First-Principles Study of the Contact Resistance at 2D Metal/2D Semiconductor Heterojunctions

Michel Houssa *, Ruishen Meng®, Valery Afanas’ev and André Stesmans

Department of Physics and Astronomy, University of Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium; ruishen.meng@kuleuven.be (R.M.); valeri.afanasiev@kuleuven.be (V.A.); andre.stesmans@kuleuven.be (A.S.)
* Correspondence: michel.houssa@kuleuven.be; Tel.: +32-16-327291

Received: 15 December 2019; Accepted: 7 February 2020; Published: 15 April 2020

Abstract: The high contact resistance at metal/two-dimensional (2D) semiconductor junctions is a major issue for the integration of 2D materials in nanoelectronic devices. We review here recent theoretical results on the contact resistance at lateral heterojunctions between graphene or 1T-MoS₂ with 2H-MoS₂ monolayers. The transport properties at these junctions are computed using density functional theory and the non-equilibrium Green’s function method. The contact resistance is found to strongly depend on the edge contact symmetry/termination at graphene/2H-MoS₂ contacts, varying between about $2 \times 10^2$ and $2 \times 10^4 \, \Omega \cdot \mu m$. This large variation is correlated to the presence or absence of dangling bond defects and/or polar bonds at the interface. On the other hand, the large computed contact resistance at pristine 1T/2H-MoS₂ junctions, in the range of $3–4 \times 10^4 \, \Omega \cdot \mu m$, is related to the large electron energy barrier (about 0.8 eV) at the interface. The functionalization of the metallic 1T-MoS₂ contact by various adsorbates is predicted to decrease the contact resistance by about two orders of magnitude, being very promising for device applications.

Keywords: 2D materials; density functional theory; non-equilibrium Green’s function method; electronic transport simulations; contact resistance

1. Introduction

Two-dimensional (2D) materials are currently attracting a lot of attention, both fundamentally and technologically [1–7]. Concerning their possible use in field-effect transistors, these materials would enable to scale the channel thickness down to the atomic level, resulting in an optimized electrostatic control of the devices. In addition, heterostructures based on 2D materials, formed by their van der Waals stacking or via the formation of 2D lateral heterojunctions, show promise for the realization of novel devices with unique electronic, optoelectronic or magnetic properties [8–13].

However, the high contact resistance ($R_cW$) in these 2D material-based devices is still a major issue [14,15]. Typical contact resistances at various metal/2D semiconductor interfaces are in the range of $10^3–10^5 \, \Omega \cdot \mu m$, severely limiting the device performances; $R_cW$ should be indeed reduced to about 100 $\Omega \cdot \mu m$ in field-effect devices [14]. Promising interfaces, based on lateral 2D metal/2D semiconductor heterojunctions, were realized recently [16–27]. Very interestingly, low $R_cW$ values, in the range of 100–200 $\Omega \cdot \mu m$, were reported at edge contacts formed between the metallic 1T-MoS₂ phase and the semiconducting 2H-MoS₂ phase [16,20].

We discuss here recent theoretical results on the contact resistance at lateral heterojunctions between graphene or 1T-MoS₂ with 2H-MoS₂ monolayers, obtained from first-principles simulations. The computed contact resistance at graphene/2H-MoS₂ junctions varies between $10^2$ and $10^4 \, \Omega \cdot \mu m$ and strongly depends on the edge contact symmetry (zigzag or armchair) and termination (Mo and/or S terminated); these results are correlated to the presence or absence of dangling bond defects and/or polar bonds at/near the interface. On the other hand, the contact resistance at pristine 1T/2H-MoS₂...
contacts weakly depends on the edge contact symmetry, and it is about \(3-4 \times 10^4 \Omega \mu \text{m}\), due to the large electron energy barrier at the interface. The functionalization of metallic 1T-MoS\(_2\), by various adsorbates, was found to decrease the contact resistance by about two orders of magnitude.

