

Supplementary Information

Quantum transport of short-gate MOSFETs based on monolayer MoSi₂N₄

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Table S1. Cartesian coordinates of the optimized MoSi₂N₄.

	Element	x(Å)	y(Å)	z(Å)
0	Nitrogen	0.728071	0.84099	11.2342
1	Nitrogen	0.728234	-0.841012	8.96366
2	Silicon	0.728244	0.840523	9.48292
3	Molybdenum	2.18436	0.000232082	12.48
4	Nitrogen	0.728057	0.841012	13.7255
5	Nitrogen	0.728232	-0.84099	15.9948
6	Silicon	0.728241	0.840552	15.4764

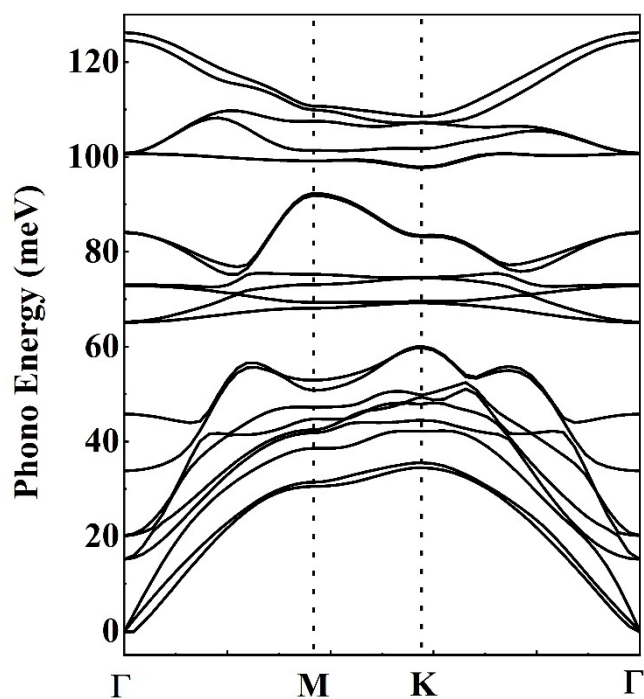


Figure S1. Phonon dispersion spectrum of ML MoSi₂N₄.

