Supplementary Materials for
Sliding ferroelectricity in bilayer phosphorus-analogue compounds: mechanisms and applications

Dong-Dong Wang,[a] Xin-Yi Gao,[a] Yan-Dong Guo,[*a] Yu-Ting Guo,[a] Zhi-Peng Huan,[a] Li-Yan Lin,[a] Yue Jiang,[*b] Zeng-Yun Gu,[a] Hong-Li Zeng,[*c] Xiao-Hong Yan[c]

[a]College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210046, China. E-mail: yandongguo@njupt.edu.cn

[b]College of Science, Jinling Institute of Technology, Nanjing 211169, China. E-mail: jiangyue@jit.edu.cn

[c]College of Natural Science, Nanjing University of Posts and Telecommunications, Nanjing 210046, China. E-mail: hlzeng@njupt.edu.cn

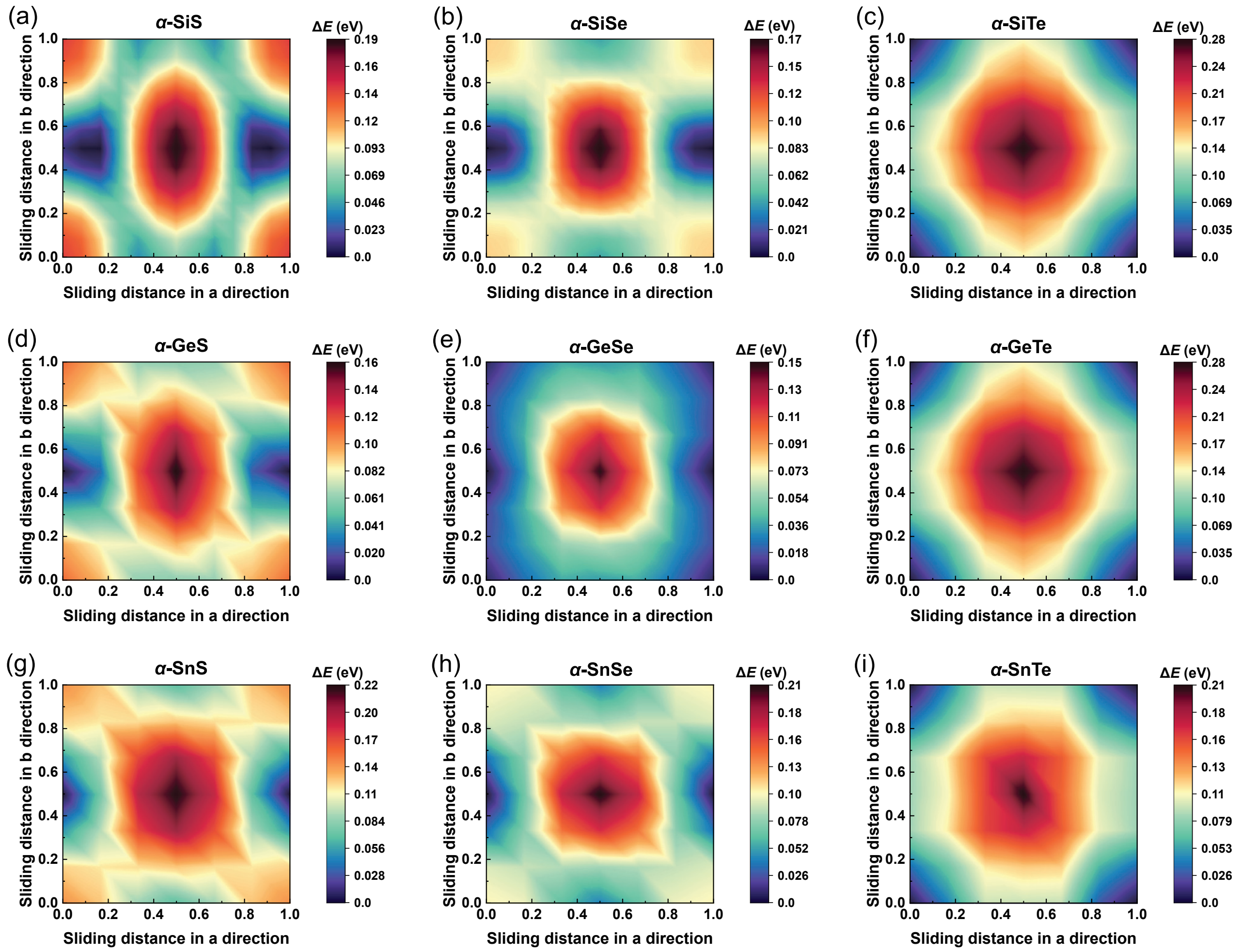

Fig. S1 (a)-(i) The energy profiles of the sliding bilayer α-phase MX materials (M = Si, Ge, and Sn; X = S, Se, and Te). Among these materials, only the bilayer α-SiS exhibits a clear double well sliding path.

Table S1 Lattice constant, ferroelectric switching barrier (E_b) and out-of-plane polarization (P_{out}) of MX materials (M = Si, Ge, Sn, and Pb; X = S, Se, and Te).

