

# Physical insight and performance metrics of monolayer MX<sub>2</sub> heterojunction TFETs

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The physics and performance of monolayer MX<sub>2</sub> heterojunction n TFETs are studied using a quantum simulation. The imaginary wave vector reveals that WTe<sub>2</sub> is the most promising source material. Results of heterojunction TFETs with WTe<sub>2</sub> source material and of WTe<sub>2</sub> homojunction TFET reveal that WTe<sub>2</sub>-MoS<sub>2</sub> heterojunction TFET is the most promising candidate with a 620 μA/μm drive current for a 0.3 volt gate swing. The energy gap between the valence band of source material and the conduction band of channel material,  $\delta E_{cv}$ , is the key parameter for high drive current. The WTe<sub>2</sub>-MoS<sub>2</sub> heterojunction has the smallest  $\delta E_{cv}$  value that results in small band bending near the heterojunction, which creates the shortest tunnel path and therefore yields the highest drive current. The WTe<sub>2</sub>-MoS<sub>2</sub> TFET has an average turn-on slope of 15.6 mV/dec, an on/off current ratio of  $6.2 \times 10^8$ , a drive current of 620 μA/μm, a transconductance of 10.98 mS/μm, a total capacitance of 0.829 fF/μm, a switching delay of 0.401 ps, and a cutoff frequency of 2.1 THz. The performance metrics closely comply with the ITRS 2026 LOP and LSTP device requirements. Its  $I_{60}$  value of 11.97 μA/μm is large enough to compete with MOSFETs.

**1. Introduction:** Increased power dissipation in nanoscaled transistors may be overcome by tunnelling field-effect transistors (TFETs) due to their sub-60 mV/dec turn-on characteristics, which allows aggressive  $V_{DD}$  scaling [1–4]. Transition metal dichalcogenides (TMDCs) are layered materials. Monolayer and a few layers of TMDCs have been used to implement field effect transistors [5, 6]. The bulk and few layers of TMDCs have an indirect bandgap. Therefore, they are not promising candidates for band to band tunnelling (BTBT) transistors. However, the monolayer TMDCs are direct gap two-dimensional (2D) materials [7, 8]. Different techniques such as mechanical exfoliation [9, 10] and lithium-based intercalation [11] can be used to extract a monolayer from the bulk metal chalcogenides family.

Superior performance of TMDC heterojunction (HTJ) TFETs over their homojunction (HJ) counterparts has been reported by Cao *et al.* [4]. According to their simulation study, WTe<sub>2</sub> and MoS<sub>2</sub> are the best combination. An experimental demonstration of BTBT in MoS<sub>2</sub>-MoTe<sub>2</sub> HTJ has been reported in [12]. They have found that the staggered band alignment at the hetero-interface boosts the BTBT compared to the HJ configuration. Vertical HTJ WTe<sub>2</sub> and MoS<sub>2</sub> TFETs are studied in [13]. Their results show that the ultra-steep turn-on characteristic is robust against atomic defects and impurity scattering. Lam *et al.* [14] reported an order of magnitude enhancement in on-state current for the common-*X* HTJ TFETs compared to the constituents' HJ TFETs. Choukroun *et al.* [15] compared several HTJs and reported that WTe<sub>2</sub>-MoS<sub>2</sub> and MoTe<sub>2</sub>-MoS<sub>2</sub> are the most promising HTJs.

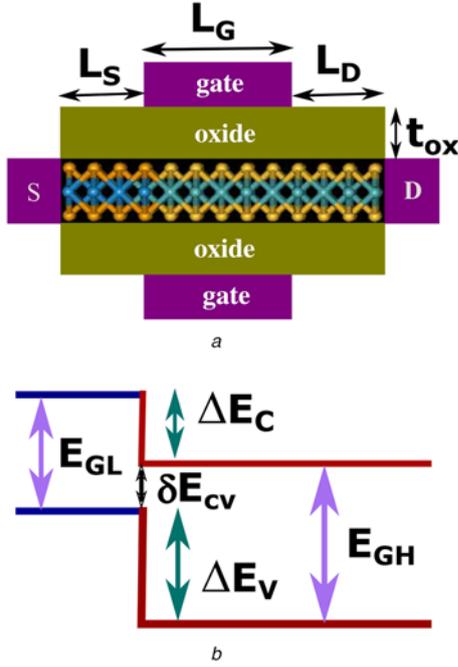
Monolayer TMDCs have been used to realise TFETs both in vertical tunnelling structure [13, 16–20] and lateral tunnelling structure [12, 14, 15, 21, 22]. However, the lateral structure is conventional and the experimental technique of the lateral structure is rapidly growing [23–26]. Although lateral HTJ TFETs of different combinations of monolayer TMDCs have been studied [4, 13–15] and a few combinations such as WTe<sub>2</sub>-MoS<sub>2</sub> and MoTe<sub>2</sub>-MoS<sub>2</sub> have been reported as the most promising combinations, the deep level physical insight of such combinations needs to be understood and the benchmark of their device performance against the technology requirements need to be assessed. In this work, we choose lateral HTJ TFETs of monolayer TMDC to