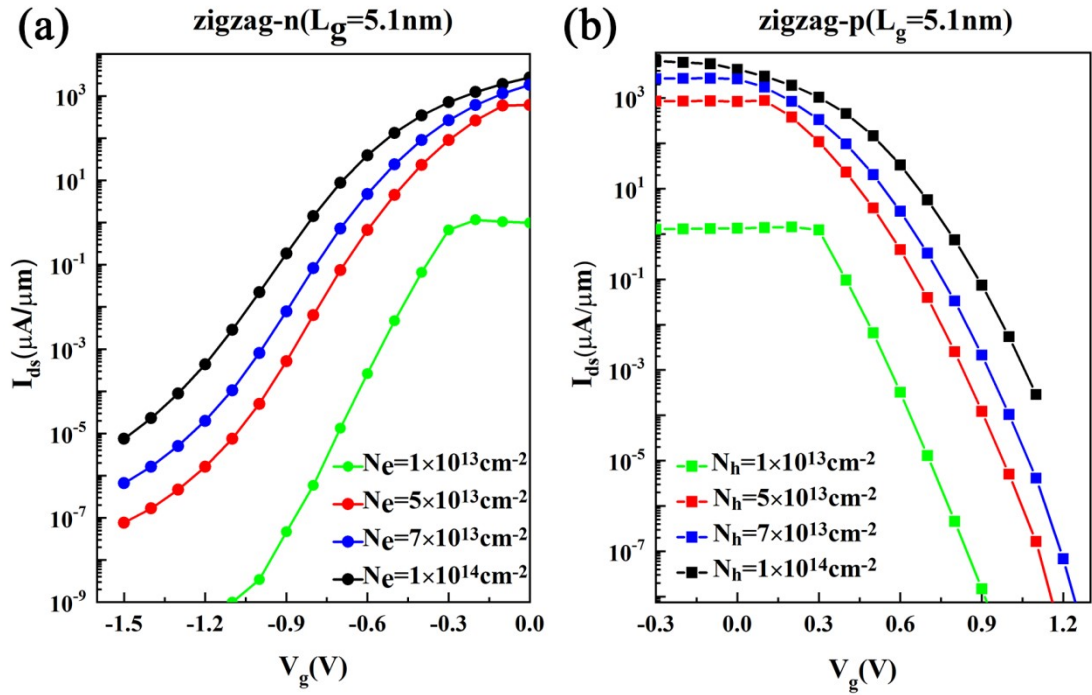


Figure S2. Comparison of the electrical characteristics of 5.1nm- L_g DG ML zigzag MoSi_2N_4 MOSFETs with different concentrations between (a) n-type and (b) p-type doping.

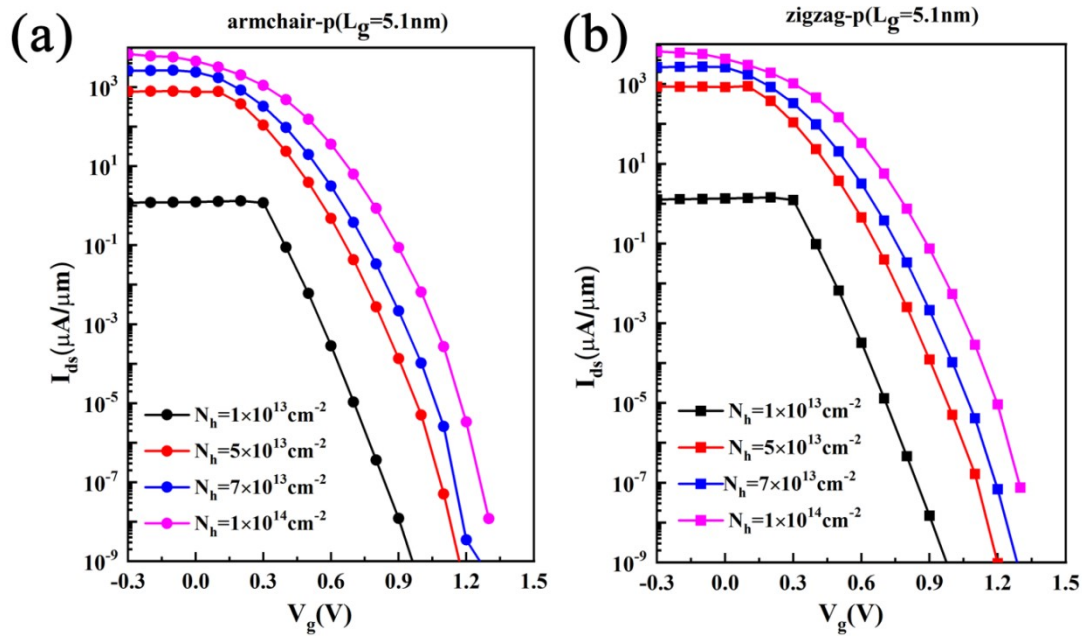


Figure S3. Comparison of electronic transport properties of DG ML MoSi_2N_4 between (a) armchair and (b) zigzag directions.

Table S2. Comparison of electrical properties of 5.1nm- L_g DG ML MoSi_2N_4 MOSFETs in different electron transport

directions with different concentrations.

	EOT (nm)	V _{dd} (V)	N _h (cm ⁻²)	SS (mV/dec)	I _{on} (μA/μm)
zigzag-p	0.41	0.64	5×10 ¹³	45	850.2
			7×10 ¹³	47	1616.5
			10 ¹⁴	48	1428.8
armchair-p	0.41	0.64	5×10 ¹³	41	753.8
			7×10 ¹³	35	1554.2
			10 ¹⁴	41	1459.9
ITRS	0.41	0.64	-	-	900

Table S3. Comparison of parameters between 2 nm, 3 nm, 4 nm, 5.1 nm gate length DG ML MoSi₂N₄ MOSFETs and

ITRS 2013 HP devices.