Configuration	Lattice constant (Å)	E_b (meV/u.c.)	P_{out} (pC/m)
bilayer α-SiS	4.32/4.10	7.8	5.6
bilayer β-SiS	3.30	3.89	0.28
bilayer β-SiSe	3.50	5.50	0.38
bilayer β-SiTe	3.82	7.50	0.55
bilayer β-GeS	3.48	4.70	0.28
bilayer β-GeSe	3.65	6.55	0.33
bilayer β-GeTe	3.94	8.85	0.55
bilayer β-SnS	3.73	6.17	0.1
bilayer β-SnSe	3.91	8.84	0.2
bilayer β-SnTe	4.16	11.14	0.5
bilayer β-PbS	3.94	9.56	0.08
bilayer β-PbSe	4.06	12.10	0.13
bilayer β-PbTe	4.30	14.20	0.53

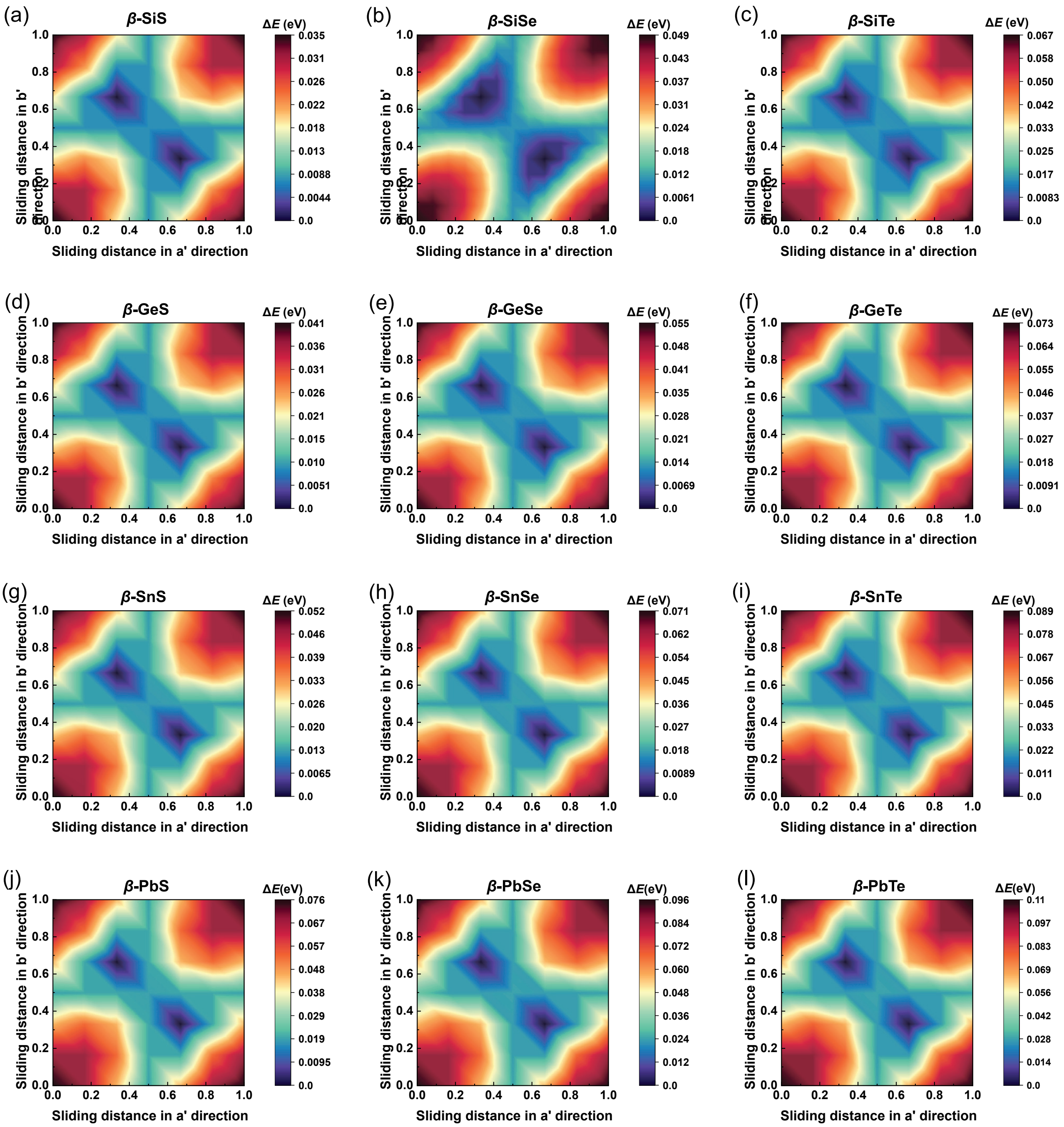

Fig. S2 (a)-(l) The energy profiles of the sliding bilayer β-phase MX materials (M = Si, Ge, Sn and Pb; X = S, Se, and Te). All materials exhibit distinct double potential energy well.

