SiC–H is different ($d_1 = 2.899$ Å and $d_2 = 2.270$ Å), the Mo–S bond lengths in the bottom and top MoS₂ sublayers ($L_{Mo–S} = 2.408$ Å) are equal to each other. The structural parameters change little, but the binding energy ($E_b = -405$ meV) is lower than that of MoS₂ on fully hydrogenated SiC by 80%. Fig. 6b shows the DOS projected on the bottom MoS₂, H–SiC–H, and top MoS₂ sublayers. For the MoS₂/H–SiC–H/MoS₂ trilayer heterostructure, the VBM is mainly contributed by the bottom MoS₂ sublayer, whereas the CBM is dominated by the electronic states from the top MoS₂ sublayer. The potential difference across the fully hydrogenated SiC sheet breaks the interfacial symmetry, resulting in a p-type (n-type) doping in the bottom (top) monolayer MoS₂. So bipolar doping might be induced without an external electric field being applied. As shown in Fig. 6c, the charge is substantially redistributed. The plane-averaged charge density difference in the MoS₂/H–SiC–H/MoS₂ heterostructure seems to be a sum of those of MoS₂/H–SiC–H and MoS₂/H–SiC–H. The charge transfer leads to a significant potential difference of 1.426 eV between the bottom and top MoS₂ monolayers (Fig. 6d). So a dipole moment from the top monolayer MoS₂ to the bottom one is generated. Accordingly, p-n junctions, field effect transistors and logic devices might be designed.

3.4. Transport properties

The MoS₂/H–SiC–H/MoS₂ device is constructed between four layers of Au in the channel region (Fig. 7a). The semi-infinite face-centered cubic Au(111) planes are used as electrodes. Electrodes with different lengths of 4.71 Å, 7.06 Å and 14.13 Å were adopted to study the effect of electrode size on the transport properties of the MoS₂/H–SiC–H/MoS₂ heterostructure. As shown in Fig. 7b, their transmission spectra are almost coincident with each other; that is, they are independent of electrode size because of the semi-infinite electrode used. So as an example, the electrode with a length of 7.06 Å is adopted. First, we examine whether the dipole moment between the bottom and top MoS₂ monolayers is maintained. Although the energy difference is increased, the VBM (CBM) is still mainly contributed by the bottom (top) MoS₂ sublayer for the MoS₂/H–SiC–H/MoS₂ trilayer heterostructure in the channel region (Fig. S6, ESI†). The Schottky barrier is evaluated from the DOS of MoS₂ to be 0.527 eV and 0.728 eV for electron and hole, respectively. Fig. 7b shows the transmission spectra of the MoS₂–H–SiC–H–MoS₂ trilayer heterostructure under zero bias, which is consistent with the electronic properties. The drain-source current of the MoS₂–H–SiC–H–MoS₂ trilayer heterostructure under a bias voltage is calculated, and the results are shown in Fig. 7c. The MoS₂–H–SiC–H–MoS₂ system exhibits current rectification, characteristic of a p-n junction.

Fig. 6 (a) Optimized structure of bilayer MoS₂ separated by a fully hydrogenated SiC sheet (MoS₂/H–SiC–H/MoS₂). (b) DOS projected on bottom MoS₂, H–SiC–H, and top MoS₂ in an MoS₂/H–SiC–H/MoS₂ trilayer heterostructure. The Fermi level is set at 0 eV and indicated by the green line. The plane-averaged (c) charge density difference and (d) electrostatic potential of MoS₂/H–SiC–H/MoS₂ trilayer heterostructure. The inset is the 3D isosurface of the charge density difference. The red and green areas represent electrons accumulation and depletion, respectively.

Fig. 7 Transfer characteristics of the MoS₂/H–SiC–H/MoS₂ trilayer heterostructure with Au electrodes: (a) optimized structure of the MoS₂/H–SiC–H/MoS₂ trilayer heterostructure by constructing between six layers of Au, (b) transmission spectrum under zero bias, and (c) I–V curve.
4. Conclusions

First-principles calculations are performed to study the influences of a hydrogenated SiC sublayer on the electronic states and charge transfer in monolayer MoS$_2$ stacked on an SiC sheet. It is found that monolayer MoS$_2$ exhibits metallic characteristics when in contact with the Si termination of SiC–H (MoS$_2$/Si–H), but exhibits ambipolar type polarization when in contact with the C termination of Si–H (MoS$_2$/C–H). Furthermore, monolayer MoS$_2$ can be switched from p-type on H-Si termination to n-type on H-C termination (MoS$_2$/H–Si and MoS$_2$/H–C). In an MoS$_2$/Si–C/H–MoS$_2$ trilayer heterostructure, the fully hydrogenated SiC is sandwiched between two monolayer MoS$_2$ charge transfer, the top or bottom MoS$_2$ sublayer and SiC occurs, resulting in p-n junctions. This implies that the electronic states of monolayer MoS$_2$ on an SiC sheet can be substantially tuned through hydrogenation and a p-n junction might be produced in the 2D heterostructure, which is crucial for electronic device applications.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

This work was jointly supported by National Natural Science Foundation of China (Grant No. 51771144, 5147130, 51501012), Natural Science Foundation of Shaanxi Province (No. 2017JZ015), Fund of the State Key Laboratory of Solidification Processing in NWPU (SKLSP201708), Fundamental Research Funds for the Central Universities. This work was carried out at HPCC Platform in Xian Jiaotong University.

References