	L _g (nm)	EOT (nm)	V _{dd} (V)	SS (mV/dec)	I _{off} (μA/μm)	I _{on} (μA/μm)	I _{off} /I _{on}	C _g (fF/μm)	τ (ps)	PDP (fJ/μm)
zigzag-n	5.1	0.41	0.64	98	0.1	833.3	8333	0.228	0.525	0.093
zigzag-p				47		1616.5	16165	0.213	0.253	0.087
ITRS	5.1	0.41	0.64		0.1	900		0.600	0.423	0.24
zigzag-n	4.0	0.41	0.64	125	0.1	570.0	5700	0.168	0.566	0.069
zigzag-p				73		1273.0	12730	0.158	0.238	0.065
zigzag-n	3.0	0.41	0.64	239	0.1	25.4	254	0.291	21.971	0.119
UL=1.0nm				167		225.8	2258	0.149	1.267	0.061
UL=2.1nm				128		467.2	4672	0.163	0.670	0.067
UL=3.7nm				99		422.6	4226	-	-	-
zigzag-p				122		605.1	6051	0.128	0.406	0.052
UL=1.0nm				91		902.5	9025	0.154	0.328	0.063
UL=2.1nm				65		895.3	8953	0.147	0.315	0.060
UL=3.7nm				54		456.5	4565	-	-	-
zigzag-n	2.0	0.41	0.64	342	0.1	3.6	36	0.081	42.843	0.033
UL=1.0nm				276		17.1	171	-	-	-
UL=2.0nm				168		205.1	2051	-	-	-
UL=4.0nm				134		225.9	2259	-	-	-
zigzag-p				154		257.9	2579	0.100	0.744	0.041
UL=1.0nm				137		429.1	4291	-	-	-
UL=2.0nm				89		432.9	4329	-	-	-
UL=4.0nm				77		265.9	2659	-	-	-

