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Impact of device scaling on the electrical properties of MoS₂ field-effect transistors

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I. Abstract

Two-dimensional semiconducting materials are considered as ideal candidates for ultimate device scaling. However, a systematic study on the performance and variability impact of scaling the different device dimensions is still lacking. Here we investigate the scaling behavior across 1300 devices fabricated on large-area grown MoS₂ material with channel length down to 30 nm, contact length down to 13 nm and capacitive effective oxide thickness (CET) down to 1.9 nm. These devices show best-in-class performance with transconductance of 185 μ S/ μ m and a minimum subthreshold swing (SS) of 86 mV/dec. We find that scaling the top-contact length has no impact on the contact resistance and electrostatics of three monolayers MoS₂ transistors, because edge injection is dominant. Further, we identify that SS degradation occurs at short channel length and can be mitigated by reducing the CET and lowering the Schottky barrier height. Finally, using a power performance area (PPA) analysis, we present a roadmap of material improvements to make 2D devices competitive with Silicon gate-all-around devices.

II. INTRODUCTION

CMOS technology has inadvertently followed Moore's law of device scaling for the past 50 years to achieve higher transistor density, higher speed and power improvements. A significant part of this device scaling, especially for the planar Metal-Oxide-Semiconductor-Field-Effect-Transistor (MOSFET) was achieved by scaling the gate length¹. This scaling is reaching its limits as short channel effects (SCE) significantly degrade the device performance. To partially overcome SCE, the tri-gate (FinFET) structure has been introduced². For future technology nodes, the gate-all-around nanosheet FET, which sandwiches thin layers of Silicon channel between multiple gates, is expected to provide additional improvements. Both configurations enhance the electrostatic control over the channel and allow for further gate length scaling. However, it has been reported³ that the required Silicon channel thickness scaling below 10 nm severely degrades the carrier mobility due to increased surface-roughness scattering. In this context, two-dimensional (2D) semiconducting materials such as transition metal-dichalcogenides (TMDs) are considered to be ideal candidates due to their naturally passivated surface and ultra-thin body (1 monolayer MoS₂ ~ 0.65 nm), providing excellent gate-control and enhanced transport^{4,5,6,7}. However, since many studies are performed with manually exfoliated flakes and collecting large datasets is very labor-intensive, there has been a strong focus on only selecting top performing devices, at the cost of less device understanding. Until recently, only a few TMD studies^{8,9,10} have focused on devices fabricated using large area grown films. Especially for device scaling¹¹, a statistically significant set of data is still lacking.

Therefore, we carry out a study of the impact of geometrical scaling on an extensive data set of large-area grown tri-layer MoS₂ MOSFETs (1300 devices). We investigate the impact of scaling the channel length (L_{ch}) and width (W_{ch}), contact length (L_{cont}) and effective oxide thickness (EOT) on various device performance metrics such as the on- and off-current (I_{on} , I_{off}), contact resistance (R_c), subthreshold swing (SS), interface trap density (D_{it}) and threshold voltage (V_T). We demonstrate that scaling the contact length down to 13 nm has no impact on the device performance. This confirms that carrier injection occurs exclusively from the edge of the metal directly into the thin TMD channel, which is in line with our TCAD simulations. Further, using our large data set, we make a detailed assessment on the scaling trends of SS and V_T with device dimensions. We identify the variation in the number of MoS₂ layers in the channel and contact regions as a possible source for SS

1 degradation and V_T variability for ultra-scaled TMD MOSFETs. Such insights are crucial for device
2 understanding and enables device architectures such as double-gate¹² or stacked TMD FETs to outperform Si
3 FETs¹³. This article is an extension of our previous work presented at IEDM 2019¹⁰.

4

5 **RESULTS AND DISCUSSION**

6 We employ large area MoS₂ grown on a 2" c-plane sapphire template by metal-organic chemical vapor
7 deposition (MOCVD) process using molybdenum hexacarbonyl and dihydrogen sulfide as the precursors.
8 Atomic force microscopy (AFM) shows the MoS₂ is composed of 3 monolayers (ML) fully closed and
9 continuous film, with nucleation of 4 ML and 5 ML island regions (Fig 1a). The average thickness is 3.6 ML,
10 measured using Rutherford backscattering spectrometry (RBS). The device schematic is illustrated in Fig 1b
11 and details of the fabrication process (Fig 1c) are discussed in the Methods section. Three different gate-oxides;
12 (1) 50 nm SiO₂ (2) 12 nm HfO₂, and (3) 4 nm HfO₂ are used. An optical image after contact deposition is shown
13 in Fig 1d and cross-section TEM images of the final fabricated device are shown in Fig 1e,f.

14 Direct current measurements are performed in N₂ ambient to avoid any impact of ambient humidity.
15 A total of 1300 devices with varying L_{ch} (30 nm to 5 μ m), L_{cont} (10 nm to 500 nm) and W_{ch} (200 nm to 10 μ m)
16 are measured at two different drain-source bias ($V_{DS} = 0.05$ V, 1 V). Back-gate leakage is low and below the
17 tool noise range (<1 pA) for the 50 nm SiO₂ and 12 nm HfO₂. Devices with 4 nm HfO₂ have higher gate-drain
18 leakage at $V_{DS} = 1$ V due to large contact pads. Therefore, the source current (I_S), instead of the drain current
19 (I_D), is used in their analysis. Channel edge effects are negligible, as confirmed by the constant on-state current
20 density for several W_{ch} (Fig. S1). Devices with short L_{ch}, wide W_{ch} and therefore high absolute current, show a
21 large parasitic voltage drop over the source-drain metal probes, and are therefore ~~are~~ omitted from the analysis.
22 The threshold voltage of the FETs for $V_{DS} = 0.05$ V, 1 V is obtained by both the linear extrapolation from peak-
23 transconductance ($V_{T,LE}$) and constant-current method ($V_{T,CC}$ extracted at $I_D = 10$ nA * W_{ch}/L_{ch}). SS is reported
24 either as SS_{min}, which is the minimum value across the entire swing, or as SS_{CC}, extracted at a current level of
25 $I_D = 1$ nA * W_{ch}/L_{ch} for the stated V_{DS} bias.

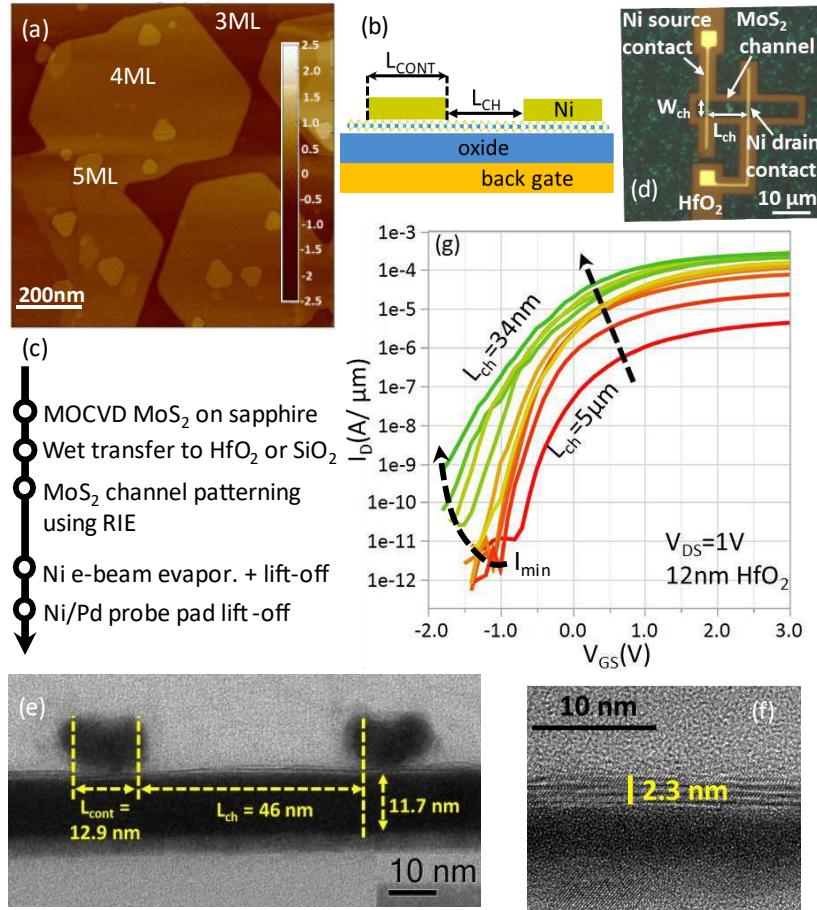


Fig 1. (a) Atomic force micrograph of CVD MoS₂ on sapphire template shows a closed 3ML layer with islands of 4 and 5 monolayers distributed randomly. (b) Device schematic with global back-gate and top source/drain contacts. (c) Fabrication flow for the back-gated devices. (d) Optical micrograph showing the patterned MoS₂ channel with 10 nm Ni contacts. (e) Cross-TEM shows a fabricated device with $L_{\text{cont}}=13$ nm and $L_{\text{ch}}=46$ nm on 12 nm HfO₂. (f) Zoom-in of the channel region for another device showing 3 monolayer MoS₂ on nominal 4 nm HfO₂ (g) Transfer characteristics at a fixed $V_{\text{DS}}=1$ V. Maximum drive current at $V_{\text{GS}}=3$ V scales with L_{ch} saturating for short-channel devices. The plot shows $L_{\text{ch}}=34$ nm, 44 nm, 50 nm, 70 nm, 100 nm, 200 nm, 300 nm, 500 nm, 1000 nm, 5000 nm.

I A. Scaling of on- and off-state currents

From the representative transfer characteristics in Fig 1g, we observe that the off-state current significantly increases as L_{ch} is scaled, as a result of a loss of gate control. Accordingly, we extract the minimum current in the entire back gate sweep (I_{min}), and we observe that it is the same for both oxides and lower than the noise floor of the tool (<1 pA). However, when comparing the I_{off} in the scatterplot Fig 2a, which is extracted at a fixed displacement field of 0.4 V/nm below $V_{\text{T,CC}}$, we note that the HfO₂ sample exhibits higher I_{off} compared to the SiO₂ sample. This suggests that the subthreshold swing is limited by the high interface trap density (see *Section D*). We also note that for both oxides, I_{off} degrades with smaller L_{ch} . This is mainly due to SS degradation observed for short L_{ch} devices, and will be further discussed in *Section E*.

