

# Sub 10 nm Bilayer Bi<sub>2</sub>O<sub>2</sub>Se Transistors

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Due to high carrier mobility and excellent air stability, emerging 2D semiconducting Bi<sub>2</sub>O<sub>2</sub>Se is attracting much attention as a potential channel candidate for the next-generation field effect transistor (FETs). Although the fabricated bilayer (BL) and few layers Bi<sub>2</sub>O<sub>2</sub>Se FETs exhibit a large current on/off ratio (>10<sup>6</sup>) and a near-ideal subthreshold swing value (≈65 mV dec<sup>-1</sup>), the performance limit of ultrashort channel Bi<sub>2</sub>O<sub>2</sub>Se FET is obscure. Here the ballistic performance upper limit of the sub 10 nm BL Bi<sub>2</sub>O<sub>2</sub>Se metal-oxide-semiconductor FETs (MOSFETs) is simulated for the first time by using *ab initio* quantum transport simulations. The optimized BL Bi<sub>2</sub>O<sub>2</sub>Se n-type MOSFETs can fulfill the high performance device requirements on the on-state current, delay time, and power dissipation of the International Technology Roadmap for Semiconductors in 2028 until the gate length is scaled down to 5 nm. Therefore, Moore's law can be extended to 5 nm by taking BL Bi<sub>2</sub>O<sub>2</sub>Se as the channel.

## 1. Introduction

Field effect transistors (FETs) with a channel length smaller than 10 nm are the compelling demand for the electronics

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DOI: 10.1002/aelm.201800720

quest in the next decade.<sup>[1–4]</sup> However, Moore's law has approached its physical limit because silicon FETs scaling down to 10 nm gate length especially for the sub 5 nm node is difficult to have satisfactory performance caused by the severe short channel effect.<sup>[1,5,6]</sup> To extend Moore's law down to sub 10 nm, 2D semiconductors are proposed as the next-generation channel candidates to replace silicon.<sup>[2,7–10]</sup> Their atomic thickness benefits the improvement of gate electrostatic controlling ability, and their uniform and free-dangling-bond structures lead to improved transporting efficiency.<sup>[5,11–14]</sup> The most extensively concerned 2D semiconductors are transition metal dichalcogenides (TMDs)

like 2D MoS<sub>2</sub> and black phosphorene (BP).<sup>[10,15–20]</sup> The 1 nm L<sub>g</sub> bilayer (BL) MoS<sub>2</sub> FET and 8.2 nm L<sub>g</sub> monolayer (ML)/9.6 nm L<sub>g</sub> multilayer MoS<sub>2</sub> FETs are successfully fabricated.<sup>[1,3,21]</sup> However, 2D MoS<sub>2</sub> FETs with low carrier mobility (≈270 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>),<sup>[22–26]</sup> suffer from low on-state current (≈20 μA μm<sup>-1</sup>)<sup>[1]</sup> and thus poor device switching speed. BP FETs possess a high carrier mobility (≈1000 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>) but are instable under ambient condition.<sup>[27–29]</sup> It is urgent to explore 2D semiconductors with high carrier mobility, air stability, and superior device performances in logic devices simultaneously.

Very recently, ML, BL, and few layers Bi<sub>2</sub>O<sub>2</sub>Se are successfully fabricated on mica substrate by means of chemical vapor deposition (CVD) method.<sup>[30–32]</sup> Bi<sub>2</sub>O<sub>2</sub>Se, as a typical bismuth-based oxychalcogenide semiconductor, is composed by Bi<sub>2</sub>O<sub>2</sub> layers and Se layers under weak electrostatic interaction.<sup>[8,22,32–34]</sup> Remarkably, 2D Bi<sub>2</sub>O<sub>2</sub>Se has an ultrahigh electron mobility (>20 000 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> at low temperature, ≈450 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> at room temperature), which exceeds that of MoS<sub>2</sub>.<sup>[30–32,35–37]</sup> 2D Bi<sub>2</sub>O<sub>2</sub>Se down to monolayer shows robust stability in air, and in moist or thermal conditions.<sup>[32]</sup> Since the stability is a precondition for large-scale production, 2D Bi<sub>2</sub>O<sub>2</sub>Se is a more feasible candidate of the next-generation channel material compared with BP. So far, the ML Bi<sub>2</sub>O<sub>2</sub>Se high performance devices have not been fabricated yet due to a big contact resistance while the long channel top-gated high performance BL and few layer Bi<sub>2</sub>O<sub>2</sub>Se FETs with Au/Pd electrode have been fabricated and exhibited a large current on/off ratio (>10<sup>6</sup>).<sup>[32]</sup> However, the performance upper limit of BL Bi<sub>2</sub>O<sub>2</sub>Se FET in ultrashort channel remains unknown. Therefore, it is highly desirable to explore whether sub 10 nm BL Bi<sub>2</sub>O<sub>2</sub>Se FET can meet the

requirements of International Technology Roadmap for Semiconductors (ITRS)<sup>[38]</sup> in the next decade.

In this work, we theoretically evaluate the device performance of the sub 10 nm double-gated (DG) BL Bi<sub>2</sub>O<sub>2</sub>Se metal-oxide-semiconductor FETs (MOSFETs) using ab initio quantum transport simulations. The highest on-state current of the BL Bi<sub>2</sub>O<sub>2</sub>Se p-MOSFETs without underlap (UL) structure could only fulfill ≈55% high performance (HP) ITRS goals at  $L_g = 9$  nm while it can increase to ≈77% HP on-state current requirement of the ITRS with help of underlap structure. The BL Bi<sub>2</sub>O<sub>2</sub>Se n-MOSFETs could not fulfill the HP ITRS goals without underlap structure while with the resort of underlap structure, they could meet the standard of on-state current, delay time, and power dissipation indicator (PDP) of ITRS goals for HP devices until  $L_g$  scaling down to 5 nm. Therefore, BL Bi<sub>2</sub>O<sub>2</sub>Se is a potential channel material for sub 10 nm transistor due to its high device performance and high stability.

## 2. Methodology

The transport properties are calculated by using the density functional theory (DFT) coupled with the nonequilibrium Green's function (NEGF) formalism, as implemented in the Atomistix ToolKit 2017 package.<sup>[39,40]</sup> The transmission coefficient  $T_{k_{||}}(E)$  ( $k_{||}$  stands for the reciprocal lattice vector along the surface-parallel direction in the irreducible Brillouin zone) is represented by<sup>[5,41]</sup>

$$T_{k_{||}}(E) = \text{Tr} \left[ \Gamma_{k_{||}}^l(E) G_{k_{||}}(E) \Gamma_{k_{||}}^r(E) G_{k_{||}}^\dagger(E) \right] \quad (1)$$

where  $G_k(E)$  and  $G_k^\dagger(E)$  stand for the retard and advanced Green's function, respectively, and  $\Gamma_{k_{||}}^r(E) = i(\Sigma_{l/r} - \Sigma_{l/r}^\dagger)$  is the broadening width originating from left/right electrode in the form of self-energy  $\Sigma_{l/r}$ . Given a certain energy,  $T_{k_{||}}(E)$  is averaged over all different  $k_{||}$ . The drain current  $I_{ds}$  is calculated through the following Landauer–Büttiker formula<sup>[42–44]</sup>

$$I_{ds}(V_b, V_g) = \frac{2e}{h} \int_{-\infty}^{+\infty} \{T(E, V_b, V_g) [f_s(E - \mu_s) - f_D(E - \mu_D)]\} dE \quad (2)$$

