Supplemental material for

Evolutional Carrier Mobility and Power Factor of Two-Dimensional Tin Telluride due to Quantum Size Effects

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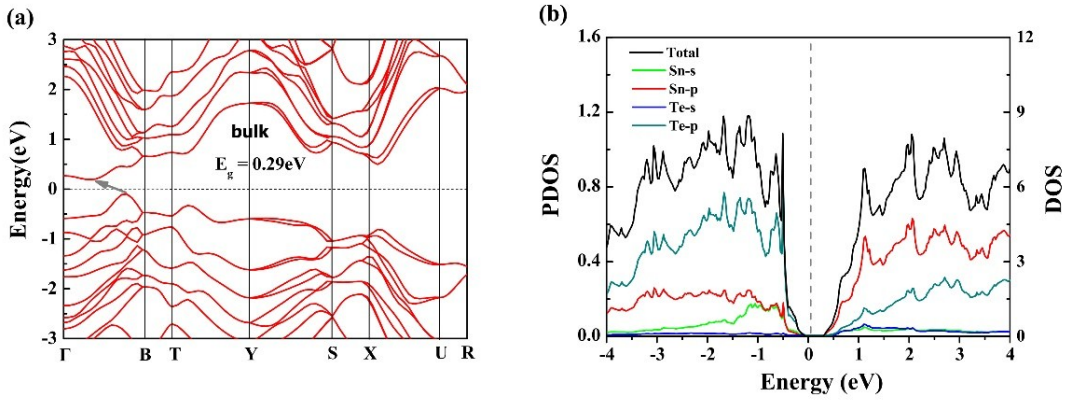
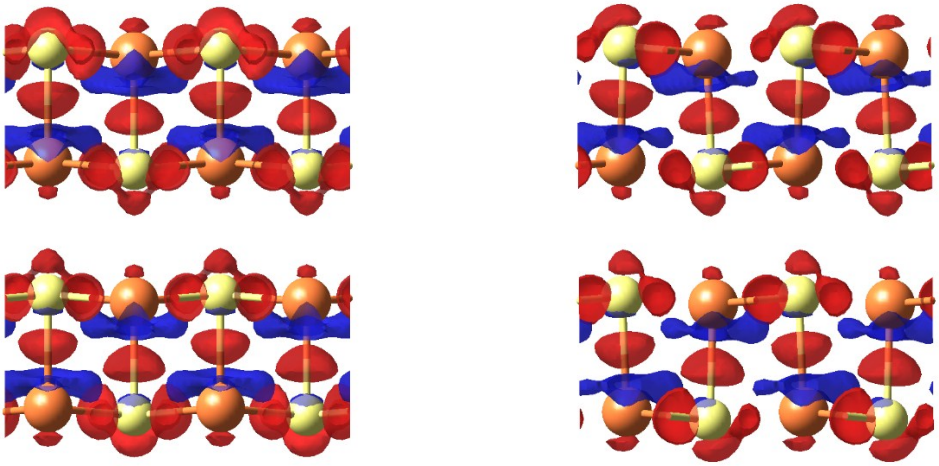


Figure S1. (a) Electronic band structure and (b) total density of states (TDOS) and the partial density of state (PDOS) of bulk SnTe extracted from optPBE-vdw functional.

(a) (b)