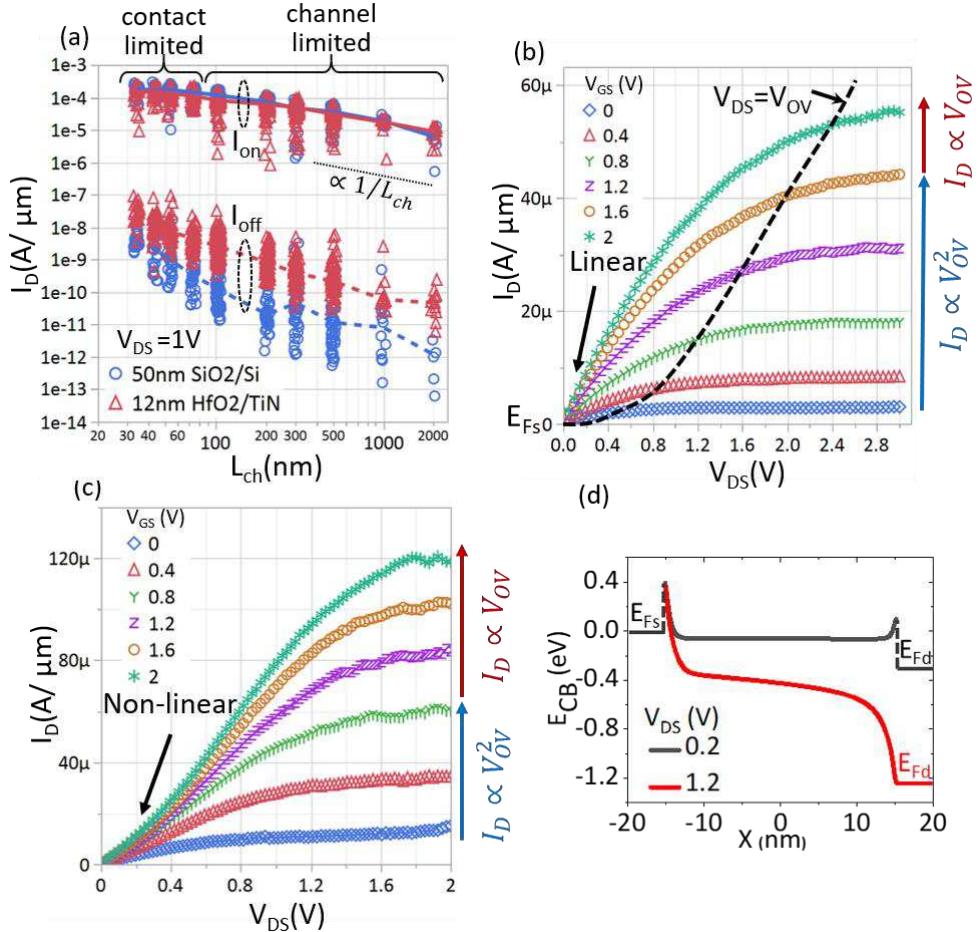


Fig 2. (a) Scatter plot (with median line) showing I_{on} extracted at $n_s = 1\text{e}13 \text{ cm}^{-2}$ and I_{off} at a fixed displacement field of 0.4 V/nm below $V_{T,CC}$ for $V_{DS} = 1$ V. I_{on} for the 50 nm SiO₂ and 12 nm HfO₂ devices overlap indicating no impact on low-field mobility and contact barrier. I_{on} roughly scales as $1/L_{ch}$ for $L_{ch} > 500$ nm and saturates for $L_{ch} < 50$ nm. I_{off} is higher for HfO₂ compared to SiO₂ due to high interface trap density. (b) I_D - V_{DS} for $L_{ch} = 500$ nm shows linear triode regime and saturation at high V_{DS} . The dashed line follows the current at $V_{DS} = V_{OV}$. While the onset of saturation follows the V_{OV} at low V_{GS} , it saturates at $V_{DS} = 2.4$ V for high V_{GS} . The saturation current roughly scales V_{OV}^2 and V_{OV}^1 , at low and high V_{GS} , respectively. (c) I_D - V_{DS} for $L_{ch} = 30$ nm shows non-linear triode regime due to Schottky contacts and saturation at high V_{DS} . Saturation current follows a similar trend as $L_{ch} = 500$ nm but V_{DS} at onset of velocity saturation is reduced to 1.4 V. (d) Conduction band profile for $L_{ch} = 30$ nm device with Schottky contacts shown for low and high V_{DS} . The Fermi-level at the source and drain are indicated by E_{FS} and E_{FD} , respectively. The Schottky barrier is shown as the abrupt potential change at the contact-channel interface. At low V_{DS} , I_D is determined by Schottky contacts. At high V_{DS} , though the potential drops significantly at the source contact, velocity saturation near the drain determines the I_D characteristics.

Next, we evaluate the I_{on} at a fixed charge density (n_s) of 10^{13} cm^{-2} and do not observe any difference between the 50 nm SiO₂ and 12 nm HfO₂ samples (Fig 2a). This indicates that the carrier transport in the MoS₂ channel is predominantly limited by charged impurities¹⁴ in the MoS₂ or at the interfaces, and not by remote phonons¹⁵ in the gate oxide.

For the I_{on} , two distinct channel length scaling regimes can be identified in Fig 2a. In the long-channel limit ($\sim L_{ch} > 500$ nm), the I_{on} increases roughly proportional to $1/L_{ch}$ and the device operates in the triode region

1 (illustrated in Fig 2b for the 12 nm HfO₂ sample and L_{ch} = 500 nm) i.e. gate-overdrive (V_{ov} = V_{GS} - V_T) > V_{DS}
2 for both oxides. The drain current also exhibits strongly linear dependence with V_{DS} in the triode region (Fig
3 2b), suggesting that the channel resistance is dominant for this L_{ch} and beyond. We also extract a low-field-
4 effect mobility of ~15 cm²/V.s (inset of Fig 3c) using the transfer length method (TLM) for both the samples
5 with 12 nm HfO₂ and 50 nm SiO₂. At higher lateral electric field (higher V_{DS}), I_D saturates (Fig 2b), and the
6 saturation current scales quadratically with V_{ov} (here V_{T,CC} = -0.4 V) due to channel pinch-off near the drain.
7 However, for the highest V_{ov} (~2 - 2.4 V), the saturation current scales roughly linear with V_{ov}, indicating that
8 it is limited by saturation of drift velocity at high lateral-field¹⁶ (F_{LATERAL} > 5 V/μm).

9 In the short-channel limit (~L_{ch} < 50 nm), the dependence of I_{on} on L_{ch} saturates (Fig 2a). Accordingly,
10 in the output characteristics for L_{ch} = 30 nm (Fig 2c), we make two observations; (1) super-linear I_D for V_{DS} <
11 0.4 V and (2) saturation of I_D for V_{DS} > 1.4V. The distinct super-linear dependence of I_D with V_{DS} (Fig 2c)
12 suggests that the Schottky contacts at the metal-MoS₂ interface limit the current even though the bias conditions
13 (V_{ov} > V_{DS}, here V_{T,CC} = -0.3V) ensure that the channel is continuously accumulated with electrons. At higher
14 V_{DS}, I_D saturates similarly to the L_{ch} = 500 nm device. The current at the onset of saturation is roughly
15 proportional to V_{ov}^{1.5-1.7} and V_{ov}^{0.8-0.9} for low and high V_{ov}, respectively, closely following the long-channel
16 characteristics. This indicates that while contact resistance dominates at low V_{DS}, velocity saturation near the
17 drain likely determines the current at high V_{DS}.

18 We can further understand both these observations from the simulated conduction band profile of
19 L_{ch} = 30 nm device (Fig 2d) for low and high V_{DS}. In the linear regime (V_{DS} = 0.2 V and V_{ov} > V_{DS}), the drain-
20 source potential is predominantly dropped across the reverse-biased source and forward-biased drain Schottky
21 contacts. With increasing V_{DS} (higher lateral field), the transmission probability across the Schottky contacts
22 increases rapidly, especially across the reverse-biased source, giving rise to the super-linear dependence of I_D
23 with V_{DS}. At even higher V_{DS} (V_{DS} = 1.2 V), the electric field in the channel near the drain is large enough that
24 the drift velocity saturates, which saturates the current.

25 B. Contact length scaling

26 Fig. 3a shows that I_{on} (@ n_s = 10¹³ cm⁻²) does not degrade as L_{cont} is scaled down to 13nm. This agrees
27 with TCAD simulations^{10,17,18} that predict contact edge injection of carriers for 1-3 layers of MoS₂ channel. This