2. Computational Methods

The first-principles simulations of the 2D metal/semiconductor lateral heterostructures were performed using density functional theory (DFT), as implemented in the Siesta code [28], using the generalized gradient approximation (GGA) for the exchange-correlation functional [29]. Valence electrons were described using double-zeta polarized basis sets, while core electrons were described by norm-conserving pseudopotentials [30]. The slab models investigated in this work may include a net dipole moment, induced by defects or adsorbates on the surface; the calculations on such systems are performed by including self-consistent dipole corrections [31]. Long-range van der Waals forces were also included, using Grimme dispersion corrections [32].

The non-equilibrium Green’s function (NEGF) method was used for the ballistic transport simulations of the heterostructures, as implemented in the TranSiesta code [33], with single-zeta polarized basis sets [34–36]. The system was divided into three different parts, i.e., the left electrode, the central channel region, and the right electrode, as schematically pictured in Figure 1.

![Figure 1](image)

**Figure 1.** Schematic two terminal device used for the non-equilibrium Green’s function (NEGF) transport simulation. The electrochemical potentials of the left (\(\mu_1\)) and right (\(\mu_2\)) electrodes are shifted by \(qV\) when a bias \(V\) is applied to the structure. The self-energies \(\Gamma_1\) and \(\Gamma_2\) at the contacts are also indicated.

The ballistic current–voltage (I–V) characteristics are computed using the Landauer equation [37,38].

\[
I = \frac{2q}{h} \int \text{Trace} \left[ \Gamma_1 G^R \Gamma_2 G^A \right] \left( f_1(E) - f_2(E) \right) dE
\]

(1)

where \(q\) and \(h\) are the electron charge and Planck constant, respectively, \(G^R\) (\(G^A\)) is the retarded (advanced) Green’s function, and \(\Gamma_i\) and \(f_i\) are the self-energies and electronic distribution functions at the contacts, respectively.

The resistance \(R\) of the 2D metal/semiconductor heterojunction is obtained from the simulated current–voltage characteristics in the linear regime (\(R = V/I\)), as shown for a typical 1T/2H/1T-MoS\(_2\) structure in Figure 2a. The calculated resistance (multiplied by the contact width \(W\)) is shown in Figure 2b as a function of the channel length. The resistance presents an almost linear dependence on the channel length, as expected in the (quasi-) ballistic regime [39,40].

\[
R(L_{channel}) W = 2(R_c W) + R_{channel}(L_{channel}) W.
\]

(2)
b-charge carrier mobilities in graphene, in the
2

\[ \sigma \]

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range of \( 10^4 \text{–} 10^6 \text{ cm}^2/\text{Vs} \) [45–47].

\( \text{MoS}_2 \) is a member of the transition metal dichalcogenide family. Monolayer and few-layer \( \text{MoS}_2 \)
were investigated recently for their potential use in 2D material-based field-effect transistors and
photonic devices [48–51]. Each molybdenum atom is bonded to six sulfur atoms in \( \text{MoS}_2 \), with three S

The factor 2 in this equation accounts for the two 1T/2H interfaces in the two-terminal device. The
contact resistance \( R_{cw} \) is then obtained by extrapolating the resistance \( RW \) to the limit \( L_{\text{channel}} \to 0 \text{ nm} \).

3. Structural and Electronic Properties of Graphene and \( \text{MoS}_2 \)

Before discussing the contact resistance at 2D metal/semiconductor interfaces, we briefly present
the structural and electronic properties of graphene and \( \text{MoS}_2 \). Graphene consists of a single (flat)
layer of carbon atoms, arranged in a hexagonal network, as shown in Figure 3a [41–44]. The C atoms
are \( sp^2 \)-hybridized in graphene, forming two single bonds (\( \sigma \)) and one double bond (\( \sigma \) and \( \pi \)) with
their first neighbors. The computed lattice parameter of graphene, using DFT-GGA simulations, is
about 2.47 Å [3], typically 0.4% larger than the experimental one, i.e., 2.46 Å [43,44].

