Supplementary Material

Sub-5 nm Monolayer Germanium Selenide (GeSe) MOSFETs: towards High Performance and Stable Device

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Table S1. Benchmark of the ballistic performances upper limit of the sub-5 nm DG ML GeSe MOSFETs (zigzag- and armchair-directed) for HP applications against the ITRS requirements (2013 version). Here, L_g = 1-5 nm, EOT = 0.41 nm, V_{dd} = 0.64 V, N_e (N_h) = 5×10^{12} cm^{-2}, and I_{off} = 0.1 μA/μm for HP applications. I_{on}: on-state current; *SS*: subthreshold swing; C_t: total capacitance; τ: delay time; and PDP: power-delay product.

	L_g (nm)	V_{dd} (V)	UL (nm)	SS (mV/dec)		I_{on} (μA/μm)		I_{on}/I_{off}		C_t (fF/μm)		τ (ps)		PDP (fJ/μm)	
ITRS HP	5.1	0.64	0	—		900		9.00×10^3		0.600		0.423		0.24	
				***n*-type**	***p*-type**	***n*-type**	***p*-type**	***n*-type**	***p*-type**	***n*-type**	***p*-type**	***n*-type**	***p*-type**	***n*-type**	***p*-type**
Armchair	1	0.64	0	170	200	117	11	1.17×10^3	1.1×10^2	0.060	0.063	0.330	3.650	0.025	0.026
			2	150	190	236	67	2.36×10^3	6.7×10^2	0.064	0.063	0.173	0.599	0.026	0.026
			4	140	160	400	219	4×10^3	2.19×10^3	0.057	0.063	0.091	0.183	0.023	0.026
	2	0.64	0	150	160	404	198	4.04×10^3	1.98×10^3	0.110	0.119	0.174	0.383	0.045	0.049
			2	130	140	518	332	5.18×10^3	3.32×10^3	0.100	0.104	0.124	0.201	0.041	0.043
			4	100	120	481	325	4.81×10^3	3.25×10^3	0.081	0.083	0.107	0.164	0.033	0.034
	3	0.64	0	120	130	433	289	4.33×10^3	2.89×10^3	0.129	0.153	0.191	0.339	0.053	0.063
			2	100	110	461	328	4.61×10^3	3.28×10^3	0.104	0.106	0.144	0.207	0.042	0.043
			4	90	100	492	307	4.92×10^3	3.07×10^3	0.105	0.117	0.137	0.244	0.043	0.048
	4	0.64	0	100	110	475	312	4.75×10^3	3.12×10^3	0.169	0.174	0.227	0.358	0.069	0.071
			2	80	90	444	301	4.44×10^3	3.01×10^3	0.148	0.154	0.214	0.328	0.061	0.063
			4	70	80	494	326	4.94×10^3	3.26×10^3	0.136	0.129	0.177	0.253	0.056	0.053
	5	0.64	0	80	100	441	309	4.41×10^3	3.09×10^2	0.247	0.201	0.358	0.417	0.101	0.083
			2	60	90	442	318	4.42×10^3	3.18×10^3	0.202	0.214	0.292	0.430	0.083	0.087
			4	60	70	483	328	4.83×10^3	3.28×10^2	0.179	0.261	0.237	0.508	0.073	0.107
Zigzag	1	0.64	0	140	130	261	21	2.61×10^3	2.1×10^2	0.073	0.069	0.180	2.095	0.030	0.028
			2	140	120	288	476	2.88×10^3	4.76×10^3	0.071	0.068	0.158	0.091	0.029	0.028
			4	130	120	308	1238	3.08×10^3	1.24×10^4	0.064	0.060	0.133	0.031	0.026	0.024
	2	0.64	0	120	110	279	1173	2.79×10^3	1.17×10^4	0.097	0.094	0.222	0.051	0.040	0.038
			2	110	90	281	1605	2.81×10^3	1.61×10^4	0.088	0.089	0.200	0.035	0.036	0.036
			4	100	90	298	1639	2.98×10^3	1.64×10^4	0.070	0.080	0.150	0.031	0.029	0.033
	3	0.64	0	100	80	266	1640	2.66×10^3	1.64×10^4	0.142	0.133	0.342	0.052	0.058	0.054
			2	90	80	274	1651	2.74×10^3	1.65×10^4	0.118	0.121	0.276	0.047	0.048	0.049
			4	80	60	295	1693	2.95×10^3	1.69×10^4	0.115	0.110	0.249	0.042	0.047	0.045
	4	0.64	0	80	80	267	1655	2.67×10^3	1.66×10^4	0.146	0.151	0.351	0.058	0.060	0.062
			2	80	80	401	1673	4.01×10^3	1.67×10^4	0.144	0.143	0.230	0.055	0.059	0.059
			4	70	60	296	1703	2.96×10^3	1.70×10^4	0.122	0.144	0.263	0.054	0.050	0.059
	5	0.64	0	80	80	258	1655	2.58×10^3	1.66×10^4	0.225	0.274	0.559	0.106	0.092	0.112
			2	80	60	266	1684	2.66×10^3	1.68×10^4	0.166	0.296	0.399	0.113	0.068	0.121
			4	60	60	302	1625	3.02×10^3	1.66×10^4	0.135	0.175	0.287	0.069	0.055	0.072