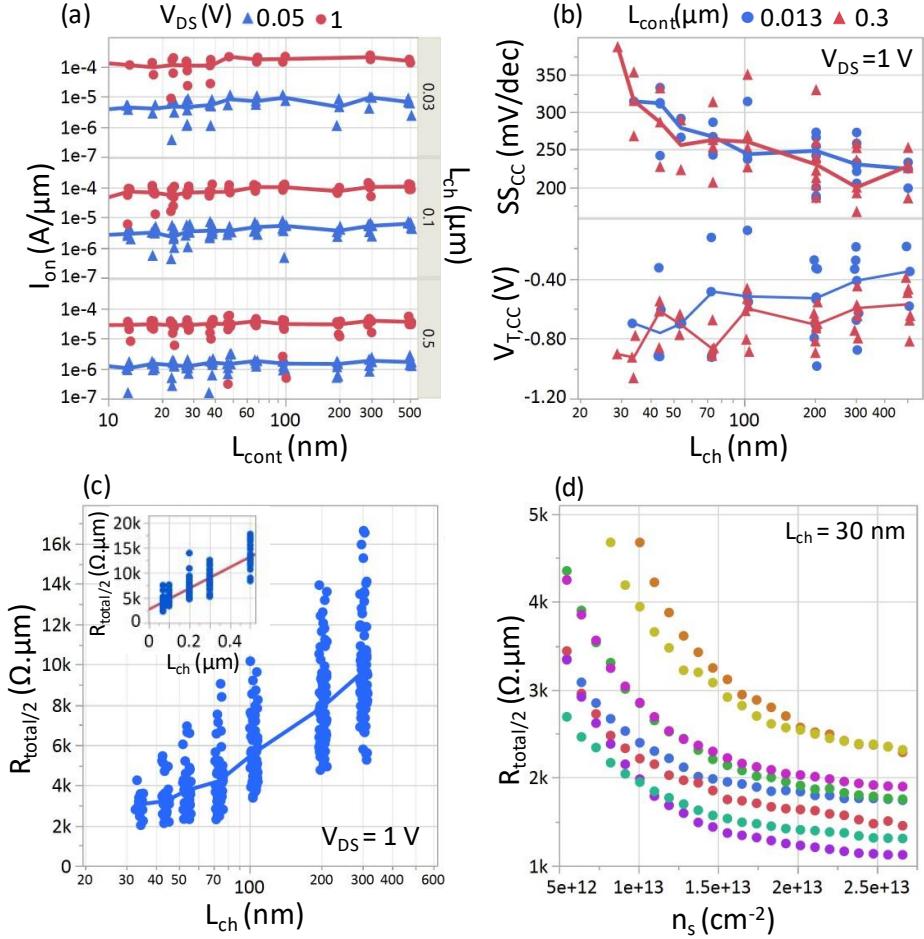


Fig 3. Scatter plot (with median line) of (a) I_{on} (at $n_s = 1 \times 10^{13} \text{ cm}^{-2}$) versus L_{cont} for $L_{\text{ch}} = 30 \text{ nm}$ (contact-limited), 100 nm (intermediate regime), and 500 nm (mobility limited). No dependence on L_{cont} down to 13 nm indicates carrier injection from the edge of the metal directly into the MoS₂ channel with $L_T < 13 \text{ nm}$. (b) SS_{CC} and $V_{T,\text{CC}}$ versus L_{ch} for $L_{\text{cont}} = 13 \text{ nm}$ and 300 nm. No systematic deviation with L_{cont} indicates identical electrostatics in both cases. (c) $R_{\text{total}/2}$ (at $n_s = 1 \times 10^{13} \text{ cm}^{-2}$) versus L_{ch} show saturation below $L_{\text{ch}} = 50 \text{ nm}$ due to contact resistance. Upper limit for R_C is obtained as median $R_{\text{total}/2}$ for $L_{\text{ch}} = 30 \text{ nm}$. Median R_C values of $3 \text{ k}\Omega.\mu\text{m}$ with best performers at $2 \text{ k}\Omega.\mu\text{m}$ are obtained. (inset) TLM fit of $R_{\text{total}/2}$ (at $n_s = 1 \times 10^{13} \text{ cm}^{-2}$) versus L_{ch} gives $R_C = 2.7 \text{ k}\Omega.\mu\text{m}$ and field-effect mobility = $15 \text{ cm}^2/\text{V.s}$ (d) $R_{\text{total}/2}$ versus n_s for $L_{\text{ch}} = 30 \text{ nm}$ at $V_{\text{DS}} = 1 \text{ V}$ of 8 devices. R_C significantly reduces at $n_s = 2 \times 10^{13} \text{ cm}^{-2}$ due to better carrier injection into the accumulated channel.

observation holds true for three different L_{ch} (30 nm, 100 nm, 500 nm) over a wide range of L_{cont} (500 nm to 13 nm) and for varying lateral field ($V_{\text{DS}} = 0.05 \text{ V}, 1 \text{ V}$). In all three cases, as predicted, we do not observe any systematic degradation of I_{on} by scaling down L_{cont} from 500 nm to 13 nm. Even for the shortest $L_{\text{ch}} = 30 \text{ nm}$, where the channel resistance is negligible and the device is Schottky contact limited (I_D-V_{DS} is super-linear at low V_{DS} in Fig 2c), the contact resistance is independent of L_{cont} . Moreover, the electrostatic properties of the device are also unaffected by scaling down L_{cont} as can be seen in Fig 3b from the trend of SS_{CC} and $V_{T,\text{CC}}$ (@ $V_{\text{DS}} = 1 \text{ V}$) with L_{ch} for two extreme contact lengths. The SS degradation and V_T roll-off with shorter L_{ch} , are independent of the contact length. The insensitivity to L_{cont} scaling also holds for other gate-oxides and charge

1 densities (plots not shown). In summary, for 3 ML MoS₂, the active region of MoS₂ under the metal contact
2 where most of the electrons get injected (called the transfer length L_T) is at least below 13 nm.

3 These results agree very well with our previous TCAD simulations. For thin MoS₂ (1-3 ML), these
4 predict L_T smaller than the minimum simulated L_{cont} of 2 nm (Fig. S2). This is caused by the Schottky barrier
5 (SB) at metal-MoS₂ interface, which depletes the MoS₂ underneath and prevents vertical electron injection.
6 Therefore, injection is only allowed from the edge of the metal contact directly into the carrier-rich channel,
7 which is also predicted in other work^{18,19}. For thicker MoS₂ (more than 5 ML), the MoS₂ region underneath the
8 contact is no longer depleted and a longer section of the contact contributes to carrier injection^{20,21,22}.

9 In other work^{21,23,24,25}, transfer lengths of 80 nm to 630 nm have been calculated using the transfer length
10 method (x-axis intercept), but those values are in contradiction with our results. As argued elsewhere²⁶, this
11 method should not be used for thin TMD layers and Schottky contacts. The Schottky barrier fully depletes the
12 TMD below, therefore the sheet resistance below the contact and in the channel are not the same, which is a
13 requirement of the transfer length method. However, the transfer length method can still be reliably used for
14 mobility calculation, because it does not have this requirement of identical TMD sheet resistance in the channel
15 and below the metal.

16 C. Contact resistance extraction

17 As we found in *Section A* that devices become more contact dominated as L_{ch} is scaled, we now take a
18 closer look at the value of the contact resistance. We extract the contact resistance (R_c) directly as half of the
19 total device resistance (R_{tot}/2) for devices with the shortest L_{ch} = 30 nm, without any need for extrapolation like
20 in the TLM method. By considering R_c ~ R_{tot}/2, an upper limit is obtained for R_c, as it assumes negligible
21 channel resistance. Fig 3c shows a plot of R_{tot}/2 at a charge density of 10¹³ cm⁻² vs L_{ch}. For L_{ch} < 50 nm, the
22 R_{tot}/2 saturates, and we obtain a median Nickel-MoS₂ R_c ~ 3 kΩ·μm (at n_s = 10¹³ cm⁻²), which is in good
23 agreement with R_c extracted using TLM (inset of Fig 3c). Our R_C values are comparable to the state-of-the-art
24 devices which have been demonstrated with Au²⁰ or Indium²⁷ contact metals. For increased V_{ov}, the contact
25 resistance further drops due to better carrier injection into the accumulated channel, and we obtain R_c ~ 1.2 - 2
26 kΩ·μm @ n_s = 2 x 10¹³ cm⁻² (Fig 3d). For even higher carrier densities (compare n_s = 2 x 10¹³ cm⁻² to 2.7 x 10¹³
27 cm⁻²), R_c no longer improves significantly. Significant device-to-device variation in contact resistance is

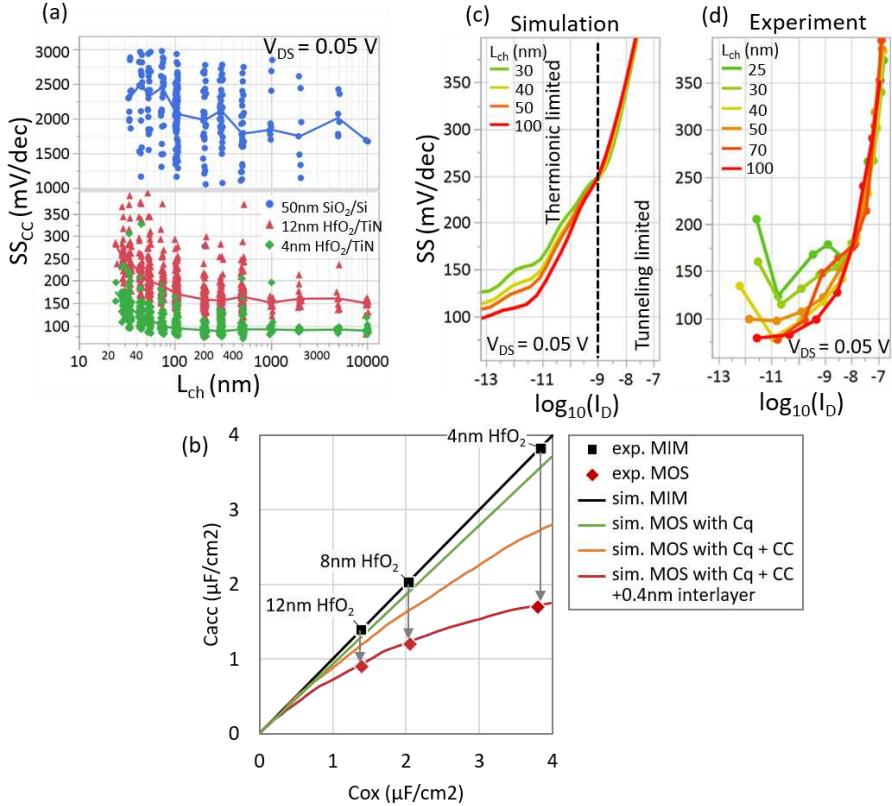


Fig 4. (a) Scatter plot (with median line) of SS_{CC} versus L_{ch} for the three different oxides. While SS improves with lower EOT, the degradation and scatter for short channel devices are attributed to electrostatic potential fluctuations caused by non-uniform thickness of MoS_2 in the contact and channel regions. (b) Experimentally measured maximum accumulation capacitance from MOScap (C_{max}) versus MIMcap capacitance (C_{ox}). Systematically, the C_{max} is lower than C_{ox} corresponding to an additional 1 nm CET over the measured EOT. Simulations show this is caused by the quantum capacitance C_q (MoS_2 having lower DOS than metal), the impact of the charge centroid (CC) further away in MOS than MIM, and additionally due to 0.4 nm of water or carbon residues stuck at the $\text{HfO}_2/\text{MoS}_2$ interface during transfer. Qualitative comparison between (c) simulated and (d) experimental SS versus $\log(I_D)$ for different L_{ch} . The simulated SS is for a uniform 3 monolayers MoS_2 with SBH = 0.45 eV. Two transport regimes at the contacts—thermionic emission and tunneling through the SB are identified. In the thermionic regime, the relative increase of field in the channel from the source/drain Schottky contacts degrades gate control for short L_{ch} devices. In the tunneling regime, the nearly equal tunneling lengths for the different L_{ch} results in a similar but degraded SS compared to the thermionic regime.

I observed, possible due to polymer residues between the contact metal and the MoS_2 , which were not completely removed after the transfer and contact lithography steps of the fabrication flow.

