Supplementary Information (SI) for Journal of Materials Chemistry C.

Supplementary Materials

Quantum Transport Simulation of α-GeTe Ferroelectric Semiconductor Transistor

Qiang Li,[1] Zongmeng Yang[2], Xingyue Yang[2], Wenjing Zhou[3], Chen Yang,[2] Xiaotian Sun,[4] Shibo Fang,[2*] and Jing Lu[2,5,6,7,8*]

[1] Department of Physics, Hubei Minzu University, Enshi, 445000, P. R. China

[2] State Key Laboratory for Mesoscopic Physics and School of Physics, Peking University, Beijing 100871, P. R. China

[3] Department of Statistics, University of Michigan, Ann Arbor 48109, USA

[4] College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang 471934, P. R. China

[5] Collaborative Innovation Center of Quantum Matter, Beijing 100871, P. R. China

[6] Beijing Key Laboratory for Magnetoelectric Materials and Devices (BKL-MEMD), Peking University, Beijing 100871, P. R. China

[7] Peking University Yangtze Delta Institute of Optoelectronics, Nantong 226010, P. R. China

[8] Key Laboratory for the Physics and Chemistry of Nanodevices, Peking University, Beijing 100871, P. R. China

*Corresponding Authors: jinglu@pku.edu.cn, botk@pku.edu.cn

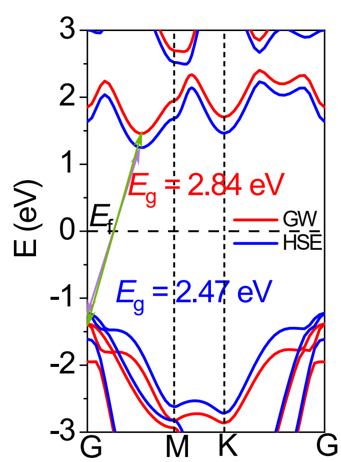

Fig. S1 Band structure of monolayer (ML) α-GeTe using hybrid functionals and the GW method.

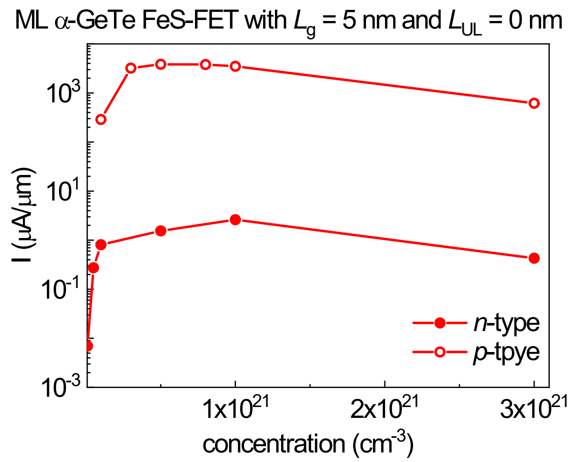

Fig. S2 Transport current of the ML α-GeTe FeS-FET (up-state) along the armchair direction with gate length L_g = 5 nm and without underlap length under different *n*-type and *p*-type doping concentrations.

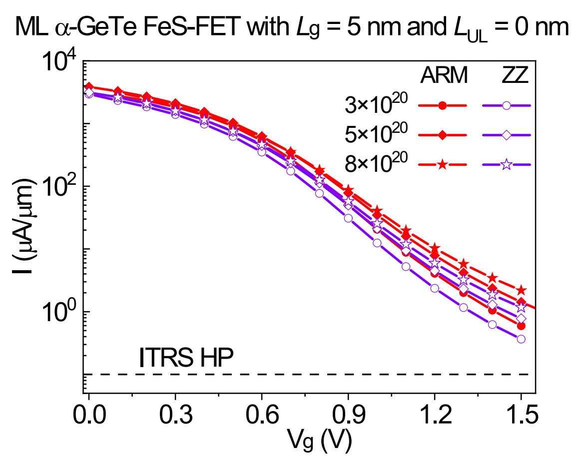

Fig. S3 Transport current of the ML α-GeTe FeS-FET (up-state) along the armchair and zigzag direction with gate length L_g = 5 nm and without underlap length under different *p*-type doping concentrations.

