

# Exploring 2D TMD pFET gate stack scalability towards 1nm electrical thickness

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**Abstract**— We report p-type compatible WO<sub>x</sub>/HfO<sub>2</sub> gate stacks for WSe<sub>2</sub>-based 2D pFET devices. 2D pFET compatible gate stacks are challenging as typical 2D gate stack processes often result in unintentional n-type doping. In this work, we preserve the p-type attributes of the channel through ALD precursor optimization, while employing interfacial layers to maintain the channel integrity. Dual-gate devices are fabricated with channel length down to 50nm and gate stacks achieving about 1.4 nm CET. We also present the first reported 2D pFET CV characteristics, including AC conductance analysis, showing successful CET scaling when thinning from 10 nm down to 4 nm HfO<sub>2</sub> physical thickness.

**Keywords**—2D pFET, gate-stack, oxygen plasma, high-k ALD, CET scaling

## I. INTRODUCTION

2D TMD channel materials are expected to extend the scalability of future technology nodes beyond Si, thanks to their atomically thin channel, enabling good electrostatic control, while not severely degrading mobility. Realization of a performant pFET device is a cornerstone in further advancing the 2D-channel materials technology. However, recent studies indicate that forming a p-type compatible gate stack requires a tailored approach, as gate stacks used in nFETs often include interfacial layers (ILs) that induce n-type doping, compromising p-type performance. In this work, we explore p-type compatible gate stacks, underlining the importance of high-k deposition process in the overall device performance, and propose a WO<sub>x</sub>/HfO<sub>2</sub> gate stack that shows promise to meet (sub-)1nm CET requirements.

## II. PROCESSES, RESULTS AND DISCUSSION

### A. Device fabrication

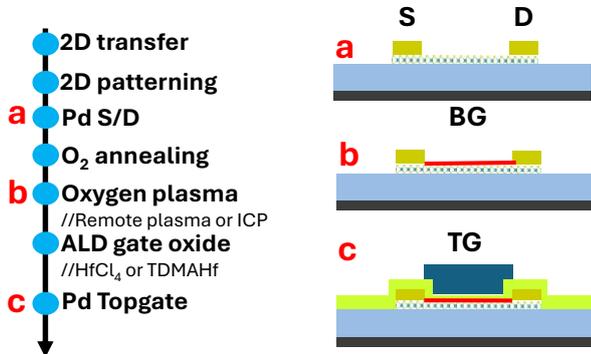


Fig. 1. Key process steps and schematic cross-sections for dual-gate 2D TMD pFET device fabrication. The labels a, b, c indicate intermediate and EOL testing points.

Fig.1 shows a schematics of a dual-gate (DG) device fabrication process flow. Unless otherwise specified, the channel material is multilayer (nML) WSe<sub>2</sub> directly grown

on SiO<sub>2</sub> substrates using a 300 mm MOCVD process [1]. Prior to device fabrication, the 2D material was transferred onto a 12 nm ALD HfO<sub>2</sub> substrate deposited over a TiN back gate (BG). A 200 C O<sub>2</sub> anneal was performed after S/D contacts definition to reduce the contact resistance. An O<sub>2</sub> plasma was used to form a WO<sub>x</sub> IL by sacrificial WSe<sub>2</sub> oxidation, followed by ALD HfO<sub>2</sub> deposition and top gate (TG) patterning.