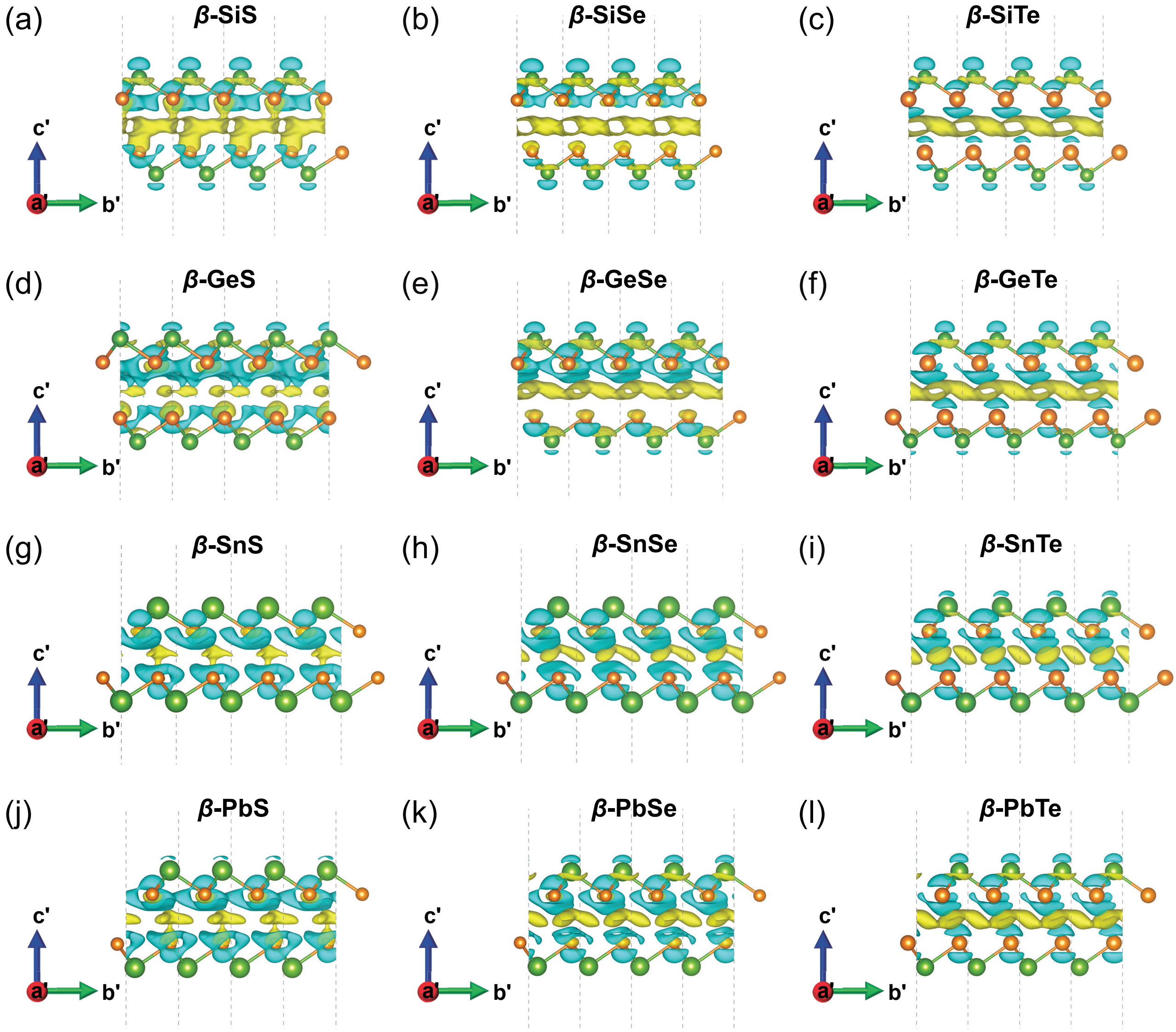

Fig. S3 (a)-(l) The differential charge density distributions of the maximum polarization in the MX materials (M = Si, Ge, Sn, and Pb; X = S, Se, and Te), where yellow indicates charge accumulation and blue indicates hole accumulation. When the M atom is fixed, with the increasing atomic number of X atom, the number of charges involved in interlayer transfer also increases significantly.