Table S2. Benchmark of the ballistic performances upper limit of the sub-5 nm DG ML GeSe MOSFETs (zigzag- and armchair-directed) for LP applications against the ITRS requirements (2013 version). Here, L_g = 1-5 nm, EOT = 0.49 nm, V_{dd} = 0.64 V, N_e (N_h) = 5×10^{12} cm^{-2}, and I_{off} = 2×10^{-5} μA/μm for LP applications. I_{on}: on-state current; *SS*: subthreshold swing; C_t: total capacitance; τ: delay time; and PDP: power-delay product.

	L_g (nm)	V_{dd} (V)	UL (nm)	SS (mV/dec)		I_{on} (μA/μm)		I_{on} /I_{off}		C_t (fF/μm)		τ (ps)		PDP (fJ/μm)	
ITRS LP	5.1	0.64	0	—		295		5.9×10^6		0.69		1.493		0.28	
Type				*n*-type	*p*-type	*n*-type	*p*-type	*n*-type	*p*-type	*n*-type	*p*-type	*n*-type	*p*-type	*n*-type	*p*-type
Armchair	5	0.64	0	—	—	—	—	—	—	0.247	0.201	—	—	0.101	—
			2	270.0	—	0.490	—	9.8×10^3	—	0.202	0.214	263.84	—	0.083	—
			4	160.0	—	84	—	1.68×10^6	—	0.179	0.261	1.36	—	0.073	—
Zigzag	3	0.64	0	—	—	—	—	—	—	0.142	0.133	—	—	0.058	—
			2	210.0	—	3.1	—	6.2×10^4	—	0.118	0.121	24.36	—	0.048	—
			4	240.0	—	6.7	—	1.34×10^5	—	0.115	0.110	10.99	—	0.047	—
	4	0.64	0	220.0	—	5.4	—	1.08×10^5	—	0.146	0.151	17.30	—	0.060	—
			2	160.0	—	97	—	1.94×10^6	—	0.144	0.143	0.95	—	0.059	—
			4	130.0	—	161	—	3.22×10^6	—	0.122	0.144	0.48	—	0.050	—
	5	0.64	0	160.0	—	100	—	2.0×10^6	—	0.225	0.274	1.44	—	0.092	—
			2	130.0	—	245	—	4.9×10^6	—	0.166	0.296	0.43	—	0.068	—
			4	90.0	—	274	—	5.48×10^6	—	0.135	0.175	0.32	—	0.055	—