![Figure 3. (a) Top view of the atomic configuration of graphene. (b) Computed electronic band structure of graphene. The Fermi level corresponds to the reference (zero energy) level.](image)

The computed electronic band structure of graphene is shown in Figure 3b. The characteristic
linear energy dispersion near the Fermi level is clearly observed, forming a so-called Dirac cone; the
valence band (corresponding to \( \pi \) orbitals) and the conduction band (corresponding to \( \pi^* \) orbitals)
touch at the Fermi level \( E_F \), resulting in a zero density of states at \( E_F \). For this reason, graphene is
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atoms above and three below, in a trigonal prismatic or octahedral structure, forming a three-layered atomic sheet [52] (see Figure 4a). In bulk MoS\textsubscript{2}, these sheets are “bonded” via weak Van der Waals forces. In its most stable form, bulk MoS\textsubscript{2} crystallizes in the 2H (trigonal prismatic) phase, with a lattice parameter of 3.16 Å; the computed lattice parameter, using DFT-GGA simulations, is about 3.17 Å [3]. Bulk 2H-MoS\textsubscript{2} is an indirect semiconductor, with an energy band-gap of about 1.2 eV. The band-gap of MoS\textsubscript{2} increases when the number of layers decreases, becoming a direct band-gap semiconductor at the limit of a MoS\textsubscript{2} single layer [53,54], with a computed DFT-GGA band-gap of about 1.8 eV [3], as shown in Figure 4b. Depending on the growth conditions and/or on the chemical treatment [17,55], 2H-MoS\textsubscript{2} can be transformed to the meta-stable 1T-MoS\textsubscript{2} phase. This octahedral phase has a computed lattice parameter of 3.15 Å, and it is metallic [3,56–58], as shown in Figure 4c.

![Figure 4](image_url)

**Figure 4.** (a) Schematic representations of 2H, 3R, and 1T phases of transition metal dichalcogenides. (b) Computed electronic band structure of a 2H-MoS\textsubscript{2} monolayer. The reference energy level corresponds to the valence band edge. (c) Computed electronic band structure of a 1T-MoS\textsubscript{2} monolayer. The reference energy level corresponds to the Fermi level.

4. **Graphene/2H-MoS\textsubscript{2} Edge Contacts**

We considered four different graphene/monolayer 2H-MoS\textsubscript{2} slab models, with various edge contact symmetries and/or terminations, as shown in Figure 5 [59]. Large supercells (with about 250 atoms) were used for the DFT simulations, to minimize the strain in the graphene and MoS\textsubscript{2} layers (which is typically below 1.5% in both materials). The zigzag and armchair interface models were built by using (36.5 × 19.4) Å\textsuperscript{2} and (36.8 × 16.8) Å\textsuperscript{2} rectangular supercells, respectively. A vacuum layer of about 20 Å was considered for each interface models, to avoid spurious interactions between adjacent cells. Model 1 was based on an armchair–edge interface, with a single graphene layer. After
relaxation, carbon–sulfur (2.14 Å average bond length) and carbon–molybdenum (1.83 Å average bond length) bonds were present at this interface, as well as sulfur dangling bonds (from the bottom sulfur sublayer). A graphene bilayer was considered in model 2, in order to saturate these dangling bonds by the formation of C–S bonds. Model 3 was based on a zigzag–edge interface, terminated by Mo atoms, where C–Mo bonds (2.13 Å average bond length) were only present after relaxation, resulting in a “defect-free” contact model. A sulfur-terminated zigzag edge contact was considered in Model 4. In this case, only C–S bonds (1.79 Å average bond length) were formed, but S dangling bonds were present in the bottom sulfur sublayer.