D. Long channel electrostatics and Dit extraction

Fig 4a shows that the subthreshold swing SS_{CC} obtained at $V_{DS} = 0.05$ V for different L_{ch} , improves with thinner back-gate oxide due to better gate control of the charge in the channel. Consequently, we achieve the best subthreshold swing for the devices on 4 nm HfO_2 substrate (Fig. S3) with median $SS_{min} = 90$ mV/dec and 110 mV/dec (at $V_{DS} = 0.05$ V) for $L_{ch} = 50$ nm and 30 nm, respectively.

In the long-channel limit i.e. $L_{ch} > 1 \mu\text{m}$, SS_{CC} saturates to a constant median value of 80 mV/dec, 150 mV/dec, 1800 mV/dec for 4 nm HfO₂, 12 nm HfO₂, and 50 nm SiO₂ respectively. This is determined by the charging of MoS₂/oxide interface and channel defects (60° grain boundaries²⁸, and point defects²⁹), for which we calculate a trap density ($D_{it,min}$) of $4.5 - 7 \times 10^{12} \text{ cm}^{-2}\text{eV}^{-1}$ from SS_{min} . We also confirm this D_{it} value using multi-frequency C-V measurements of TiN/HfO₂/MoS₂ MOScap³⁰, where we obtain an acceptor-type trap density of $3.2 - 6 \times 10^{12} \text{ cm}^{-2}\text{eV}^{-1}$ with energy levels near the midgap.

From C-V measurements, we find that the MOS capacitance is systematically lower than the target oxide capacitance due to exposure to water and/or atmospheric carbon during the wet transfer process from the sapphire template to the target substrates. Fig 4b shows how the maximum accumulation capacitance (C_{max}) measured from TiN/HfO₂/MoS₂ MOScap (shown as the red diamonds) is lower than the value of C_{ox} measured from TiN/HfO₂/TiN MIMcap (without MoS₂, shown as the black line). Equivalently, the capacitance equivalent oxide thickness (CET) values for MOScap (1.9 nm, 2.7 nm, and 3.8 nm) are systematically 1 nm higher than the EOT values of the MIMcaps (0.9 nm, 1.7 nm, and 2.6 nm). We calculate that the effect of quantum capacitance due to the limited density of states in MoS₂, and the effect of charge centroid being a few angstrom away from the interface, are insufficient to account for this 1 nm difference. As the MIMcaps are not exposed to water or polymer during the fabrication, Fig 4b shows the difference between the CET and EOT values can be explained by a 0.4nm thick layer of water or hydrocarbons adsorbed from the ambient, or a combination thereof. In the future, we expect dry transfer in a controlled ambient will lower the CET, closer to the nominal EOT.

E. Short channel electrostatic degradation and variability

In the short-channel limit, i.e. $L_{ch} < 100 \text{ nm}$, Fig 4a shows a degradation of median SS_{CC} but also increased scatter (SS_{CC} at $V_{DS} = 1 \text{ V}$ in Fig. S4). A similar trend is also seen for SS_{min} (Fig. S3). We hypothesize that the increased median and scatter could both be caused by the Schottky contacts, where the median SS degradation with shorter L_{ch} is related to the relative increase of depletion regions from the Schottky contacts, while the scatter could be due to the variation in Schottky barrier height³¹ (SBH) induced by the non-uniform thickness of the MoS₂, seen in the AFM image in Fig.1a.

We first verify the hypothesis of degraded median SS for shorter L_{ch} by comparing representative experimental SS versus I_D curves to simulations in Fig 4c. We consider full SS - I_D curves instead of extracting SS at a single current level to understand the injection mechanism in a wider operation range. The simulations are performed for a $SBH = 0.45$ eV and uniform 3 ML MoS₂ channel. We observe two different regimes for SS for both the simulated and experimental data. In the first low-current regime ($I_D < 1e-9$ A/ μ m), the current is limited by the thermionic emission of carriers from the metal into the channel. Here, the barrier for electrons consists of the highest position of conduction band edge inside the channel determined by the gate-bias. In this low-current regime, SS is determined by the change in the conduction band edge with gate-bias. As discussed in section D, the lower limit for SS (which corresponds to SS_{min} in fig.S3), is defined by the interface trap density. The degradation of SS_{min} for short- L_{ch} devices is due to the electrostatic potential of the source and drain metallurgical junctions influencing the channel potential and degrading the gate control. This is illustrated

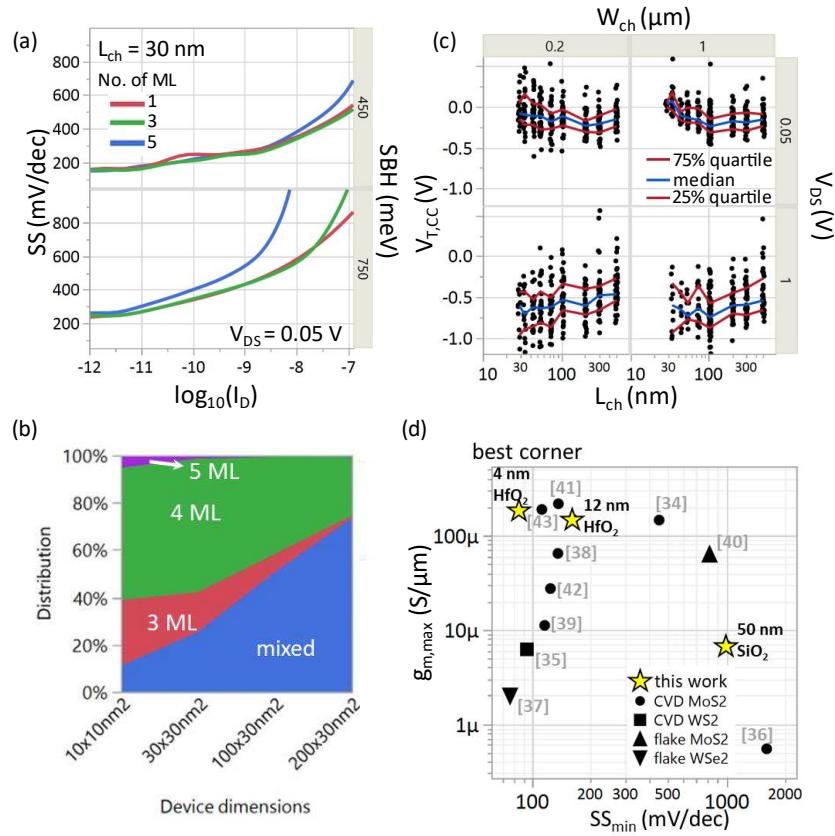


Fig 5. (a) Simulated SS versus $\log(I_D)$ for a uniform layer of 1, 3 and 5 monolayers of MoS₂ for SBH = 0.45 eV and 0.75 eV. For $I_D > 1e-9$ A/ μ m, tunneling through Schottky barrier determines the SS. Subsequently, a thinner channel results in better gate control, shorter tunneling length and therefore better SS. (b) Probability distribution versus device dimensions ($L_{ch} \times W_{ch}$). AFM from Fig 1a was used to compute the probability distribution for fabricating devices on only 3, 4, 5 or a combination of those (mixed). Our experimental devices have a 60-70% probability of being mixed, leading to non-uniform gate control across the channel and contact regions. (c) $V_{T,CC}$ versus L_{ch} for two different W_{ch} (200 nm, 1000 nm) and V_{DS} (0.05 V, 1 V). No V_T roll-off at $V_{DS} = 0.05$ V due to excellent gate control over the channel for 12 nm HfO₂. V_T roll-off of about 200 mV for $V_{DS} = 1$ V due to higher lateral-field at the source contact allowing for more carrier injection. No systematic V_T deviation between $W_{ch} = 1$ μ m and 200 nm. (c) Benchmark plot showing $g_{m,max}$ versus SS_{min} . All values are at $V_{DS} = 1$ V except [39] - $V_{DS} = 0.1$ V, [34] - $V_{DS} = 0.5$ V, [40] - $V_{DS} = 1.2$ V, [37] - $V_{DS} = 1.5$ V. In this work, 4 nm HfO₂ provides best SS = 86 mV/dec and $g_{m,max} = 185$ μ S/ μ m.

in Fig. S5 where the conduction band energy is flat over most of the device for $L_{ch} = 100$ nm, while it is lowered for $L_{ch} = 30$ nm with the region of maximum barrier reducing to a small portion near the center of the device. Note that this effect is similar to conventional MOSFETs. The second regime ($I_D > 1e-9$ A/ μ m) is reached when the conduction band in the channel is lowered further, and carriers can efficiently tunnel through the SB (Fig. S6). Here, the thermionic component over the barrier saturates and the tunneling path length determines the current. Because it continuously changes with higher V_g , the SS is worse than the first regime. Correspondingly, in the experimental devices, the SS_{CC} extracted at $I_D > 1e-8$ A/ μ m (for $L_{ch} < 100$ nm) shows a higher value than SS_{min} and stronger degradation with L_{ch} . The SS for a given I_D also becomes nearly independent of L_{ch} , because the tunneling path length depends

1 only on the gate voltage and the thicknesses and dielectric permittivities of the TMD³² and oxide, for the low
2 lateral electric field ($V_{DS} = 0.05$ V). This is illustrated in Fig. S6 where the conduction band energy and tunneling
3 rate are plotted along the edge carrier injection path for $L_{ch} = 30$ nm and 100 nm, showing no significant
4 difference. With further reduction in SBH, the SS value in the second regime improves, reaching closer to the
5 thermionic limit of the first regime.

6 We study the increased SS scatter for short L_{ch} seen experimentally, using simulations of devices with
7 different uniform MoS₂ channel thickness and SBH. Fig 5a shows the simulated SS value for two different SBH
8 (0.45 eV, 0.75 eV) and three different uniform thicknesses (1,3 and 5 layers) of MoS₂ for $L_{ch} = 30$ nm. Similar
9 to the above case, we note two different regimes for SS irrespective of the barrier height. For the first regime of
10 low I_D (< 1e-8 A/ μ m for SBH = 0.45 eV and < 1e-11 A/ μ m for SBH = 0.75 eV), the SS is determined only by
11 thermionic emission over the channel barrier. Therefore, the SS is independent on the channel thickness.
12 However, the SS degrades for SBH=0.75 eV compared to 0.45 eV, because the higher Schottky barrier field
13 penetrates deeper into the channel. For the second regime of high I_D (> 1e-8 A/ μ m for SBH = 0.45 eV and > 1e-
14 10 A/ μ m for SBH = 0.75 eV), the SS is dependent on the tunneling length which is sensitive to the thickness of
15 the semiconductor among other parameters³³. Subsequently, the gate control over the Schottky barrier, and
16 hence the tunneling length, reduces with thicker MoS₂, resulting in poor SS for the 5 ML MoS₂ (Fig. S7). In
17 agreement with this observation, we also note that the difference in SS between the layers is more pronounced
18 for the higher SBH of 0.75 eV.

