Quantum Simulations of MoS_2 FETs Including Contact Effects

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2D materials have attracted considerable interest for applications in field-effect transistors (FETs) given their potential for high packing densities and excellent electrostatic control. Transition metal dichalcogenides (TMDs) have been extensively studied due to their promising electron transport properties down to monolayer thicknesses. MoS2 represents the most studied material in this class, with recent advances in its processing steadily bringing TMD-based technology closer to industrial applications [1]. One of the main challenges remains achieving low contact resistances due to Fermi level pinning at metal-TMD interfaces. Recently, the use of semimetals has been proposed to circumvent this issue. The combination of lower densities of states around the Fermi level and weaker interaction at semimetal-TMD interfaces results in contact resistances close to requirements for competing with Si technology [2]. The properties of semimetal-TMD interfaces have been studied using *ab-initio* simulations, providing insight into their electronic and charge transport characteristics [3]. However, such simulation frameworks are of limited use in device simulations due to their high computational cost. In this study we demonstrate a modelling approach that enables simulation of TMD-based devices with lengths of up to hundreds of nanometers with explicit descriptions of semimetal contacts.

In this work we simulate the electrical properties of field-effect transistors (FETs) based on monolayer (ML) MoS2 using a non-equilibrium Green's function (NEGF) solver [4]. Our approach enables computationally efficient simulations including quantum mechanical treatment of phonon scattering and electron tunneling phenomena. The electronic structure of Bi and ML-MoS2 are described by fitting atomistic simulations to continuum models based on k.p and the effective mass approximation. The properties of Bi/ML-MoS2 interfaces have been fitted to reproduce *ab-initio* simulations. Figure 1 illustrates simulated device geometries, where periodic boundary conditions have been applied along the width direction to simulate infinitely wide devices. Contact resistances have been extracted using the transmission line model. A back-gated architecture has been employed to emulate typical experimental setups for characterizing similar contact stacks.

Figure 2 shows the local density of states for a device in a state near its threshold voltage V_{TH}. Regions on either side of the channel explicitly describe source/drain junctions between semimetallic Bi and ML-MoS_2. Ohmic contacts between Bi and a metal are described via self-energies, as per the usual NEGF framework. Figure 3 shows the spectral current for the same state. As previously reported, inelastic phonon scattering is found to assist injection of carriers into ML-MoS2. Figure 4 shows the resistance across devices for gate lengths in the 20 nm – 50 nm range. A contact resistance of R_C=169 Ω.µm is extracted for a contact length L_C=10 nm and a channel carrier density of 10^{13} cm^{-2}, in good agreement with previous literature. Neglecting the effects of phonon scattering is found to increase contact resistance to R_C=390 Ω.µm, in excellent agreement with *ab-initio* simulations [3]. Figure 5 shows the contact resistance extracted for devices with varying contact lengths. R_C is

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observed to sharply increase for L_C < 15 nm, indicating a transfer length on the order of 10 nm. Figure 6 shows the transfer characteristics for a device with L_C=10 nm and L_{CH}=20 nm, where excellent switching characteristics are observed as the subthreshold swing remains at the thermodynamic limit.

The simulation framework presented here is capable of capturing physical phenomena relevant for reproducing the electrical characteristics of Bi/ML-MoS2 contacts reported in experimental studies. Its low computational cost allows simulating length scales well-beyond that of atomistic frameworks and can be used to derive insight into device operation, opening an avenue for device and contact engineering in 2D materials using efficient quantum simulations.

[1] B.-J. Chou et al., "High-performance monolayer MoS2 nanosheet GAA transistor," Nanotechnology, 2023. [2] P.-C. Shen et al., "Ultralow contact resistance between semimetal and monolayer semiconductors," Nature, 2021. [3] D. Lizzit et al., "Ab-initio transport simulations unveil the Schottky versus Tunneling barrier trade-off in metal-TMD contacts," IEDM, 2022. [4] *Q* Simulator*. (2024). EOLAS Designs. [Online]. Available: https://eolasdesigns.com/home/qstar/

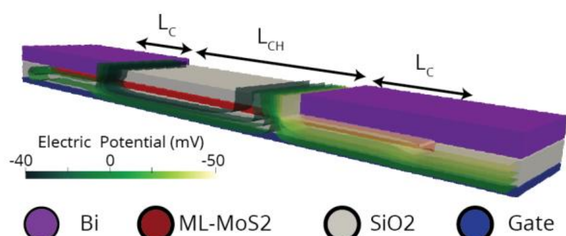

Figure 1: Simulated device geometry. L_C is the Bi/ML-MoS2 contact length, and L_{CH} the channel length. SiO2 thickness is 1 nm. Contour surfaces correspond to electric potential for V_{GS}≈V_{TH}.