The computed interface formation energies of the slab models are shown in Table 1. The formation energy \( \gamma \) of the graphene/MoS\(_2\) interface is calculated using the following equation [24,60]:

\[
\gamma = \frac{1}{2L} \left( E_{\text{total}} - \sum_{i} n_{i} \mu_{i} - n_{\text{MO}} \mu_{\text{MoS}_2} - \Delta n_{S} \mu_{S} \right),
\]

where \( L \) is the interface length, \( E_{\text{total}} \) is the total energy of the graphene/MoS\(_2\)/graphene system, \( n_{i} \) and \( \mu_{i} \) are the number of atoms and their chemical potentials, respectively, \( \mu_{\text{MoS}_2} \) is the total energy of a MoS\(_2\) (single layer) unit cell, and \( \Delta n_{S} = n_{S} - 2n_{\text{Mo}} \). The chemical potential \( \mu_{\text{Mo}} \) was fixed to that of body-centered cubic Mo, while \( \mu_{S} = \frac{1}{2} (\mu_{\text{MoS}_2} - \mu_{\text{Mo}}) \) in the Mo-rich limit, and \( \mu_{S} = \mu_{S}^{\text{bulk}} \) in the S-rich limit, where \( \mu_{S}^{\text{bulk}} \) corresponds to the sulfur chemical potential of a S\(_8\) ring [24].

The computed interface formation energies of the slab models are shown in Table 1. The Mo-terminated zigzag interface model (model 3 in Figure 5) was the most stable one, in the molybdenum-rich limit. On the other hand, the armchair interface model, with a bilayer graphene layer, had the lowest \( \gamma \) in the sulfur-rich limit. Note that the Mo and S-terminated zigzag edge contacts,
with a graphene monolayer (model 3 and 4), also had comparable interface formation energies in the S-rich limit, with both interfaces likely produced during such a growth process.

Table 1. Computed interface formation energies $\gamma$ of the different graphene/MoS$_2$ interface models shown in Figure 5, in the Mo-rich and S-rich limit, respectively. The value of the computed contact resistance $R_{cW}$ of each interface model is also given.

| Interface Model | $\gamma$ (eV/Å) Mo-Rich Limit | $\gamma$ (eV/Å) S-Rich Limit | $R_{cW}$ (Ω·µm) |
|-----------------|-------------------------------|-------------------------------|------------------|
| Model 1         | 2.4                           | 2.4                           | $8.1 \times 10^3$ |
| Model 2         | 1.5                           | 1.5                           | $5.6 \times 10^2$ |
| Model 3         | 1.2                           | 1.8                           | $2.2 \times 10^2$ |
| Model 4         | 2.6                           | 1.9                           | $2.3 \times 10^4$ |

The computed $R_{cW}$ of the different edge-contact models is also shown in Table 1. The contact resistances for the “defect-free” interfaces (model 2 and 3) were typically between 220 and 560 Ω·µm. These values are comparable to those reported at graphene/metal edge contacts [61]. On the other hand, the $R_{cW}$ at interfaces with sulfur dangling bonds was about two orders of magnitude larger.

The transmission probabilities of the Mo and S terminated zigzag interface models are discussed below, in order to gain further insight into these results. The computed (zero-bias) transmission spectrum of the molybdenum-terminated zigzag interface model (model 3) is shown in Figure 6a. The onset of transmission is at about 0.1 eV from the Fermi level, a result which is in agreement with the energy barrier height $\Phi_B$ of about 0.1 eV, calculated from the electrostatic potential profile of the heterostructure [59], as well as from the graphene and MoS$_2$ contributions to the electronic density of states, shown in Figure 6b. Note that the computed graphene work function and MoS$_2$ electron affinity were about 4.4 eV and 4.2 eV, respectively, resulting in an “ideal” interface barrier of 0.2 eV. The barrier height at the Mo-terminated interface model was reduced by about 0.1 eV from the ideal value, due to the presence of polar C–Mo bonds (electrons transferred from Mo to C atoms), forming a dipole layer at the interface, as illustrated in Figure 7a. These C–Mo bonds significantly contributed to the electronic density of states near the Fermi level, as indicated from the isosurface charge density plot shown in the inset of Figure 6b. The resulting low energy barrier at the Mo-terminated zigzag interface led to a low $R_{cW}$ in the range of 200 Ω·µm.