19 In our experiments, we have even more variability due to non-uniform thickness within a single device.
20 Even for the smallest functional device footprint ($L_{ch} \sim 30$ nm * $W_{ch} \sim 200$ nm), we always have a high probability
21 (~70%) of having a mixed device i.e. regions of 3, 4 and 5 layers of MoS₂ within the same device. This is
22 illustrated in Fig 5b where the representative AFM (Fig 1a) image of the material was used to compute the
23 probability of fabricating devices with different dimensions on only 3 (or) 4 (or) 5 or a mix of those layers.
24 These mixed-thickness devices, together with the associated SBH variations, would result in non-uniform gate
25 control and large scatter in the SS values of experimental devices.

| **F. Threshold voltage control**

2 We analyse V_T control for decreasing channel length, and Fig 5c shows that there is no significant
3 median V_T roll-off at $V_{DS} = 0.05$ V. With a higher $V_{DS} = 1$ V, we notice a V_T roll-off of about 200 mV from L_{ch}
4 = 500 nm to 30 nm. We attribute this roll-off to the higher lateral electric field across the reverse-biased Schottky
5 contact, because V_{DS} is fixed at 1 V for all L_{ch} . This higher electric field allows for increased carrier injection
6 in short channel devices, which lowers V_T . This roll-off could be mitigated by improving the gate control
7 through gate-oxide scaling, or by reducing the amount of defects at the MoS_2 /oxide interface.

8 V_T control for decreasing channel width is also shown in Fig 5c, and no systematic impact is seen as
9 W_{ch} is scaled from 1 μm down to 200 nm. However, we note that there is an increased V_T variability for all L_{ch}
10 devices with $W_{ch} = 200$ nm compared to $W_{ch} = 1 \mu\text{m}$, especially at $V_{DS} = 0.05$ V. This increased V_T variability
11 could be attributed to the higher probability of finding devices on discrete layers (Fig 5b) for narrower channel
12 compared to a wider channel where the devices are always mixed. Other sources of variability such as bias-
13 temperature instability, non-uniformity of the MoS_2 grains etc. could also impact the V_T variability and more
14 dedicated experiments are required.

15

16 **IV. BENCHMARK, PROJECTION AND CONCLUSION**

17 We present a benchmark chart (Fig 5d) to compare the performance of our devices against flake and
18 CVD 2D material FETs in literature^{34,35,36,37,38,39,40,41,42,43}. We choose the peak of transconductance ($g_{m,\max}$)
19 measured at $V_{DS} = 1$ V and SS_{\min} as the two metrics for comparison, similar to conventional Si transistors. The
20 best corner is on the top-left since low SS_{\min} and high $g_{m,\max}$ are desired. Our SiO_2 devices, owing to the thick
21 EOT, provide low transconductance even for the shortest L_{ch} devices. Scaling the EOT (12 nm HfO_2 and 4 nm
22 HfO_2) and using an optimized process flow (see Methods), we gain both in transconductance and SS, achieving
23 a $R_c < 2 \text{ k}\Omega.\mu\text{m}$ for Ni contact metal and $D_{it} < 5 \times 10^{12} \text{ cm}^{-2}$ for a CET of 1.9 nm. We demonstrate the highest

1 $g_{m,\max} = 185 \mu\text{S}/\mu\text{m}$ at $V_{DS} = 1 \text{ V}$ and a minimum SS of 86 mV/dec for 4 nm HfO_2 . We also achieve $I_{\max} = 400$
 2 $\mu\text{A}/\mu\text{m}$ at $V_{DS} = 1 \text{ V}$ and $V_{GS} = 4 \text{ V}$ for our 12 nm HfO_2 samples (Fig. S8).

3

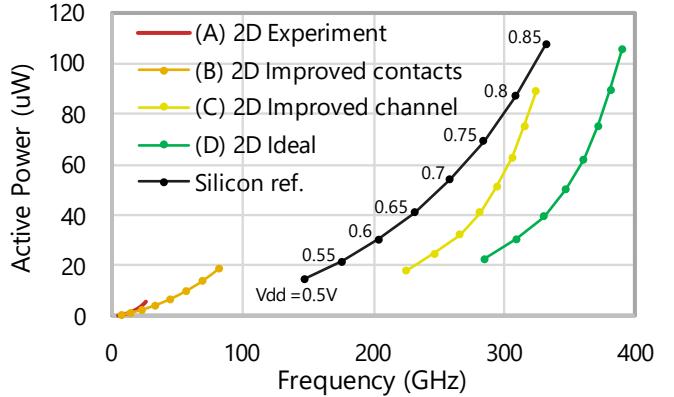
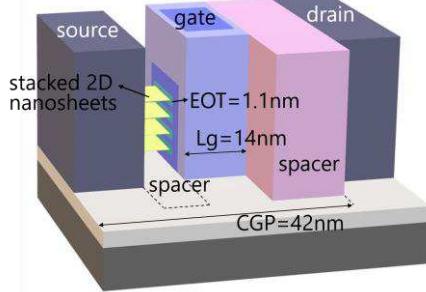


Figure 6: (a) Power performance area (PPA) analysis comparing Silicon and 2D in the same configuration of 4 stacked nanosheets with gate-all-around. (b) The baseline (A) is set with experimental values, $R_c=1.5\text{k}\Omega\cdot\mu\text{m}$ (corresponding to $\Phi_{SB}=0.45\text{eV}$), $\mu=15\text{cm}^2/\text{Vs}$, $D_{it}=3\times10^{12}\text{cm}^{-2}\text{eV}^{-1}$, $t_{channel}=3$ layers. For (B) the contacts are improved with $R_c\leq50\Omega\cdot\mu\text{m}$ (corresponding to $\Phi_{SB}=0.2\text{eV}$). For (C) the channel is further improved with $\mu=200\text{cm}^2/\text{Vs}$, $D_{it}=1\times10^{12}\text{cm}^{-2}\text{eV}^{-1}$, $t_{channel}=1$ layer. For (D), more aggressive improvements are done with $\mu=450\text{cm}^2/\text{Vs}$ and no R_c . For all curves, the area is the same and the bias conditions are such that at $V_{dd}=0.7\text{V}$, I_{off} is fixed at 2nA .

Methodology from [45].

4

5 Despite the fact our 2D performance is among the best in literature, significant improvements are still needed
 6 to make 2D materials competitive with Silicon channel devices for high-performance logic applications.
 7 Therefore we propose a roadmap using the Power Performance Area (PPA) metric for technology comparison
 8 in figure 6. 2D-FET and Silicon nanosheet technology are compared using an inverter-based ring oscillator
 9 circuit, where each device consists of 4 vertically stacked sheets with scaled $L_g=14\text{nm}$ and gate-all-around
 10 structure, corresponding to the imec 2nm node [45]. All devices are retargeted to an $I_{off} = 2\text{nA}$ at 0.7V V_{dd} and
 11 the inverter-circuit area is kept the same for fairer comparison between technologies. Starting from the baseline
 12 case (A) where experimental channel and contact parameters are assumed, the performance strongly improves
 13 in (B) when the Schottky barrier height is reduced. In (C), improvements to the 2D channel mobility results in
 14 higher ring-oscillator operating frequency compared to Silicon, owing to superior electrostatic control of the
 15 2D devices at shorter gate lengths. In (D), the ideal performance is simulated with more aggressively optimized
 16 material parameters.

17

In conclusion, we have scaled down the different device dimensions of CVD-grown MoS₂ FETs and demonstrated $g_{m,\max} = 185 \mu\text{S}/\mu\text{m}$ and $SS_{\min} = 86 \text{ mV/dec}$ which are among the best in literature. Using our large dataset, we systematically identified the key obstacles to be tackled to outperform Silicon. First, we showed that scaling L_{cont} for thin MoS₂ does not impact the short channel performance, which allows for an overall reduction in the device footprint. Second, we identified that for $L_{\text{ch}} < 100\text{nm}$, the on-current is currently limited by high Schottky contact resistance ($R_c = 1-2 \text{ k}\Omega.\mu\text{m}$) at low V_{ds} , and by a combination of velocity saturation and the Schottky barriers at high V_{ds} . Third, we identified that our devices suffer from short channel effects (SS degradation), caused by the Schottky barrier at intermediate current level and the thick CET at low current level. Reducing the CET is therefore crucial to keep optimal electrostatic control of the thin channel. We established that a 0.4nm layer of water or adsorbed hydrocarbons (or combination thereof) at the HfO₂/MoS₂ interface is the root cause of a lower-than-expected CET. This value is consistent across different thicknesses of HfO₂. Therefore, an optimized transfer process free of water and carbon is needed to enable gate stack scaling below 1nm, and additionally allow upscaling to 300mm-wafer processing. Finally, we have demonstrated using a PPA analysis that if the obstacles of Schottky contacts, gate stack scaling and mobility improvement can be tackled, MoS₂ FETs will significantly outperform Silicon GAA FETs at the imec 2nm node and beyond, and are therefore excellent candidates to continue logic scaling.

V. METHODS

A. Device fabrication

For the device design, we use the back-gate configuration with top-contacts (Fig 1b). The fabrication flow is summarized in Fig 1c. The MoS₂ is delaminated from the sapphire growth substrate using water intercalation and transferred to three different target substrates; (1) Si/50 nm SiO₂ (2) Si/50 nm SiO₂/5 nm TiN/12 nm HfO₂, or (3) Si/50 nm SiO₂/5 nm TiN/4 nm HfO₂. Before transfer, the target substrates are pre-cleaned using a solvent rinse, followed by an optimized forming gas anneal (FGA) or soft O₂ plasma, for SiO₂ and HfO₂ back-gate oxides, respectively. The active channels are patterned using PMMA mask and e-beam lithography, followed by reactive ion etching (Cl₂ + O₂) of MoS₂. Source and drain contacts of different lengths (L_{cont}) with different channel lengths (L_{ch}) are subsequently defined on the active channel by another e-beam

1 lithography exposure of ZEP520A-2 resist (ZEON Corp.), e-beam evaporation of 10nm Ni, and metal lift-off
2 in anisole. We ensure a low vacuum pressure $< 10^{-6}$ Torr while depositing the Ni contact metal. Finally, in a
3 third e-beam lithography step, thicker Ni/Pd contact pads are lifted off.

