Effect of monolayer supports on the electronic structure of single-layer MoS₂

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Abstract. We present results of density functional theory based calculations of the electronic structure of a single-layer of MoS₂, as modified by three different single-layer materials used as support: hexagonal boron nitride (h-BN), graphene, and silicene, using the local density approximation (LDA), on the one hand, and a functional that explicitly includes van der Waals interactions (optB88-vdW), on the other hand. Because the lattice mismatch between the primitive cell of MoS₂ and those of the supports is large, calculations are performed with as large a supercell as computationally feasible, so as to reduce the incommensurability between lattices. Even though van der Waals interactions are expected to play an important role in the binding between MoS₂ and h-BN and graphene, we find that the band structure and related conclusions obtained by optB88-vdW and LDA are quite similar for the three heterostructures considered here. Single-layer MoS₂ interacts weakly with h-BN and graphene, while covalent bonds are formed with silicene. Detailed analysis of the electronic density of states also indicates little effect of h-BN and graphene, while silicene severely modifies it by introducing additional states within the band gap. Furthermore, adsorption on graphene brings the conduction bands of MoS₂ down to the Fermi level of graphene as a result of charge transfer from graphene to MoS₂, while adsorption on silicene shifts both valence and conduction bands towards the Fermi level, in addition to inducing a gap of ~50 meV in silicene itself.

1. Introduction

The experimental production of graphene on 2004 [1] has sparked tremendous interest in the study of two-dimensional (2D) atomic crystals. Layered materials in which the bonding within layers is covalent and that between them is of the van der Waals (vdW) type are a rich source of 2D materials. One set of such materials is the transition-metal dichalcogenide, of which molybdenum disulfide (MoS₂) is a prototype. When MoS₂ is reduced from bulk to a single layer its electronic properties change drastically. Both forms have been experimentally and theoretically shown to be semiconductors, but while in the bulk the gap is indirect (~1.3 eV), in the single layer the optical and fundamental gap are direct (~1.8 eV [2-4] and 2.15 eV [5], respectively) making MoS₂ attractive for electronic and optical applications. Figure 1a shows the structural features of a single layer of MoS₂: this material is formed by an atomic plane of molybdenum sandwiched between two atomic planes of sulfur. Even though single-layer MoS₂ has an thickness of three atomic layers, researchers have successfully found its usage in fabricating electronic devices such as field-effect transistor [6, 7], phototransistors [8].

Evidently, the properties of MoS₂ are affected by the substrate on which it is. For example, h-BN is a good choice as support in order to get higher photoluminescence quantum yield in a single layer of
MoS$_2$ [9]. Also, the efficiency and properties of MoS$_2$-based field-effect transistors vary depending upon the substrates used in device fabrications [6, 10]. Understanding the effect of support on properties of MoS$_2$ is thus important for MoS$_2$-based device designing and manufacturing. It would be also helpful to locate supports whose interactions with an adsorbed MoS$_2$ film are either negligible (with virtually no effect on the intrinsic properties of the film) or tunable in ways that produce desired effects. We are interested in the effect of three 2D materials, h-BN, graphene, and silicene, as supports on electronic properties of single-layer MoS$_2$ because these 2D material substrates share with MoS$_2$ a hexagonal lattice and because such heterostructures have been experimentally realized [9].

Hexagonal boron nitride has proven to be an attractive dielectric substrate for improving the mobility of charge carriers and stability in graphene [11]. Among its features are its large band gap (~5.97 eV) [12] and its relative lack of dangling bonds, which reduces charge traps. Graphene, on the other hand, is a zero-gap material in which charge carriers near Dirac points behave as massless particles [13]. At the same time, silicene the analogue of graphene for silicon, has been predicted to be stable with a low buckled-honeycomb geometry rather a planar structure owing to the strong tendency of Si atoms to adopt $sp^3$ hybridization [14]. Just as graphene, silicene is a zero-gap material whose conduction and valence bands meet at the K point of the 2D Brillouin zone.