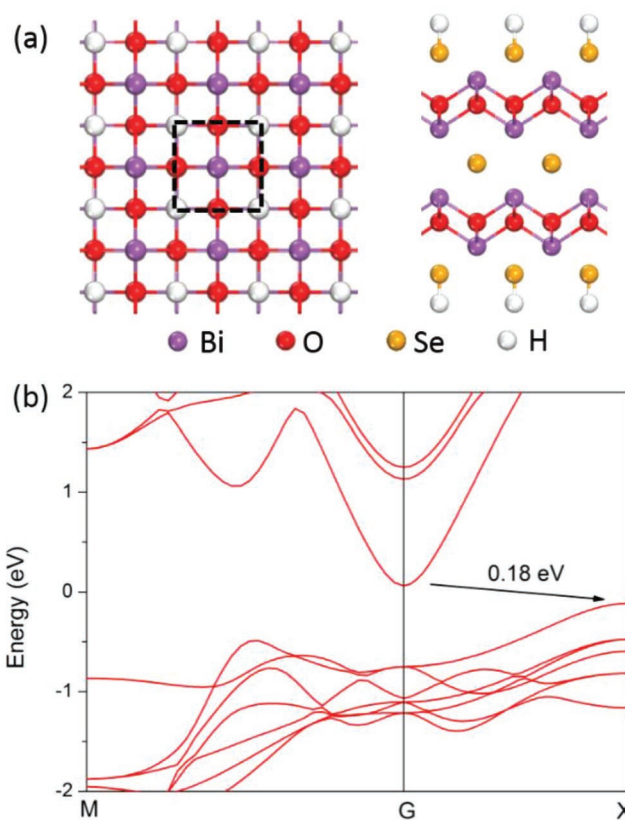
where  $f_s$  and  $f_D$  are the Fermi–Dirac distribution function for the source and drain, respectively,  $\mu_s$  and  $\mu_D$  are the Fermi level of the source and drain, respectively. The double zeta polarized basis set (DZP) is adopted. The temperature is set to 300 K, and the real-space mesh cutoff is taken as 75 hartree. The  $k$ -point meshes for the electrode region and the central region are  $35 \times 1 \times 35$  and  $35 \times 1 \times 1$ , respectively. The generalized gradient approximation (GGA) in the form of Perdew–Burke–Ernzerhof (PBE) potential is employed to describe the exchange correlation interaction.<sup>[45]</sup> In the FET configuration, electron–electron interaction of the channel is heavily weakened by the introduced carriers. The DFT-GGA method based on single electron approximation approaches the quasiparticle method and is accurate enough to describe the electronic structure of this case.<sup>[46–48]</sup> For example, the bandgap of degenerately doped ML MoSe<sub>2</sub> is 1.52 eV at DFT-GGA level,<sup>[49]</sup> which is in great consistency with the value of 1.59 eV calculated by quasiparticle method within GW approximation<sup>[48]</sup> and 1.58 eV obtained

by angle-resolved photoemission spectroscopic.<sup>[50]</sup> For another example, the calculated transport gap of ML, BL, and trilayer BP with Ni electrode at the DFT-GGA level is 0.65, 0.81, and 0.68 eV, in good accordance with the experimentally measured value of 1.00, 0.71, and 0.61 eV respectively.<sup>[51–53]</sup>

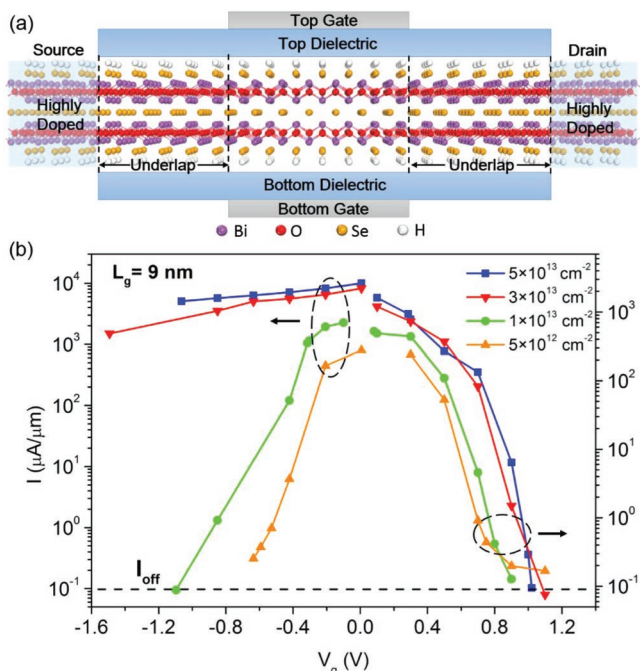
## 3. Results and Discussions

### 3.1. Model and Device

Unlike the well-known 2D materials, such as few layers MoS<sub>2</sub> and BP, which are stacked via interlayer van der Waals interaction, 2D Bi<sub>2</sub>O<sub>2</sub>Se is separated by charge-compensating cations and anions. Se<sup>2-</sup> anionic layer is sandwiched by (Bi<sub>2</sub>O<sub>2</sub>)<sup>2+</sup> cationic layers via electrostatic interaction.<sup>[30]</sup> To balance the non-stoichiometry caused by additional Se layer in 2D Bi<sub>2</sub>O<sub>2</sub>Se, hydrogen atoms are added to passivate the outmost Se atoms.<sup>[35]</sup> The bulk Bi<sub>2</sub>O<sub>2</sub>Se has a tetragonal structure with lattice constants of  $a = b = 3.88$  Å and  $c = 12.16$  Å.<sup>[32]</sup> The optimized lattice parameters of BL Bi<sub>2</sub>O<sub>2</sub>Se is  $a = b = 3.98$  Å (Figure 1a). The calculated bandgap of BL Bi<sub>2</sub>O<sub>2</sub>Se is 0.18 eV at the DFT-GGA level (Figure 1b), which is in agreement with the previously calculated value at the DFT-GGA level.<sup>[32]</sup> The two-probe DG BL Bi<sub>2</sub>O<sub>2</sub>Se MOSFET is constructed with intrinsic BL Bi<sub>2</sub>O<sub>2</sub>Se as channel and n-doped or p-doped BL Bi<sub>2</sub>O<sub>2</sub>Se as electrode in semi-infinite length, as shown in Figure 2a. The segments



**Figure 1.** Lattice and electronic structure of BL Bi<sub>2</sub>O<sub>2</sub>Se. a) Top and side views of BL Bi<sub>2</sub>O<sub>2</sub>Se structure. b) Band structure of BL Bi<sub>2</sub>O<sub>2</sub>Se.