4 **B. TCAD calibration**

5 All simulations⁴⁴ are performed in Sentaurus Synopsys Device. The low-field mobility (μ_{eff}) is
6 calibrated from an experimental TLM fit shown in Fig 3c and implemented under a constant mobility model.
7 An estimate for D_{it} is obtained from multi-frequency CV measurements as discussed in section D. An acceptor
8 trap distribution uniform over the entire bandgap is assumed with $D_{it} = 3e12 \text{ cm}^{-2}\text{eV}^{-1}$. With μ_{eff} and D_{it} fixed
9 by experiments, the Schottky barrier height is fitted to median transfer characteristics of $L_{ch} = 30 \text{ nm}$ devices
10 which are predominantly contact-limited. For the Schottky injection, the non-local tunneling model based on
11 the Wentzel-Kramers-Brillouin approach is used.

12

13 **Data availability:** The data that support the findings of this study are available from the corresponding
14 author upon reasonable request.

15 **Additional information:** The authors declare that there are no competing interests.

16 **Author contributions:** Goutham Arutchelvan and Quentin Smets conceived the experiments. Goutham
17 Arutchelvan, with support from Quentin Smets and Surajit Sutar, performed the device fabrication,
18 characterization and analysis. Goutham Arutchelvan and Devin Verreck performed the TCAD simulations.
19 Zubair Ahmad performed the PPA analysis. C-V measurements and analysis were performed by Abhinav
20 Gaur, with support from Dennis Lin. The CVD MoS2 was grown by Benjamin Groven and e-beam litho
21 support was provided by Julien Jussot. Prof. Marc Heyns, Inge Asselberghs and Iuliana Radu managed the
22 overall activities and allocation of resources under the beyond CMOS program at imec, Belgium. The
23 manuscript was written by Goutham Arutchelvan with contributions from Quentin Smets and Devin Verreck.
24 The manuscript was revised by all co-authors.

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Figures

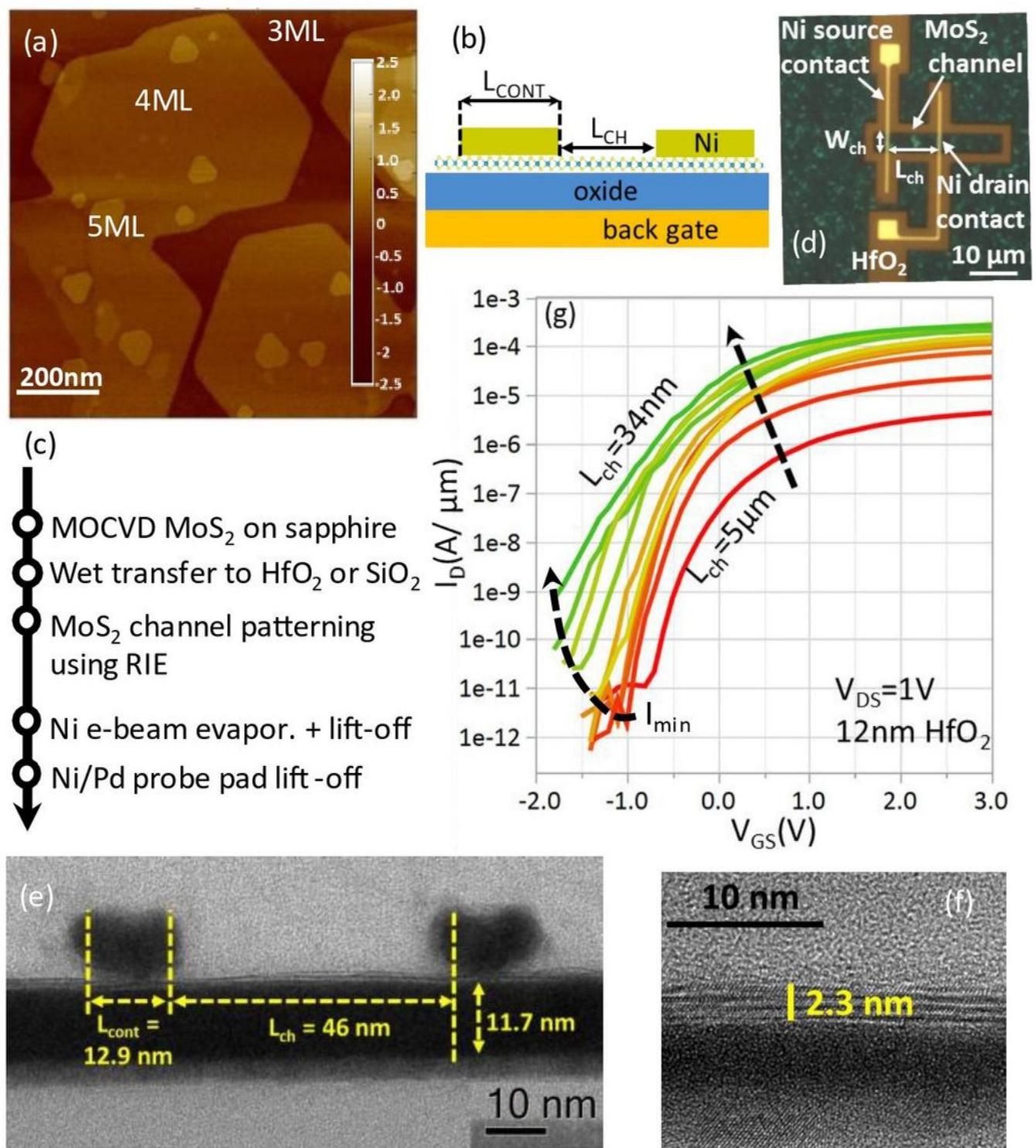


Figure 1

(a) Atomic force micrograph of CVD MoS₂ on sapphire template shows a closed 3ML layer with islands of 4 and 5 monolayers distributed randomly. (b) Device schematic with global back-gate and top source/drain contacts. (c) Fabrication flow for the back-gated devices. (d) Optical micrograph showing

the patterned MoS₂ channel with 10 nm Ni contacts. (e) Cross-TEM shows a fabricated device with L_{cont} = 13 nm and L_{ch} = 46 nm on 12 nm HfO₂. (f) Zoomin of the channel region for another device showing 3 monolayer MoS₂ on nominal 4 nm HfO₂ (g) Transfer characteristics at a fixed VDS = 1 V. Maximum drive current at VGS = 3 V scales with L_{ch} saturating for short-channel devices. The plot shows L_{ch} = 34 nm, 44 nm, 50 nm, 70 nm, 100 nm, 200 nm, 300 nm, 500 nm, 1000 nm, 5000 nm.

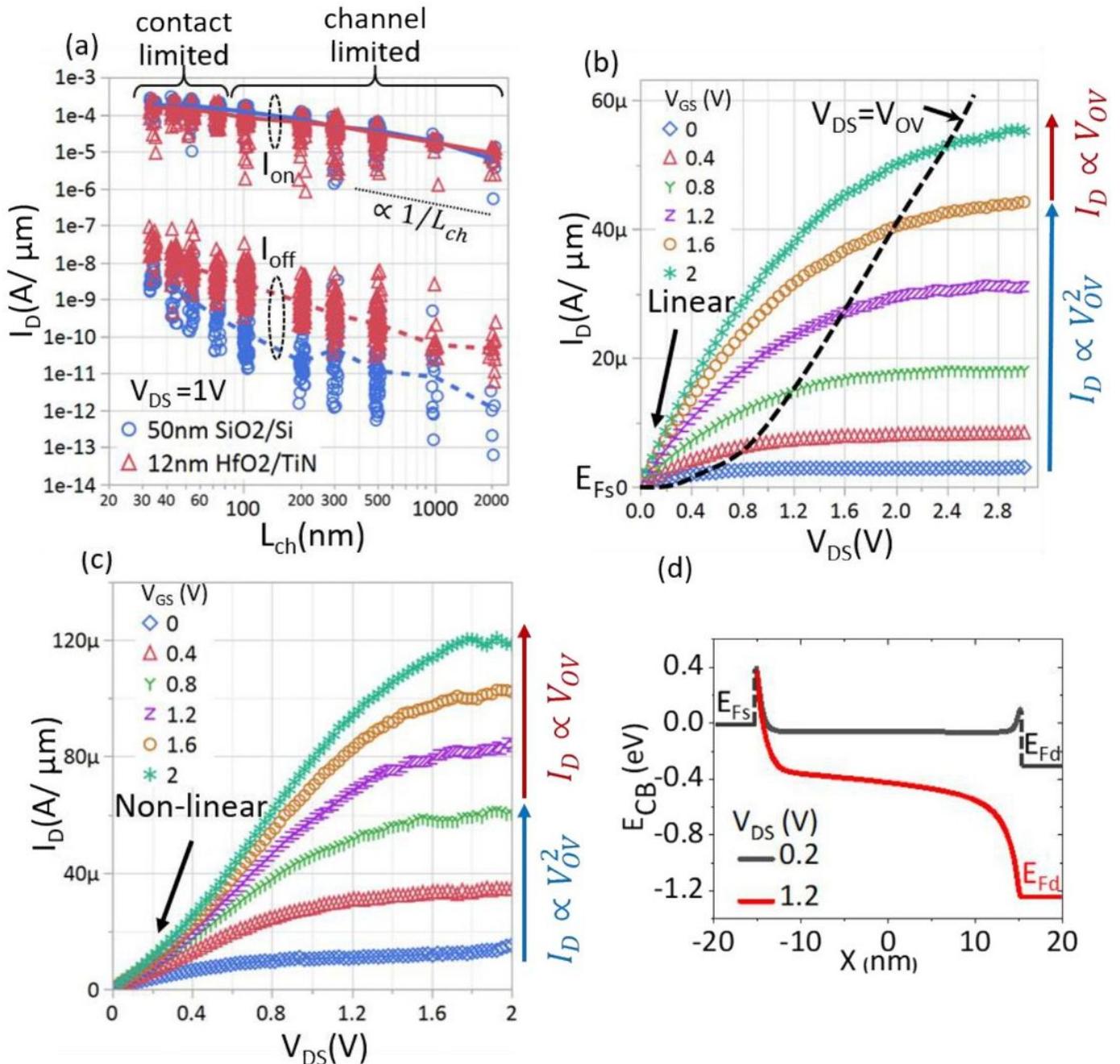


Figure 2

(a) Scatter plot (with median line) showing I_{on} extracted at $n_s = 1 \text{ e}^{13} \text{ cm}^{-2}$ and I_{off} at a fixed displacement field of 0.4 V/nm below VT,CC . for $V_{DS} = 1$ V. I_{on} for the 50 nm SiO₂ and 12 nm HfO₂ devices overlap indicating no impact on low-field mobility and contact barrier. I_{on} roughly scales as