understand the physical insight of BTBT in such structures and to evaluate the performance metrics of such a TFET. We also benchmark its performance metrics against the ITRS 2026 low operating power (LOP) and low standby power (LSTP) technology requirements [27].

**2. Device structure and simulation approach:** The double gate TFET device structure that we use for simulation is shown in Fig. 1a. The gate oxide is HfO<sub>2</sub> with a dielectric constant of 20 and a thickness value of 2.56 nm. This is equivalent to an effective oxide thickness of 0.5 nm. The source and drain are doped with a doping density of  $10^{21}$  and  $5 \times 10^{20}$  cm<sup>-3</sup>, respectively, and the channel is intrinsic. The effective doping can be done by surface adatoms [28] and absorption of atoms such as potassium [29], rhenium [30], gold [30], niobium [31], chlorine [32], and hydrogen [32, 33]. The monolayer MX<sub>2</sub> HTJ is formed at the source-channel interface with a staggered band alignment as schematically shown in Fig. 1b. The monolayer MX<sub>2</sub> materials used for source, drain, and channel have hexagonal honeycomb lattice structures (1H-MX<sub>2</sub>), which are semiconductors and have a finite gap at the K-point of the 2D hexagonal Brillouin zone (BZ). The source is a lower bandgap MX<sub>2</sub> while the channel MX<sub>2</sub> has a relatively higher bandgap. The source-channel HTJ uses monolayer MX<sub>2</sub> with different combinations.

For simulation, we solve Poisson's equation and non-equilibrium Green's functions (NEGF) self-consistently. The 2D Poisson's equation uses a finite difference scheme for discretisation over the entire device domain and is solved using a Newton-Raphson method. Discretisation uses a 0.2 nm grid in the channel and a 0.5 nm grid in oxide and other parts of the device domain. Under boundary conditions, we fixed the voltage at gate electrodes and set the normal component of electric field to zero at all other boundaries. We use a recursive Green's function algorithm (RGFA) [34] to solve NEGF for electron and hole densities under ballistic transport

$$n(x, z) = n_s n_v \int_{-\infty}^{\infty} dk_y \int_{E_C}^{\infty} \frac{dE}{2\pi} [A_S(E, k_y) f(E, k_y, \mu_S) + A_D(E, k_y) f(E, k_y, \mu_D)], \quad (1)$$



**Fig. 1** The schematics of device cross section and heterojunction band alignment

*a* Cross section of the TFET structure used for simulation. The channel is an axial hetero-structure of  $\text{MX}_2$  2D material. Different dimensions are  $L_S = L_G = L_D = 20 \text{ nm}$  and  $t_{\text{ox}} = 2.56 \text{ nm}$ , which is corresponding to an effective oxide thickness of  $0.5 \text{ nm}$

*b* Sketch of staggered band alignment along the transport direction.  $E_G$ 's are the band gaps of low- and high-bandgap materials,  $\Delta E_C$  and  $\Delta E_V$  are the conduction and valence band offsets, and  $\delta E_{cv}$  is the offset between valence band of low-bandgap material and conduction band of high-bandgap material

$$p(x, z) = n_s n_v \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{E_V} \frac{dE}{2\pi} [A_S(E, k_y)(1 - f(E, k_y, \mu_S)) + A_D(E, k_y)(1 - f(E, k_y, \mu_D))] \quad (2)$$

Here  $n_s$  and  $n_v$  account for spin and valley degeneracies, respectively,  $A$ 's are the source and drain spectral functions,  $f$  is the Fermi function, and  $\mu$ 's are the source and drain Fermi levels. The RGFA and calculation procedures of  $A_S$  and  $A_D$  are discussed in detail in [34, 35]. The BZ of monolayer  $\text{MX}_2$  is hexagonal, and the band edges happen at the  $K$ -points of the BZ. As there are six  $K$ -points in the hexagonal BZ and each  $K$ -point is shared by three adjacent units, we set  $n_v$  to 2.