While we were motivated by the work of Ma et al. [15] who used density functional theory (DFT) to show that for the graphene/MoS$_2$ heterostructure a gap opens in graphene, we have become aware of a few other related studies in the course of preparation of this manuscript. Komsa and Krasheninnikov [16] using DFT and a semi-empirical correction for van der Waals interactions through the DFT-D2 approach [17] show that for the bilayer heterostructures MoS$_2$/BN and MoS$_2$/graphene, the electronic structure of MoS$_2$ is not modified. The MoS$_2$/BN heterostructure was found to be a semiconductor while MoS$_2$/graphene was a semimetal, with the Dirac point of graphene slightly below of the conduction bands of MoS$_2$. Unlike Ma et al. [15], they did not report any gap opening in graphene. Li et al. [18], on the other hand, report a gap opening of the graphene/MoS$_2$ superlattice which varies with the stacking of the two materials, and that the graphene/MoS$_2$ superlattice turns metallic and conduction bands of MoS$_2$ are aligned with the Fermi level. Likewise, a number of other authors [19-22] have carried out calculations for one or more of the heterostructures considered here and their results depend very much of the amount of strain in the system and the choice of the functional used for the DFT calculations.

Our interest in this work is two-fold: 1) carry out a comparative study of the changes in the electronic structure of single-layer MoS$_2$ brought about by each of three single-layer materials used as a substrate, when the lattice match is small; 2) compare the results obtained using LDA with those from more accurate treatment of van der Waals interactions (as in the code optB88-vdW). It is well known that the LDA overestimates bonding. The general gradient approximation (GGA) designed to correct this deviation, has had reasonable success. On the other hand, both functionals fail to take into account dispersion forces. However, unlike GGA which gives only repulsive interactions in weakly bond systems, LDA frequently gives reasonable results [23-25]. As we shall see, LDA, perhaps fortuitously, provides reasonably good description of the three systems in question here. While it would have been most attractive to have considered systems sizes in which the MoS$_2$ layer had zero strain, the results presented here have very small (<1.6% for MoS$_2$/BN and MoS$_2$/silicene and <3% for MoS$_2$/graphene) lattice mismatch.

2. Computational procedure

Our calculations are based on DFT as implemented in the Vienna ab initio Simulation Package (VASP) [26, 27], and Quantum Espresso package (QE) [28]. For VASP calculations, we use projector augmented wave (PAW) [29, 30] pseudopotentials generated using Perdew-Burke-Ernzerhof parameterization (PBE) [31] and plane-wave basis set (with a cut-off energy of 500 eV) methods. We utilize the optB88-vdW [32, 33] version of the van der Waals density functional (vdW-DF) [34, 35] because of its success in the treatment of dispersion bonded systems [33]. For simplification in the text and for emphasizing the explicit inclusion of vdW interaction, we refer herein opbtB88-vdW as vdW.
For QE calculations, the exchange and correlation effects are treated within the local density approximation (LDA), using the Perdew-Zunger (PZ) functional [36]. Electronic wave-functions are expanded using a plane-wave basis set with a kinetic energy cutoff of 60 Ry. We used norm-conserving pseudo-potentials [37].

The lattice mismatch between primitive cell of MoS$_2$ and the supports here considered is large (experimental lattice parameters of MoS$_2$, h-BN, and silicene are 3.16 Å [38], 2.504 Å [39], and 2.46 Å [40], respectively). Previous theoretical studies have shown that the use of strong or free strained heterostructures lead to different results [15, 16, 20]. In order to minimize the changes in the electronic structure coming from the artificial strain introduced to get commensurability between lattices, we have considered, for each MoS$_2$/substrate combination, supercells with large periodicities in which the lattice mismatch is small and is computationally feasible for DFT calculations. Additionally, because we consider the single-layer MoS$_2$ as the adsorbate, in all cases its lattice parameter will be slightly adjusted to get commensurability with the single-layer supports, while the lattice parameters of the supports will be fixed to their optimized values. Parameters of supercells were generated using our calculated lattice constant of support materials and will be described more in details in the next section. A vacuum of ~15 Å was used to separate normal periodical images to minimize the interaction between them. Models were fully relaxed until all components of force acting on each ion are smaller than 0.01 eV/Å. The reciprocal space was sampled with a 6×6×1 mesh generated through Monkhorst-Pack scheme [41] for MoS$_2$/graphene and MoS$_2$/BN, while with a 3×3×1 mesh for MoS$_2$/silicene.

### 3. Structural properties

![Figure 1](image1.png)  
![Figure 2](image2.png)

Figure 1. Structural representations of (a) single-layer MoS$_2$, (b) single-layer boron nitride, (c) graphene, and (d) silicene. For the supports (b-d), the high-symmetry adsorptions sites are labeled as H (hole), T4 (tetrahedral), and T (top).