**Figure 2.** a) Schematic view of the DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFET. b) Transfer characteristics for different source and drain doping concentration of electron ( $N_e$ ) (left-hand axis) and hole ( $N_h$ ) (right-hand axis) with  $L_g = 9$  nm.

between the gate and the electrode are UL constitutions. Symmetric UL lengths ( $L_{UL}$ ) of 0, 2, and 4 nm are considered. The equivalent oxide thicknesses (EOTs) of the  $\text{SiO}_2$  dielectric is set to 0.41–0.56 nm, and the supply voltage ( $V_{dd}$ ) of each device is 0.64–0.72 V ( $=V_b$ ), which are adapted to the ITRS requirements for HP devices in different  $L_g$ . Off-state current  $I_{off}$  is fixed at

$0.1 \mu\text{A} \mu\text{m}^{-1}$ , the OFF current for HP application requirement of ITRS. Only HP devices are considered, because  $I_{ds}$  is difficult to converge to the order of magnitude of  $10^{-5} \mu\text{A} \mu\text{m}^{-1}$ , the low power (LP) goal of ITRS.  $I_{on}$  is evaluated at a specific supply gate voltage ( $V_g$  (on) =  $V_b + V_g$  (off)). The key figures of merit of the ballistic performance are benchmarked against the ITRS requirements for HP devices in **Tables 1** and **2**.

In order to ensure the most efficient carrier injection, it is critical to employ the optimal doping concentration on the checked BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs. The doping concentration ranging from  $5 \times 10^{12}$  to  $5 \times 10^{13} \text{ cm}^{-2}$  are considered.<sup>[5]</sup> The transfer characteristics of the 9 nm gate length BL  $\text{Bi}_2\text{O}_2\text{Se}$  n- and p-MOSFETs without UL at the bias of 0.72 V in four doping concentrations are plotted in Figure 2b. The optimized electron (hole) doping concentration of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n (p)-MOSFET is  $N_e = 1 \times 10^{13} \text{ cm}^{-2}$  ( $N_h = 5 \times 10^{13} \text{ cm}^{-2}$ ) because the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n (p)-MOSFET in this circumstance can not only reach the off-state of the HP requirement of ITRS in 2022 horizon but also possess the maximum  $I_{on}$  and the minimum subthreshold swing (SS) compared with other cases (Table S1, Supporting Information) simultaneously.

### 3.2. Current

In a logic switch, a high on-state current implies a high operating speed and is one of the key figures of merit of the device performance, especially for the HP servers.<sup>[54,55]</sup> The typical transfer characteristics of the n- and p-type sub 10 nm DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs without UL at biases of  $V_b = 0.72, 0.69, 0.64,$  and  $0.64$  V with  $L_g = 9, 7, 5,$  and  $3$  nm, respectively, are shown in **Figure 3**. All p-MOSFETs have small enough source–drain leakage currents to fulfill the OFF state requirement

**Table 1.** Benchmark of the ballistic performance of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n-MOSFETs against the ITRS 2013 requirements for HP transistors of the next decades.

	$L_g$ [nm]	$L_{UL}$ [nm]	EOT [nm]	$V_{dd}$ [V]	SS [mV dec <sup>-1</sup> ]	$I_{on}$ [ $\mu\text{A} \mu\text{m}^{-1}$ ]	$I_{off}$ [ $\mu\text{A} \mu\text{m}^{-1}$ ]	$C_t$ [fF $\mu\text{m}^{-1}$ ]	$\tau$ [ps]	PDP [fJ $\mu\text{m}^{-1}$ ]
	9	0	0.54	0.72	111	1144	0.1	0.558	0.351	0.289
		2			102	1794	0.1	0.522	0.210	0.270
		4			112	– <sup>a)</sup>	– <sup>a)</sup>	0.486	– <sup>a)</sup>	– <sup>a)</sup>
ITRS 2022	8.8	0	0.49	0.69	117	– <sup>a)</sup>	– <sup>a)</sup>	0.87	0.463	0.45
		2			100	938	0.1	0.356	0.261	0.169
		4			118	1302	0.1	0.437	0.231	0.208
ITRS 2024	7.3	0	0.41	0.64	146	– <sup>a)</sup>	– <sup>a)</sup>	0.77	0.451	0.36
		2			105	– <sup>a)</sup>	– <sup>a)</sup>	0.302	– <sup>a)</sup>	– <sup>a)</sup>
		4			114	916	0.1	0.343	0.240	0.141
ITRS 2028	5.1	0	0.41	0.64	322	– <sup>a)</sup>	– <sup>a)</sup>	0.60	0.423	0.24
		2			141	– <sup>a)</sup>	– <sup>a)</sup>	0.253	– <sup>a)</sup>	– <sup>a)</sup>
		4			134	– <sup>a)</sup>	– <sup>a)</sup>	0.235	– <sup>a)</sup>	– <sup>a)</sup>

<sup>a)</sup>ITRS  $I_{off}$  standard cannot be reached in our investigate gate voltage region.  $L_g$ : the gate length. EOT: the equivalent oxide thickness. SS: the subthreshold swing.  $V_{dd}$ : the supply voltage.  $I_{on}$ : the on-state current.  $I_{off}$ : the off-state current.  $C_t$ : the total capacitance.  $\tau$ : the delay time. PDP: the power dissipation.

**Table 2.** Benchmark of the ballistic performance of the BL Bi<sub>2</sub>O<sub>2</sub>Se p-MOSFETS against the ITRS 2013 requirements for HP transistors of the next decades.

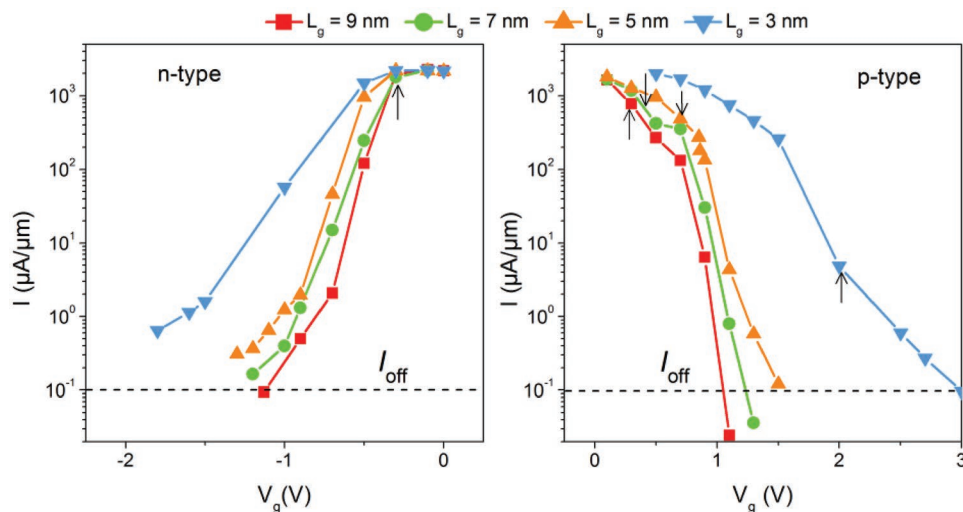
	$L_g$ [nm]	$L_{UL}$ [nm]	EOT [nm]	$V_{dd}$ [V]	SS [mV dec <sup>-1</sup> ]	$I_{on}$ [ $\mu\text{A } \mu\text{m}^{-1}$ ]	$I_{off}$ [ $\mu\text{A } \mu\text{m}^{-1}$ ]	$C_t$ [fF $\mu\text{m}^{-1}$ ]	$\tau$ [ps]	PDP [f $\mu\text{m}^{-1}$ ]	
	9	0	0.54	0.72	86	779	0.1	0.729	0.675	0.378	
		2			65	958	0.1	0.553	0.414	0.289	
		3			84	1039	0.1	0.525	0.363	0.272	
		4			73	631	0.1	0.420	0.486	0.218	
ITRS 2022	8.8					1350	0.1	0.87	0.463	0.45	
		7	0	0.49	0.69	102	729	0.1	0.599	0.567	0.285
		2				83	720	0.1	0.474	0.456	0.226
ITRS 2024	7.3	4			65	477	0.1	0.345	0.414	0.164	
		5	0	0.41	0.64	181	275	0.1	0.467	1.077	0.190
		2				96	585	0.1	0.342	0.375	0.140
ITRS 2028	5.1	4			60	540	0.1	0.276	0.327	0.113	
		3	0	0.41	0.64	400	2	0.1	0.311	99.387	0.127
		2				320	18	0.1	0.272	9.984	0.111
		4			172	221	0.1	0.219	0.624	0.090	

$L_g$ : the gate length. EOT: the equivalent oxide thickness. SS: the subthreshold swing.  $V_{dd}$ : the supply voltage.  $I_{on}$ : the on-state current.  $I_{off}$ : the off-state current.  $C_t$ : the total capacitance.  $\tau$ : the delay time. PDP: the power dissipation.