The monolayer  $\text{MX}_2$  is modelled using a two-band Hamiltonian at  $K$ -point [36]

$$H(k_x, k_y) = \begin{bmatrix} E_C & tf(k_x, k_y) \\ tf^*(k_x, k_y) & E_V \end{bmatrix}, \quad (3)$$

where  $E_C$  and  $E_V$  represent the band edges,  $t = (\hbar/a)\sqrt{2E_G/2m^*}$ , and  $f(k_x, k_y)$  is given by

$$f(k_x, k_y) = \exp\left(\frac{ik_y a}{\sqrt{3}}\right) + 2 \exp\left(-\frac{ik_y a}{2\sqrt{3}}\right) \cos\left(\frac{k_x a}{2}\right). \quad (4)$$

The lattice constant  $a$ , the bandgap  $E_G$  at  $K$ -point and the effective mass  $m^*$  are taken from [37]. The strain is not considered in this work. The source and channel are modelled using their unstrained Hamiltonians, and the interface coupling matrix is the average of the two.

The self-consistent loop starts with an initial guess of the potential profile based on the equilibrium calculation. The potential update for subsequent iterations uses an Anderson mixing scheme [38] to expedite the convergence. Once the profile is converged, the direct BTBT current is calculated from

$$I_D = n_s n_v \left(\frac{e}{\hbar}\right) \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} \frac{dE}{2\pi} T(E, k_y) \cdot [f(E, k_y, \mu_S) - f(E, k_y, \mu_D)], \quad (5)$$

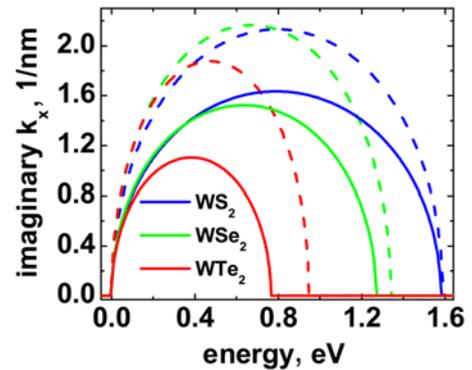
where  $e$  is the electronic charge,  $\hbar$  is the reduced Planck's constant, and we use RGFA [34, 35] to calculate the transmission coefficient

$$T = \text{tr}(\Gamma_{1,1}^S [A_{1,1} - G_{1,1} \Gamma_{1,1}^S G_{1,1}^\dagger]), \quad (6)$$

where  $G$  is the retarded Green's function and  $\Gamma^S$  is the source broadening function [34, 35].

**3. Results and discussions:** The imaginary wave vector that connects the conduction band to the valence band through the energy gap is the key factor for evaluating the direct BTBT probability. As the current flow in a tunnel field-effect transistor is controlled by the direct BTBT, we first need to examine the imaginary wave vector that connects the band edges of a monolayer  $\text{MX}_2$ . The imaginary wave vector versus energy curves of six monolayer  $\text{MX}_2$  materials is shown in Fig. 2. The solid lines are for  $M=W$  and the corresponding dashed lines are for  $M=\text{Mo}$ . The area under the imaginary wave vector curve has an inverse relation with the direct BTBT probability. The lesser the area is, the more the tunnelling probability is. Clearly,  $\text{WTe}_2$  has the highest tunnelling probability as it has the lowest area. Taking  $\text{WTe}_2$  as the reference, the area ratios for Mo materials are  $\text{MoS}_2:\text{MoSe}_2:\text{MoTe}_2 = 4.03:3.46:2.11$ , and for W materials are  $\text{WS}_2:\text{WSe}_2:\text{WTe}_2 = 3.06:2.29:1$ . Therefore, as source material, the best choice is obviously  $\text{WTe}_2$ , the next one is  $\text{MoTe}_2$ , and so on.