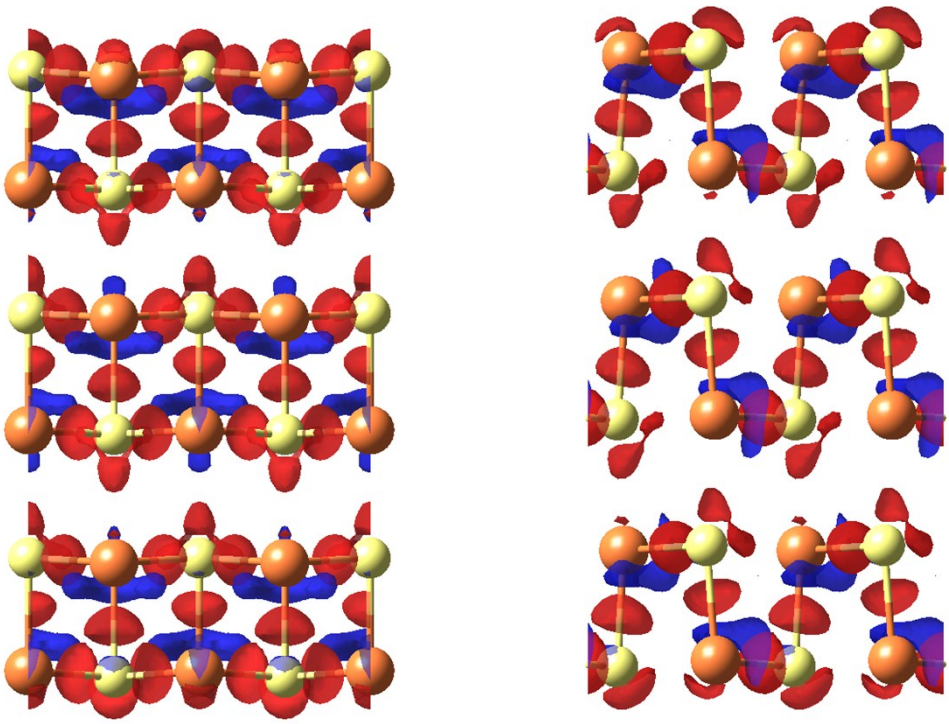
Monolayer

(c) (d)