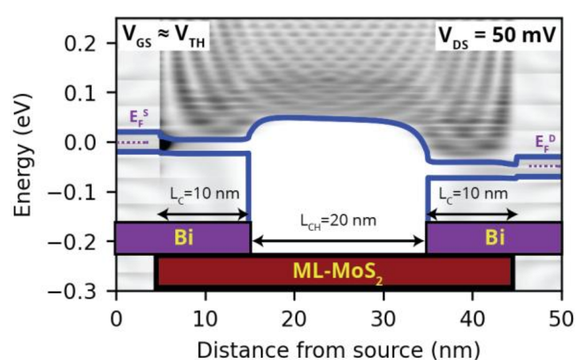

Figure 2: Local density of states. Coloured regions indicate active materials in each region.

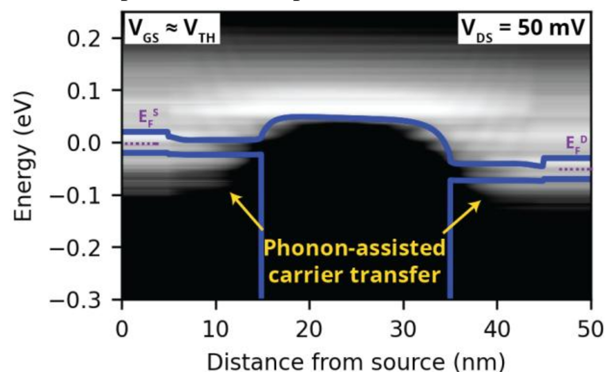

Figure 3: Spectral current. Brighter regions indicate higher current. L_C=10 nm and L_{CH} = 20 nm.

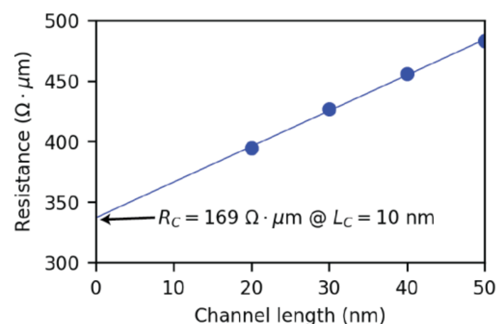

Figure 4: Contact resistance extracted using the transmission line model.

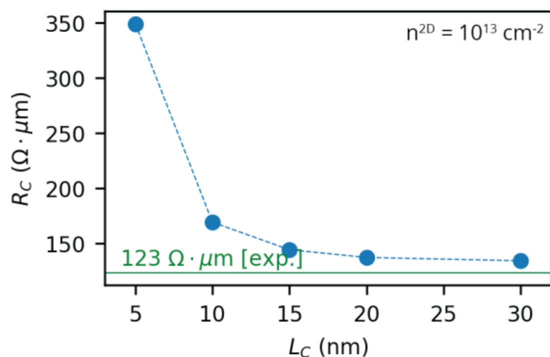

Figure 5: Contact resistance vs. contact length.

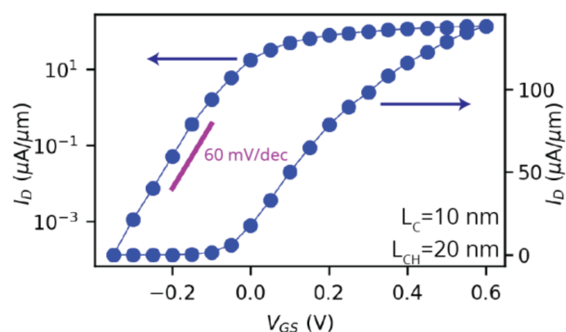

Figure 6: Device transfer characteristics.