### B. Precursors impact

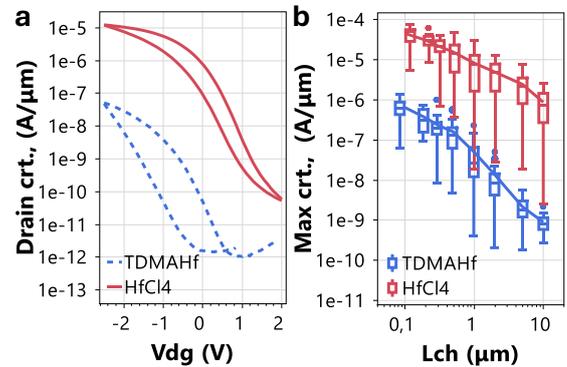


Fig. 2. (a) DG median IV characteristics for fully-processed DG devices (Fig. 1,c), with a plasma-formed WO<sub>x</sub> IL and 10nm ALD HfO<sub>2</sub> deposited with 2 different processes, using TDMAHF and HfCl<sub>4</sub> precursors, respectively ( $L_{ch} = 1 \mu m$ ). (b) Maximum current scaling with channel length ( $L_{ch}$ ), evidencing a major impact of the ALD precursor. In DG operation mode, the BG and TG are connected together,  $V_{bg} = V_{tg} = V_{dg}$ .

Formation of WO<sub>x</sub> IL by a plasma-based oxidation process on nML WSe<sub>2</sub> is essential to protect the WSe<sub>2</sub> channel, induce p-type doping, and promote ALD nucleation and growth [2]. Nevertheless, severe drive current reduction was observed, after high-k (HfO<sub>2</sub>) deposition. To find the root cause, we used 2 different ALD processes to fabricate DG devices, with organic/inorganic precursors, i.e. TDMAHF and HfCl<sub>4</sub>. IV characteristics (Fig.2) show a major difference, with around 2 orders of magnitude higher drive current and better hysteresis for HfCl<sub>4</sub>-based HfO<sub>2</sub> and otherwise identical-process devices. This difference in current was maintained across the entire channel length range. We attribute this outcome to the chemistry of the ALD process, where the organic byproducts of the TDMAHF-based HfO<sub>2</sub> may interact with the WO<sub>x</sub> IL, resulting in W with a lower oxidation state, and compromise the quality of the IL and/or the WO<sub>x</sub>/HfO<sub>2</sub> inner interface.. This is suggested by the hard-XPS (HAXPES) W3d spectra, where a slightly larger shift of the W-O peak to lower binding energies was observed for the TDMAHF case compared to the HfCl<sub>4</sub> (Fig.3). Degradation of the WO<sub>x</sub> IL is also seen in SS data, which have higher values for the TDMAHF case (not shown). Separate experiments, performed on monolayer (ML) WSe<sub>2</sub>, where the WSe<sub>2</sub> material was exposed to the HfO<sub>2</sub> deposition

process directly (without any  $\text{WO}_x$  IL) (Fig.4) showed that while the  $\text{HfCl}_4$  process degrades the channel, the TDMAHf process induced n-type doping, suppressing the p-type branch. This is consistent with chemical action on  $\text{WSe}_2$  by HCl byproduct ( $\text{HfCl}_4$  process), while dimethylamine ( $\text{HN}(\text{CH}_3)_2$ ) byproduct adsorbs into and functionalizes  $\text{WSe}_2$  (TDMAHf process), respectively. Hence, when present, the  $\text{WO}_x$  IL acts as a protective layer, which can only withstand the  $\text{HfCl}_4$ -based ALD process.

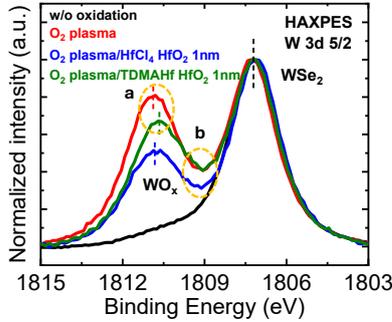


Fig. 3. W3d HAXPES spectra with plasma surface treatment and different ALD processes on multilayer (nML)  $\text{WSe}_2$ . The decrease of the  $\text{HfCl}_4$ -based W-O peak is attributed to a limited removal of  $\text{WO}_x$  during the ALD process, while features **a** and **b** suggest an increased fraction of W suboxides formation for the TDMAHf-based ALD process. A 1nm-only ALD  $\text{HfO}_2$  has been employed to form the  $\text{WO}_x/\text{HfO}_2$  interface on blanket samples to allow HAXPES probing resolution.