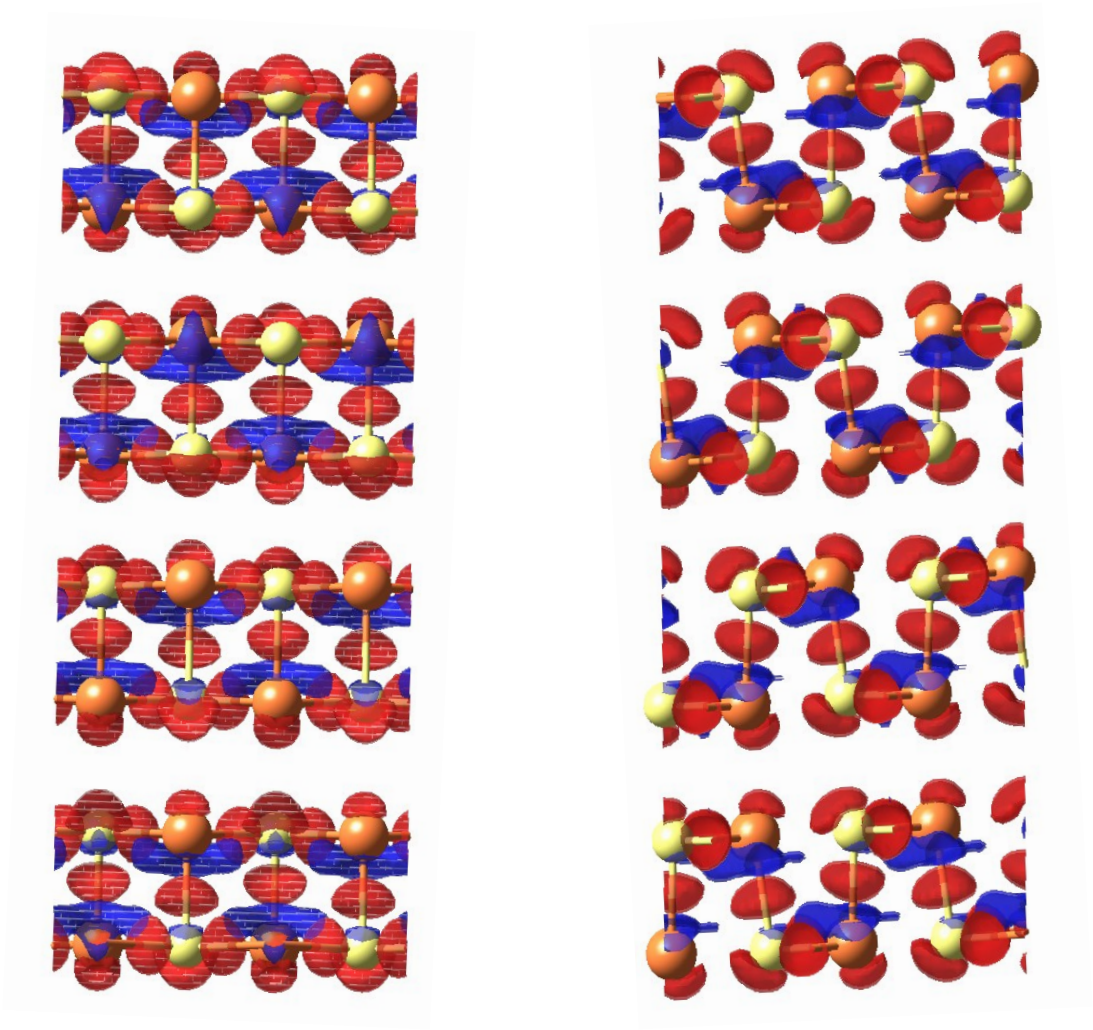
Bilayer

(e) (f)