$1/L_{ch}$ for $L_{ch} > 500$ nm and saturates for $L_{ch} < 50$ nm. I_{off} is higher for HfO₂ compared to SiO₂ due to high interface trap density. (b) ID-VDS for $L_{ch} = 500$ nm shows linear triode regime and saturation at high VDS. The dashed line follows the current at $V_{DS} = V_{OV}$. While the onset of saturation follows the V_{OV} at low VGS, it saturates at $V_{DS} = 2.4$ V for high VGS. The saturation current roughly scales V_{OV2} and V_{OV1} , at low and high VGS, respectively. (c) ID-VDS for $L_{ch} = 30$ nm shows non-linear triode regime due to Schottky contacts and saturation at high VDS. Saturation current follows a similar trend as $L_{ch} = 500$ nm but VDS at onset of velocity saturation is reduced to 1.4 V. (d) Conduction band profile for $L_{ch} = 30$ nm device with Schottky contacts shown for low and high VDS. The Fermi-level at the source and drain are indicated by EFS and EFD, respectively. The Schottky barrier is shown as the abrupt potential change at the contact-channel interface. At low VDS, IDS is determined by Schottky contacts. At high VDS, though the potential drops significantly at the source contact, velocity saturation near the drain determines the ID characteristics.

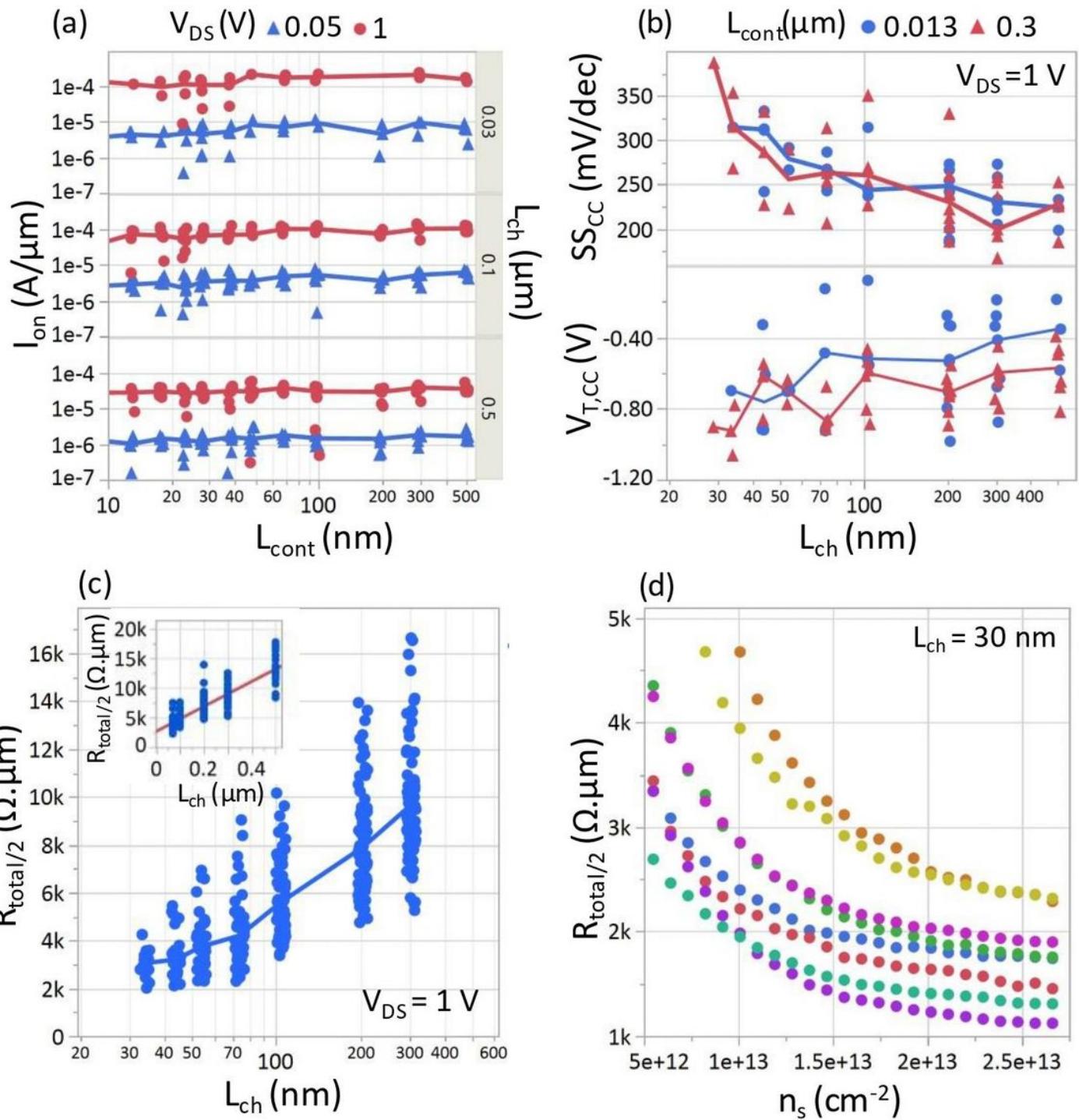


Figure 3

Scatter plot (with median line) of (a) I_{on} (at $n_s = 1e13 \text{ cm}^{-2}$) versus L_{cont} for $L_{ch} = 30 \text{ nm}$ (contact-limited), 100 nm (intermediate regime), and 500 nm (mobility limited). No dependence on L_{cont} down to 13 nm indicates carrier injection from the edge of the metal directly into the MoS₂ channel with $LT < 13 \text{ nm}$. (b) SS_{CC} and $V_{T,CC}$ versus L_{ch} for $L_{cont} = 13 \text{ nm}$ and 300 nm . No systematic deviation with L_{cont} indicates identical electrostatics in both cases. (c) $R_{total/2}$ (at $n_s = 1e13 \text{ cm}^{-2}$) versus L_{ch} show saturation below $L_{ch} = 50 \text{ nm}$ due to contact resistance. Upper limit for RC is obtained as median

$R_{\text{total}}/2$ for $L_{\text{ch}} = 30 \text{ nm}$. Median RC values of $3 \text{ k}\Omega.\mu\text{m}$ with best performers at $2 \text{ k}\Omega.\mu\text{m}$ are obtained. (inset) TLM fit of $R_{\text{total}}/2$ (at $n_s = 1e13 \text{ cm}^{-2}$) versus L_{ch} gives $R_c = 2.7 \text{ k}\Omega.\mu\text{m}$ and field-effect mobility = $15 \text{ cm}^2/\text{V.s}$ (d) $R_{\text{total}}/2$ versus n_s for $L_{\text{ch}} = 30 \text{ nm}$ at $V_{DS} = 1 \text{ V}$ of 8 devices. RC significantly reduces at $n_s = 2e13 \text{ cm}^{-2}$ due to better carrier injection into the accumulated channel.

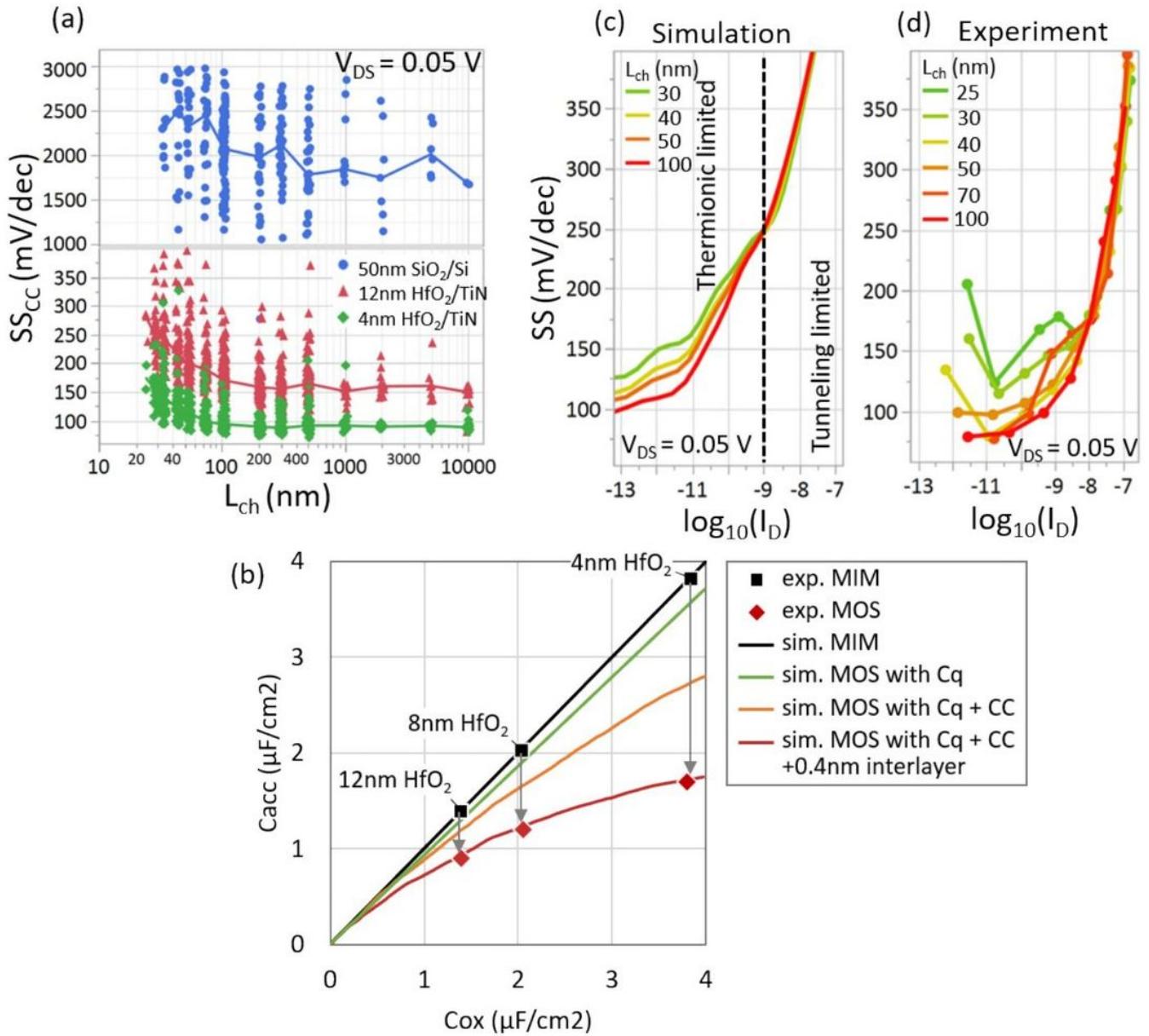


Figure 4

(a) Scatter plot (with median line) of SS_{CC} versus L_{ch} for the three different oxides. While SS improves with lower EOT, the degradation and scatter for short channel devices are attributed to electrostatic potential fluctuations caused by non-uniform thickness of MoS₂ in the contact and channel regions. (b) Experimentally measured maximum accumulation capacitance from MOScap (C_{max}) versus MIMcap capacitance (C_{ox}). Systematically, the C_{max} is lower than C_{ox} corresponding to an additional 1 nm CET over the measured EOT. Simulations show this is caused by the quantum capacitance C_q (MoS₂ having

