

Engineering of n -type metal-TMD contacts via ferroelectric polarization: an *ab-initio* transport study

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Abstract—In this paper, we investigate by means of *ab-initio* quantum transport simulations the possibility of engineering top metal-monolayer transition metal dichalcogenide contacts by exploiting the polarization of ferroelectric oxides.

We show that the electrostatic doping induced in MoS₂ by a ferroelectric oxide can unpin the Fermi level at the metal-semiconductor interface, thus lowering the Schottky barrier height and effectively reducing the contact resistance to enable n -type ohmic contacts. Recent experimental evidence of a successful integration of TMDs on ferroelectric oxide supports the feasibility of the contact design option proposed in this paper.

Complete device simulations of MoS₂ FETs with engineered contacts suggest that these devices can attain very competitive drive current values.

Index Terms—*ab-initio*, NEGF, MoS₂, Contact Resistance

I. INTRODUCTION

The integration in CMOS technologies of transition metal dichalcogenides (TMDs) requires Ohmic contacts between metals and TMDs with a low contact resistance (R_C). However, even in defect-free metal-TMD interfaces, metal-induced gap states (MIGS) are responsible for Fermi level pinning [1]–[3], which results in large R_C values and a non-Ohmic behavior. As a consequence, the engineering of metal-TMD contacts is a topic of major interest for the leading semiconductor companies [4]–[8]. Following the experimental validation of the integration of TMDs on top of ferroelectric oxides [9]–[11], in this work we propose and explore an approach to engineer metal-MoS₂ contacts whereby MoS₂ is electrostatically doped by an underlying ferroelectric material. Thanks to the MoS₂ ability of accommodating free-electron densities up to several units in 10^{14} cm^{-2} [10], the proposed technique is found to be very effective for a metal-MoS₂ contact. Our analysis is based on Density Functional Theory (DFT) calculations for the influence of the ferroelectric polarization on the metal-MoS₂ vertical heterojunction (VHJ), and on *ab-initio* quantum transport simulations based on the Nonequilibrium Green's Functions (NEGF) formalism. The metal-MoS₂ VHJ is studied in terms of R_C and included in I-V simulations for MoS₂

nanoscale FETs, and by accounting also for the influence of Image Force Barrier Lowering (IFBL) effects [12], [13].

The paper proceeds as follows. Section II describes the material and geometrical parameters of the devices studied in this work and, moreover, it provides details about the *ab-initio* transport methodology used for our self-consistent NEGF simulations. Section III presents the results that we obtained for the contact resistance of an In-MoS₂ contact engineered by means of an underlying layer of ferroelectric Hafnium Zirconium Oxide (HZO). Section IV reports the simulated transfer characteristics of a MoS₂ FET with engineered In-MoS₂ contacts. Finally, in Section V we provide a few concluding remarks.

II. DEVICES AND SIMULATION METHODOLOGY

The n -type FET with engineered contacts simulated in this work is sketched in Fig. 1.

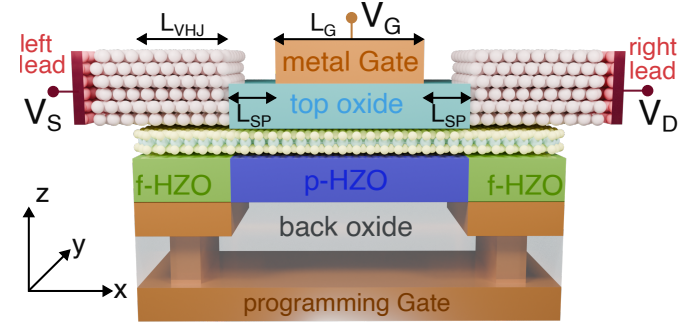


Fig. 1. Sketch of the simulated device, including the source and drain leads for the In-MoS₂ contact. The ferroelectric f-HZO is used to engineer the In-MoS₂ contact, while the p-HZO below the channel is paraelectric. The programming gate is used to set the ferroelectric polarization, which modulates the Schottky barrier height (SBH) and thus the contact resistance.