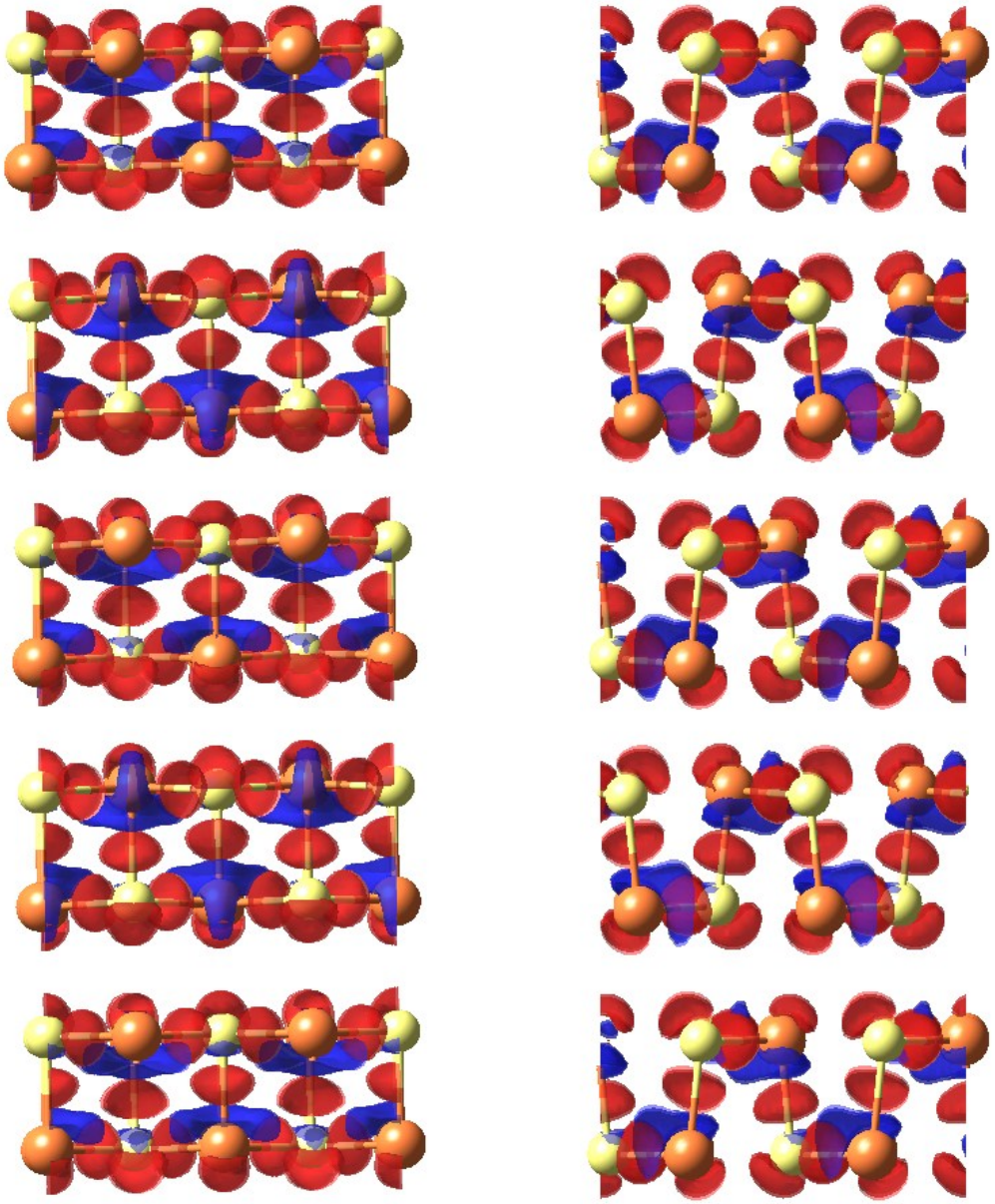
Triple layer

(g) (h)