lower DOS than metal), the impact of the charge centroid (CC) further away in MOS than MIM, and additionally due to 0.4 nm of water or carbon residues stuck at the HfO₂/MoS₂ interface during transfer. Qualitative comparison between (c) simulated and (d) experimental SS versus log (ID) for different Lch. The simulated SS is for a uniform 3 monolayers MoS₂ with SBH = 0.45 eV. Two transport regimes at the contacts— thermionic emission and tunneling through the SB are identified. In the thermionic regime, the relative increase of field in the channel from the source/drain Schottky contacts degrades gate control for short Lch devices. In the tunneling regime, the nearly equal tunneling lengths for the different Lch results in a similar but degraded SS compared to the thermionic regime.

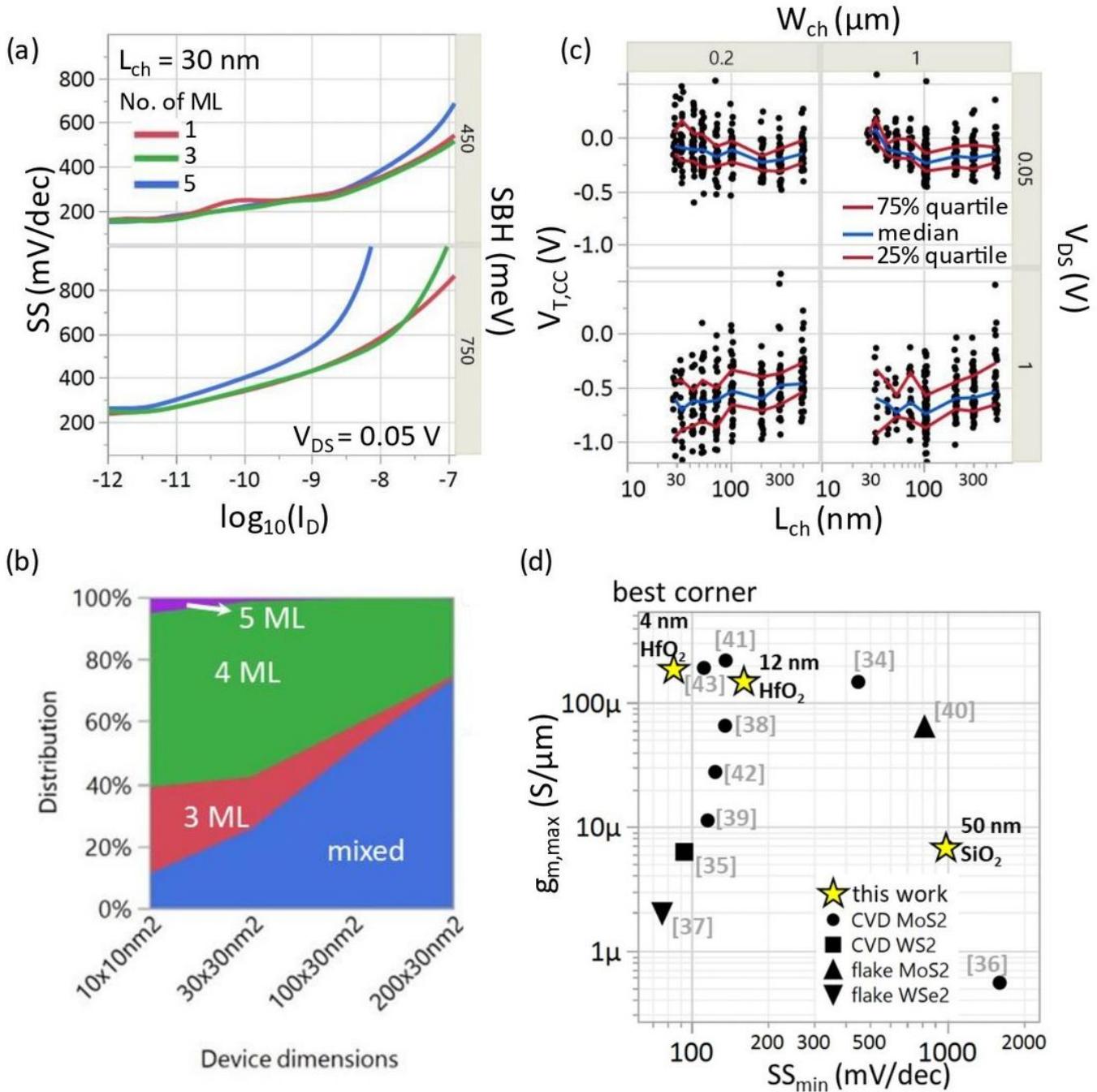


Figure 5

(a) Simulated SS versus log (ID) for a uniform layer of 1, 3 and 5 monolayers of MoS₂ for SBH = 0.45 eV and 0.75 eV. For ID > 1e-9 A/um , tunneling through Schottky barrier determines the SS. Subsequently, a thinner channel results in better gate control, shorter tunneling length and therefore better SS. (b) Probability distribution versus device dimensions (Lch x Wch). AFM from Fig 1a was used to compute the probability distribution for fabricating devices on only 3, 4, 5 or a combination of those (mixed). Our experimental devices have a 60-70% probability of being mixed, leading to non-uniform gate control across the channel and contact regions. (c) VT,CC versus Lch for two different Wch (200 nm, 1000 nm) and VDS (0.05 V, 1 V). No VT roll-off at VDS = 0.05 V due to excellent gate control over the channel for 12 nm HfO₂. VT roll-off of about 200 mV for VDS = 1 V due to higher lateral-field at the source contact allowing for more carrier injection. No systematic VT deviation between Wch = 1 μ m and 200 nm. (c) Benchmark plot showing gm,max versus SSmin. All values are at VDS = 1 V except [39] - VDS = 0.1 V, [34] - VDS = 0.5 V, [40] - VDS = 1.2 V, [37] - VDS = 1.5 V. In this work, 4 nm HfO₂ provides best SS = 86 mV/dec and gm,max = 185 μ S/ μ m.

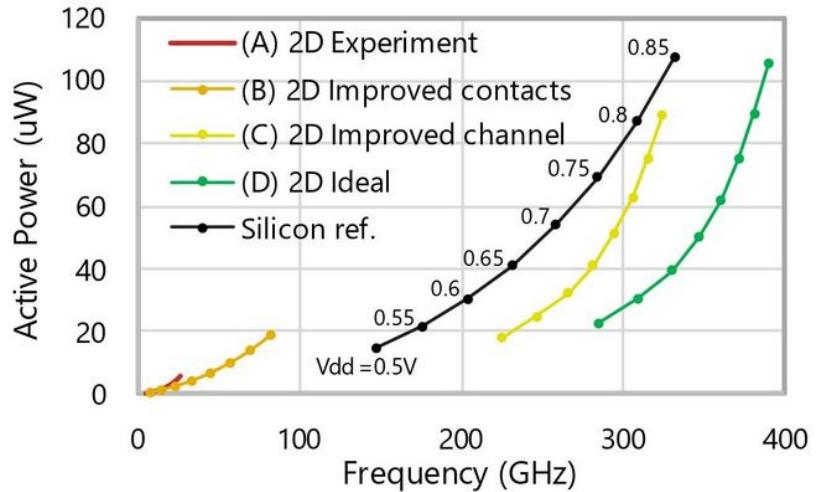
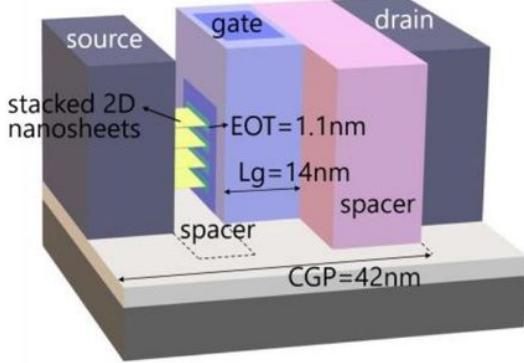


Figure 6

(a) Power performance area (PPA) analysis comparing Silicon and 2D in the same configuration of 4 stacked nanosheets with gate-all-around. (b) The baseline (A) is set with experimental values, $R_c=1.5\text{k}\Omega\cdot\mu\text{m}$ (corresponding to $\Phi_{SB}=0.45\text{eV}$), $\mu=15\text{cm}^2/\text{Vs}$, $Dit=3\times10^{12}\text{cm}^2\text{eV}^{-1}$, $t_{channel}=3$ layers. For (B) the contacts are improved with $R_c\leq50\Omega\cdot\mu\text{m}$ (corresponding to $\Phi_{SB}=0.2\text{eV}$). For (C) the channel is further improved with $\mu=200\text{cm}^2/\text{Vs}$, $Dit=1\times10^{12}\text{cm}^2\text{eV}^{-1}$, $t_{channel}=1$ layer. For (D), more aggressive improvements are done with $\mu=450\text{cm}^2/\text{Vs}$ and no R_c . For all curves, the area is the same and the bias conditions are such that at $V_{dd}=0.7\text{V}$, I_{off} is fixed at 2nA. Methodology from [45].

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- [Supplementaryinfo.pdf](#)