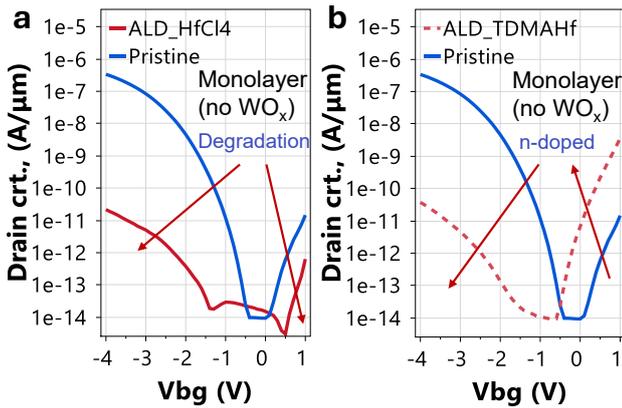


Fig. 4.  $I_d V_g$  curves of monolayer  $\text{WSe}_2$  devices and without  $\text{WO}_x$  IL evidence the direct impact of the as-deposited  $\text{HfO}_2$ : the  $\text{HfCl}_4$ -precursor induces a degradation of the current level, while TDMAHf precursor induces an n-type doping, commonly observed with other dielectrics, e.g.  $\text{AlO}_x$  or Si-seed ( $\text{SiO}_x$ ).

### C. Plasma impact

$\text{O}_2$  plasma treatment forms the  $\text{WO}_x$  IL by  $\text{WSe}_2$  oxidation. A direct plasma leads to a stronger p-type doping, resulting in large current increase and  $V_T$ -shift, limiting the on/off ratio ( $I_{\text{max}}/I_{\text{min}}$ ) of the device. A remote  $\text{O}_2$  plasma process produces a soft doping, mainly resulting in  $V_T$ -shift (Fig.5, for test point “b” in Fig. 1). Forming the TG with ALD  $\text{HfO}_2$  (test point “c”, Fig.1) results in good TG control, able to counteract the channel doping and turn off the devices, while retaining the advantage of higher drive current achieved with direct  $\text{O}_2$  plasma treatment (Fig.6). When operated in the DG mode (BG and TG tied together),  $I_{\text{max}}/I_{\text{min}}$  ratio for the samples that received a direct plasma  $\text{WO}_x$  IL exceeds 7 decades.

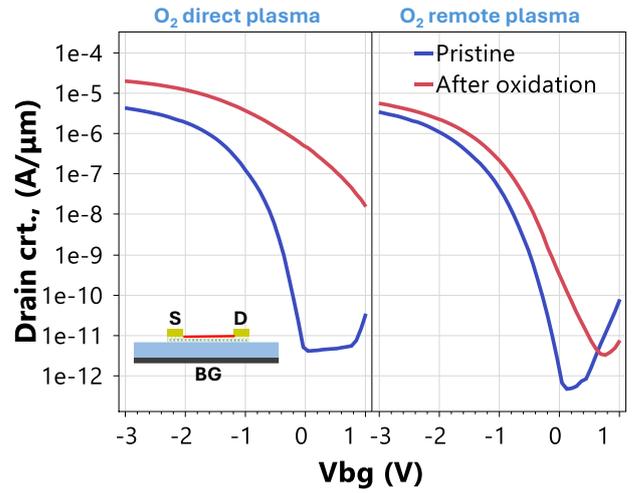


Fig. 5.  $\text{WO}_x$  ILs produced by  $\text{O}_2$  plasma oxidation, induce p-type doping, in contrast with  $\text{HfO}_2$  (Fig.4) or other ILs. A strong doping is achieved with a direct  $\text{O}_2$  plasma, leading to a noticeable increase of the drive current and a  $V_T$ -shift. A soft doping is achieved with a remote  $\text{O}_2$  plasma, resulting mainly in a  $V_T$ -shift. Data show median  $I_V$  curves, for devices of  $L_{\text{ch}} = 2 \mu\text{m}$ .