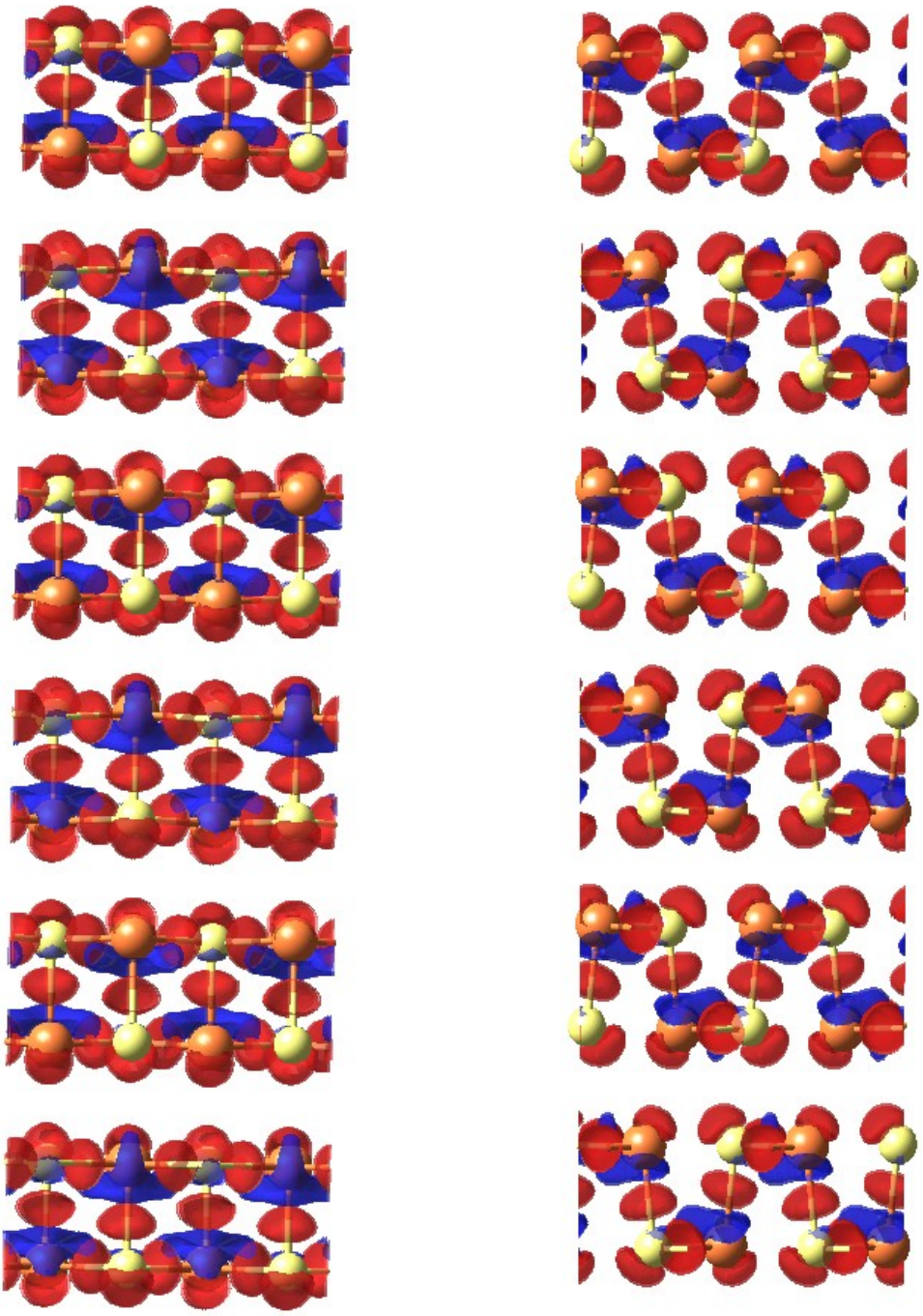
Four layer

(i) (j)



Five layer

(k) (l)



Six layer

Figure S2. (a)-(l) The side views of calculated difference charge density distribution for the 1L-6 L SnTe , with a constant density of 0.02 /-0.02 e/Å^3 for the electrons accumulation and depletion respectively.