First, a TFET is well known to have bipolar characteristics, i.e. current flows for both positive and negative gate biases. Second, a TFET generally has a poor drive current. One of the effective ways to block the bipolar characteristics and to boost the drive current is to use a source-channel HTJ [12, 14, 20, 39, 40] with a staggered band alignment. As  $\text{WTe}_2$  has the highest BTBT probability (the lowest area of the imaginary wave vector curve), we choose  $\text{WTe}_2\text{-WS}_2$  HTJ for the same M,  $\text{WTe}_2\text{-MoTe}_2$  HTJ for the same X, and  $\text{WTe}_2\text{-MoS}_2$  mixed HTJ. In all three cases, the HTJ band alignment is TYPE-II as shown in Fig. 1b and  $\text{WTe}_2$  is the source material for the highest possible drive current. We took the band alignment parameters,  $\Delta E_C$  and  $\Delta E_V$  from [41].



**Fig. 2** Imaginary wave vector  $k_x$  versus energy plots for six monolayer  $\text{MX}_2$  materials. The solid lines are for  $M=W$  and the corresponding dashed lines are for  $M=\text{Mo}$ . The valence band top is the reference energy

The drain current,  $I_D$ , versus the gate bias,  $V_{GS}$ , characteristics for three HTJ together with the  $WTe_2$  HJ channels are shown in Fig. 3. We set drain bias,  $V_{DS}$  to 0.3 V and swing  $V_{GS}$  over a wide range. Then the  $I$ - $V$  curves are shifted along the voltage axis to set  $V_{GS} = 0$  at  $I_D = 10^{-6}$   $\mu A/\mu m$ . Note that the bipolar part (negative  $V_{GS}$ ) of the HJ channel is not shown in the figure for better visibility. In terms of on-state current and turn-on slope, the  $WTe_2$ - $MoTe_2$  HTJ TFET and the  $WTe_2$  HJ TFET have very similar characteristics, whereas,  $WTe_2$ - $MoS_2$  and  $WTe_2$ - $WS_2$  HTJ TFETs have improved characteristics. As off-state is set at  $I_D = 10^{-6}$   $\mu A/\mu m$  and  $V_{GS} = 0$ , we defined on-state as  $V_{GS} = V_{DS} = 0.3$  V, and found that the on-state currents are, respectively, 620, 7.6, 0.63, and 0.43  $\mu A/\mu m$  for  $WTe_2$ - $MoS_2$  HTJ,  $WTe_2$ - $WS_2$  HTJ,  $WTe_2$ - $MoTe_2$  HTJ, and  $WTe_2$  HJ TFETs. The corresponding average turn-on slopes are 15.6, 17.8, 28.3, and 31.3 mV/dec over the drain current range of  $10^{-6}$  to  $10^{-2}$   $\mu A/\mu m$ . Clearly, the  $WTe_2$ - $MoTe_2$  HTJ and the  $WTe_2$  HJ TFETs have similar turn-on and on-state behaviour. However, the on-state current of  $WTe_2$ - $MoS_2$  TFET is far better than other three TFETs, although its turn-on slope is close to that of  $WTe_2$ - $WS_2$  TFET, i.e. the  $WTe_2$ - $MoS_2$  HTJ has the highest drive current with an on/off current ratio of  $6.2 \times 10^8$  for a 0.3 V swing. Lam *et al.* [14] simulated various HJ and HTJ TFETs and reported that  $MoTe_2$ - $WTe_2$  HTJ has the highest drive current for p-TFET and  $WTe_2$  HJ is best for n-TFET. The HTJ combinations that have been used for n-TFETs are  $WS_2$ - $MoS_2$ ,  $WSe_2$ - $MoSe_2$ , and  $WTe_2$ - $MoTe_2$ , i.e.  $MX_2$  HTJs with the same X. However, Cao *et al.* [4] reported that  $WTe_2$ - $MoS_2$  is the best HTJ combination, which is consistent with our results. Lateral HTJs of  $WTe_2$ - $MoS_2$  and  $MoTe_2$ - $MoS_2$  have also been reported as the most promising combinations [15]. Li *et al.* [20] reported very steep turn-on characteristics of  $WTe_2$ - $MoS_2$  vertical HTJ.

