Contact Resistance at MoS₂-based 2D Metal/Semiconductor Lateral Heterojunctions

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The contact resistance at lateral 1T-MoS₂/2H-MoS₂ heterostructures is theoretically studied, using first-principles simulations based on density functional theory and the non-equilibrium Green's function method. The computed contact resistance lies between 30 and 40 kΩ μm and is weakly dependent on the contact edge symmetry (armchair or zigzag). These values are about two orders of magnitude larger than the experimental ones reported recently on MoS₂-based metal/semiconductor lateral heterojunctions. This discrepancy can be explained by considering the interaction of 1T-MoS₂ with various chemical species (H, Li or H₂O) present during the local transformation of semiconducting 2H-MoS₂ into metallic 1T-MoS₂. The functionalization of 1T-MoS₂ by these atoms or molecules results in the decrease of its workfunction, leading to contact resistances in the range of few hundreds Ω μm.

Keywords: 2D metal/semiconductor heterostructures, graphene, transition metal dichalcogenides, first-principles simulations, electronic transport properties.

1. Introduction

Two dimensional (2D) materials are currently triggering a lot of interest, due to their potential applications in future nanoelectronic devices.¹⁻⁵ These materials indeed offer the possibility to scale the channel thickness of field-effect transistors down to the atomic level, leading to an optimized electrostatic control of the charge carriers in these devices. The formation of 2D heterostructures, either by the van der Waals stacking of different 2D materials, or via the formation of 2D lateral heterojunctions, also pave the way to the fabrication of novel devices with unique electronic, optoelectronic or magnetic properties.⁶⁻¹¹

The contact resistance is a critical issue in these 2D materials-based devices. Typical contact resistances at various metal/2D semiconductor interfaces are in the range of 10^3 - $10^5 \text{ } \Omega \text{ } \mu\text{m}$ [12], severely limiting the device performances; for field-effect transistor applications, the contact resistance should be reduced to about $100 \text{ } \Omega \text{ } \mu\text{m}$.¹² Promising interfaces, with potentially much reduced contact resistances, consist in lateral 2D-metal/2D-semiconductor heterojunctions; such interfaces have been fabricated recently¹³⁻¹⁸ and also studied theoretically.¹⁹⁻²⁴ Very interestingly, low contact resistances, in the range of 100 - $200 \text{ } \Omega \text{ } \mu\text{m}$, have been recently reported at lateral heterostructures formed between the metallic 1T-MoS₂ (octahedral) phase and the semiconducting 2H-MoS₂ (trigonal prismatic) phase.^{13,17}

In this work, we have theoretically studied the contact resistance of 1T-MoS₂/2H-MoS₂ lateral heterostructures, using density functional theory (DFT) and the non-equilibrium Green's function method (NEGF). The computed contact resistance lies between 30 and $40 \text{ k}\Omega \text{ } \mu\text{m}$, and depends weakly on the edge contact symmetry (zigzag or armchair). These values are about two orders of magnitude larger than the experimental values reported in

ref. 13 and 17. This discrepancy can be explained by considering the interaction of 1T-MoS₂ with various atoms (H, Li) or molecules (H₂O) which are present during the local transformation of semiconducting 2H-MoS₂ into metallic 1T-MoS₂; ^{13,17,25} the adsorption of these species on 1T-MoS₂ leads to the lowering of the energy barrier at the 1T-MoS₂/2H-MoS₂ interface and reduces the contact resistance by about 2 orders of magnitudes. These results highlight the beneficial effect of the functionalization of metallic 1T-MoS₂, in order to achieve low contact resistances at MoS₂-based lateral heterojunctions.

2. Computational methods

The atomic relaxation and electronic structure calculations of the 1T-MoS₂/2H-MoS₂ interface models (shown in Fig. 1) are performed using DFT, as implemented in the Siesta package.²⁶ The generalized gradient approximation (GGA) is used for the exchange-correlation functional.²⁷ Core electrons are described by norm-conserving pseudopotentials²⁸ and valence electrons are described using double-zeta polarized basis sets. The energy cut-off is fixed to 300 Ry and a (2x2x1) and (15x15x1) Monkhorst-Pack k-point mesh is used for the structural relaxations and electronic structure calculations, respectively. The convergence threshold for the residual atomic forces is fixed to 0.01 eV/Å. The calculations are performed by including self-consistent dipole corrections, which are particularly important for computing the workfunction of slab models including a net dipole moment, induced e.g. by the presence of adsorbates on a surface.²⁹ Long-range van der Waals forces are also included, using Grimme semi-empirical dispersion corrections.³⁰ The ballistic transport simulations are performed using NEGF, as implemented in the TranSiesta package.³¹ Single-zeta polarized basis sets, which are commonly used for the transport simulations using Transiesta,^{31,32} were employed. Test calculations with larger