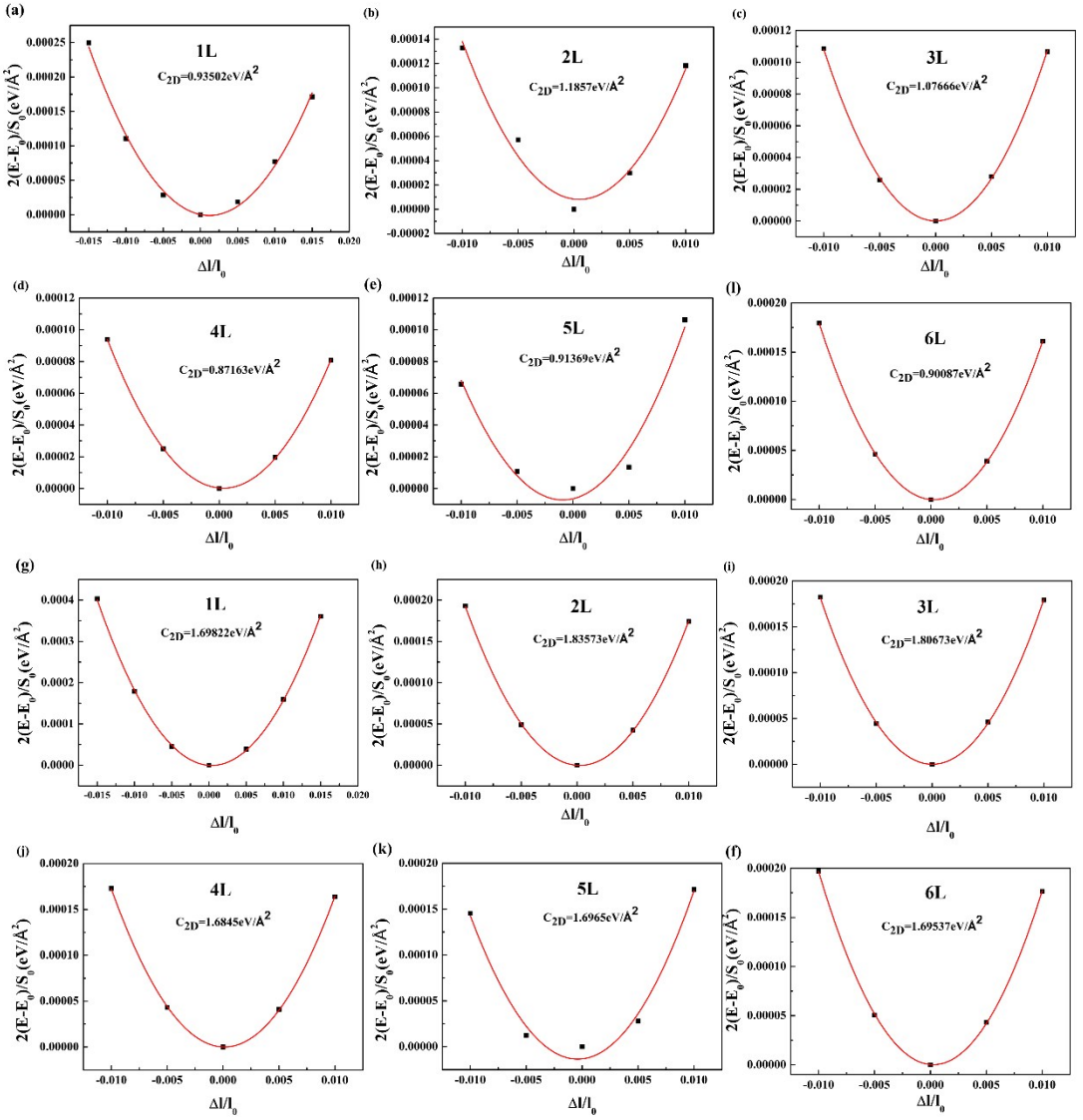


Figure S3. Calculated elastic constants (C_{2D}) by fitting the energy difference to quadratic polynomial functions for monolayer (1 L) and few layer (2 L, 3 L, 4 L, 5 L and 6 L) SnTe along armchair (a-f) and zigzag (g-l) directions.