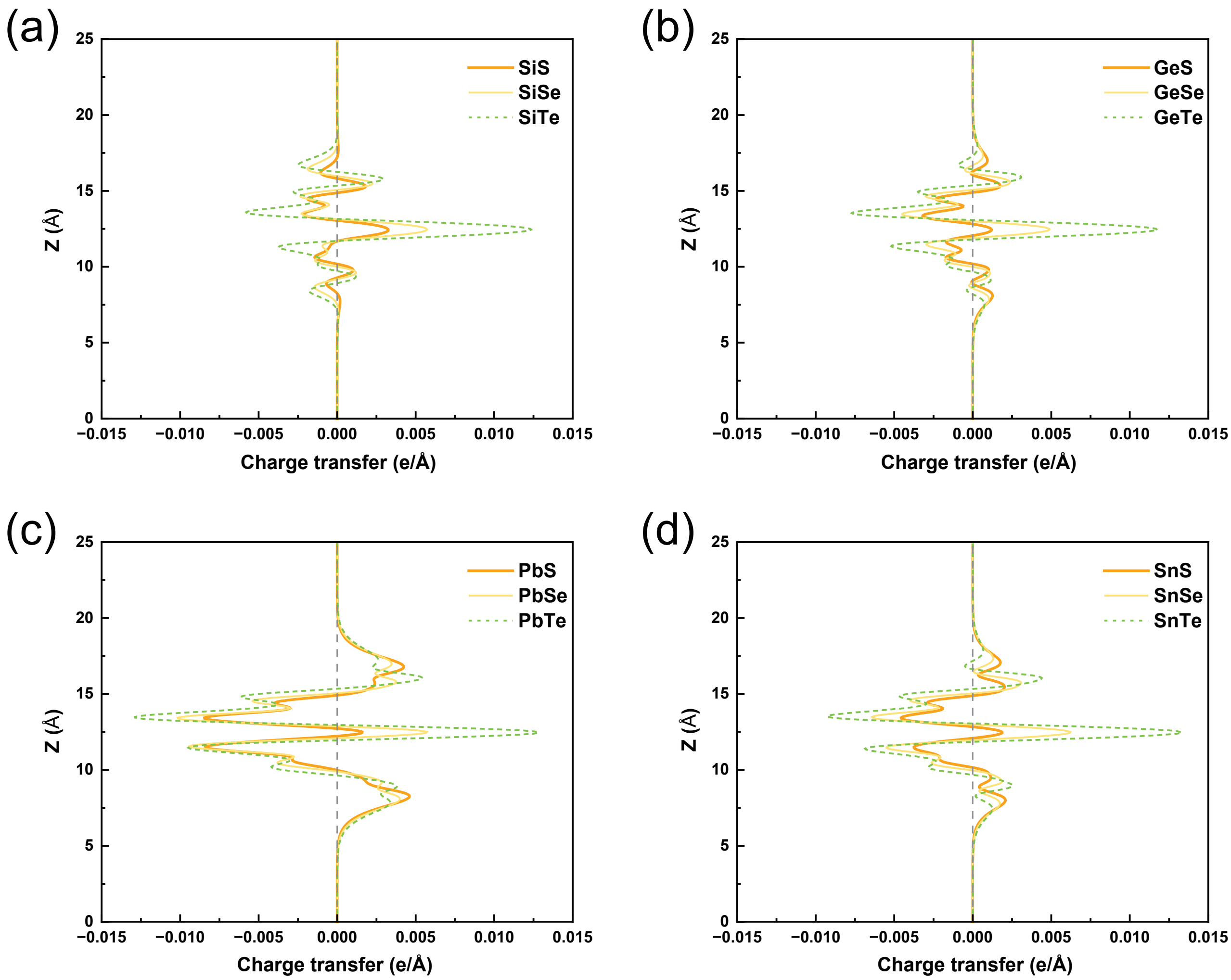

Fig. S4 (a)-(l) The planar differential charge density distributions of the maximum polarization in the MX materials (M = Si, Ge, Sn, and Pb; X = S, Se, and Te). By using contrast to highlight, as the atomic number of X atom increases, the overall amount of charge involved in charge transfer also increases.

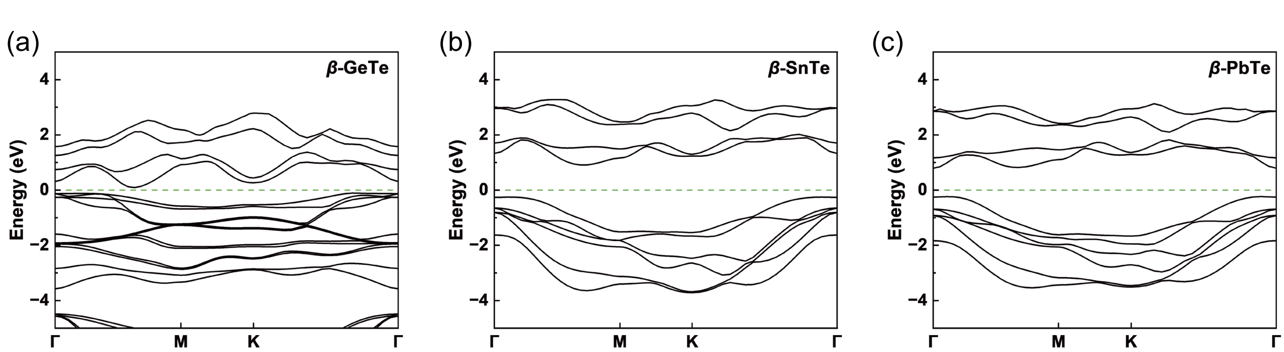

Fig. S5 (a)-(c) The band structure diagrams of β-GeTe, β-PbTe, and β-SnTe, which are used as channel materials.