basis sets gave almost identical results. The system is separated into three different parts along the transport direction, namely the left electrode (1T-MoS₂), the central channel region (2H-MoS₂) and the right electrode (1T-MoS₂), as shown in Fig. 1. The ballistic current-voltage (I-V) characteristics are computed using the Landauer equation^{31,33,34}

$$I = \frac{2q}{h} \int \text{Trace}[\Gamma_1 G^R \Gamma_2 G^A] (f_1(E) - f_2(E)) dE \quad (1)$$

where q is the electron charge, h the Planck constant, G^R and G^A are the retarded and advanced Green's functions, Γ_1 and Γ_2 are the self-energies of the left and right contacts, respectively, and f_1 and f_2 are the distribution function of the left and right contacts, respectively. For the complex contour integration, ten points on the line part and thirty points along the arc part are used.

The resistance R of the 1T/2H MoS₂ heterostructure is extracted from the computed I-V curves in the linear regime ($R=V/I$), as shown in Fig. 2 (a) for a typical 1T/2H-MoS₂ heterostructure. The resistance (multiplied by the contact width W) is shown in Fig. 2 (b), for three different 2H-MoS₂ channel lengths (L_{channel}). The resistance shows a (weak) linear dependence on L_{channel} , as expected in the quasi-ballistic transport regime,^{35,36}

$$R(L_{\text{channel}}) W = 2(R_c W) + R_{\text{channel}}(L_{\text{channel}}) W \quad (2)$$

The factor two in equation (2) accounts for the two 1T/2H interfaces in the simulated structures (cf. Fig. 1). The contact resistance $R_c W$ is then extracted by extrapolating the resistance RW to the limit $L_{\text{channel}}=0$ nm.

3. Results and discussion

The calculated in-plane lattice parameters of monolayer 2H-MoS₂ and 1T-MoS₂ are $a=b=3.17$ Å and $a=b=3.15$ Å, respectively, in good agreement with previous DFT results.³⁷ The computed (direct) energy band gap of monolayer 2H-MoS₂ is about 1.7 eV, while the 1T-MoS₂ phase is predicted to be metallic. Lateral 1T-MoS₂/2H-MoS₂/1T-MoS₂ heterostructures, with armchair or zigzag edges, were built for the ballistic transport simulations. The armchair interface model (198 atoms) was formed by using a rectangular supercell with cell parameters $a=35$ Å and $b=16.5$ Å. The lengths of the 1T-MoS₂ contacts and 2H-MoS₂ channel are 9.5 Å and 16 Å, respectively, and the contact width is 16.5 Å. The zigzag interface model (216 atoms) was formed by using a rectangular supercell with $a=34$ Å and $b=19$ Å. The lengths of the 1T-MoS₂ contacts and 2H-MoS₂ channel are 9 Å and 16 Å, respectively, and the contact width is 19 Å. In both models, a vacuum layer of 20 Å was used, to avoid spurious interactions between adjacent supercells. The residual strain in the 2H-MoS₂ and 1T-MoS₂ layers is typically less than 0.25 %; such a low strain has a minimal impact on the electronic structure of the two MoS₂ polymorphs.

The relaxed 1T/2H-MoS₂ heterostructures with armchair and zigzag edge contacts, are shown in Fig. 1 (a) and (b), respectively. The atomic relaxation of the entire system was performed using the conjugate gradient method, with double-zeta polarized basis sets. Atomically sharp and defect free interfaces are obtained, due to the very good lattice matching between 1T-MoS₂ and 2H-MoS₂, in agreement with previous first-principles calculations.²³ The Mo-S bond length near the interface varies typically between 2.35 and 2.55 Å, corresponding to a bond length variation of about $\pm 4\%$, as compared to the Mo-S bond length in 2H-MoS₂ (2.42 Å) and 1T-MoS₂ (2.44 Å).