To understand the physics behind the high drive current in  $WTe_2$ - $MoS_2$  HTJ TFET, we plot the on-state electric field distribution along the channel in Fig. 4 and the band profiles together with the current spectrum in Fig. 5. The HTJ is located at  $x=0$ . The negative electric field in Fig. 4 indicates that the electrons move in the positive  $x$  direction (from source to drain). The electric field magnitude at the  $WTe_2$ - $WS_2$  junction is 15.77 MV/cm and it is 11.46 MV/cm at  $WTe_2$ - $MoS_2$  junction, i.e. in on-state, the junction field value is higher at  $WTe_2$ - $WS_2$  junction. Clearly, the electric field is not the origin of the high drive current of  $WTe_2$ - $MoS_2$  HTJ.

From current density profiles of Fig. 5 we see that  $WTe_2$ - $MoS_2$  HTJ TFET has a peak current density of  $8.65 \times 10^3$   $\mu A/\mu m/eV$  at energy  $E = -0.093$  eV (source Fermi level is the reference). The tunnel path at this energy is 1.93 nm long, whereas, the  $WTe_2$ - $WS_2$  HTJ TFET has the peak current density of 67.6  $\mu A/\mu m/eV$  and the corresponding tunnel path is 5.74 nm long. Clearly, the shortest tunnel path results in high drive current

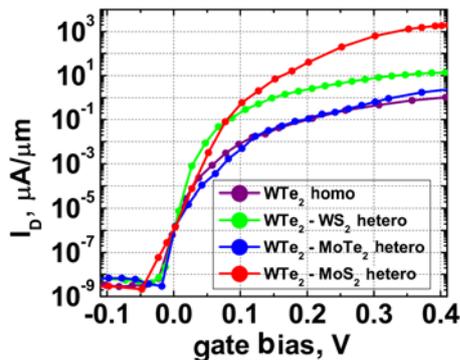


Fig. 3 Drain current versus gate bias plots for  $MX_2$  homo and hetero junction n-channel TFETs. The drain to source bias  $V_{DS} = 0.3$  V

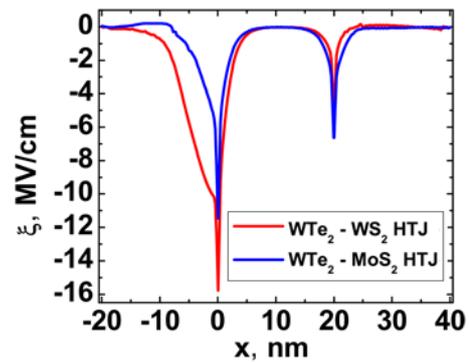


Fig. 4 On-state electric field along the transport direction of  $WTe_2$ - $MoS_2$  and  $WTe_2$ - $WS_2$  HTJ TFETs

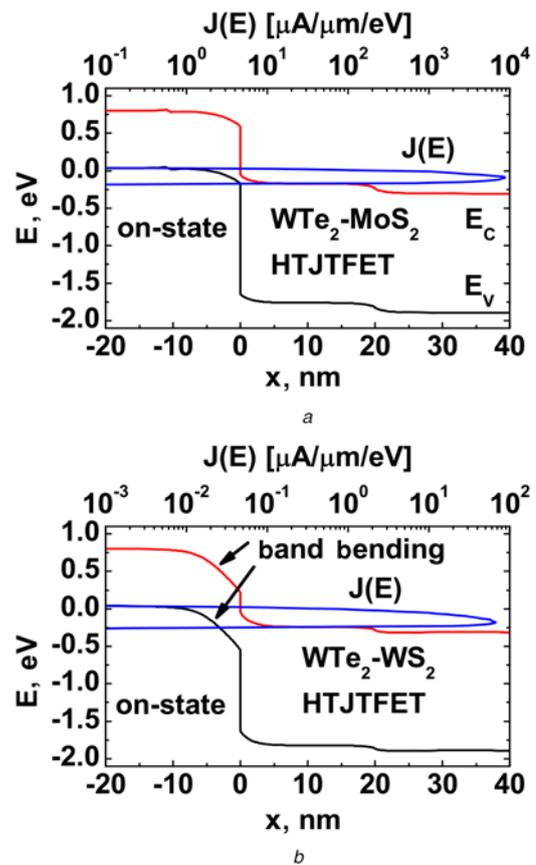


Fig. 5 On-state band profiles and current spectrum  
a  $WTe_2$ - $MoS_2$  HTJ TFET  
b  $WTe_2$ - $WS_2$  HTJ TFET. Source Fermi level is the energy reference

in  $WTe_2$ - $MoS_2$  HTJ TFET. Despite the same source material and same type (TYPE-II) of band alignment, a longer tunnel path is created in  $WTe_2$ - $WS_2$  junction due to the high junction field (see Fig. 4). The high junction field creates larger band bending near the junction (see two arrows in Fig. 5b) which results in longer tunnelling path.