Figure 2. Relaxed models to represent the adsorption of a single layer of MoS$_2$ on different supports. $h$ in the figure represents the distance between layers, and $\Delta Z$ is the height difference between Si atoms.

We found a lattice parameter of 3.187 Å (3.167 Å) with the vdW (LDA) functional for single-layer MoS$_2$ which is less than 1% difference from experimental value [38], of 2.508 Å (2.502 Å) for h-BN, of 2.465 Å (2.448 Å) for graphene, and of 3.863 Å (3.81 Å) silicene. We considered in this work the system consisting of (4×4) MoS$_2$ and (5×5)h-BN, (3×3) MoS$_2$ and (4×4)graphene, (6×6) MoS$_2$ and (5×5) silicene with lattice mismatches of -1.65% (-1.32%), 3.03% (2.91%), and 0.99% (0.18%), respectively. The LDA always gives a lower lattice mismatch. Here, we defined the lattice mismatch as $1-(n/n_0a/a_0)$; where $(n_0, a_0)$ and $(n, a)$ are the (number of periodical units, lattice parameters) of the support and of the adsorbed MoS$_2$ film, respectively. Positive (negative) lattice mismatch indicates
that the adsorbed film is under tensile (compressive) strain. To find the optimal adsorption structures of a single-layer MoS$_2$ on the support in question, we constructed several models on the basis of the periodicities listed above. To fit the single-layer MoS$_2$ over the support we choose a sulfur atom or a molybdenum atom belonging to the single-layer MoS$_2$ as an initial point of reference, and place it on a high-symmetry site of the support (see Figure 1. b, c, and d) allowing the single-layer MoS$_2$ and the support to have the same orientation. We repeated this process for each possible combination of S or Mo atom and types of high-symmetry sites. It is important to note that we adjusted the MoS$_2$ lattice parameter to make it commensurable with the support.

We obtained three non-equivalent models for MoS$_2$ on h-BN (ST$_{TB}$, ST$_{TN}$, and SH, those are equivalent with MoTN, MoHt, and MoTB, respectively), two on graphene (ST and MoTr, those are equivalent with SH, ST$_4$ and MoHt, MoT$_4$, respectively). Herein, Name of each configuration is simplified by X$Y$, where X (= S or Mo) is the reference atom of MoS$_2$, Y is the high-symmetry site of support on top of which X is placed. See figure 1 for explanations of Y subscripts. For the same support, the difference of the total energy between non-equivalent models is very small, of the order of only tenths of meV resulting in that we can regard these conformations of the three systems as isoenergetic. It is worth mentioning that the total energy of vdW-heterostructures are generally insensitive to the stacking order between layers [15, 18, 19, 21]. Nerveless, we chose to study in details the configurations with the lowest energy. For the case of vdW functional, they are S on hole (SH) for MoS$_2$/BN, S on top (ST) for MoS$_2$/graphene, and S on top of a tetrahedral site (ST$_4$) for MoS$_2$/silicene, as presented in Figure 2. For the case of LDA functional, they are and S on top of B (ST$_{TB}$) for MoS$_2$/BN, S on top (ST) for MoS$_2$/graphene, and Mo on top of a tetrahedral site (MoT$_4$) for MoS$_2$/silicene. We find the average vertical distance ($h$) between MoS$_2$ and support is always lower in LDA approximation. The structural parameters of the heterostructures are summarized in Table 1.

| Length (Å)         | MoS$_2$/BN (vdW) | MoS$_2$/graphene (vdW) | MoS$_2$/silicene (vdW) | MoS$_2$/BN (LDA) | MoS$_2$/graphene (LDA) | MoS$_2$/silicene (LDA) |
|--------------------|-------------------|------------------------|------------------------|------------------|------------------------|------------------------|
| Mo-Mo              | 3.136             | 3.128                  | 3.286                  | 3.264            | 3.219                  | 3.174                  |
| Mo-S               | 2.406             | 2.412                  | 2.440                  | 2.439            | 2.425                  | 2.423                  |
| MoS$_2$/support ($h$) | 3.353             | 2.379                  | 3.373                  | 3.318            | 3.205,3.742            | 2.882,3.406            |
| B-N                | 1.448             | 1.445                  | -                      | -                | -                      | -                      |
| C-C                | -                 | -                      | 1.423                  | 1.413            | -                      | -                      |
| Si$_{up}$/Si$_{down}$ | -                 | -                      | -                      | -                | 2.294                  | 2.261                  |
| ΔZ                 | -                 | -                      | -                      | -                | 0.50-0.57              | 0.43-0.60              |