The computed contact resistances at the pristine 1T-MoS₂/2H-MoS₂ interfaces are shown in Fig. 2 (c). Note that the resistance is multiplied by the contact width W , such that the contact resistance is expressed in $\Omega \mu\text{m}$. $R_c W$ lies in the range of 30-40 $\text{k}\Omega \mu\text{m}$, and does not depend much on the edge symmetry. The high contact resistance can be explained by the large interface energy barrier ($\Phi_B \approx 0.8 \text{ eV}$), resulting from the difference between the calculated workfunction of 1T-MoS₂ ($\Phi_m \approx 5 \text{ eV}$) and the calculated electron affinity of 2H-MoS₂ ($\chi \approx 4.2 \text{ eV}$), as shown schematically in the energy band diagram presented in Fig. 3. Note that the workfunction of 1T-MoS₂ was calculated from the difference between the average value of the deformation potential in the vacuum region and the Fermi energy of the slab model.³⁸ The calculated interface barrier $\Phi_B \approx 0.8 \text{ eV}$ at the 1T/2H-MoS₂ interface is in excellent agreement ($\Phi_B = 0.82 \text{ eV}$) with previous DFT simulations.²³

The computed $R_c W$ is about 2 orders of magnitude larger than experimental values reported recently on 1T-MoS₂/2H-MoS₂ lateral heterostructures.^{13,17} This discrepancy can be explained by assuming that the workfunction of 1T-MoS₂ is much lower than 5 eV, possibly due to the interaction of MoS₂ with different chemical species during the local transformation of semiconducting 2H-MoS₂ into metallic 1T-MoS₂. As a matter of fact, during device processing, 2H-MoS₂ is exposed to n-butyllithium solutions to induce the transformation to the 1T metallic phase.^{13,17,25}

We suppose that during the n-butyllithium treatment and subsequent processing (such as washing in H₂O), chemical species like H, Li and/or H₂O could be adsorbed on the 1T-MoS₂ surface. Consequently, we have investigated the effect of these adsorbates on its workfunction. As shown in Fig. 4 (a), a H atom is adsorbed on the 1T-MoS₂ surface, by forming a S-H bond (1.37 Å bond length). Li is most favorably adsorbed on top of a Mo atom (with average Li-Mo distance of 3.07 Å), see Fig. 4(b), like in 2H-MoS₂.³⁹

Interestingly, the adsorption of H and Li on 1T-MoS₂ results in the formation of the more stable distorted 1T'-phase,⁴⁰ as indicated by the distorted Mo atoms forming "1D zigzag chains", which are connected by red dashed lines on the side views of the atomic structures in Fig. 4 (a) and (b). We have also considered the possible interaction of a H₂O molecule with a sulfur vacancy in 1T-MoS₂. In this case, an O-H group fills the vacant site, the O atom forming bonds with the neighbor Mo atoms (with average Mo-O bond length of 2.22 Å); this leads to a local distortion of the 1T-MoS₂ lattice near the O atom, as shown in Fig. 4 (c). A neighbor S-H bond (1.38 Å bond length) is also formed.

The adsorption energies E_{ads} of these various chemical species on 1T-MoS₂ were computed using the expression

$$E_{ads} = E_{tot}(MoS_2 + adsorbate) - E_{tot}(MoS_2) - E_{tot}(adsorbate) \quad (3)$$

where the first, second and last term represents the total energy of the 1T-MoS₂ surface with the adsorbate, the total energy of the 1T-MoS₂ surface, and the total energy of the adsorbate, respectively. For this last term, we used $\frac{1}{2}E_{tot}(H_2)$ for H, $\frac{1}{2}E_{tot}(\text{bulk-Li})$ for Li (considering its body-centered cubic lattice), and $E_{tot}(H_2O)$ for H₂O.

The calculated adsorption energies are compared in Table 1. The values are found to be negative, suggesting that all these species are favorably adsorbed on the 1T-MoS₂ surface. As also indicated in Table 1, partial electron transfer is taking place from the adsorbate to MoS₂, resulting in a "n-type doping" of the 2D material.

The change in the electrostatic potential of 1T-MoS₂ induced by the adsorption of H, Li, and H₂O is shown in Fig. 5 (a)-(c), respectively. An upward shift of the electrostatic potential induced by the adsorbates is clearly observed on these figures, indicating that the

workfunction of 1T-MoS₂ is decreased after the adsorption of these species. As shown in Fig. 5 (d)-(f), the workfunction shift $\Delta\Phi_m$ is almost a linear function of the adsorbate surface coverage; in fact, $\Delta\Phi_m$ depends almost linearly on the partial charge transferred from the adsorbate to the 1T-MoS₂ layer, as illustrated in Fig. 6.