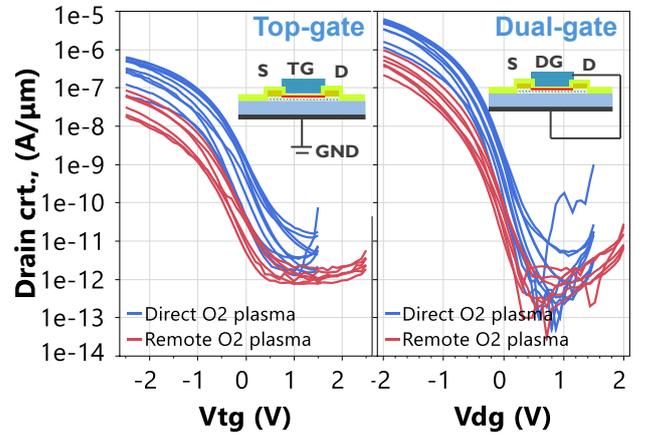


Fig. 6. (Top) gate stacks formed with  $\text{HfCl}_4$ -based  $\text{HfO}_2$ , for both plasma treatments, show very good TG control, which can turn off the direct plasma-treated devices, while retaining the advantage of a higher drive current (left plot). Operating the devices in DG mode (TG and BG shorted) further improves the channel modulation, increasing  $I_{\text{max}}/I_{\text{min}}$  ratio to over 7 orders of magnitude (right plot). ( $L_{\text{ch}} = 2 \mu\text{m}$ )

### D. Gate stack scaling

We adopted an direct  $\text{O}_2$  plasma treatment and a  $\text{HfCl}_4$ -based  $\text{HfO}_2$  process to explore gate scalability. We fabricated devices with  $\text{HfO}_2$  thickness down to 3 nm (Fig.7). HR-TEM cross-sections through 50 nm channel devices show well formed, uniform gate stacks for both 4nm and 3nm  $\text{HfO}_2$ , and nML  $\text{WSe}_2$  channel. Line profiles of EDS maps on a 3 nm- $\text{HfO}_2$  device evidence presence of the  $\text{WO}_x$  IL, by shifts of W profile relative to Se, and that of O relative to Hf. Very good electrostatic control of both TG and BG is shown, down to 3 nm  $\text{HfO}_2$  layer (Fig.8).

Gate dielectric thickness scaling shows improved modulation of the drain current ( $I_d$ ), at similar bias, and for the same  $\Delta V_{tg}$  swing.

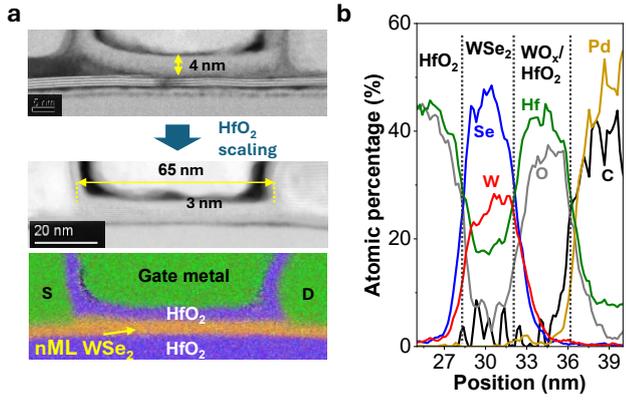


Fig. 7. (a) TEM cross-sections and elemental map of fabricated DG devices of  $L_{ch}=50\text{nm}$ , featuring a  $\text{WO}_x/\text{HfO}_2$  gate stack with 4nm (top) and 3nm (bottom)  $\text{HfCl}_4$ -based  $\text{HfO}_2$ . The  $\text{WSe}_2$  channel consists of several (4-8) monolayers (nML). (b) Integrated line scans, evidencing existence of a thin  $\text{WO}_x$  IL between the channel and  $\text{HfO}_2$  dielectric.