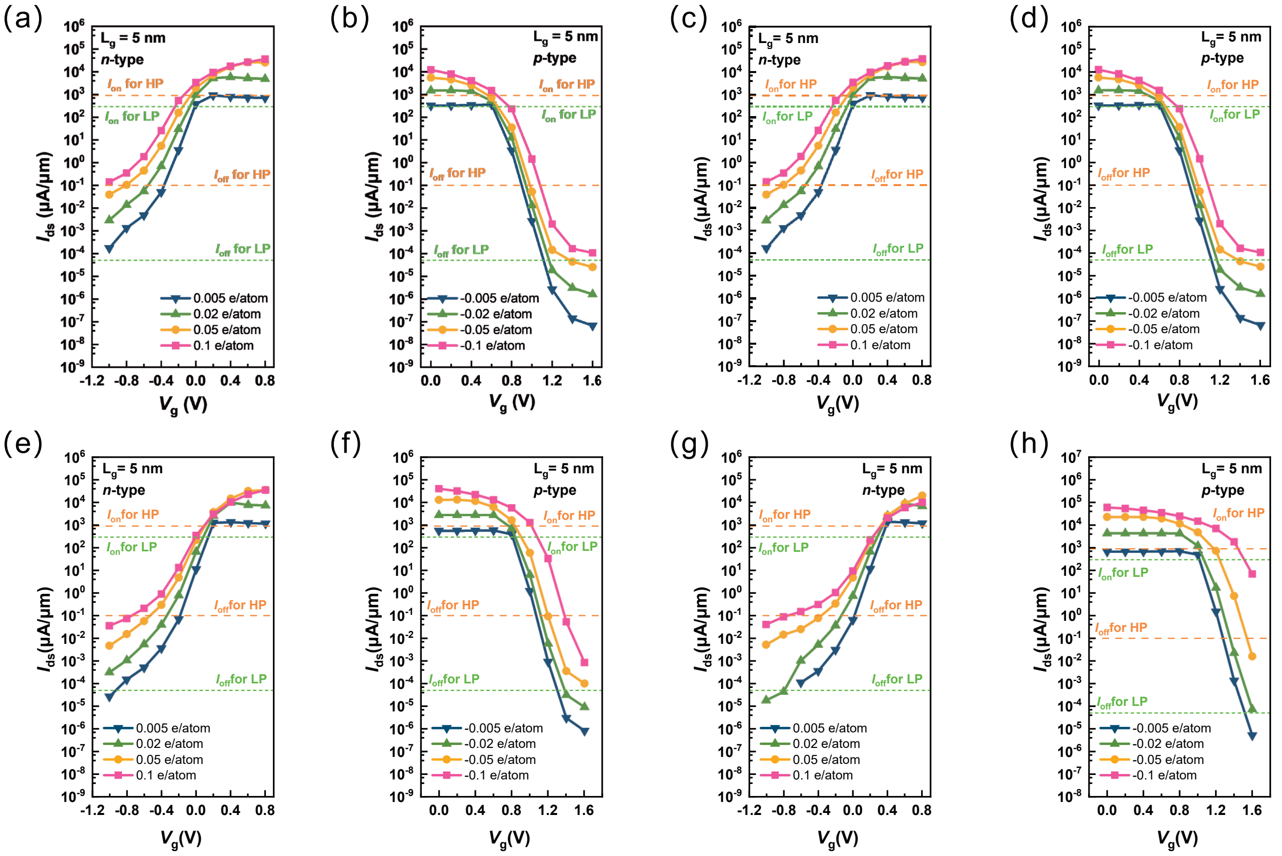

Fig. S6 (a)-(b) The doping concentration testing of bilayer α-SiS. (c)-(d) The doping concentration testing of bilayer β-SiTe. (e)-(f) The doping concentration testing of bilayer β-SnTe. (g)-(h) The doping concentration testing of bilayer β-PbTe. The black dashed lines represent the ITRS off-state current standards for high performance (HP) and low power (LP) devices, respectively.

Table S2 The device performance of the sub-5-nm-gate bilayer α-SiS FETs against the ITRS 2013 requirements for HP and LP application, including on-state current (I_{on}), off-state current (I_{off}) and on-off-ratio ($I_{\mathrm{on}}/I_{\mathrm{off}}$). The data in bold black indicates compliance with the ITRS standards, while the data represented by hyphens indicates that the curve struggles to reach the cutoff current.