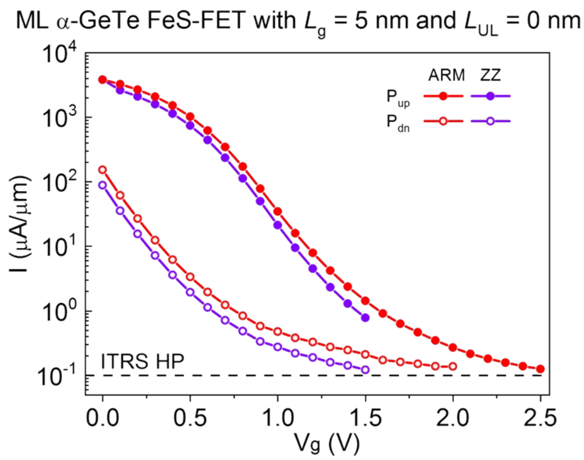

Fig. S4 Transport current of the ML α-GeTe FeS-FET (up-state and down-state) along the armchair and zigzag direction with gate length L_g = 5 nm and without underlap length under 5×10^{20} cm^{-3} doping concentration.

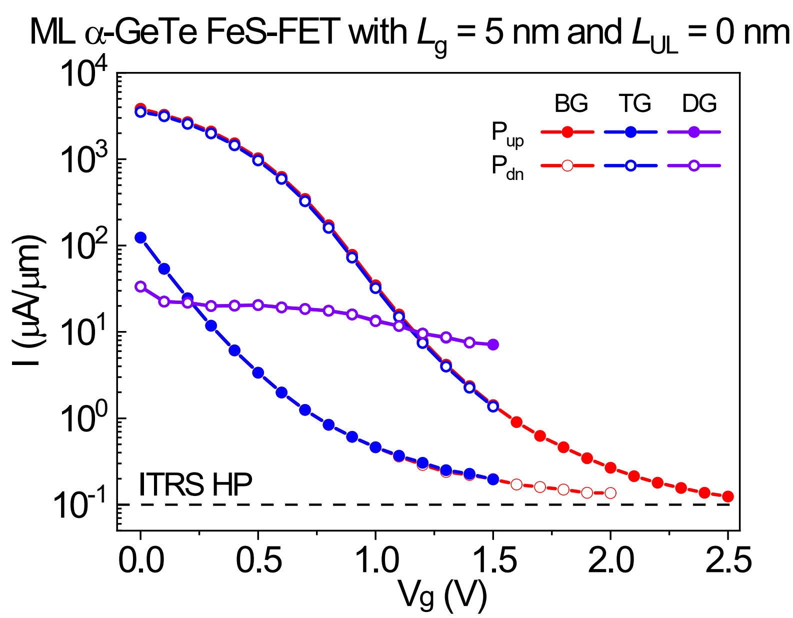

Fig. S5 Transport current of the bottom gate (BG), top gate (TG), and double (DG) ML α-GeTe FeS-FET (up-state and down-state) along the armchair direction with gate length L_g = 5 nm and without underlap length 5×10^{20} cm^{-3} doping concentration.