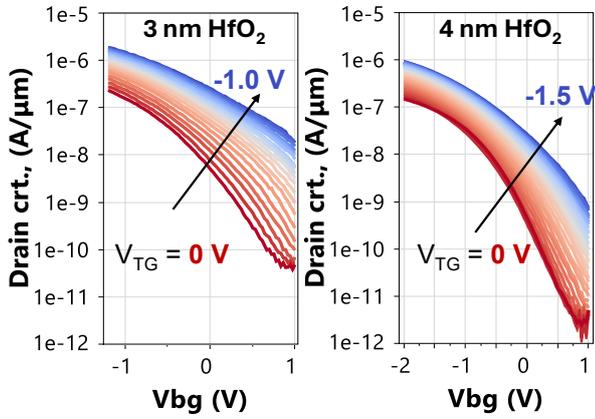


Fig. 8. IV transfer curves of back-gated devices with  $\text{WO}_x/\text{HfO}_2$  gate stacks, at various TG biases. Very good control is achieved, even for the thinnest TG stack (3nm  $\text{HfO}_2$ ). Devices have  $L_{ch} = 5 \mu\text{m}$ .

Dual-sweep IV plots show that the hysteresis is small (Fig.9), with an extracted  $|\Delta V/V_{dg,max}| < 60 \text{ mV/V}$ .  $I_{max}$  exceeds  $100 \mu\text{A}/\mu\text{m}$ , with the best performing devices showing a maximum current of up to  $\sim 170 \mu\text{A}/\mu\text{m}$ , for 4 nm  $\text{HfO}_2$  thickness.  $I_{max}-L_{ch}$  plots (Fig.10) show that the contact resistance limits the actual device performance; contact optimization would project current levels well over  $500 \mu\text{A}/\mu\text{m}$  at below 50 nm channel length, if contact resistance is reduced sufficiently.

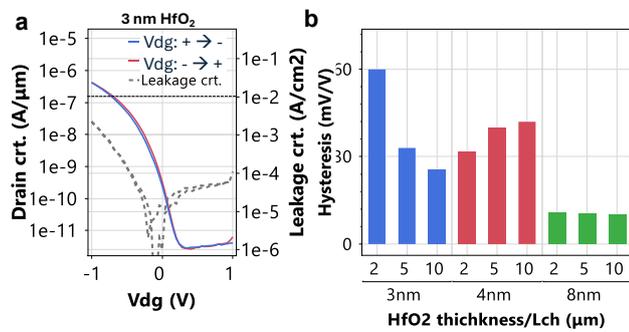


Fig. 9. (a) Double-sweep IV's for  $\text{HfCl}_4$ -based  $\text{WO}_x/3\text{nm HfO}_2$  gate stacks, measured on large area DG devices, evidencing very small hysteresis and low leakage current, with margin for further  $\text{HfO}_2$  thickness scaling (DG operation,  $L_{ch}=10\mu\text{m}$ ,  $W_{ch}=5\mu\text{m}$ ). (b) Median hysteresis  $|\Delta V/V_{dg,max}|$  extracted at a current level  $I_d=10^{-7}$

$\mu\text{A}/\mu\text{m}$  for several  $\text{HfCl}_4$ -based  $\text{WO}_x/\text{HfO}_2$  TG stacks show values below  $60\text{mV/V}$ .