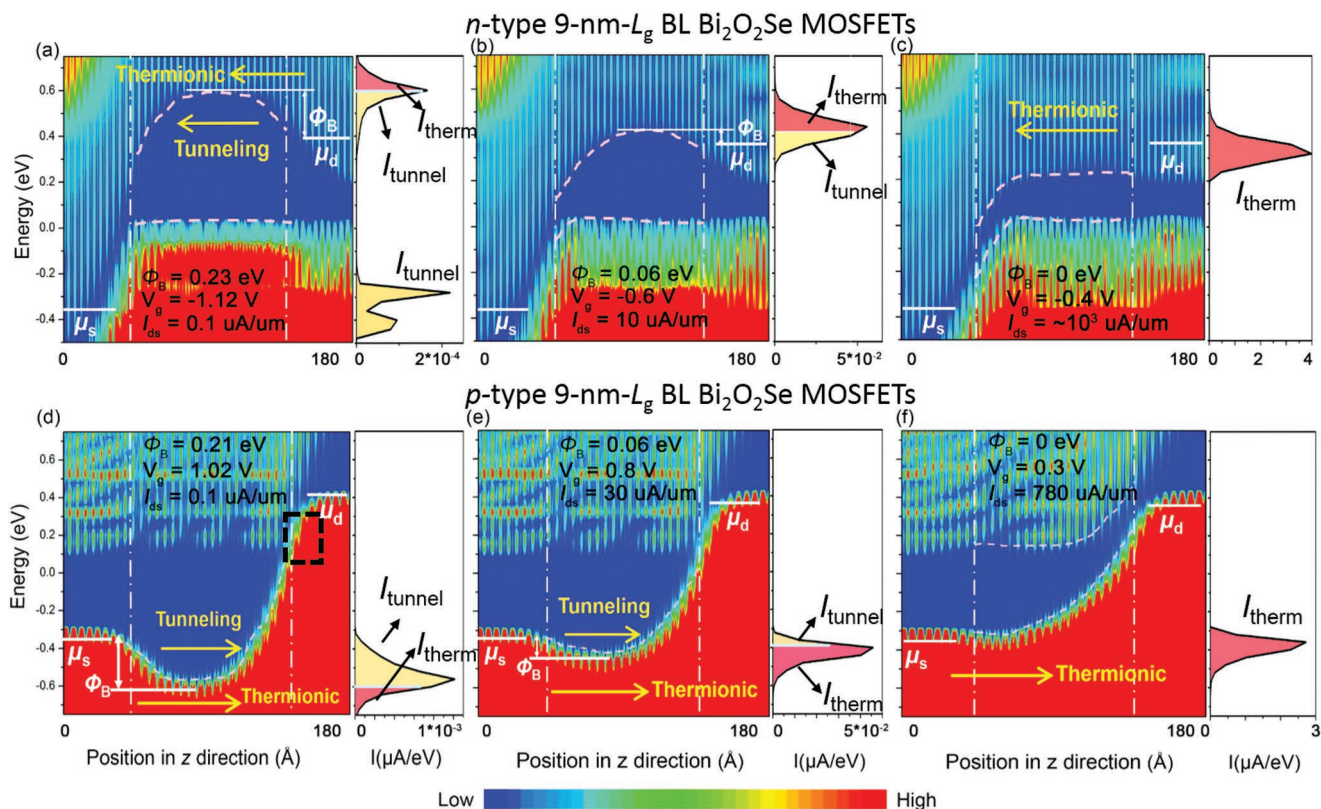
of HP device ( $0.1 \mu\text{A } \mu\text{m}^{-1}$ ) and share the similar maximal current  $I_{max}$ .<sup>[8,54]</sup> However, the on current  $I_{on}$  is different from  $I_{max}$  because it is evaluated at a specific gate voltage window ( $V_g(\text{on}) = V_b + V_g(\text{off})$ ), where  $V_b$  is the bias voltage,  $V_g(\text{on})$  and  $V_g(\text{off})$  are the gate voltage of ON state and OFF state, respectively.  $I_{on}$  of these p-MOSFETS at  $L_g = 9, 7, 5,$  and  $3 \text{ nm}$  is  $779, 729, 275,$  and  $2 \mu\text{A } \mu\text{m}^{-1}$ , respectively, much lower than the corresponding ITRS HP required  $1350, 1170, 900,$  and  $900 \mu\text{A } \mu\text{m}^{-1}$ . All the checked n-MOSFETS could not reach the OFF state except for the  $9 \text{ nm}$   $L_g$  device.  $I_{on}$  of BL Bi<sub>2</sub>O<sub>2</sub>Se n-MOSFET at  $L_g = 9 \text{ nm}$  is  $1144 \mu\text{A } \mu\text{m}^{-1}$ , fulfilling the 85% ITRS requirement ( $1350 \mu\text{A } \mu\text{m}^{-1}$ ) for HP devices.

It is noteworthy that the n-MOSFET possesses a higher on-state current than that of the p-MOSFET at  $L_g = 9 \text{ nm}$ . The reason lies in the smaller electron effective mass and the faster electron velocity of the n-MOSFET. The effective mass is proportional to the reciprocal of the curvature of the band dispersion spectrum. From the perspective of the band dispersion spectrum of Figure 1b, the electron effective mass is smaller than the hole one in BL Bi<sub>2</sub>O<sub>2</sub>Se ( $m_e^* = 0.11 m_0$  and,  $m_h^* = 0.81 m_0$ ,  $m_0$  is the free-electron mass). Smaller effective mass increases the carrier velocity according to  $v = \frac{1}{\hbar} \frac{dE}{dk} = \frac{\hbar k}{m^*}$  and thus the current.

It is also worth mentioning that larger effective mass can more



**Figure 3.** Transfer characteristics for the n- and p-type DG BL Bi<sub>2</sub>O<sub>2</sub>Se MOSFETS at different  $L_g$ . The black dash line represents  $I_{off}$  required by the ITRS 2013 for HP devices. The black arrow labels the position of  $I_{on}$  in different  $L_g$ .



**Figure 4.** Position resolved local density of states (LDOS) and the spectrum current in the channel region for the n-type and p-type 9 nm  $L_g$  DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs under  $V_b = 0.72$  V. a–c) 9 nm  $L_g$  n-MOSFET at  $V_g = -1.12$ ,  $-0.6$ , and  $-0.4$  V for OFF state, the intermediate state and ON state, respectively. e–g) 9 nm  $L_g$  p-MOSFET at  $V_g = 1.02$ ,  $0.8$ , and  $0.3$  V for OFF state, the intermediate state and ON state, respectively.  $\mu_s$  and  $\mu_d$  are the electrochemical potential of the source and drain, respectively.  $\Phi_B$  is the effective barrier height. The white dash dot lines are the edges of gate. The yellow dash arrows represent the thermionic and tunneling electron transports.