Type	Expansion direction	L_{g}(nm)+UL(nm)	HP			LP		
			I_{on} (μA/μm)	I_{off} (μA/μm)	$I_{\mathrm{on}}/I_{\mathrm{off}}$	I_{on} (μA/μm)	I_{off} (μA/μm)	$I_{\mathrm{on}}/I_{\mathrm{off}}$
ITRS 2013			900.00	0.10		295.00	5E-5	
n-type	along a direction	5+0	**1892.00**	**0.10**	**1.89E+04**	-	-	-
n-type	along a direction	5+1	**3189.46**	**0.10**	**3.19E+04**	**567.04**	**5E-5**	**1.13E+07**
n-type	along a direction	5+2	**2761.85**	**0.10**	**2.76E+04**	**888.98**	**5E-5**	**1.77E+07**
n-type	along a direction	5+3	**1878.52**	**0.10**	**1.88E+04**	**638.77**	**5E-5**	**1.27E+07**
n-type	along a direction	3+0	-	-	-	-	-	-
n-type	along a direction	3+1	-	-	-	-	-	-
n-type	along a direction	3+2	**1963.41**	**0.10**	**1.96E+04**	-	-	-
n-type	along a direction	3+3	**1293.07**	**0.10**	**1.29E+04**	-	-	-
n-type	along a direction	1+0	-	-	-	-	-	-
p-type	along a direction	5+0	**1187.24**	**0.10**	**1.18E+04**	-	-	-
p-type	along a direction	5+1	**2454.24**	**0.10**	**2.45E+04**	0.01	5E-5	1.30E+02
p-type	along a direction	5+2	**2321.13**	**0.10**	**2.32E+04**	**340.32**	**5E-5**	**6.80E+06**
p-type	along a direction	5+3	738.98	0.10	7.38E+03	**334.19**	**5E-5**	**6.60E+06**
p-type	along a direction	3+0	-	-	-	-	-	-
p-type	along a direction	3+1	534.95	0.10	5.34E+03	-	-	-
p-type	along a direction	3+2	**1180.43**	**0.10**	**1.18E+04**	-	-	-
p-type	along a direction	3+3	878.07	0.10	8.78E+03	4.24	5E-5	8.48E+04
p-type	along a direction	1+0	-	-	-	-	-	-

Table S3 The device performance of the sub-5-nm-gate bilayer β-SiTe FETs against the ITRS 2013 requirements for HP and LP application, including on-state current (I_{on}), off-state current (I_{off}) and on-off-ratio (I_{on}/I_{off}). The data in bold black indicates compliance with the ITRS standards, while the data represented by hyphens indicates that the curve struggles to reach the cutoff current.

Type	Expansion direction	L_g(nm)+UL(nm)	HP			LP		
			I_{on} (μA/μm)	I_{off} (μA/μm)	I_{on}/I_{off}	I_{on} (μA/μm)	I_{off} (μA/μm)	I_{on}/I_{off}
ITRS 2013			900.00	0.10		295.00	5E-5	
n-type	along a direction	5+0	**3417.69**	**0.10**	**3.42E+04**	-	-	-
n-type	along a direction	5+1	**5026.35**	**0.10**	**5.63E+04**	-	-	-
n-type	along a direction	5+3	**2329.51**	**0.10**	**2.23E+04**	**719.13**	**5E-5**	**1.44E+07**
n-type	along a direction	5+5	**916.99**	**0.10**	**9.17E+03**	291.92	5E-5	5.84E+06
n-type	along a direction	3+0	-	-	-	-	-	-
n-type	along a direction	3+1	166.08	0.10	1.66E+03	-	-	-
n-type	along a direction	3+3	**1967.96**	**0.10**	**1.97E+04**	-	-	-
n-type	along a direction	3+5	739.04	0.10	7.39E+03	87.48	5E-5	1.75E+06
n-type	along a direction	1+0	-	-	-	-	-	-
n-type	along b direction	5+0	**2380.46**	**0.10**	**2.38E+04**	-	-	-
n-type	along b direction	5+1	**5311.86**	**0.10**	**5.31E+04**	-	-	-
n-type	along b direction	5+3	**2189.99**	**0.10**	**2.19E+04**	226.58	5E-5	4.53E+06
n-type	along b direction	5+5	848.95	0.10	8.49E+03	243.52	5E-5	4.87E+06
n-type	along b direction	3+0	-	-	-	-	-	-
n-type	along b direction	3+1	-	-	-	-	-	-
n-type	along b direction	3+3	**3430.98**	**0.10**	**3.43E+04**	-	-	-
n-type	along b direction	3+5	**1512.03**	**0.10**	**1.51E+04**	0.76	5E-5	1.52E+04
n-type	along b direction	1+0	-	-	-	-	-	-
p-type	along a direction	5+0	**1647.56**	**0.10**	**1.65E+04**	**879.85**	**5E-5**	**1.76E+07**
p-type	along a direction	5+1	**1597.34**	**0.10**	**1.60E+04**	**750.03**	**5E-5**	**1.50E+07**
p-type	along a direction	5+3	672.14	0.10	6.72E+03	291.08	5E-5	5.82E+06
p-type	along a direction	5+5	329.01	0.10	3.29E+03	-	-	-
p-type	along a direction	3+0	**1498.10**	**0.10**	**1.50E+04**	-	-	-
p-type	along a direction	3+1	**1462.40**	**0.10**	**1.46E+04**	**348.04**	**5E-5**	**6.96E+06**
p-type	along a direction	3+3	614.98	0.10	6.15E+03	255.69	5E-5	5.11E+06
p-type	along a direction	3+5	305.89	0.10	3.06E+03	138.20	5E-5	2.76E+06
p-type	along a direction	1+0	-	-	-	-	-	-
p-type	along b direction	5+0	**1484.71**	**0.10**	**1.48E+04**	**889.62**	**5E-5**	**1.78E+07**
p-type	along b direction	5+1	**1462.13**	**0.10**	**1.46E+04**	**769.30**	**5E-5**	**1.54E+07**
p-type	along b direction	5+3	634.35	0.10	6.34E+03	289.93	5E-5	5.80E+06
p-type	along b direction	5+5	310.64	0.10	3.11E+03	128.02	5E-5	2.56E+06
p-type	along b direction	3+0	**2360.72**	**0.10**	**2.36E+04**	-	-	-
p-type	along b direction	3+1	**2625.63**	**0.10**	**2.62E+04**	**518.76**	**5E-5**	**1.04E+07**
p-type	along b direction	3+3	**941.67**	**0.10**	**9.42E+03**	**408.90**	**5E-5**	**8.18E+06**
p-type	along b direction	3+5	474.78	0.10	4.75E+03	236.50	5E-5	4.73E+06
p-type	along b direction	1+0	-	-	-	-	-	-

