Supporting Information

The Anisotropic Transport Property of Antimonene MOSFETs

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Table S1. The transmission directions calculated in this paper.

Transmission direction θ (°)	0°	4.7°	8.9°	10.9°	13.9°	14.7°
(m,n)	(1,0)	(1,10)	(1,5)	(1,4)	(1,3)	(5,14)
Transmission direction θ (°)	15.3°	16.1°	19.1°	21.1°	25.3°	30°
(m,n)	(3,8)	(2,5)	(1,2)	(4,7)	(3,4)	(0,1)

Table S2. Requirements of ITRS for HP transistors.

	L_g (nm)	EOT (nm)	V_{dd} (V)	I_{off} (μA/μm)
ITRS HP 2028	5.1	0.41	0.64	0.1
	I_{on}/I_{off}	C_g (fF/μm)	τ (ps)	PDP (fJ/μm)
ITRS HP 2028	9×10^3	0.60	0.423	0.24

Transfer I-V curves of 4nm gate length ML antimonene MOSFETs along 0° direction are taken as examples to compare the performance three different doping concentrations and UL length ranging from 0 to 2 nm. The results of transfer I-V curves are shown in Figure S1. The detailed I_{on} and SS data are shown in Table S3. The influence of different doping concentrations on leakage and on-state current can be seen in Table S4 below. The I_{DS8}/I_{DS6} is the ratio of I_{DS} with 8.0×10^{13} cm^{-2} and 6.0×10^{13} cm^{-2} doping concentration, respectively. I_{DS6}/I_{DS4} is the ratio of I_{DS} with 6.0×10^{13} cm^{-2} and 4.0×10^{13} cm^{-2} doping concentration, respectively. It can be seen clearly that the promotion to leakage current (V_{GS} from -0.6 V to -0.3 V) is much higher than to the maximum current (V_{GS} from 0.2 V to 0.5 V) by increasing doping concentrations. Inversely, devices can effectively suppress SCE by extending UL length at the cost of I_{on}. Therefore, the 6.0 $\times$ 10^{13} cm^{-2} doping concentration coupled with 0 nm and 1 nm UL are selected to guarantee a sufficient drain current and relatively low leakage current.

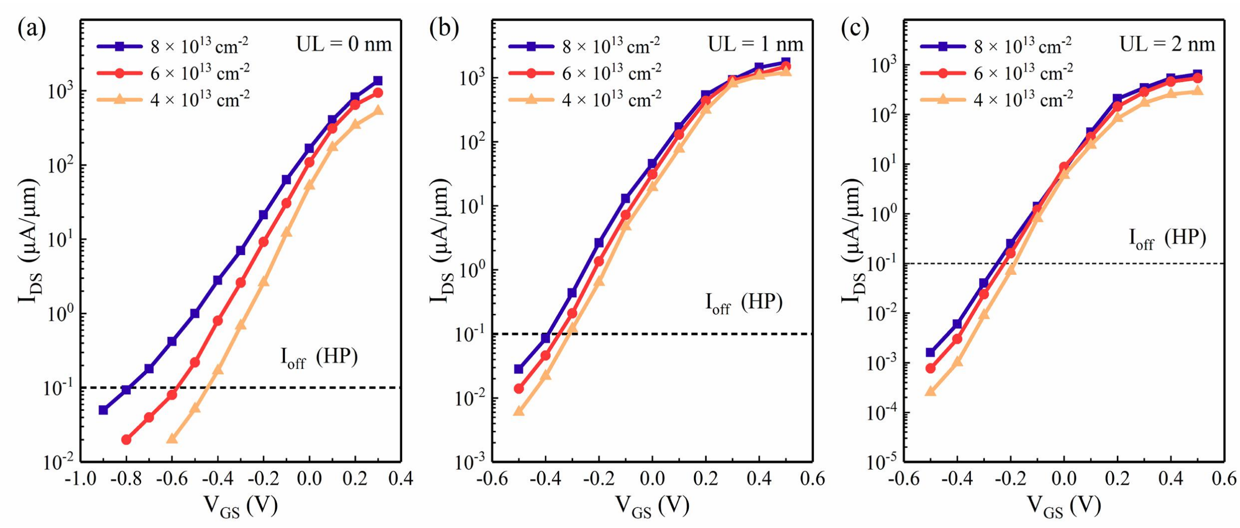

Figure S1 The transfer I-V curves of antimonene MOSFETs along 0° direction as functions of doping concentrations and UL length. The dashed lines represent ITRS HP off-state (I_{off} (HP)) threshold current in (a-c).

Table S3. I_{on} and SS of MOSFETs along 0° direction as functions of doping concentrations and UL length.

