## **Electronic Supplementary Information (ESI)**

## **Promising ultra-short channel transistors based on OM2S (M=Ga, In)**

## **monolayer for high performance and low power consumption**

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Fig. S1 (a) Projected band structures of OIn<sub>2</sub>S monolayer. Band-decomposed chargedensity distributions relevant to conduction band minimum and valence band maximum of (b)  $OGa_2S$  and (c)  $Oha_2S$ . Isovalue is  $0.008$  e/bohr<sup>3</sup>.

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**Fig.** S2 Projected density of states (PDOS) of (a)  $OGa<sub>2</sub>S$  and (b)  $OIn<sub>2</sub>S$ .



**Fig.** S3 Transfer characteristics of dual-gate (DG) and single-gate (SG) *n*-type OGa<sub>2</sub>S MOSFETs with  $L<sub>g</sub>$  equal to 5nm. The doping concentration in the electrode region is  $3 \times 10^{13}$  e/cm<sup>-2</sup>. The gray and orange lines stand for ITRS off-state current standards for HP and LP applications, respectively. The SG\_O and SG\_S indicate that the gate electrode is added to the oxygen and sulfur terminals, respectively.



**Fig.** S4 Transfer characteristics of *n*-type and *p*-type OIn<sub>2</sub>S MOSFETs with diverse  $L_{\rm g}$ under supply voltage  $V_{ds} = 0.64$  V. The doping concentration in the electrode region is  $3 \times 10^{13}$  e/cm<sup>-2</sup>. The gray and orange lines stand for ITRS off-state current standards for HP and LP applications, respectively.



Fig. S5 Transfer characteristics of monolayer (a-e) OGa<sub>2</sub>S and (f-j) OIn<sub>2</sub>S MOSFETs under supply voltage  $V_{ds} = 0.64$  V with diverse electrode doping concentrations of electron.



**Fig.** S6 Transmission spectra of the (a-b) 2nm and (c-d) 3nm OGa<sub>2</sub>S MOSFETs with different doping concentrations and  $V_g$ . The  $V_{ds}$  is 0.64 V and the bias window is an energy window of -0.32~0.32 eV. The  $\mu_R$  is the electrochemical potential of the right electrode.



**Fig.** S7 The spectral current of the (a-c) 2nm and (d-f) 3nm OGa<sub>2</sub>S MOSFETs with different doping concentrations. The insets in (a), (d) and (e) are enlarged images of the sections in dashed boxes.



Fig. S8 Transfer characteristics of monolayer OGa<sub>2</sub>S (a) and OIn<sub>2</sub>S MOSFETs (b) with diverse underlap (UL) length at  $V_{ds} = 0.64$  V.



Fig. S9 Transfer characteristics of OGa<sub>2</sub>S MOSFETs with  $L_g$  equal to 12nm. The doping concentration in the electrode region is  $3 \times 10^{13}$  e/cm<sup>-2</sup> and the  $V_{ds}$  is 0.65 V. The red and blue dashed lines stand for IRDS off-state current standards for HP and LP applications, respectively.

**Table S1.** Performance metrics of OGa<sub>2</sub>S MOSFETs with  $L<sub>g</sub>$  equal to 12nm in our work against the requirements of the IRDS in 2028.  $L_g$ : Gate length;  $V_{ds}$ : Supply voltage; SS: Subthreshold swing; *τ*: Delay time; and PDP: Power dissipation, respectively.

	$L_{\rm g}$	$V_{\rm ds}$	$I_{\rm off}$	$I_{\text{on}}$	<b>SS</b>	τ	<b>PDP</b>
	(nm)	(V)	$(\mu A/\mu m)$		$(\mu A/\mu m)$ (mV/dec)	(ps)	$(fJ/\mu m)$
<b>IRDS</b> 2028(HP)	12	0.65	0.01	1979	75	0.122	0.156
OGa <sub>2</sub> S	12	0.65	0.01	2570.7	59.6	0.085	0.140
<b>IRDS</b> 2028(LP)	12	0.65	$1 \times 10^{-4}$	1336	68	0.180	0.156
OGa <sub>2</sub> S	12	0.65	$1 \times 10^{-4}$	2279.8	58.7	0.088	0.128