To gain further insight into the physics of high drive current in  $WTe_2$ - $MoS_2$  HTJ TFET, we look into the band alignment again. We denoted the energy gap between the conduction band of the channel material and the valence band of the source material as  $\delta E_{cv}$  as shown in Fig. 1b. Taking  $WTe_2$  as the source material in all HTJs, the  $\delta E_{cv}$  values for  $MoS_2$ ,  $MoSe_2$ ,  $MoTe_2$ ,  $WS_2$ , and  $WSe_2$  are, respectively, 0.13, 0.51, 0.60, 0.51, and 0.82 eV [41]. The lowest value of  $\delta E_{cv}$  in  $WTe_2$ - $MoS_2$  HTJ is the origin for

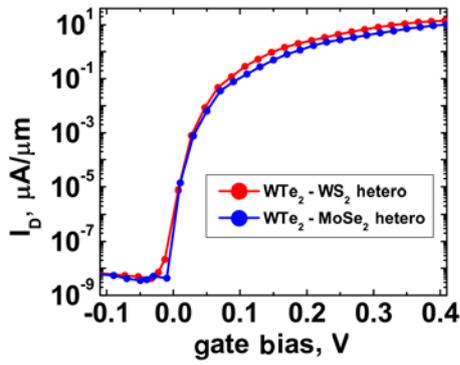


Fig. 6 Comparison of  $I$ - $V$  characteristics of  $WTe_2$ - $WS_2$  and  $WTe_2$ - $MoSe_2$  HTJ TFETs. Both HTJs have the same  $\delta E_{cv}$  value

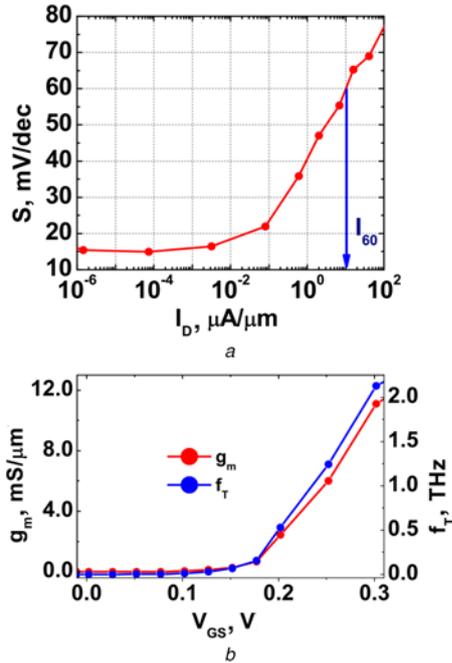


Fig. 7 Turn-on slope, transconductance, and cut-off frequency plots  
a Subthreshold slope versus drain current plot  
b Transconductance  $g_m$  and cut-off frequency  $f_T$  versus gate bias plots for the  $WTe_2$ - $MoS_2$  HTJ TFET

lower on-state electric field, which results in the shortest tunnel path. The origin can be further verified from the values of  $\delta E_{cv}$ . We see that both the  $WTe_2$ - $WS_2$  and  $WTe_2$ - $MoSe_2$  HTJs have the same  $\delta E_{cv}$  values. Therefore, both TFETs should have very similar  $I$ - $V$  characteristics. This is, in fact, the case. The results are compared in Fig. 6. The slight difference may come from different dielectric values of  $WS_2$  and  $MoSe_2$ .

After gaining the insight of high current in  $WTe_2$ - $MoS_2$  HTJ TFET, we next evaluate the performance metrics of this structure. For a 0.3 V swing in  $V_{GS}$ , we find that the on-state current is  $620 \mu A/\mu m$ , which is corresponding to an on/off current ratio of  $6.2 \times 10^8$ . The subthreshold slope  $S$ , transconductance  $g_m$ , and unity current gain frequency  $f_T$  are shown in Fig. 7. The subthreshold slope  $S$  is below 60 mV/dec over seven decades change in current. The average  $S = 15.6$  mV/dec in the  $I_D$  range of  $10^{-6}$ - $10^{-2} \mu A/\mu m$ . A reference independent figure of merit for sub-60 mV/dec devices is  $I_{60}$ , i.e. the drain current at 60 mV/dec. According to Vandenberghe *et al.* [42], the  $I_{60}$  value of a HJ TFET should be in the range of 1-10  $\mu A/\mu m$  to compete with metal oxide semiconductor field effect transistors (MOSFETs).