Doping concentration (e/cm^{-2})		UL = 0 nm	UL = 1 nm	UL = 2 nm
4.0×10^{13}	I_{on} (μA/μm)	323	470	251
	SS (mV/dev)	127	110	102
6.0×10^{13}	I_{on} (μA/μm)	312	1002	494
	SS (mV/dev)	148	124	113
8.0×10^{13}	I_{on} (μA/μm)	68	926	533
	SS (mV/dev)	201	143	128

Table S4. I_{DS} ratio of zigzag antimonene MOSFETs with different UL length.

V_{GS}		-0.6V	-0.5V	-0.4V	-0.3V	…	0.2V	0.3V	0.4V	0.5V
UL = 0nm	I_{DS8}/I_{DS6}	5.3	4.5	3.5	2.7	…	1.3	1.4	-	-
	I_{DS6}/I_{DS4}	4.0	4.2	4.7	3.8	…	1.9	1.8	-	-
UL = 1nm	I_{DS8}/I_{DS6}		2.0	1.9	1.8	…	1.2	1.0	1.3	1.2
	I_{DS6}/I_{DS4}		2.3	2.1	2.0	…	1.4	1.1	1.1	1.2
UL = 2nm	I_{DS8}/I_{DS6}		2.1	2.0	1.7	…	1.4	1.2	1.2	1.2
	I_{DS6}/I_{DS4}		3.0	3.0	2.7	…	1.7	1.7	1.8	1.9

Table S5. Benchmark of 4 nm gate length ML antimonene MOSFETs performance compares with ITRS HP goals.

	Transmission direction θ (°)	I_{on} (μA/μm)	SS (mV/dec)	C_g (fF/μm)	τ (ps)	PDP (fJ/μm)
ITRS HP goals	-	900	-	0.600	0.423	0.240
UL = 0 nm	0°	312	148	0.297	0.609	0.069
	10.9°	247	150	0.369	0.948	0.067
	16.1°	236	152	0.390	0.898	0.068
	19.1°	394	141	0.317	0.545	0.063
	30°	154	165	0.357	1.437	0.079
UL = 1 nm	0°	1002	124	0.125	0.080	0.069
	10.9°	842	130	0.332	0.252	0.073
	16.1°	832	131	0.362	0.278	0.069
	19.1°	1483	118	0.213	0.092	0.073
	30°	664	134	0.204	0.197	0.071

The transmission pathway in channel regions of ML antimonene MOSFETs along 10.9°, 16.1° and 19.1° are shown in Figure S2. All the transmission pathway is obtained at on-state. The number and strength of red transmission arrows disturbing the transmission efficiency is proportional with the effective mass. Particularly there is only few red arrows in 10.9° case blocking the transmission of blue arrows, indicating the scattering intensity in channel region varies proportional with the effective mass.