Indium (In) is used as the metal for the source and drain contacts, by virtue of its relatively low thermal energy for evaporation, and of the experimentally reported weak interaction with MoS₂, resulting in a van der Waals (vdW) type contact [10], [14]–[16]. Concerning the geometrical parameters, similarly to the design fabricated and discussed in [17],

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we set $L_G = 18$ nm, and $L_{SP} = 3$ nm for the gate and spacer lengths, respectively, and the EOT of the top gate oxide is 0.65 nm [18]. The bottom HZO oxide under the In-MoS₂ contact is ferroelectric (f-HZO), while the p-HZO below the channel is paraelectric. The coexistence of ferroelectric and paraelectric HZO phases has been experimentally demonstrated by engineering the metal-HZO contact, whereby the metal-induced in-plane stress favors a local formation of the ferroelectric HZO phase [19].

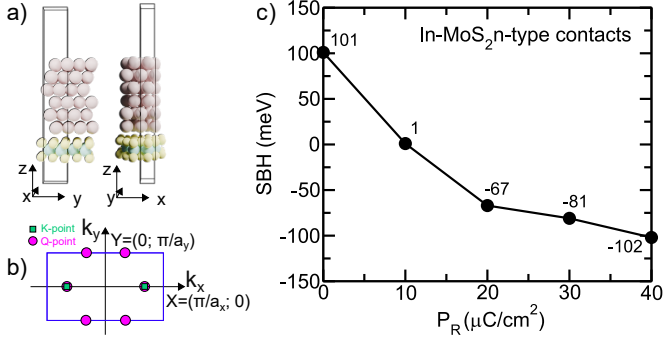


Fig. 2. (a) Side views of the orthorhombic In-MoS₂ supercell used for transport simulations. The distance between the top-most sulfur atoms and the lowest indium layer is $d=3.5$ Å. (b) Orthorhombic BZ and position of the high-symmetry points corresponding to K- and Q-valleys in the primitive cell of the MoS₂. (c) n -type Schottky barrier height (SBH) for the In-MoS₂ contact versus P_R of the underlying ferroelectric HZO (see Fig. 1) derived from DFT calculations of the supercell in plots (a),(b).

The first step of our simulation methodology consists of DFT calculations for the In-MoS₂ VHJ [see Fig. 2(a)], which were carried out by using Quantum ESPRESSO [20], and an orthorhombic unit cell necessary for subsequent transport simulations [see Fig. 2(b)]. The out-of-plane orientation of the six In layers is the (101), and it is consistent with reported XRD spectra of In deposited on bare silicon [15]. To have a commensurate lattice for In and MoS₂, which is indispensable for DFT calculations, we used a mean absolute strain of 3.3% in the In cell, so as to fit the unstrained MoS₂ cell. A 1.3 nm-thick vacuum region and dipole corrections have been employed to suppress spurious coupling with periodic replicas along the z -axis direction [20]. After relaxation, the extracted minimum energy interlayer distance (d) between In and MoS₂ is 3.0 Å, in agreement with [14], [16]. In the following of this work, however, we used $d=3.5$ Å to reduce the density of MIGS, namely a d value that is 0.5 Å larger than the calculated minimum energy distance. In actual devices, d is likely influenced by several factors, such as the orientation of the layers and the deposition technique [21]: the $d=3.5$ Å is consistent with experimental observations in systems using sacrificial interlayers during metal deposition [21]. Since DFT simulations have shown that even a strain of very few percent has a sizeable influence on the ferroelectricity of an HZO thin film [22], and given the prohibitive computational cost of the simulation of the entire In-MoS₂-HZO supercell, in our DFT calculations the HZO polarization was emulated by using a charged plate. As for the treatment of the HZO-MoS₂

interface, several experimental studies have reported very well-behaved $I_{DS} - V_{GS}$ curves for FeFETs employing an MoS₂ channel and a ferroelectric HZO or AlScN oxide [10], [11]. This is an evidence of weak orbital interactions and Fermi level-pinning in the HZO-MoS₂ system, which legitimates our simplified approach. The Hamiltonian matrices corresponding to DFT calculations were transformed from the plane-wave to a unit-cell restricted Bloch functions (URBF) basis set, and then used for electrical simulations by using the Green-Tea NEGF solver [23]. Our simulations also account for IFBL [12], [13], by using an effective, homogeneous permittivity $\epsilon_{\text{diel}} = 9.7\epsilon_0$ to describe the dielectric environment.