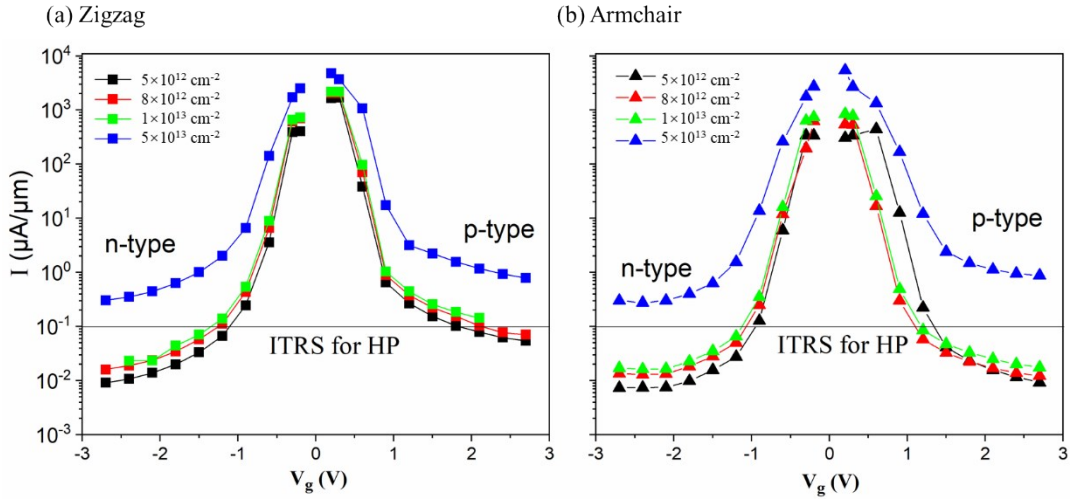

Figure S1. Transfer characteristics of the *n*- and *p*-type 5 nm gate-length DG ML GeSe MOSFETs for different source and drain doping concentrations of electron/hole (N_e (N_h)) along the zigzag (a) and armchair (b) directions.

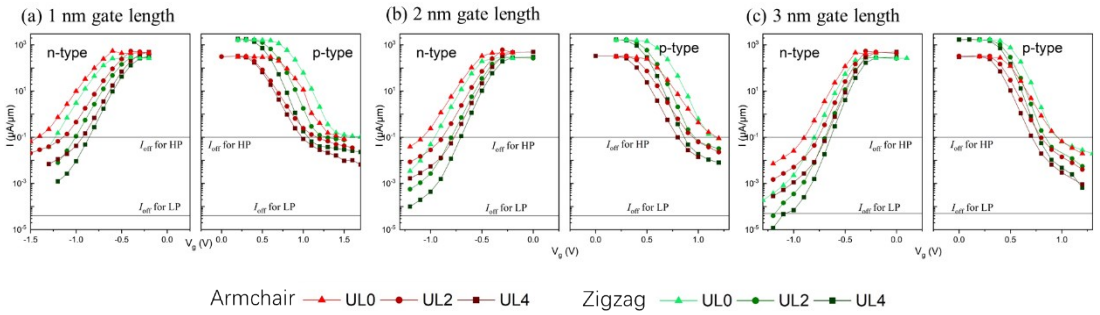

Figure S2. Transfer characteristics of the *n*- and *p*-type 1-3 nm gate-length DG ML GeSe MOSFETs with different underlaps along the armchair (red lines) and zigzag (green lines) directions, respectively. The electron (hole) concentration of the source and drain is N_e (N_h) = 5×10^{12} cm^{-2}.