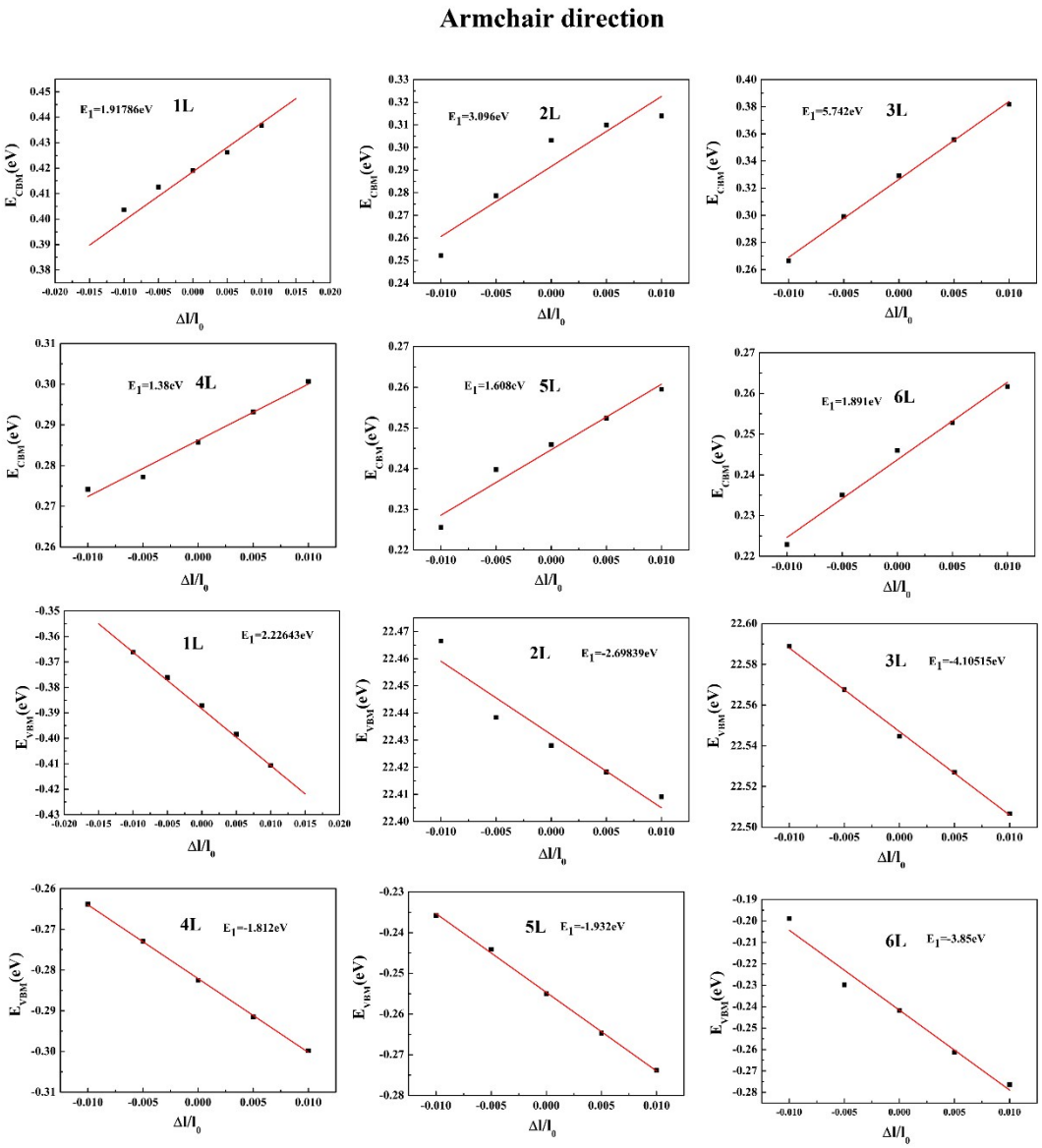


Figure S4. Calculated deformation constants (E_1) for n- and *p*-type SnTe monolayer (1 L) and few-layer (1 L, 2 L, 3 L, 4 L, 5 L and 6 L) along armchair direction