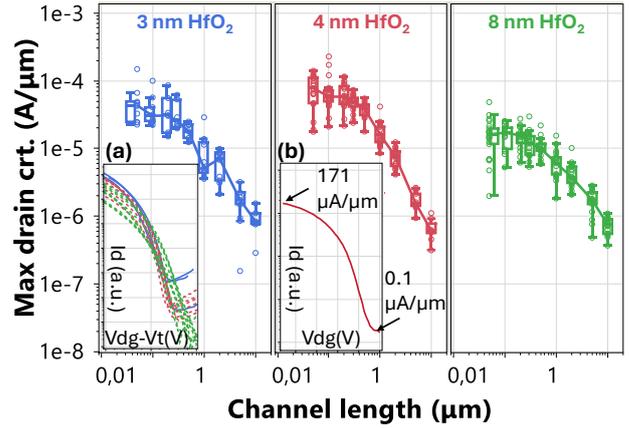


Fig. 10. Maximum current scaling with  $L_{ch}$ , indicating contact-limited conduction for devices below  $1\mu\text{m}$  channel length. This hinders observation of higher currents for short channel devices. Contact optimization may enable currents of hundreds  $\mu\text{A}/\mu\text{m}$ , at below  $50\text{nm}$ -channels, as inferred from an ideal  $I_{max}-L_{ch}$  scaling trend. The apparent drop of  $I_{max}$  at 3nm  $\text{HfO}_2$  is mainly due to lower overdrive ( $V_{dg}-V_t$ ) sweep range (corrected for in the inset a). The inset b shows an IV selected from best performing devices with 4nm  $\text{HfO}_2$  thickness ( $L_{ch} = 100\text{nm}$ ).

TABLE I.  $I_{dmax}$ , hysteresis and CET benchmarking of 2D pFET DG devices with grown-TG stack showing best-in-class  $I_{dmax}$ , hysteresis and electrical thickness. Our work is summarized in the first 3 table lines.

Gate stack	$I_{dmax}$ ( $\mu\text{A}/\mu\text{m}$ )	Hysteresis (mV/V)	$t_{\text{HfO}_2}$ (nm)	$\text{EOT}_{\text{TG}}$ (nm)
$\text{WO}_x$ (Direct) + $\text{HfCl}_4 \text{ HfO}_2$	171	30	4	1.7
$\text{WO}_x$ (Remote) + $\text{HfCl}_4 \text{ HfO}_2$	112	88	3	n/a
$\text{WO}_x$ (Direct) + TDMAHf $\text{HfO}_2$	1.23	240	10	2.8
Ref. [3] - $\text{HfO}_2$	123	n/a	12	n/a
Ref. [4] - $\text{HfO}_2$	2	n/a	10	n/a
Ref. [5] - $\text{HfO}_2$	$\sim 10$	n/a	$\sim 10$	n/a
Ref. [6] - $\text{HfO}_2$	132	n/a	n/a	n/a

Multi-frequency CV data showed well-behaved capacitances, as measured for BG-only, as well as for DG configurations on large area devices (Fig.11). TG capacitance was extracted by subtracting BG capacitance from DG capacitance, correcting for parasitic (e.g. pads) components. A CV tool was then used to extract TG electrical thickness (CET), by fitting experimental CV curves in the accumulation region. Extracted values for 10 nm down to 4 nm  $\text{HfO}_2$  gate stacks were used to extract the  $\text{HfO}_2$  dielectric constant (16) and extrapolated to an  $\text{WO}_x$  IL CET of 0.7 nm (Fig. 12). Projected CET of 3 nm  $\text{HfO}_2$  gate stack yielded a value of about 1.4 nm.

Frequency-scaled ( $G_p/\omega$ ) conductance plots on structures with 10 nm  $\text{HfO}_2$  gate stacks were taken for devices processed with both  $\text{HfO}_2$  precursors (Fig. 13) and showed an important contribution of the interface traps, of similar magnitude (expected, given the similar  $\text{WO}_x$  interface), but manifesting at different biases, consistent with the IV curves (Fig.2). We estimated a  $D_{it}$  density in the order of  $(5-6) \cdot 10^{12}/\text{cm}^2 \cdot \text{eV}$ , which leaves room for further improvement.