Table 1 Benchmarking performance metrics of  $WTe_2$ - $MoS_2$  HTJ TFET against ITRS requirements for 2026 LOP and LSTP devices

Parameter	$WTe_2$ - $MoS_2$ TFET	2026 LOP FET	2026 LSTP FET
$I_{on}$ , $\mu A/\mu m$	620	666	286
$I_{on}/I_{off}$	$6.2 \times 10^8$	$1.3 \times 10^5$	$2.86 \times 10^7$
$S$ , mV/dec	15.6	—	—
$g_m$ , mS/ $\mu m$	10.98	—	—
$C_f$ , fF/ $\mu m$	0.194	0.18	0.18
$C_{tot}$ , fF/ $\mu m$	0.829	0.402	0.383
$\tau_s$ , ps	0.401	0.26	0.73
$CV^2$ , fJ/ $\mu m$	0.0746	0.07	0.11

From Fig. 7a, we see that the  $I_{60}$  value is  $11.97 \mu A/\mu m$ , which is large enough to battle against the MOSFET competitor. The transconductance plotted in Fig. 7b is also high due to high drive current. The on-state value of transconductance is  $g_m = 10.98$  mS/ $\mu m$ , which is significantly higher than its 60 mV/dec competitors  $MoS_2$  and Si ultra-thin body MOSFETs [43].

The gate capacitance has the components of oxide capacitance, quantum capacitance, and fringing field capacitance. While the quantum capacitance is computed from  $\delta Q_{ch}/\delta \phi_s$ , where  $Q_{ch}$  is the channel charge and  $\phi_s$  is the surface potential, the fringing field capacitance is obtained from

$$C_f = \epsilon_{ext} \frac{\partial}{\partial V_{GS}} \int dz [\mathcal{E}_{GS}(z) + \mathcal{E}_{GD}(z)]. \quad (7)$$

Here,  $\mathcal{E}_{GS}(z)$  and  $\mathcal{E}_{GD}(z)$  are the electric field components in the axial direction that come out of the gate metal towards the source and drain contacts, respectively, and  $\epsilon_{ext}$  is the dielectric constant of the extended dielectric. The fringing field capacitance in parallel with the series combination of the quantum and oxide capacitances gives the total gate capacitance  $C_g$ . The unity current gain frequency (or cut-off frequency) calculated from  $f_T = g_m/2\pi C_g$  is shown in Fig. 7b. The on-state value of  $f_T$  is 2.1 THz. The switching delay time obtained from  $\tau_s = C_g V_{DD}/I_{on}$  is 0.401 ps in on-state. In Table 1, we benchmark the performance metrics of  $WTe_2$ - $MoS_2$  HTJ TFET against the ITRS requirements for 2026 LOP logic and LSTP logic. Although the gate capacitance and the delay time are slightly high, the dynamic power dissipation ( $CV^2$ ) meets the requirement.

**4. Conclusion:** In conclusion, we have performed simulation studies of monolayer  $MX_2$  HJ and HTJ tunnel FETs. The complex band structures of different  $MX_2$  monolayer materials show that  $WTe_2$  is the most promising source material for BTBT. Simulation results of different HTJ structures with  $WTe_2$  as the source material and of the  $WTe_2$  HJ structure show that the  $WTe_2$ - $MoS_2$  HTJ TFET supplies the highest drive current. The energy gap between the valence band of  $WTe_2$  and the conduction band of  $MoS_2$  is very small. Therefore, band alignment for BTBT happens at the junction at a relatively lower electric field. This results in small band bending near the HTJ which creates the shortest tunnel path and hence the highest drive current. The  $WTe_2$ - $MoS_2$  HTJ TFET has high on-current, high transconductance, and very low subthreshold slope that meet the ITRS 2026 LOP requirements. However, the switching delay is slightly larger due to the high gate capacitance.

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