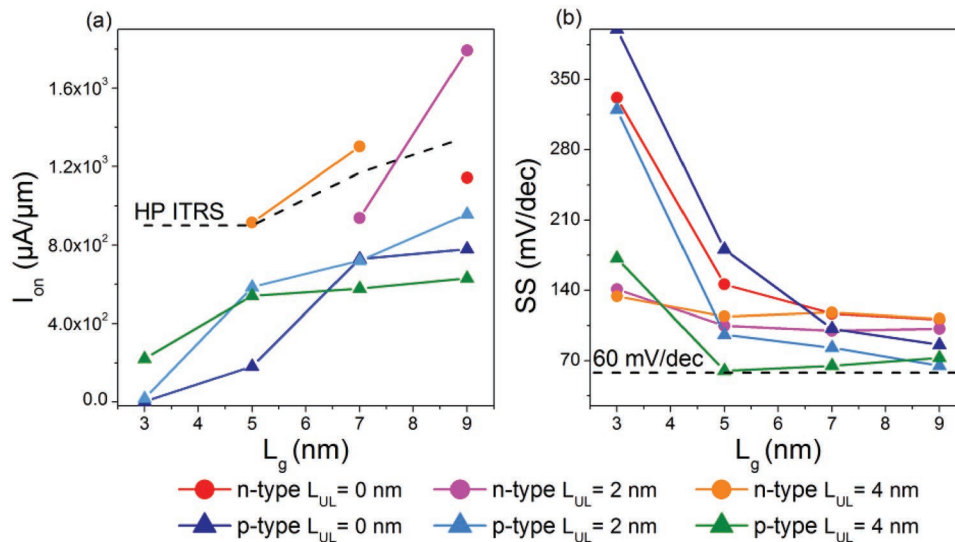
easily block the tunneling leakage because  $I_{\text{tunnel}}$  decreases exponentially with the effective mass, i.e.,  $I_{\text{tunnel}} \propto e^{-l\sqrt{m^*}\Phi_B}$ , where  $l$  and  $\Phi_B$  are the width and the height of the barrier respectively. As a result, the BL  $\text{Bi}_2\text{O}_2\text{Se}$  p-MOSFETs are much easier to reach OFF state than the n-MOSFETs.

To unveil the gate modulation and the current change mechanism, the position resolved local density of states (LDOS) and the spectrum current of the 9 nm  $L_g$  n-MOSFET and the 9 nm  $L_g$  p-MOSFET at different gate voltages ( $V_g$ ) are shown in **Figure 4**.  $I_{\text{ds}}$  is composed by tunneling current ( $I_{\text{tunnel}}$ ) and thermionic current ( $I_{\text{therm}}$ ).  $I_{\text{tunnel}}$  and  $I_{\text{therm}}$  are separated by the top of  $\Phi_B$ . In the OFF state ( $I_{\text{ds}} = 0.1 \mu\text{A} \mu\text{m}^{-1}$ ) of the 9 nm  $L_g$  n-MOSFET (Figure 4a) with  $V_g = -1.12$  V and  $\Phi_B = 0.23$  eV, the conduction band minimum (CBM) and the valence band maximum (VBM) of the channel are lifted by  $V_g$ .  $I_{\text{tunnel}}$  at low energy level stems from the tunneling from the VB to the CB within the left electrode (Figure 4a). In the intermediate state ( $I_{\text{ds}} = 10 \mu\text{A} \mu\text{m}^{-1}$ ) of the 9 nm  $L_g$  n-MOSFET with  $V_g = -0.6$  V (Figure 4b), the upward degree of the CBM of the channel is alleviated and  $\Phi_B$  decreases to 0.06 eV.  $I_{\text{tunnel}}$  and  $I_{\text{therm}}$  sharply increase by two orders of magnitude. In the ON state ( $I_{\text{ds}} = \approx 1000 \mu\text{A} \mu\text{m}^{-1}$ ) of the 9 nm  $L_g$  n-MOSFET (Figure 4c), the supply  $V_g = -0.4$  V releases the upward degree of the CBM of the channel and diminishes  $\Phi_B$ .  $I_{\text{therm}}$  dominates the total current. The VBM of the channel in the intermediate state and

ON state is not lifted upward.  $I_{\text{tunnel}}$  at the VB is much smaller than  $I_{\text{tunnel}}$  and  $I_{\text{therm}}$  at the CB.

The gate modulation of the 9 nm  $L_g$  p-MOSFET (Figure 4d–f) is similar to that of the 9 nm  $L_g$  n-MOSFET. From the OFF state (Figure 4d) to the intermediate state (Figure 4e) and to the ON state (Figure 4f), the downward degree of the VBM of the channel is gradually alleviated,  $\Phi_B$  decreases from 0.21 to 0 eV, and  $I_{\text{therm}}$  dominates the total current. Even if  $\Phi_B$  is vanished,  $I_{\text{on}}$  can only reach few hundreds of  $\mu\text{A} \mu\text{m}^{-1}$  because of the heavier hole effective mass. In spite of the fact that the CB connects to the VB at the right edge of the gate, no current component is observed at this energy range (labeled a black dash square in Figure 4d). This is because the local and discontinuous states in the VB impede electrons moving from the LDOS in Figure 4d–f.

To get a high on-state current, UL as an improvement method can extend the effective channel length, impede the short channel effects and thus effectively boost the device performance. On the other hand, the gate controlling capacity to the uncovered channel region is weaker than the covered one, and too long UL will degrade the device performance. Therefore, the length of UL has to be optimized.<sup>[54]</sup> The transfer characteristics of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n- and p-MOSFETs with different  $L_{\text{UL}}$  are compared in Figures S2 and S3 in the Supporting Information respectively. We benchmark  $I_{\text{on}}$  versus  $L_g$  for the HP DG BL



**Figure 5.** a) HP- $I_{on}$  and b) SS versus  $L_g$  for the n- and p-type DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs at different  $L_{UL}$  as indicated in the legend.

$\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs against the ITRS standards in Figure 5a.  $L_{UL} = 2$  nm is the optimal length for the 9 nm  $L_g$  n-MOSFET because  $I_{on}$  is maximized with a value of  $1794 \mu\text{A} \mu\text{m}^{-1}$  (Table 1), which exceeds the ITRS HP goal ( $1350 \mu\text{A} \mu\text{m}^{-1}$ ), while  $L_{UL} = 4$  nm is so long that the leakage current could not meet the HP OFF state requirement.  $L_{UL} = 4$  nm is the optimal length for both the 7 and 5 nm  $L_g$  n-MOSFETs because  $I_{on}$  is maximized with values of 1302 and  $916 \mu\text{A} \mu\text{m}^{-1}$  and exceeds the ITRS required 1170 and  $900 \mu\text{A} \mu\text{m}^{-1}$  for HP applications, respectively. Hence, the n-MOSFETs with proper UL could extend the Moore's law down to 5 nm. The 3 nm  $L_g$  n-MOSFETs with different  $L_{UL}$  are still vulnerable to the short channel effect and the ITRS required OFF state could not be fulfilled.