![Figure 6](image-url) Figure 6. (a) Computed transmission spectrum (at zero bias) of a graphene/MoS$_2$ lateral heterostructure with Mo-terminated zigzag edge contacts (model 3 in Figure 5). The Fermi level corresponds to the reference (zero) energy. (b) Partial electronic density of states (PDOS) of graphene and MoS$_2$. The inset shows the isosurface charge density (0.01 e/Å$^3$) near the Fermi level. Adapted from Reference [59].
Figure 7. (a) Schematic energy band diagram of (a) Mo-terminated and (b) S-terminated zigzag edge graphene/MoS$_2$ interfaces.

The (zero-bias) transmission probability of the S-terminated zigzag interface model, with a large density of sulfur dangling bonds (model 4), is shown in Figure 8a. The onset of the transmission probability was at about 0.4 eV from the Fermi level at this interface, and the transmission was much reduced, in comparison to the molybdenum-terminated interface model. The energy barrier $\Phi_B$, extracted from the electrostatic potential profile [59] and the partial electronic density of states, shown in Figure 8b, was increased by about 0.3 eV at the S-terminated contact, due to the presence of S dangling bonds, which produced gap states at about 0.4–0.5 eV below the MoS$_2$ conduction band. The isosurface charge density (see the inset of Figure 8b) indicates that the sulfur dangling bonds significantly contributed to the electronic DOS near the Fermi level, which was pinned by these gap states, resulting in an interface barrier $\Phi_B$ of about 0.4 eV, as illustrated in Figure 7b. Consequently, the $R_cW$ was increased by about two orders of magnitude at this S-terminated zigzag interface, as compared to the Mo-terminated one.

Figure 8. (a) Computed transmission spectrum (at zero bias) of a graphene/MoS$_2$ lateral heterostructure with S-terminated zigzag edge contacts (model 4 in Figure 3). The Fermi level corresponds to the reference (zero) energy. (b) Partial electronic density of states (PDOS) of graphene and MoS$_2$. The inset shows the isosurface charge density ($0.01 \text{e/Å}^3$) near the Fermi level. Adapted from Reference [59].
5. T/2H MoS$_2$ Edge Contacts

We considered 1T/2H-MoS$_2$ heterostructures (also based on MoS$_2$ monolayers) with armchair or zigzag edges [62], as shown in Figure 9. The armchair-edge (198 atoms) and zigzag-edge (216 atoms) interface models were obtained by using (35 × 16.5) Å$^2$ and (34 × 19) Å$^2$ rectangular supercells, respectively, with a vacuum layer of 20 Å; the residual strain in the MoS$_2$ layers was typically less than 0.25%.

![Figure 9](image_url)

**Figure 9.** Top views of the relaxed atomic configurations of lateral 1T-MoS$_2$/2H-MoS$_2$ interface models with (a) armchair and (b) zigzag edge contacts. Blue and yellow spheres correspond to Mo and S atoms, respectively.

The relaxed 1T/2H-MoS$_2$ interface models, with armchair and zigzag edges, are shown in Figure 9a,b, respectively. Since the lattice parameters of 1T- and 2H-MoS$_2$ are almost identical, atomically sharp and defect-free interfaces were obtained, in agreement with previous DFT simulations [26].