In order to compare the relative stability of our models configurations we calculated the binding energy (BE) per unit area of MoS$_2$ for each system, i.e., the difference between the energy of the relaxed heterostructure and that of relaxed single-layer components, divided by the number of unit areas of MoS$_2$, as summarized in the equation $BE = \frac{\left[ E_t - (E_s + E_i) \right]}{n}$, where $E_t$, $E_s$, and $E_i$ are the total energy of, respectively, the system, the support, and the isolated MoS$_2$ layer prior to adsorption, and $n$ is the number of unit cells of adsorbed MoS$_2$ layer in the considered supercell. Negative values of $BE$ indicate adsorption of MoS$_2$ on the substrate. For the considered heterostructures we find $BE$ (calculated using vdW functional) to be -160 meV per unit-cell of MoS$_2$ for MoS$_2$/BN, -120 meV for MoS$_2$/graphene, and -190 meV for MoS$_2$/silicene. The respective values calculated with LDA functional are -77, -79, and -142 meV. Both vdW and LDA approximations indicate that MoS$_2$ binds most strongly on silicene. Although the vertical distance between MoS$_2$ and support is always lower in LDA, the absolute value of binding energy is always larger in vdW case.
4. Electronic structure of heterostructures

Our calculated band structures for the three heterostructures considered here, together with that of simple layer MoS$_2$ (for comparison) are presented in Figure 3 for vdW case and in Figure 4 for LDA case. In agreement with previous findings [15, 20], single-layer MoS$_2$ is a direct band gap semiconductor, with a band gap $\sim$1.67 eV for vdW and $\sim$1.81 eV for LDA (this latter one coincides with the experimental optical gap) at the K point. It is important to mention that the calculated band gaps reported here are much smaller than that calculated using GW method [42] ($\sim$2.75 eV [43]) and that measured experimentally ($\sim$2.15 eV [5]).

![Figure 3. Calculated band structure in vdW case of (a) isolated single-layer MoS$_2$ (Blue dots correspond to Mo states, while magenta dots are sulfur states), (b) MoS$_2$-(4×4)/ BN-(5×5), (c) MoS$_2$-(3×3)/ graphene-(4×4), and (d) MoS$_2$-(6×6)/ silicene-(5×5). In (b), (c), and (d), blue and green dots show the contribution from MoS$_2$, and from support materials, respectively.](image)

![Figure 4. Calculated band structure in LDA case of (a) isolated single-layer MoS$_2$, (b) MoS$_2$-(4×4)/ BN-(5×5), (c) MoS$_2$-(3×3)/ graphene-(4×4), and (d) MoS$_2$-(6×6)/ silicene-(5×5).](image)

In order to understand the band structure of these systems it is useful to recall that when the periodicity of a supercell increases, the first Brillouin zone of the supercell diminishes in size, so that bands of the normal cell are folded into a smaller Brillouin zone. The first Brillouin zones of all films treated here have hexagonal geometry which allows us adopt the 3N-rule [44] to comprehend how $k$-points in the extended Brillouin zones can be folded into the primitive one: for $(3N\pm1) \times (3N\pm1)$ periodicities, K points of the primitive cell are folded to K points of the supercell’s Brillouin zone; for $(3N) \times (3N)$ periodicities, K points of the primitive cell are folded to $\Gamma$ point of the supercell.

Calculated band structure of the MoS$_2$/BN heterostructure with the vdW approximation (see Figure 3b) shows a direct gap of approximately 1.86 eV, 0.19 eV larger than that of an isolate single-layer MoS$_2$ (figure 3a) while that with LDA functional also indicates a direct band gap that is slightly (0.03 eV) larger than that of a single layer (see figure 4a, 4b). The difference in the band gap values can be traced to the artificial strain effect [45]. Apart from this, the band structures of each single layer components do not exhibit significant changes from its isolate ones.