The effect of these adsorbates on the contact resistance of 2H-MoS₂/1T-MoS₂ interfaces is shown in Fig. 2 (c). Armchair-edge contacts were considered, with the following adsorbate coverage on the 1T-MoS₂ electrodes: 8 % Li, 12% H₂O and 22% H; we point out that adsorbate coverages in the range of 10 to 25 % have been reported on the surface of functionalized transition metal dichalcogenide monolayers.⁴¹ The workfunction of 1T-MoS₂ is about 4.3 eV for these coverages, corresponding to an energy barrier at the 2H-MoS₂/1T-MoS₂ interface of about 0.1 eV. As shown in Fig. 2 (c), the contact resistance is reduced by more than 2 orders of magnitude at these “functionalized” 1T-MoS₂ contacts, being comparable to the experimental values ($R_c W \approx 100\text{-}200 \text{ } \Omega \text{ } \mu\text{m}$) reported in ref. 13 and 17.

4. Conclusions

The contact resistance at lateral 1T-MoS₂/2H-MoS₂ heterostructures has been computed using first-principles simulations, based on DFT and the NEGF method. The computed contact resistance at pristine interfaces lies between 30 and 40 k $\Omega \text{ } \mu\text{m}$, being almost independent of the contact edge symmetry. These high contact resistances arise from the large energy barrier (about 0.8 eV) at the 1T-MoS₂/2H-MoS₂ interface, and are typically two orders of magnitude larger than experimental values recently reported in the literature. The disagreement between the computed and experimental contact resistances can be explained by considering the interaction of 1T-MoS₂ with H, Li or H₂O, which are present

during the local transformation of semiconducting 2H-MoS₂ into metallic 1T-MoS₂. The functionalization of 1T-MoS₂ by these atoms or molecules results in contact resistances in the range of few hundreds $\Omega \mu\text{m}$. Such contact resistances are very promising for the fabrication of nanoscale MoS₂-based field effect devices.

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Table Caption

Table 1. Computed adsorption energies and electron transfer (Hirshfeld population analysis) of the different adsorbates on 1T-MoS₂. Both quantities were computed for one adsorbed atom or molecule on a (4x4) MoS₂ supercell.

Adsorbate	E _{ads} (eV)	Electron transfer to 1T-MoS ₂
H	-0.75	0.05 e
Li	-1.46	0.18 e
H ₂ O	-2.43	0.08 e

Figure 1. Top views of the relaxed atomic configurations of lateral 1T-MoS₂/2H-MoS₂/1T-MoS₂ interface models with (a) armchair and (b) zigzag edge contacts. Cyan and yellow spheres correspond to Mo and S atoms, respectively. The contact lengths (L_c), channel lengths (L_{channel}) and contact widths (W) are indicated in the figures. The 1T/2H-MoS₂ interfacial regions are highlighted by the red rectangles.

Figure 2. (a) Computed I-V characteristics of a 1T-MoS₂/2H-MoS₂/1T-MoS₂ heterostructure, with Li-doped 1T-MoS₂ contacts. The resistance R of the structure is extracted from a linear fit to the data (solid line), in the voltage range between 0.2 and 0.8 V. (b) Resistance (multiplied by the channel width W) of the same heterostructure, for three different 2H-MoS₂ channel lengths. The dashed line is a linear fit to the data. (c) Computed contact resistance $R_c W$ at different 1T-MoS₂/2H-MoS₂ interface models. The two edge contact symmetries shown in Fig. 1 were considered for the pristine interface models. For the 1T-MoS₂ electrodes with adsorbed chemical species, the surface coverage was fixed to 8 %, 12 %, and 22 % for Li, H₂O and H, respectively.

Figure 3. Schematic energy band diagram of a pristine 1T-MoS₂/2H-MoS₂ interface.

Figure 4. Top and side views of the relaxed atomic configurations of 1T-MoS₂ surfaces with different adsorbates: (a) a H atom, (b) a Li atom and (c) a H₂O molecule, interacting with a sulfur vacancy. Cyan, yellow, orange, gray and red spheres correspond to Mo, S, H, Li and O atoms, respectively.

Figure 5. Electrostatic potential of 1T-MoS₂ with (a) H atoms (surface coverage between 0 and 75%), (b) Li atoms (surface coverage between 0 and 25 %), and (c) H₂O molecules (surface coverage between 0 and 25 %) adsorbed on the surface. Calculated workfunction shift $\Delta\Phi_m$ of 1T-MoS₂ with H atoms (d), Li atoms (e) and H₂O molecules (f) adsorbed on the surface, as a function of the adsorbate surface coverage.

Figure. 6. Computed workfunction shift $\Delta\Phi_m$ as a function of the charge transferred to the 1T-MoS₂ layer (calculated as the product of the adsorbate coverage and partial charge transferred to 1T-MoS₂ from Table 1). Blue, green and red circles correspond to H, Li and H₂O adsorbed on 1T-MoS₂, respectively. The dashed line guides the eye.

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