III. ENGINEERING OF R_C VIA HZO POLARIZATION

Figure 2(c) reports the DFT calculations for the Schottky barrier height (SBH) of the n -type In-MoS₂ contact versus the remnant polarization P_R of the underlying f-HZO layer (see Fig. 1). As it can be seen, the n -type SBH of about 100 meV observed at $P_R = 0$ can be essentially canceled by a P_R larger than $\approx 10 \mu\text{C}/\text{cm}^2$.

Figure 3(a) displays the spectrum $G(E)$ of the conductance of the n -type In-MoS₂ contact, which we defined and numerically calculated as

$$G(E) = \frac{n_{sp} q^2}{2\pi h} \int_{k_y} T_{k_y}(E) \left(-\frac{df_0}{dE} \right) dk_y, \quad (1)$$

where g_{sp} is the spin degeneracy, f_0 the Fermi-Dirac distribution and T_{k_y} the k_y -resolved transmission probability. The conductance spectrum is reported in Figure 3(a) for different P_R values, and it was obtained from ballistic NEGF simulations. Consistently with Fig. 2(c), a positive P_R can effectively reduce the SBH and vastly increase $G(E)$ for energies down to below the Fermi level E_F . Moreover, Fig. 3(b) shows that the inclusion in transport calculations of the IFBL can further reduce the SBH by some tens of meV, and thus correspondingly enhance $G(E)$.

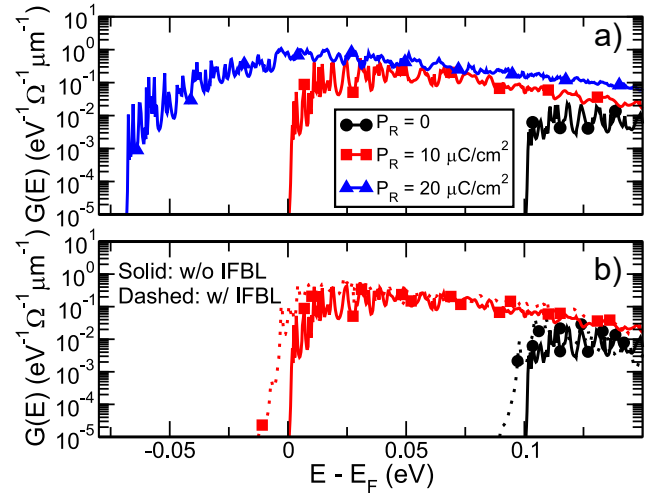


Fig. 3. (a) Ballistic conductance spectrum, $G(E)$, computed with *ab-initio* transport simulations (see Eq. 1) for In-MoS₂ n -type contacts and for different values $P_R = 0, 10, 20 \mu\text{C}/\text{cm}^2$ for the polarization of the underlying f-HZO layer. (b) Comparison of the $G(E)$ calculated either including IFBL (dotted) or neglecting IFBL (solid).

Figure 4 shows the R_C versus P_R curves for the n -type In-MoS₂ contact calculated by using the expressions

$$G_{k_y}(E) = \frac{g_{sp} q^2}{h} T_{k_y}(E) \left(-\frac{df_0}{dE} \right) \quad (2a)$$

$$\frac{1}{R_C} = \int_{-\infty}^{+\infty} G(E) dE = \frac{1}{2\pi} \int_{k_y} \left[\int_{-\infty}^{+\infty} G_{k_y}(E) dE \right] dk_y \quad (2b)$$

For a P_R around 20-30 $\mu\text{C}/\text{cm}^2$, which are typical P_R values for the f-HZO and other CMOS compatible ferroelectrics [9], [24], the ferroelectric-engineered In-MoS₂ contacts exhibit R_C values below 100 $\Omega\mu\text{m}$, which makes them compliant with IRDS specifications [25]. IFBL has a fairly small influence at large P_R and small SBH values, when the corresponding R_C is not far from the MoS₂ ballistic resistance (green dashed line).