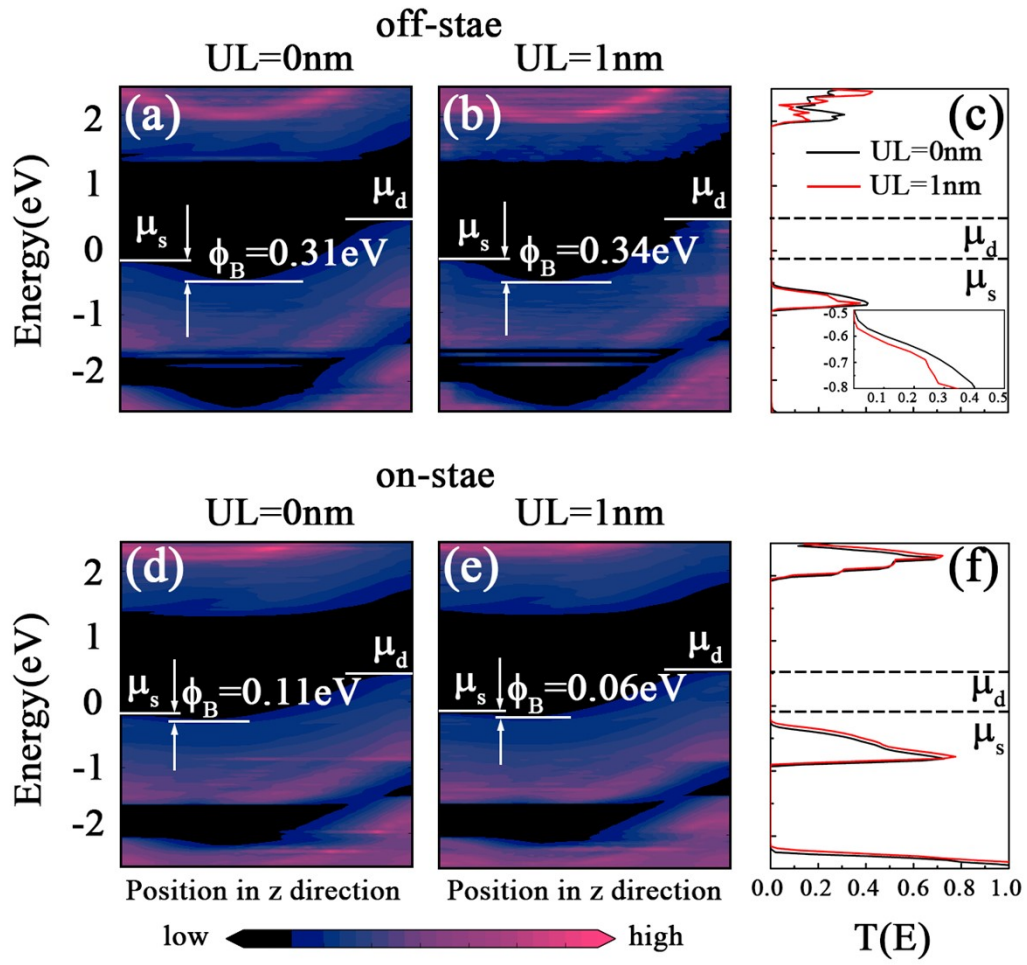


Figure S4. LDOS and transmission spectra of 2.0 nm- L_g MoSi₂N₄ p-MOSFETs with UL=0 and 1 nm along zigzag direction at HP (a-c) off- and (d-f) on-states, respectively, with $N_h = 7 \times 10^{13} \text{ cm}^{-2}$.

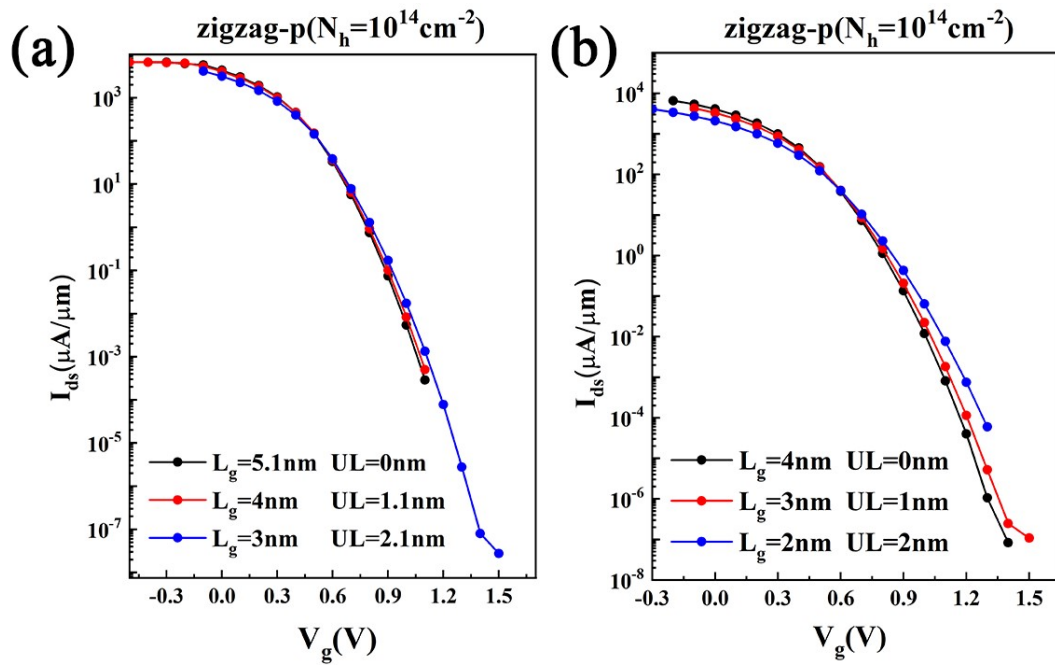


Figure S5. Comparison of electrical properties of DG ML MoSi₂N₄ MOSFETs with different gate lengths and UL under the same channel lengths of (a) 5.1 nm and (b) 4 nm.