$L_{UL} = 3$  nm is the optimal length for the 9 nm  $L_g$  p-MOSFET because  $I_{on}$  is maximized with the value of  $1039 \mu\text{A} \mu\text{m}^{-1}$ , which reaches 77% of the ITRS HP requirement, while  $L_{UL} = 4$  nm is so long that  $I_{on}$  is decreased to 49% of the ITRS HP requirement. The 7 nm  $L_g$  p-MOSFETs with different  $L_{UL}$  could not produce higher  $I_{on}$  ( $720 \mu\text{A} \mu\text{m}^{-1}$  for  $L_{UL} = 2$  nm,  $577 \mu\text{A} \mu\text{m}^{-1}$  for  $L_{UL} = 4$  nm) compared with the 7 nm  $L_g$  p-MOSFET without UL ( $729 \mu\text{A} \mu\text{m}^{-1}$ ).  $I_{on}$  of the 5 nm  $L_g$  p-MOSFETs doubles to 584 and  $570 \mu\text{A} \mu\text{m}^{-1}$ , respectively, when  $L_{UL} = 2$  and 4 nm are adopted. As  $L_{UL}$  extends from 0 to 2 and to 4 nm,  $I_{on}$  of the 3 nm  $L_g$  p-MOSFET increases dramatically from 2 to 18 and to  $221 \mu\text{A} \mu\text{m}^{-1}$ , respectively. However, even if in some cases the p-MOSFETs with UL induces higher  $I_{on}$ , none of these  $I_{on}$  could meet the ITRS goals for HP applications.

### 3.3. Subthreshold Swing

Apart from  $I_{on}$ , SS is also one of the key figures of merit for device performance evaluation. SS is expressed as  $SS = \frac{\partial V_g}{\partial \lg I_{ds}}$ , which means the incremental gate voltage applied to change the current by one decade and indicates the device gate controlling ability.<sup>[8]</sup> The smaller SS, the better gate controlling. The SS values versus different  $L_g$  of DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  n- and p-MOSFETs are plotted in Figure 5b. As  $L_g$  scales down, SS sharply increases

with values of 111, 117, 146, and  $322 \text{ mV} \text{ dec}^{-1}$  (86, 105, 181, and  $400 \text{ mV} \text{ dec}^{-1}$ ) for  $\text{Bi}_2\text{O}_2\text{Se}$  n (p)-MOSFETs with  $L_g = 9, 7, 5,$  and 3 nm, respectively.

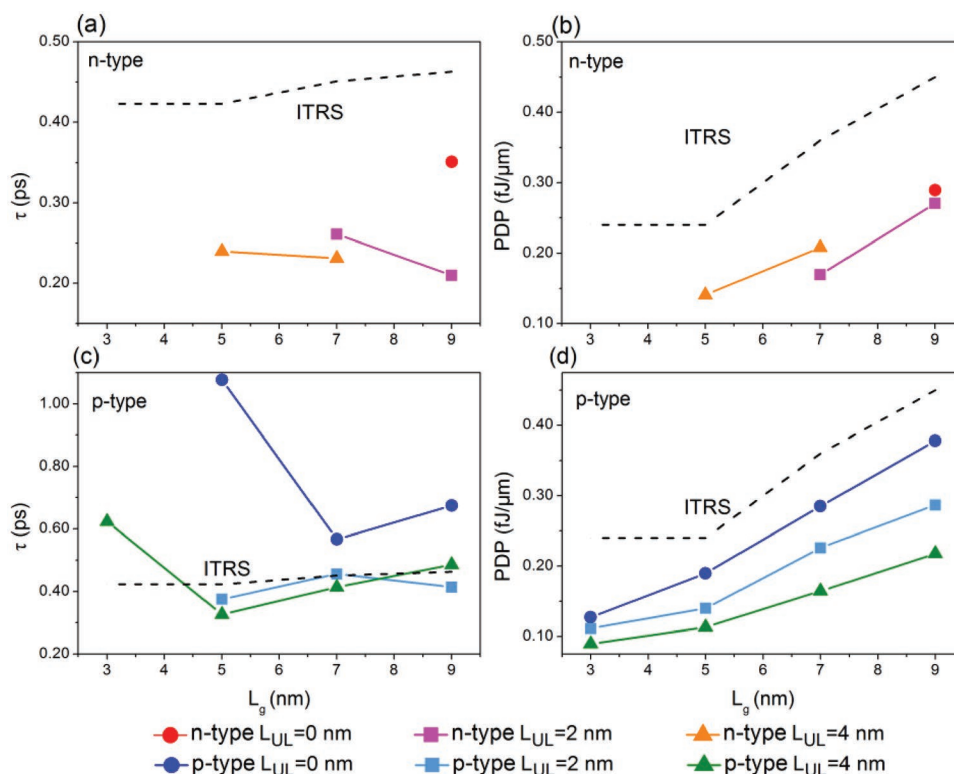
The UL helps reduce SS and improve the gate electrostatics. The effect of UL on the SS of  $L_g \leq 5$  nm n-MOSFETs is remarkable. SS of the 5 nm (3 nm)  $L_g$  n-MOSFET with  $L_{UL} = 2$  nm is reduced by 28% (58%). However, with the increasing  $L_g$ , the improvement on SS by UL is less apparent. Despite of the improvement of UL on the n-MOSFETs, the SS value still surpasses  $100 \text{ mV} \text{ dec}^{-1}$  and far exceeds the ideal  $60 \text{ mV} \text{ dec}^{-1}$ .

The 9 nm  $L_g$  p-MOSFETs with UL has smaller SS value and better gate electrostatics in the subthreshold region. This difference stems from the heavier hole effective mass ( $m_h^* : m_e^* = 8:1$ ), which prefers to suppress the source-drain leakage current and to form smaller SS. SS of the 7, 5, and 3 nm  $L_g$  p-MOSFETs with  $L_{UL} = 4$  nm is reduced by 36%, 67%, and 57%, respectively. Notably, the SS of the 7 nm  $L_g$  p-MOSFET in  $L_{UL} = 4$  nm is  $65 \text{ mV} \text{ dec}^{-1}$  and the 5 nm  $L_g$  p-MOSFET in  $L_{UL} = 4$  nm is  $60 \text{ mV} \text{ dec}^{-1}$ , near to the limit of the ideal thermionic transistors ( $60 \text{ mV} \text{ dec}^{-1}$ ).<sup>[2,8,56,57]</sup>

Above threshold region, we extract transconductance ( $g_m$ ) to evaluate the gate control (Figure S1, Supporting Information). All n-MOSFETs have larger  $g_m$  (2.6–7.0  $\text{mS} \mu\text{m}^{-1}$ ) than the p-MOSFETs (1.8–3.4  $\text{mS} \mu\text{m}^{-1}$ ), which indicates a better superthreshold gate control of the n-MOSFETs.