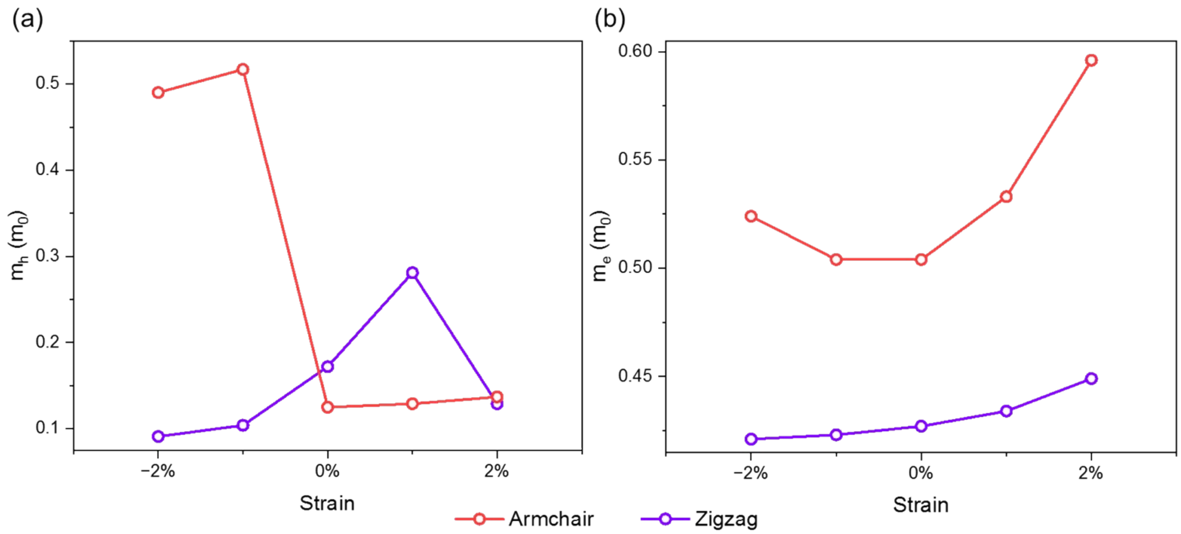

Fig. S6 The effective mass of (a) holes and (b) electrons for ML α-GeTe under compressive and tensile stress along armchair and zigzag directions.

Tab. S1 Benchmark of the ballistic performance of the sub-5 nm L_g ML α-GeTe FeS-FET with up-state against the 2028 requirements of the ITRS 2013 for the HP applications.

	L_g (nm)	L_{UL} (nm)	SS (mV/dec)	I_{off} (μA/μm)	I_{on} (μA/μm)	I_{on}/I_{off}	C_t (fF/μm)	τ (ps)	PDP (fJ/μm)
***p*-type HP**	5	0	312.47	0.1	0.34	3.4	0.35	655.71	0.14
		1	195.53	0.1	243.97	2.44×10^3	0.40	1.05	0.16
		2	144.52	0.1	802.53	8.03×10^3	0.22	0.17	0.09
	3	0		0.1	-	-			
		1		0.1	-	-			
		2	240.30	0.1	13.90	1.39×10^2	0.13	6.13	0.05
		3	181.17	0.1	257.05	2.57×10^3	0.10	0.26	0.04
	1	0		0.1	-	-			
		1		0.1	-	-			
		2		0.1	-	-			
		3		0.1	-	-			
		4	277.83	0.1	20.34	2.03×10^2	0.04	1.29	0.02
ITRS HP 2028	5.1	-	-	0.1	900	9.00×10^3	0.6	0.423	0.24

Tab. S2 Comparison of the I_{on} and *SS* values of the sub-5 nm L_g ML α-GeTe FeS-FET with up-state for the HP application between with and without NC dielectric.

	L_g (nm)	L_{UL} (nm)	without NC		with NC				
			SS (mV/dec)	I_{on} (μA/μm)	SS (mV/dec)	I_{on} (μA/μm)	C_t (fF/μm)	τ (ps)	PDP (fJ/μm)
HP	5	0	312.47	0.34	224.75	0.34	0.60	1137.84	0.25
		1	195.53	243.97	154.14	564.67	0.29	0.33	0.12
		2	144.52	802.53	120.59	1933.52	0.17	0.06	0.07
	3	0	-	-	-	-	-	-	-
		1	-	-	-	-	-	-	-
		2	240.30	13.90	216.14	247.99	0.13	0.34	0.05
		3	181.17	257.05	167.95	257.05	0.11	0.28	0.05
	1	0	-	-	-	-	-	-	-
		1	-	-	-	-	-	-	-
		2	-	-	-	-	-	-	-
		3	-	-	-	-	-	-	-
		4	277.83	20.34	267.38	42.22	0.04	0.62	0.02
ITRS	5.1			900		900	0.60	0.423	0.24