The computed R$_c$W at the pristine 1T/2H-MoS$_2$ interfaces was about 3–4 × 10$^4$ Ω·μm for the armchair and zigzag edges (see Table 2). The high contact resistance was due to the large interface energy barrier (Φ$_B$ ≈ 0.8 eV), which corresponds to the difference between the computed work function of 1T-MoS$_2$ (Φ$_{m}$ ≈ 5 eV) and the computed electron affinity of 2H-MoS$_2$ (χ = 2248 4.2 eV), as schematically illustrated in Figure 10. The calculated interface barrier Φ$_B$ ≈ 0.8 eV is in very good agreement (Φ$_B$ = 0.82 eV) with other DFT simulations performed on similar 1T/2H-MoS$_2$ heterojunctions [26].

| Interface Model       | $R_c W$ (Ω·μm) | $E_{ads}$ (eV) | Electron Transfer to 1T-MoS$_2$ (e) |
|-----------------------|---------------|---------------|-----------------------------------|
| Pristine armchair contact   | 3.8 × 10$^4$       | /             | /                                 |
| Pristine zigzag contact    | 2.9 × 10$^4$       | /             | /                                 |
| H$_2$O-adsorbed contact   | 2.8 × 10$^2$       | −0.75         | 0.05                              |
| Li-adsorbed contact       | 1.9 × 10$^2$       | −1.46         | 0.18                              |
| H$_2$O-adsorbed contact   | 4.7 × 10$^2$       | −2.43         | 0.08                              |

Table 2. Computed contact resistance, adsorption energies $E_{ads}$ and electron transfer (Hirshfeld population analysis) of the different 1T/2H-MoS$_2$ interface models. The adsorption energies and charge transfer were computed for one adsorbed atom or molecule on a (4 × 4) 1T-MoS$_2$ supercell.
It should be pointed out that the calculated $R_\text{tot}W$ was about two orders of magnitude larger than experimental values reported on 1T-MoS$_2$/2H-MoS$_2$ edge contacts [16,20]. The discrepancy may be explained by assuming that 1T-MoS$_2$ has a lower effective work function, which could arise from its interaction with chemical species during the local semiconducting (2H) to metallic (1T) MoS$_2$ transformation. During device processing, 2H-MoS$_2$ is indeed exposed to $n$-butyllithium solutions, to induce its transformation to the 1T metallic phase [16,20,63]. During this chemical treatment, chemical species like H, Li, and/or H$_2$O could be adsorbed onto the 1T-MoS$_2$ surface. We, thus, investigated the effect of these adsorbates on the 1T-MoS$_2$ work function. An H atom was adsorbed onto 1T-MoS$_2$ by forming an S–H bond, with a bond length of 1.37 Å (see Figure 11a). On the other hand, Li was most favorably adsorbed onto of an Mo atom, with average Li–Mo distance of 3.07 Å, as indicated in Figure 11b, as in 2H-MoS$_2$ [64]. Interestingly, the formation of the more stable distorted 1T'-phase of MoS$_2$ [56] was promoted by the adsorption of H and Li, as indicated by the distorted Mo atoms forming “one-dimensional (1D) zigzag chains”, which are connected by red dashed lines in Figure 11a,b. We also studied the interaction between a sulfur vacancy and an H$_2$O molecule. An O–H group tended to fill the vacant site, with the O atom bonding to neighbor Mo atoms (2.22 Å average Mo–O bond length); this resulted in the local distortion of the 1T-MoS$_2$ lattice, as indicated in Figure 11c. A neighbor S–H bond was also formed, with a bond length of 1.38 Å.

The adsorption energies $E_{\text{ads}}$ of these atoms or molecules on 1T-MoS$_2$ are computed using the following equation:

$$E_{\text{ads}} = E_{\text{tot}}(\text{MoS}_2 + \text{adsorbate}) - E_{\text{tot}}(\text{MoS}_2) - E_{\text{tot}}(\text{adsorbate}),$$

(4)

where the last term, representing the total energy of the adsorbate, was fixed to $\frac{1}{2}E_{\text{tot}}($H$_2$) for H, $\frac{1}{2}E_{\text{tot}}($bulk-Li) for Li, and $E_{\text{tot}}($H$_2$O) for H$_2$O [62].