Figure 3c and 4c show band structures of MoS$_2$ on graphene system calculated using vdW and LDA functionals, respectively. Since graphene is a zero-gap material, it introduces states inside the gap of the single-layer MoS$_2$ and the heterostructure is a semimetal. From these band structures calculated using vdW functional (figure 3c), it is clear that graphene is $p$-doped and MoS$_2$ is $n$-doped.
because the Dirac point of graphene aligns above the Fermi level while the bottom of conduction bands (BCB) of MoS$_2$ has occupation suggesting a charge transfer from graphene to MoS$_2$. In LDA case (figure 4c), the effect is not that pronounced. However, BCB of MoS$_2$ and the Dirac point of graphene are also alignment to Fermi level indicating a much smaller charge transfer than that in the case of vdW functional. It is also worth mentioning that results from both functionals do not show any gap-opening in graphene, in contradiction with results reported by Ma et al. [15], suggesting that the interaction between MoS$_2$ and graphene is not strong enough to break symmetry of graphene.

Figures 3d and 4d show band structures of MoS$_2$ on silicene system calculated using vdW and LDA functionals, respectively. As in the case of MoS$_2$/graphene, silicene introduces states inside the MoS$_2$ gap. Interestingly, there is a small gap opening at the Dirac point of silicene and the entire system turns out to be a semiconductor with a small gap of $\sim$50 meV for vdW, and 55 meV for LDA. The gap opening indicates that the interaction between MoS$_2$ and silicene is strong enough to break symmetry of silicene similar to what has been reported in by Li et al. [21]. This result is in good agreement with that from Gao et al. [46]. However, they found a gap of 70 meV for silicene/MoS$_2$ system. The difference can be mainly traced to the functional (DFT-D2) and the lattice mismatch of 2.42% and PBE-D functional used by Gao et al. [46] resulting in the stronger interaction between MoS$_2$ and silicene. The parameter $\Delta Z$ (which indicates the difference in height between Si-up and Si-down, see Figure 2) was 0.50 Å in vdW, and 0.44 Å in LDA for our relaxed cell of isolate silicene, while in relaxed MoS$_2$/silicene heterostructure $\Delta Z$ has several values distributed in the range 0.50-0.57 Å in vdW and 0.43-0.60 in LDA (as shown in the Table 1). These values imply that the LDA-calculated interactions between MoS$_2$ and silicene causes a stronger modification to silicene than vdW-calculated one does attesting once again that the silicene opening is larger in the LDA case.

Further insights into the band structure may be obtained from the electronic density of states (DOS), with information about the contribution of the orbitals of each species, through the projected density of states (PDOS). Because PDOS obtained by both approximations, vdW and LDA, are very similar, we only present the vdW results. Figure 5a shows the DOS of an isolated single-layer MoS$_2$: states on both sides of and near the band gap mainly have Mo-$d$ character, and a strong orbital mixing between S-$p$ and Mo-$d$ states can be appreciated (we have used our 4x4 supercell to compare with the MoS$_2$/BN system explicitly).

Figure 5b shows total DOS and various partial contributions (only orbitals with major contributions) for MoS$_2$/BN system. Not surprisingly, the shape of the DOS of an isolated single-layer MoS$_2$ (figure 5a) and of a MoS$_2$/BN heterostructure (figure 5b) are somewhat similar (in the range of energy shown). Additionally the top valence band (TVB) of h-BN is almost aligned with the TVB of MoS$_2$. Hence no electronic state is introduced in the gap of the single-layer MoS$_2$ and no occupied states of the BN appear until around of 4.7 eV. Comparing PDOS of S and Mo atoms in the single-layer MoS$_2$ and those in the MoS$_2$/BN system, we can appreciate their similarities, including the width of band gap and the majority Mo-$d$ character in the top of the valence bands and bottom of the conduction bands, indicating that the BN does not cause any significant effect on the electronic structure of MoS$_2$.