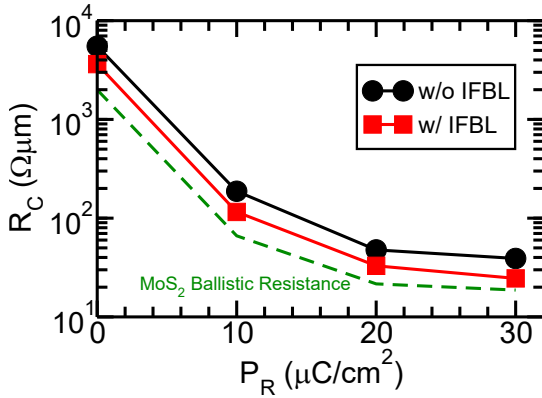


Fig. 4. Contact resistance versus the f-HZO polarization P_R for an n -type In-MoS₂ contact and calculated from Eqs.(2). Results are compared for ballistic transport and by either accounting for IFBL (red squares), or neglecting IFBL (black circles). The green dashed line shows the MoS₂ ballistic resistance.

IV. MoS₂ FETs WITH ENGINEERED CONTACTS

To go beyond the R_C analysis of Fig. 4, we simulated the I_{DS} curves of n -type FETs by self-consistently solving the NEGF equations and the Poisson problem for the electrostatics. Given the metallic nature of In, we did not solve the Poisson equation in the In-MoS₂ VHJ, and we simply set appropriate Dirichlet boundary conditions at the source and drain edges.

Figure 5 compares the ballistic $I_{DS}-V_{GS}$ for the n -type FET obtained either for engineered In-MoS₂ contacts (i.e. for $P_R=20 \mu\text{C}/\text{cm}^2$ in the underlying f-HZO, see Fig. 1) or for *non* engineered contacts (i.e. for $P_R=0$). Our results show that the ferroelectric-based contact engineering can vastly enlarge I_{DS} , consistently with the R_C improvements reported in Fig. 4(a). Qualitatively similar results have been experimentally reported for MoS₂ FeFETs with an AlScN ferroelectric [10], [26]. At $V_{GS}=0.6\text{V}$ and $V_{DS}=0.1\text{V}$, the inclusion of IFBL results in an increase of I_{DS} from $4\mu\text{A}/\mu\text{m}$ to $40\mu\text{A}/\mu\text{m}$ when $P_R=0$, and from $500\mu\text{A}/\mu\text{m}$ to $800\mu\text{A}/\mu\text{m}$ when $P_R=20 \mu\text{C}/\text{cm}^2$.

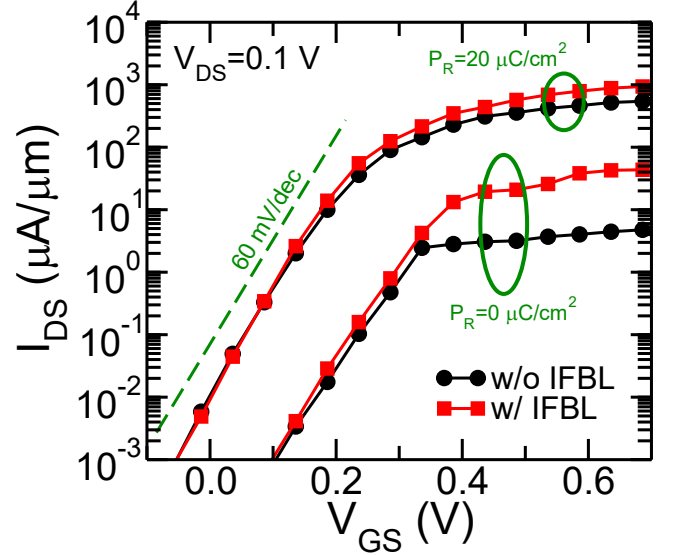


Fig. 5. Ballistic $I_{DS}-V_{GS}$ curves with IFBL (red squares) or without IFBL (black circles). The metal gate workfunction has been set to have $I_{OFF} = 10 \text{ nA}/\mu\text{m}$ at $V_{GS} = 0 \text{ V}$ (for the FET with engineered contacts), compliant with IRDS projections [25].

V. CONCLUSIONS

By using an in-house developed *ab-initio* quantum transport simulator, we proposed and validated a design option to engineer the contact resistance in top metal-TMD contacts exploiting the polarization of an underlying ferroelectric oxide.

Our results highlight how the adequate choice of P_R can turn an otherwise Schottky contact into a low R_C Ohmic contact. Full device simulations for n -type MoS₂ FETs, including image force barrier lowering, confirm the high quality of the optimized contacts.

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