All the calculated adsorption energies were negative (see Table 2), indicating that these atoms/molecules were favorably adsorbed onto 1T-MoS$_2$. A partial electron transfer, from the adsorbate to 1T-MoS$_2$, also occurred, which led to its “$n$-type doping”. Consequently, the adsorption of all these chemical species led to the reduction of the 1T-MoS$_2$ work function; an almost linear decrease of $\Phi_m$ was indeed computed for all the adsorbates considered here [62]. In fact, as shown in Figure 12, the work function shift $\Delta\Phi_m$ depended almost linearly on the partial charge transferred between the adsorbate and 1T-MoS$_2$. 
Figure 11. Side views of the relaxed atomic configurations of 1T-MoS$_2$ surfaces with different adsorbates: (a) H atom, (b) Li atom, and (c) H$_2$O molecule, interacting with a sulfur vacancy [62].

Figure 12. Computed work function shift $\Delta \Phi_m$ as a function of the charge transferred to the 1T-MoS$_2$ layer (calculated as the product of the adsorbate coverage and partial charge transferred to 1T-MoS$_2$ from Table 2) [62]. The dashed line guides the eye.

The impact of these adsorbates on the contact resistance of 1T/2H-MoS$_2$ heterojunctions is highlighted in Table 2. The adsorbate coverages were fixed to 8% Li, 12% H$_2$O, and 22% H; such coverages are consistent with experimental values obtained during the functionalization of transition-metal dichalcogenide monolayers [65]. The corresponding 1T-MoS$_2$ work function was about 4.3 eV, resulting in an energy barrier at the 1T/2H-MoS$_2$ interface of about 0.1 eV. The functionalization of 1T-MoS$_2$ by the adsorbates subsequently resulted in the decrease of the contact resistance by more than two orders of magnitude (see Table 2), being comparable to the experimental values (100–200 Ω·μm) reported in References [16] and [20].

6. Concluding Remarks

The potential integration of 2D materials in nanoscale field-effect transistors will require the formation of metal/2D semiconductor contacts with contact resistances in the range of few hundreds of
First-principles simulations predict that the contact resistance of graphene/monolayer 2H-MoS$_2$ lateral heterostructures strongly depends on the edge contact symmetry and termination. A low contact resistance, in the range of 200 $\Omega \cdot \mu$m, was computed at Mo-terminated zigzag edges, due to the possible formation of a “defect-free” interface with a low electron energy barrier. However, the presence of a large density of sulfur dangling bonds at S-terminated (zigzag or armchair) edge contacts resulted in a larger electron energy barrier, with the contact resistance being increased by two orders of magnitude. Obtaining a low contact resistance at graphene/MoS$_2$ lateral heterostructures will, thus, critically depend on the control of the edge symmetry and/or termination.

Another promising 2D metal/2D semiconductor edge contact consists of 1T/2H-MoS$_2$ lateral heterostructures. Low contact resistances, in the range of 200 $\Omega \cdot \mu$m, were also predicted from first-principles simulations at such interfaces based on MoS$_2$ monolayers, resulting from the functionalization (electron doping) of the 1T-MoS$_2$ contact by various adsorbates (H, Li, H$_2$O), likely present during the transformation of the stable 2H-MoS$_2$ phase into the meta-stable 1T-MoS$_2$ polymorph. These simulations importantly highlight the beneficial effect of the functionalization of metallic 1T-MoS$_2$ in order to achieve low contact resistances in MoS$_2$-based nanoscale devices.

Author Contributions: DFT simulations, M.H. and R.M.; supervision and project administration, M.H., V.A., and A.S.; writing—review and editing, M.H., V.A., and A.S. All authors have read and agreed to the published version of the manuscript.

Funding: Part of this work was financially supported by the KU Leuven Research Funds (project C14/17/080), and by the European project “2DFun”, an ERA-NET project in the framework of the Graphene Flagship.

Acknowledgments: Fruitful discussions with G. Pourtois, M. Heyns, M. Caymax, and D. Lin (imec) are gratefully acknowledged.

Conflicts of Interest: The authors declare no conflicts of interest.

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