## *Supporting Note: Comparison between dual-gate and single-gate OGa2S MOSFETs and analysis of SS*

The transfer characteristics of the single-gated (SG) and double-gated (DG) *n*-type OGa<sub>2</sub>S MOSFETs with  $L<sub>g</sub>$  equal to 5nm are calculated, as shown in Fig. S3. The off-state current of the SG\_O device (the gate electrode is added to the oxygen terminal) is difficult to meet the highperformance (HP) requirement of ITRS 2028 level. The DG and SG\_S devices (the gate electrode is added to the sulfur terminal) can approach this requirement at  $V_g = -0.51$  V and  $-0.08$  V, respectively. What's more, the off-state current of the DG and SG\_S devices even can satisfy the

low-power (LP) consumption standard of ITRS 2028 level at the  $V_g$  = -0.76 V and -0.45 V, respectively. However, the LP on-state current of the SG S device (137.1  $\mu$ A/ $\mu$ m) is unable to reach the ITRS requirement (295  $\mu$ A/ $\mu$ m). By contrast, the LP on-state current of the DG device (1300.2  $\mu$ A/ $\mu$ m) exceeds the ITRS demand and is about 10 times larger than that of the SG\_S configuration. In addition, the subthreshold swing (SS) of DG  $OGa<sub>2</sub>S$  MOSFET (63.6 mV/dec) is smaller than that of the SG counterpart (73.0 mV/dec).

The above phenomenon can be illustrated by the natural length  $\lambda$ , which is calculated by the formula  $\lambda = (\varepsilon_{ch} \cdot t_{ch} \cdot t_{ox} / N \varepsilon_{ox})^{1/2}$ . The  $t_{ch}$  ( $t_{ox}$ ) is the thickness of channel (dielectric layer),  $\varepsilon_{ch}$  and  $\varepsilon_{ox}$  are the dielectric constant of channel and dielectric layer separately, and N is the gate numbers. Compared with the SG configuration, the DG device possesses a larger N and thus a smaller λ. Therefore, the gate controllability of the DG device is better than that of the SG device, which leads to lower leakage current and larger on-state current of DG device. Similar conclusions have been reported in previously published studies.59-61 For example, the DG  $MoS<sub>2</sub> FET$  shows a smaller SS (65.5 mV/dec) than that of the SG counterpart (130 mV/dec) at the same drain voltage in the experiment.<sup>60</sup>

Fig. S6 and Fig. S7 plot the transmission spectra and spectral current of the 2nm and 3nm  $OGa<sub>2</sub>S$  MOSFETs with different doping

concentrations. When the doping concentration increases, the edge of the transmission spectrum gradually shifts towards the left, and the transmission possibility inside the bias window is larger, thus the larger  $I_{ds}$  can be gotten at high doping concentration. At the  $V_g$ = -0.4V, the OGa2S MOSFETs with 2nm *L*<sup>g</sup> possesses a larger transmission possibility inside the bias window than that of 3nm devices, which is consistent with the higher  $I_{ds}$  of the 2nm devices in Fig. S5. However, when  $V_g = -0.6V$ , a higher *I*<sub>ds</sub> value is not conducive to the devices reaching the off-state. As can be seen from Fig.  $S6(b)$  and (d), the 3nm  $OGa<sub>2</sub>S$  MOSFETs feature a lower transmission possibility within the bias window, so the 3nm  $OGa<sub>2</sub>S$ MOSFETs are easier to approach the off-state than the 2nm devices. Moreover, for the  $OGa<sub>2</sub>S$  MOSFETs with a doping concentration of  $1 \times 10^{13}$  e/cm<sup>2</sup>, the edge of the transmission spectrum is far away from the  $\mu_{\rm R}$ , indicating the lower leakage current. The above conclusion can also be seen from Fig. S7, the spectral current of the  $3nm OGa<sub>2</sub>S MOSFETs$  is lower than 2nm devices, corresponding to the higher  $I_{ds}$  of the 2nm devices. And the spectral current of the  $OGa<sub>2</sub>S$  MOSFETs with the doping concentration of  $1 \times 10^{13}$  e/cm<sup>2</sup> is lower than that with a doping concentration of  $3 \times 10^{13}$  e/cm<sup>2</sup> and  $1 \times 10^{14}$  e/cm<sup>2</sup>. According to the

 $\frac{\partial V_{\text{g}}}{\partial g I_{ds}}$ , for the same  $V_{\text{g}}$  difference ( $\Delta V_{\text{g}}$ ), a large  $I_{ds}$  difference leads  $SS = \frac{S}{21}$ , for the same  $V_g$  difference (  $I_{ds}$ <sup>2</sup>, tot the same  $r_g$  and  $r_g$  $=\frac{\partial V_{\rm g}}{\partial L_{\rm g}}$ , for the same  $V_{\rm g}$  difference ( $\Delta V_{\rm g}$ ),  $\partial \lg I_{ds}$ , for the same r g difference ( $\Delta r$ )

to a small SS. Fig S7 (a) and (d) show that the 3nm  $OGa<sub>2</sub>S$  MOSFETs

have a larger difference of *I* (at the same  $V_g$  difference,  $\Delta V_g = -0.4V - (-1)$ 0.6V)) compared to the 2nm devices, resulting in a lower SS. This conclusion is applicable to other doping concentrations. Moreover, with the decrease of doping concentration, the difference of *I* increases gradually, thus the SS decreases with the doping concentration declines

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