### 3.4. Intrinsic Delay Time and Power Consumption

The capacitance ( $C_i$ ) and the intrinsic delay time ( $\tau$ ) are another two crucial factors of logic switch.  $C_i$  is defined as the total capacitance composed by gate capacitance ( $C_g$ ) and fringing capacitance ( $C_f$ ).  $C_g$  is calculated by  $C_g = \frac{\partial Q_{ch}}{\partial V_g}$ , where  $Q_{ch}$  is the total charge of the central region.  $C_f$  is the twice of  $C_g$  according to the ITRS standards. The  $C_i$  of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n- and p-MOSFETs in different  $L_g$  is 0.213–0.558 and 0.219–0.729  $\text{fF} \mu\text{m}^{-1}$ , respectively. The switching speed is directly characterized by  $\tau$ , which is calculated by the formula:  $\tau = \frac{C_i V_{dd}}{I_{on}}$ , where  $V_{dd}$  is the



**Figure 6.** a) Intrinsic delay time and b) the power dissipation as functions of the gate length in the n-type DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs with different  $L_{\text{UL}}$ . c) Same as (a) but for the p-type DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs. d) Same as (b) but for the p-type DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs. The black dash lines are the ITRS HP requirements for delay time and PDP.

supply voltage. If  $I_{\text{on}}$  is effectively defined (Tables 1 and 2),  $\tau$  of a device can be figured out. The calculated  $\tau$  (0.210–0.351 ps) of all the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n-MOSFETs can meet the ITRS requirement for HP devices in next decade horizons. Only  $\tau$  of the 5 nm  $L_g$  with  $L_{\text{UL}} = 0$  and 2 nm, 7 nm  $L_g$  with  $L_{\text{UL}} = 4$  nm, and 9 nm  $L_g$  with  $L_{\text{UL}} = 2$  nm p-MOSFETs can meet the ITRS HP requirements. UL could effectively shorten  $\tau$ , as shown in **Figure 6a,c**. For example,  $\tau$  of the 5 nm  $L_g$  p-MOSFETs with  $L_{\text{UL}} = 0, 2,$  and 4 nm is 0.599, 0.474, and 0.325 ps, respectively. As a result of small  $\tau$ , BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs with UL will be a logic transistor with a fast switching speed.

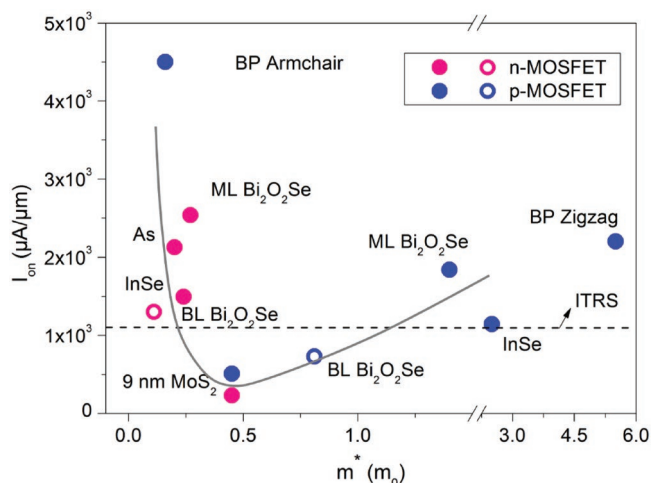
Power consumption is an important indicator concerning the switching energy.  $\text{PDP} = V_{\text{dd}} I_{\text{on}} \tau$ . If  $I_{\text{on}}$  can be effectively defined, PDP of a device can be calculated. From **Figure 6b,d**, PDP of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  p-MOSFETs monotonically decreases with the decreasing  $L_g$ . The longer  $L_{\text{UL}}$ , the smaller PDP. All the calculated PDP (0.090–0.378  $\text{fJ } \mu\text{m}^{-1}$ ) of the sub 10 nm  $L_g$  BL  $\text{Bi}_2\text{O}_2\text{Se}$  n- and p-MOSFETs could meet the ITRS HP requirement. For example, the largest PDP is 0.378  $\text{fJ } \mu\text{m}^{-1}$  for the case of 9 nm  $L_g$  BL  $\text{Bi}_2\text{O}_2\text{Se}$  p-MOSFET, much lower than the minimum value of the ITRS HP required 0.45  $\text{fJ } \mu\text{m}^{-1}$ .

## 4. Discussion

The heavily doped BL  $\text{Bi}_2\text{O}_2\text{Se}$  is employed as electrodes in our calculated BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs, and there is no Schottky barrier in the interface between the electrode and the channel.

However, there is no reliable substitutional method to dope 2D materials directly in the experiment.<sup>[5]</sup> Experimentally, metal electrode is often chosen to directly contact with 2D semiconductors and inject carriers to 2D semiconducting channel. Such a configuration often leads to a formation of Schottky barrier at the metal-semiconductor interface, and the corresponding FET is called Schottky barrier FET (SBFET). However, Schottky barrier could be eliminated by formation of Ohmic contacts with proper metal electrodes. In this case, the device performance of the SBFET may approach that of the corresponding MOSFET. For instance, when graphene as an electrode is employed in the ML BP SBFET,  $I_{\text{on}}$  of this device reaches  $\approx 90\%$  of that of the BP MOSFET because graphene forms an Ohmic contact with BP.<sup>[28,54]</sup> The fabricated long-channelled BL  $\text{Bi}_2\text{O}_2\text{Se}$  FET using Au/Pd as the electrode forms Ohmic contacts, which is in great accordance with our calculation.<sup>[58]</sup> Besides, Au, Pd, Pt, Ti, and Sc could also lead Ohmic contacts with BL  $\text{Bi}_2\text{O}_2\text{Se}$  based on ab initio quantum transporting calculations.<sup>[58]</sup> With these Ohmic contacts, the performance of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  SBFET is expected to approach the MOSFET limit.

Next, we compare the BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs with the most commonly studied BP and  $\text{MoS}_2$  counterparts. ML BP MOSFETs are predicted to show on-currents that could meet the ITRS HP/LP goals and extend Moore's law down to 2 nm on the basis of the previous calculations.<sup>[54]</sup> This device performance is superior to that of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs. However, the BL  $\text{Bi}_2\text{O}_2\text{Se}$  has more excellent air stability than BP. Since the stability is a precondition for large-scale production,



**Figure 7.** On-state current of the n- and p-MOSFETs at  $L_g = 7$  nm versus the effective mass of 2D channel materials. All data is calculated by ab initio quantum transport simulations.<sup>[5,54,60,61]</sup> The dash line is the ITRS HP requirement of the 2013 edition. The solid line is guidance to the eyes.

BL  $\text{Bi}_2\text{O}_2\text{Se}$  is more feasible to be a candidate of the next-generation channel material. Compared with the air-stable ML  $\text{MoS}_2$  MOSFET, BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFET shows an advantage in the on-current. The optimal  $I_{\text{on}}$  of the ML  $\text{MoS}_2$  n-MOSFET with  $L_{\text{UL}}$  only fulfill 50% of the ITRS HP goal,<sup>[59]</sup> but the optimal  $I_{\text{on}}$  of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n-MOSFET with  $L_{\text{UL}}$  exceeds the HP requirement based on our calculations given  $L_g = 5$  nm.