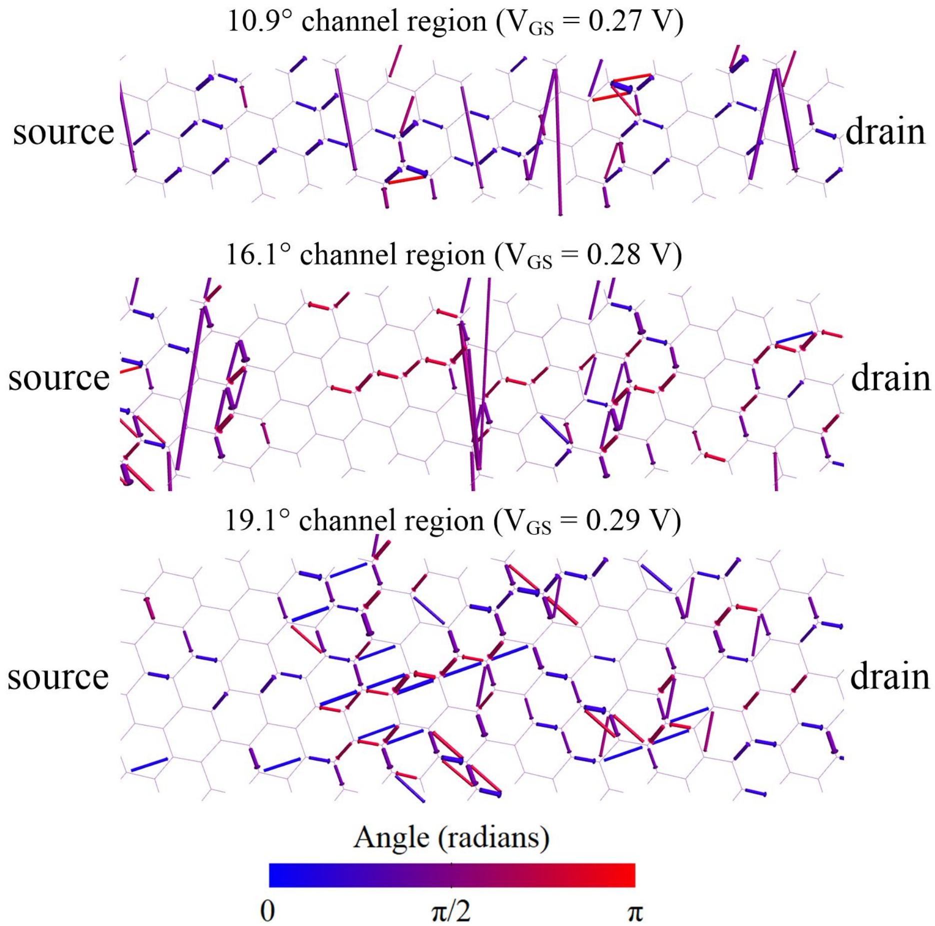

Figure S2. Transmisson pathway in channel regions of ML antimonene along 10.9°, 16.1° and 19.1° directions, with the threshold set to 0.15 au.

Band structures along different transmission directions and the unit cells along these directions are shown in Figure S3. Bandgap changed by the SOC effect are shown in Table S6. The dispersion in valence band is more obvious than that of conduction band consistent with the previous calculation.[1]

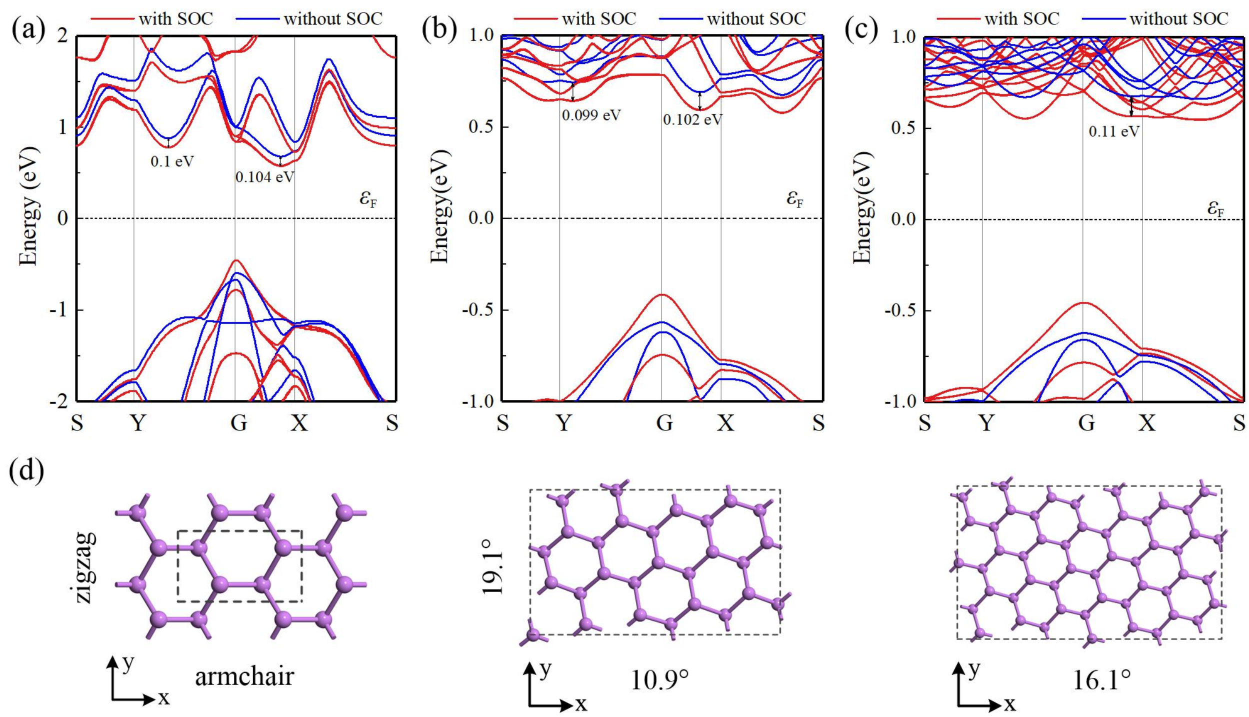

Figure S3. Comparisons of band structures along (a) 0° and 30°, (b) 10.9° and 19.1°, (c) 16.1° directions ML antimonene with and without SOC.

Table S6. Comparisons of bandgap along different transmission directions with and without SOC.

	Transmission direction θ (°)	0°	10.9°	16.1°	19.1°	30°
Without SOC	Bandgap (eV)	1.472	1.242	1.3	1.311	1.274
With SOC	Bandgap (eV)	1.233	0.992	1.023	1.057	1.031

REFERENCES

1. Pizzi, G.; Gibertini, M.; Dib, E.; Marzari, N.; Iannaccone, G.; Fiori, G. Performance of Arsenene and Antimonene Double-Gate MOSFETs from First Principles. *Nat. Commun.* **2016,** *7* (12), 12585.