Table S4 The device performance of the sub-5-nm-gate bilayer β-SnTe FETs against the ITRS 2013 requirements for HP and LP application, including on-state current (I_{on}), off-state current (I_{off}) and on-off-ratio (I_{on}/I_{off}). The data in bold black indicates compliance with the ITRS standards, while the data represented by hyphens indicates that the curve struggles to reach the cutoff current.

Type	Expansion direction	L_g(nm)+UL(nm)	HP			LP		
			I_{on} (µA/µm)	I_{off} (µA/µm)	I_{on}/I_{off}	I_{on} (µA/µm)	I_{off} (µA/µm)	I_{on}/I_{off}
ITRS 2013			900.00	0.10		295.00	5E-5	
n-type	along a direction	5+0	**4227.00**	**0.10**	**4.23E+04**	-	-	-
n-type	along a direction	5+1	**4787.28**	**0.10**	**4.79E+04**	36.02	5E-5	7.20E+05
n-type	along a direction	5+3	**2136.27**	**0.10**	**2.14E+04**	**1187.34**	**5E-5**	**2.37E+07**
n-type	along a direction	5+5	770.38	0.10	7.70E+03	**518.20**	**5E-5**	**1.04E+07**
n-type	along a direction	3+0	10.91	0.10	1.09E+02	-	-	-
n-type	along a direction	3+1	**1086.89**	**0.10**	**1.09E+04**	-	-	-
n-type	along a direction	3+3	**1737.27**	**0.10**	**1.74E+04**	4.37	5E-5	8.73E+04
n-type	along a direction	3+5	**1259.89**	**0.10**	**1.26E+04**	**659.25**	**5E-5**	**1.32E+07**
n-type	along a direction	1+0	-	-	-	-	-	-
n-type	along b direction	5+0	**5123.68**	**0.10**	**5.12E+04**	-	-	-
n-type	along b direction	5+1	**6031.19**	**0.10**	**6.03E+04**	0.39	5E-5	7.73E+03
n-type	along b direction	5+3	**2524.02**	**0.10**	**2.52E+04**	**1082.62**	**5E-5**	**2.17E+07**
n-type	along b direction	5+5	**1040.30**	**0.10**	**1.04E+04**	**520.60**	**5E-5**	**1.04E+07**
n-type	along b direction	3+0	-	-	-	-	-	-
n-type	along b direction	3+1	881.90	0.10	8.82E+03	-	-	-
n-type	along b direction	3+3	**2297.39**	**0.10**	**2.30E+04**	-	-	-
n-type	along b direction	3+5	**2485.34**	**0.10**	**2.49E+04**	**1326.67**	**5E-5**	**2.65E+07**
n-type	along b direction	1+0	-	-	-	-	-	-
p-type	along a direction	5+0	**1544.27**	**0.10**	**1.54E+04**	**1207.42**	**5E-5**	**2.41E+07**
p-type	along a direction	5+1	**1559.89**	**0.10**	**1.56E+04**	**1077.46**	**5E-5**	**2.15E+07**
p-type	along a direction	5+3	834.68	0.10	8.35E+03	**371.08**	**5E-5**	**7.42E+06**
p-type	along a direction	5+5	491.51	0.10	4.92E+03	-	-	-
p-type	along a direction	3+0	**1422.49**	**0.10**	**1.42E+04**	-	-	-
p-type	along a direction	3+1	**1485.04**	**0.10**	**1.49E+04**	-	-	-
p-type	along a direction	3+3	826.31	0.10	8.26E+03	**305.26**	**5E-5**	**6.11E+06**
p-type	along a direction	3+5	379.82	0.10	3.80E+03	176.76	5E-5	3.54E+06
p-type	along a direction	1+0	-	-	-	-	-	-
p-type	along b direction	5+0	**1487.32**	**0.10**	**1.49E+04**	**1049.17**	**5E-5**	**2.10E+07**
p-type	along b direction	5+1	**1461.78**	**0.10**	**1.46E+04**	**1067.34**	**5E-5**	**2.13E+07**
p-type	along b direction	5+3	775.61	0.10	7.76E+03	**356.25**	**5E-5**	**7.12E+06**
p-type	along b direction	5+5	363.22	0.10	3.63E+03	-	-	-
p-type	along b direction	3+0	**1440.30**	**0.10**	**1.44E+04**	-	-	-
p-type	along b direction	3+1	**1444.49**	**0.10**	**1.45E+04**	-	-	-
p-type	along b direction	3+3	767.39	0.10	7.67E+03	**308.60**	**5E-5**	**6.17E+06**
p-type	along b direction	3+5	361.19	0.10	3.61E+03	-	-	-
p-type	along b direction	1+0	-	-	-	-	-	-