To get the dependence of  $I_{\text{on}}$  on different effective masses, we plot the function of  $I_{\text{on}}$  of the n- and p-MOSFETs versus the effective mass of different 2D channel materials at  $L_g = 7$  nm in **Figure 7** (the ML  $\text{MoS}_2$  MOSFETs are at  $L_g = 9$  nm), on the basis of previous simulations.<sup>[54,55,60,61]</sup> Along with  $m^*$  increasing,  $I_{\text{on}}$  has a decreasing tendency when  $m^* \leq 0.45 m_0$  for n-MOSFETs and an increasing tendency when  $m^* \geq 0.45 m_0$  for p-MOSFETs. This is because a contradiction exists between small  $m^*$  and large  $I_{\text{on}}$ . Small  $m^*$  speeds up carrier velocity and thus large  $I_{\text{on}}$ . However, small  $m^*$  goes against to sufficient density of states (DOS) near the VBM and CBM ( $\text{dos} = \frac{g_s g_v}{2\pi\hbar^2} \sqrt{m_x^* m_y^*}$ , where  $g_s$  and  $g_v$  stand for the spin and valley degeneracies, respectively, and  $x$  and  $y$  represent for the transverse and transport directions, respectively). Insufficient DOS could not guarantee sufficient current drive.<sup>[61]</sup> It's noteworthy that the anisotropic ML armchair-directed BP p-MOSFET, whose  $m_x^* = 0.16 m_0$  and  $m_y^* = 5.40 m_0$  for the holes, possesses small  $m^*$ , adequate DOS simultaneously, and thus achieves extremely high  $I_{\text{on}}$  ( $4500 \mu\text{A} \mu\text{m}^{-1}$ ).<sup>[28]</sup> In the cases of ML  $\text{MoS}_2$ , ML/BL  $\text{Bi}_2\text{O}_2\text{Se}$ , InSe, and zigzag-directed BP p-MOSFETs, the large DOS near the VBM produces benefits to  $I_{\text{on}}$ . For other cases of ML  $\text{MoS}_2$ , ML/BL  $\text{Bi}_2\text{O}_2\text{Se}$ , InSe, and arsenene n-MOSFETs, the high carrier velocity gives advantage on their  $I_{\text{on}}$ . It's intriguing that BL  $\text{Bi}_2\text{O}_2\text{Se}$  has smaller  $m_e^*$  and higher carrier velocity but its MOSFET has a comparably lower  $I_{\text{on}}$  compared with tendency curve of the ML FETs.

As the semiconductor channel thickness increases, the carrier of channel increases, but the control ability of the gate on the channel is weakened. Generally, the device performance is degraded with the increasing layer number, reflecting the dominative role of the reduced gate control ability. For example,

as the channel thickness increases from 1.3 to 12 nm, SS of the 1 nm  $L_g$   $\text{MoS}_2$  FET extremely raises up to  $170 \text{ mV dec}^{-1}$ , and the device could not be turned off when the thickness of  $\text{MoS}_2$  is increased to  $\approx 31 \text{ nm}$ .<sup>[1]</sup> But for monolayer and bilayer 2D materials, these two effects are compelling with each other. The ML and BL BP FETs exhibit similar gate electrostatics abilities (SS =  $62\text{--}66 \text{ mV dec}^{-1}$ ) and  $I_{\text{on}}$  (a few thousand microampere per micrometer).<sup>[62]</sup> By contrast, bilayer  $\text{MoS}_2$  FET (SS =  $109 \text{ mV dec}^{-1}$  and  $I_{\text{on}}/I_{\text{off}} = 10^4$ ) shows a weaker gate control and less on/off ratio compared with monolayer  $\text{MoS}_2$  (SS =  $84 \text{ mV dec}^{-1}$  and  $I_{\text{on}}/I_{\text{off}} = 10^5$ ) based on tight-binding models.<sup>[63]</sup>

There are two causes for the poorer device performance for the BL  $\text{Bi}_2\text{O}_2\text{Se}$  FETs than the ML counterpart. One is the reduced gate electrostatics, and the other is the much smaller bandgap of  $\approx 0.18 \text{ eV}$  in BL  $\text{Bi}_2\text{O}_2\text{Se}$  (compared with a bandgap of  $\approx 1.14 \text{ eV}$  in ML  $\text{Bi}_2\text{O}_2\text{Se}$ ). The much smaller bandgap greatly increases the leakage current, making the off state difficult to access in the BL  $\text{Bi}_2\text{O}_2\text{Se}$  FETs. As the layer number continuously increases to 11, the bandgap continuously decreases nearly to 0 eV in terms of the previous calculation.<sup>[32]</sup> Hence the leak current issue becomes more serious in addition to the reduced gate electrostatics. Thus, the device performance of the sub 10 nm few layer  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs is expected to degrade.

The light effective mass and sizeable bandgap might be applicable to other bismuth oxychalcogenides, such as  $\text{Bi}_2\text{O}_2\text{S}$  and  $\text{Bi}_2\text{O}_2\text{Te}$ . The band structures of  $\text{Bi}_2\text{O}_2\text{S}$  and  $\text{Bi}_2\text{O}_2\text{Te}$  are shown in Figure S5 in the Supporting Information. The bandgaps of the ML and BL  $\text{Bi}_2\text{O}_2\text{S}$  are evaluated as  $\approx 1.77$  and  $0.83 \text{ eV}$ , respectively, larger than the BL  $\text{Bi}_2\text{O}_2\text{Se}$ . ML (BL)  $\text{Bi}_2\text{O}_2\text{S}$  has a small electron effective mass with the value of  $0.15 m_0$  ( $0.13 m_0$ ). The bandgaps of the ML and BL  $\text{Bi}_2\text{O}_2\text{Te}$  are evaluated as  $\approx 0.20$  and  $0 \text{ eV}$ , respectively. The electron effective mass of ML  $\text{Bi}_2\text{O}_2\text{Te}$  is also small ( $0.09 m_0$ ). Combining the sizeable bandgap with the quite light effective mass, ML/BL  $\text{Bi}_2\text{O}_2\text{S}$  might show performance even better than BL  $\text{Bi}_2\text{O}_2\text{Se}$ .

## 5. Conclusion

Inspired by the emerging air-stable 2D  $\text{Bi}_2\text{O}_2\text{Se}$  FET with high performance, the device performance of sub 10 nm  $L_g$  DG BL  $\text{Bi}_2\text{O}_2\text{Se}$  MOSFETs has been studied using ab initio quantum transport simulations for the first time. All the checked BL  $\text{Bi}_2\text{O}_2\text{Se}$  p-MOSFETs have smaller on-state current with respect to the n-MOSFETs due to the heavier hole effective mass. In absence of underlap structure,  $I_{\text{on}}$  of the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n-MOSFETs can not meet ITRS requirement, and the highest  $I_{\text{on}}$  can only reach  $\approx 80\%$  ITRS HP requirement at  $L_g = 9$  nm. However, with the resort of underlap, the BL  $\text{Bi}_2\text{O}_2\text{Se}$  n-MOSFETs can fulfill the HP requirements of ITRS 2013 edition until the gate length is scaled down to 5 nm. Hence, BL  $\text{Bi}_2\text{O}_2\text{Se}$  is a potential channel material for sub 10 nm FETs.

## Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.



## Acknowledgements

This work was supported by the National Key Research and Development Program of China (No. 2017YFA206303), the National Natural Science Foundation of China (Nos. 11674005 and 5173100), the National Materials Genome Project of China (No. 2016YFB0700600) and supported by the High Performance Computing Platform of Peking University, China. L.X. was supported by the Key Research and Development Program of Ningxia in China (No. 2018BEE03023).

## Conflict of Interest

The authors declare no conflict of interest.

## Keywords

ab initio quantum transport calculations, bilayer Bi<sub>2</sub>O<sub>2</sub>Se, high performance limit, sub 10 nm transistors

Received: October 13, 2018

Revised: December 27, 2018

Published online: February 4, 2019

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