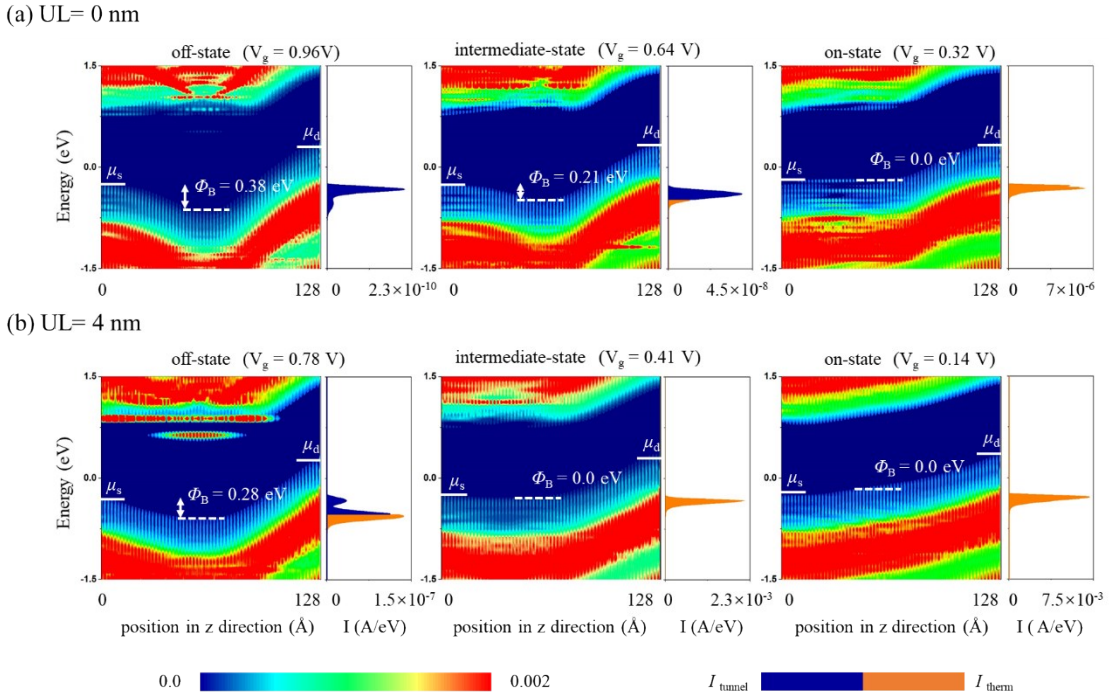

Figure S3. Local density of states (LDOS) (left panel) and the spectral current (right panel) for the *p*-type 3 nm gate-length DG ML GeSe MOSFETs (zigzag directed) with UL = 0 (a) / UL = 4 (b) under V_b = 0.64 V at different V_g, respectively. μ_s and μ_d are the electrochemical potential of the source and drain, respectively. Φ_B is the effective barrier height.

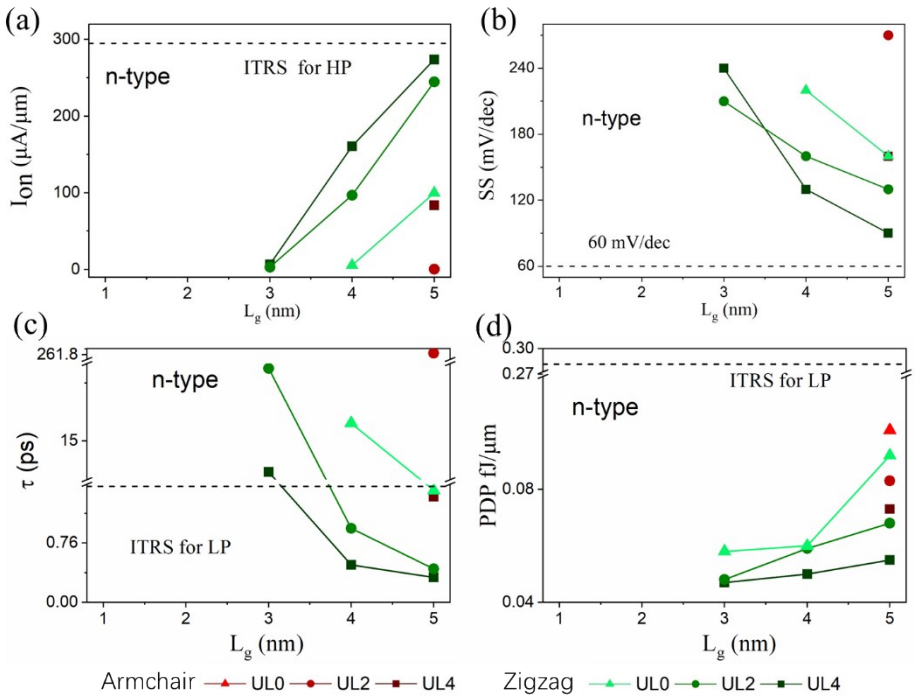

Figure S4. On-state current (a), subthreshold swing (b), intrinsic delay time (τ) (c), and power-delay product (PDP) (d) of the sub-5 nm *n*-type DG ML GeSe MOSFETs as a function of the L_g. The set of red and green lines indicate the armchair and zigzag directions, respectively.