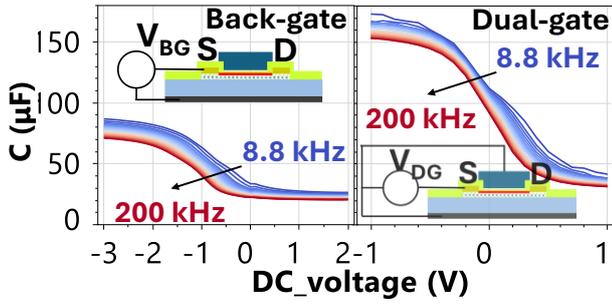


Fig. 11. Multi-frequency CV curves obtained on BG and DG large area ( $5.76 \cdot 10^{-5} \text{cm}^2$ ) devices with  $\text{HfCl}_4$ -based  $\text{WO}_x/4\text{nm HfO}_2$  TG stacks. Pad-free TG capacitance is extracted as explained in the text.

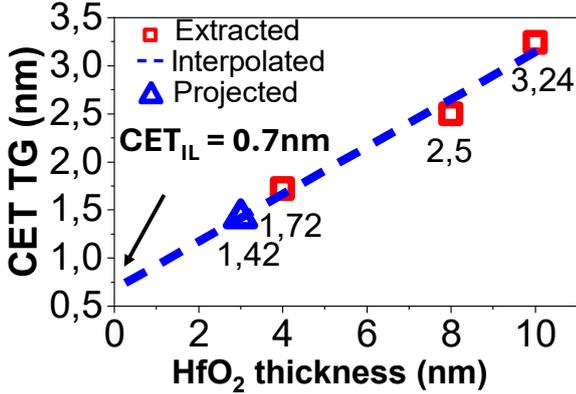


Fig. 12. CET plot, based on extracted CET values for 4nm, 8nm and 10nm  $\text{HfCl}_4$ -based  $\text{HfO}_2$  gate stacks, extrapolates to an  $\text{WO}_x$  IL of  $\sim 0.7\text{nm}$  EOT. A CET of  $\sim 1.4\text{nm}$  for  $\text{WO}_x/3\text{nm HfO}_2$  TG stacks is projected by the linear fitting curve (direct CET extraction is hindered by the leakage of the large area devices used).

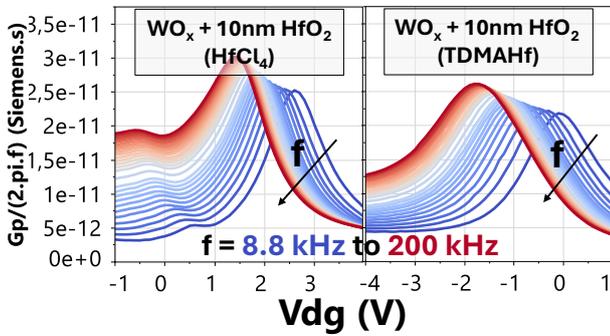


Fig. 13. Multi-frequency  $G_p/\omega$  curves for  $\text{HfCl}_4$  and TDMAHF-based gate stacks, evidencing interface traps most active at biases around their respective  $V_{FB}$ 's, consistent with the IVs in Fig.2. The peaks of the curves were used to extract the interface trap density ( $D_{it}$ ).

### III. CONCLUSION

We demonstrated p-type tailored  $\text{WO}_x/\text{HfO}_2$  gate stacks by optimizing the formation of an  $\text{WO}_x$  IL and by utilizing a suitable ALD process chemistry to preserve good pFET device performance. While the  $\text{WO}_x$  IL can be optimized to improve the p-type benefits, it is also essential to protect the  $\text{WSe}_2$  channel from secondary processes that can be induced during the ALD. Besides that, it provides an alternative method to produce an interface, which avoids using slow physisorption processes, commonly employed to enhance high-k nucleation/growth on 2D surfaces, but pose a manufacturability challenge.

Gate stack scalability was explored by IV & CV analysis, showing controllable gate stacks down to at least 3 nm  $\text{HfO}_2$  thickness. Further scalability may be achieved by optimizing the IL formation, while performance can significantly benefit from S/D contact engineering, currently limiting short-channel device performance.

### ACKNOWLEDGMENTS

This work has been partly performed within imec's core CMOS industrial affiliation program (IIAP) on Exploratory Logic devices.

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