Figure 5c shows the electronic DOS of MoS$_2$/graphene system. The PDOS confirms that BCB of the single-layer MoS$_2$ are shifted towards the Fermi level of graphene (see figure 5c). The states inside of the MoS$_2$ gap come mainly from C-$p$ orbitals. The V-shape in the DOS of graphene remains intact after MoS$_2$ adsorption (see the inset in figure 5c). The shape of the total DOS above the Fermi level is not surprisingly determined mainly by Mo-$d$ orbitals. The artificial strain applied to single-layer MoS$_2$ when conjoined with graphene causes the valence-band maximum of MoS$_2$ to move to the $\Gamma$ point; thus MoS$_2$ behaves as an indirect semiconductor, with TVB and BCB in $\Gamma$ and K points respectively giving a gap of $\sim$1 eV in vdW, and $\sim$1.2 eV in LDA. The alignment of conduction bands of MoS$_2$ to Fermi level of graphene can be exploited for fabrication of phototransistors [47] or photovoltaic devices [48], in which electron-hole pairs are produced in MoS$_2$ by absorption of light, and electrons move to graphene, while holes are trapped in MoS$_2$. 
Examination of the PDOS in MoS$_2$/silicene system (Figure 5d) reveals that MoS$_2$ and Si states extend towards the middle of the original gap of the isolated single-layer MoS$_2$. At around -1.9, -1.6 and -1.1 eV it is possible observe a slight orbital mixing (hybridization) between MoS$_2$ and silicene, consequently we expect not only vdW interactions between layers in this system but also covalent bonds. The shape of the total DOS near the Fermi level is dominated by Si-$p$ orbitals. However, beyond this region the shape of total DOS is determinate mainly by Mo-$d$ orbitals.

Figure 6. Plots of 3D electron density difference ($\Delta \rho$), for (a) MoS$_2$/BN at the isosurface value of $2\times10^{-4}$ e/Å$^3$, (b) MoS$_2$/graphene at the isosurface value of $3\times10^{-4}$ e/Å$^3$, (c) MoS$_2$/silicene at the isosurface value of $5\times10^{-4}$ e/Å$^3$. The red (green) areas represent electron density increase (decrease).

Bader-charge analysis [49-51] for vdW case indicates no charge transfer from h-BN to MoS$_2$ or vice versa and about 0.01 and 0.04 electrons from graphene and silicene, respectively, to an unit cell of a single-layer MoS$_2$. Löwdin-charge analysis [52] in LDA case indicates that there is no charge transfer from graphene or BN to MoS$_2$ and 0.02 electrons from silicene to MoS$_2$, causing it n-doped. Heterostructure with silicene shows the greatest charge transfer. In order to investigate the density redistribution in our systems, and to confirm the nature of bonding between the single layers we calculated the electron density difference $\Delta \rho = \rho_T - \rho_{Sup} - \rho_{MoS_2}$; where $\rho_T$, $\rho_{Sup}$, $\rho_{MoS_2}$ are the electron density of the heterostructure, the support in question and the single layer of MoS$_2$, respectively. Figure 6 shows the 3D electron density difference plots for each system at different isosurface values. In MoS$_2$/BN and MoS$_2$/graphene heterostructures charge redistribution is observed. However, according to Bader and Löwdin-charge analysis, the charge transfer is very small, thus in these systems vdW interactions are dominant. In MoS$_2$/silicene significant density rearrangement in MoS$_2$ layer occurs. Furthermore there is an accumulation of charge in the interlayer region suggesting orbital overlap between layers. These results confirm that unlike the vdW-dominance in MoS$_2$/BN and MoS$_2$/graphene systems, in MoS$_2$/silicene system besides the vdW interactions weak covalent interactions exist.

5. Conclusions

Results of DFT calculations of the structural and electronic properties of a single-layer MoS$_2$ supported on single-layer of: h-BN, graphene or silicene show the DFT-vdW (optB88-vdW) and LDA approximations for the XC functional to lead to very similar conclusions. For the both functionals we find the total energy to be insensitive to the stacking order between layers. Of the three considered supports, h-BN is an excellent option to preserve the electronic structure of single-layer MoS$_2$ because
it leaves the band structure virtually the same as that of an isolated single-layer. On the other hand, graphene and silicene modify the electronic structure of MoS2 by introducing states into its band gap and causing it to become n-doped. We find that in MoS2/BN, single-layer MoS2 has a direct band gap whose value is somewhat modified because of the artificial strain in the system. The MoS2/graphene heterostructure is a semimetal, where bottom of conduction bands of MoS2 is shifted to the Fermi level. The expansion applied on MoS2 to match with graphene results in the indirect gap of MoS2. In MoS2/silicene, silicene introduces states inside the gap of isolated MoS2 and MoS2 states themselves are extended towards the middle of its original gap. The interaction between MoS2 and silicene opens a gap in silicene. Thus, the heterostructure has a direct band gap of ~0.05 eV at K point. Though small, ideally this gap is sufficient to prevent electronic transitions at low temperature. The analysis of binding energy, charge transfer, and electron density difference indicate that the interaction between a single-layer MoS2 and silicene includes weak covalent interactions and is stronger than that on BN or graphene.

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