Table S5 The device performance of the sub-5-nm-gate bilayer β-PbTe FETs against the ITRS 2013 requirements for HP and LP application, including on-state current (I_{on}), off-state current (I_{off}) and on-off-ratio (I_{on}/I_{off}). The data in bold black indicates compliance with the ITRS standards, while the data represented by hyphens indicates that the curve struggles to reach the cutoff current.

Type	Expansion direction	L_g(nm)+UL(nm)	HP			LP		
			I_{on} (µA/µm)	I_{off} (µA/µm)	I_{on}/I_{off}	I_{on} (µA/µm)	I_{off} (µA/µm)	I_{on}/I_{off}
ITRS 2013			900.00	0.10		295.00	5E-5	
n-type	along a direction	5+0	**3388.01**	**0.10**	**3.39E+04**	-	-	-
n-type	along a direction	5+1	**3434.10**	**0.10**	**3.43E+04**	-	-	-
n-type	along a direction	5+3	**1529.83**	**0.10**	**1.53E+04**	**887.78**	**5E-5**	**1.78E+07**
n-type	along a direction	5+5	540.81	0.10	5.41E+03	**320.73**	**5E-5**	**6.41E+06**
n-type	along a direction	3+0	22.70	0.10	2.27E+02	-	-	-
n-type	along a direction	3+1	823.13	0.10	8.23E+03	-	-	-
n-type	along a direction	3+3	**1395.73**	**0.10**	**1.40E+04**	-	-	-
n-type	along a direction	3+5	456.40	0.10	4.56E+03	195.98	5E-5	3.92E+06
n-type	along a direction	1+0	-	-	-	-	-	-
n-type	along b direction	5+0	**4240.21**	**0.10**	**4.24E+04**	-	-	-
n-type	along b direction	5+1	**4834.59**	**0.10**	**4.83E+04**	-	-	-
n-type	along b direction	5+3	**2573.55**	**0.10**	**2.57E+04**	**1251.89**	**5E-5**	**2.50E+07**
n-type	along b direction	5+5	**999.78**	**0.10**	**1.00E+04**	**508.67**	**5E-5**	**1.02E+07**
n-type	along b direction	3+0	1.94	0.10	1.94E+01	-	-	-
n-type	along b direction	3+1	706.57	0.10	7.07E+03	-	-	-
n-type	along b direction	3+3	**1201.14**	**0.10**	**1.20E+04**	-	-	-
n-type	along b direction	3+5	**2397.92**	**0.10**	**2.40E+04**	**1286.66**	**5E-5**	**2.57E+07**
n-type	along b direction	1+0	-	-	-	-	-	-
p-type	along a direction	5+0	**2167.58**	**0.10**	**2.17E+04**	**1092.60**	**5E-5**	**2.19E+07**
p-type	along a direction	5+1	**2242.60**	**0.10**	**2.24E+04**	**1251.06**	**5E-5**	**2.50E+07**
p-type	along a direction	5+3	**1082.05**	**0.10**	**1.08E+04**	**423.18**	**5E-5**	**8.46E+06**
p-type	along a direction	5+5	488.88	0.10	4.89E+03	146.00	5E-5	2.92E+06
p-type	along a direction	3+0	**1462.20**	**0.10**	**1.46E+04**	-	-	-
p-type	along a direction	3+1	**2017.09**	**0.10**	**2.02E+04**	-	-	-
p-type	along a direction	3+3	885.29	0.10	8.85E+03	**297.16**	**5E-5**	**5.94E+06**
p-type	along a direction	3+5	446.41	0.10	4.46E+03	147.76	5E-5	2.96E+06
p-type	along a direction	1+0	-	-	-	-	-	-
p-type	along b direction	5+0	**2174.14**	**0.10**	**2.17E+04**	**1059.83**	**5E-5**	**2.12E+07**
p-type	along b direction	5+1	**2150.27**	**0.10**	**2.15E+04**	**1122.54**	**5E-5**	**2.25E+07**
p-type	along b direction	5+3	**1123.35**	**0.10**	**1.12E+04**	**508.01**	**5E-5**	**1.02E+07**
p-type	along b direction	5+5	490.41	0.10	4.90E+03	242.35	5E-5	4.85E+06
p-type	along b direction	3+0	705.04	0.10	7.05E+03	-	-	-
p-type	along b direction	3+1	**2082.52**	**0.10**	**2.08E+04**	-	-	-
p-type	along b direction	3+3	**942.49**	**0.10**	**9.42E+03**	**330.24**	**5E-5**	**6.60E+06**
p-type	along b direction	3+5	476.58	0.10	4.77E+03	-	-	-
p-type	along b direction	1+0	-	-	-	-	-	-