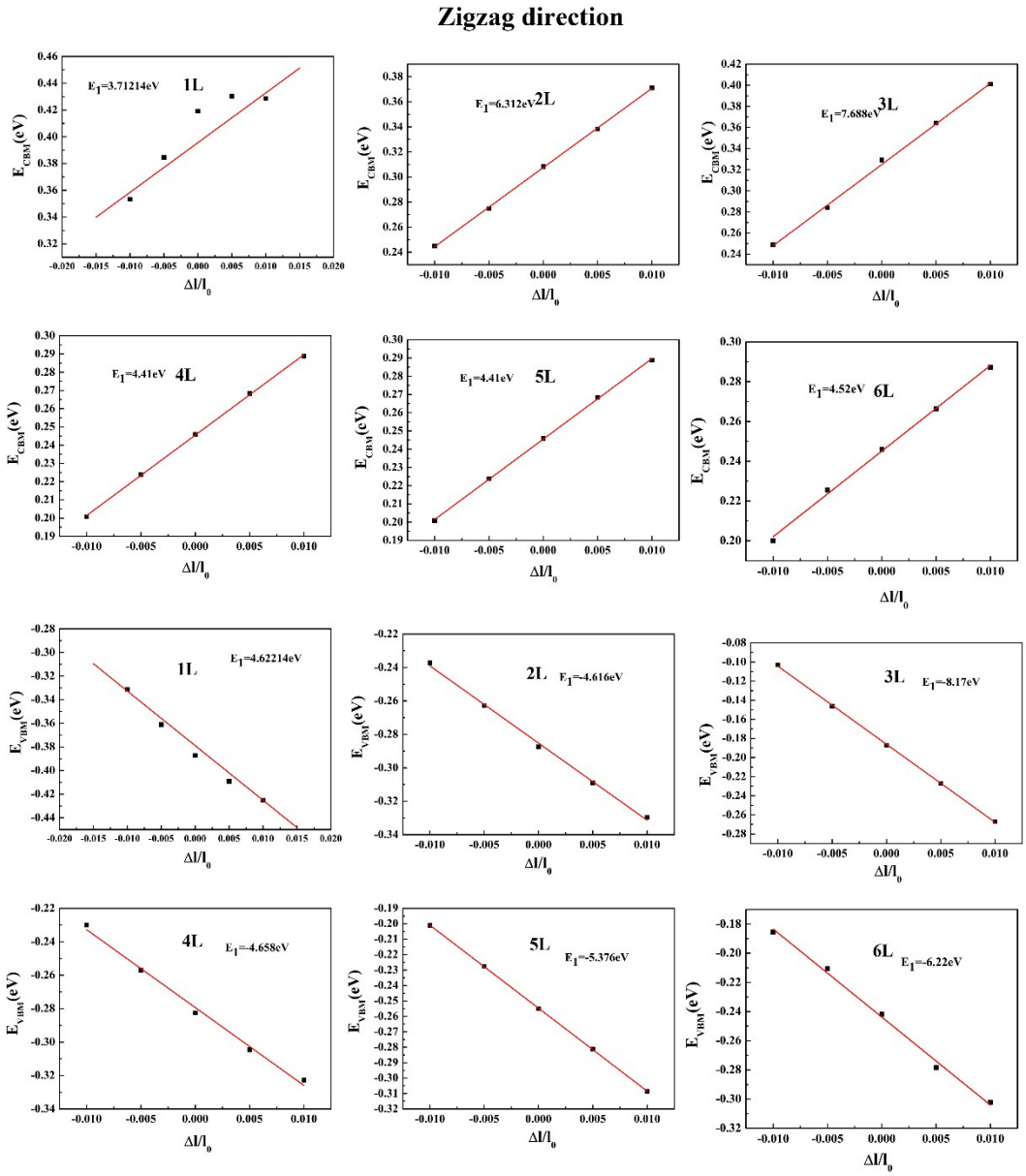


Figure S5. Calculated deformation constants (E_1) for n- and *p*-type SnTe monolayer (1 L) and few-layer (2 L, 3 L, 4 L, 5 L and 6 L) along zigzag direction.

Table S1. Deformation potential constant (E_1), elastic constant (C_{2D}), effective mass (m*), carrier mobility (μ) and relaxation time (τ) at 300 K, 500 K, 700 K and 900 K, in the armchair and zigzag directions of the 1-6 L SnTe.

1L

Carrier type	Direction	C_{2D} (J/m^2)	E_1 (eV)	m^* (m_0)	T = 300K		T = 500K		T = 700K		T = 900K	
					μ $(cm^2V^{-1}s^{-1})$	τ (fs)	μ $(cm^2V^{-1}s^{-1})$	τ (fs)	μ $(cm^2V^{-1}s^{-1})$	τ (fs)	μ $(cm^2V^{-1}s^{-1})$	τ (fs)
hole	Armchair	15.0	1.9	0.31	1037	183	622	109	444	78	346	61
	Zigzag	27.2	3.7	0.23	677	89	406	53	290	38	226	30
electron	Armchair	15.0	2.2	0.23	1866	244	1119	146	799	104	622	81
	Zigzag	27.2	4.6	0.10	1809	103	1085	62	775	44	603	34

2L

Carrier type	Direction	C_{2D} (J/m^2)	E_1 (eV)	m^* (m_0)	T = 300K		T = 500K		T = 700K		T = 900K	
					μ $(cm^2V^{-1}s^{-1})$	τ (fs)	μ $(cm^2V^{-1}s^{-1})$	τ (fs)	μ $(cm^2V^{-1}s^{-1})$	τ (fs)	μ $(cm^2V^{-1}s^{-1})$	τ (fs)
hole	Armchair	19.0	3.1	0.26	560	83	336	50	240	36	187	28
	Zigzag	29.4	6.3	0.32	170	31	102	19	73	13	56	10
electron	Armchair	19.0	2.7	0.20	1983	226	1189	135	850	96	661	75
	Zigzag	29.4	4.6	0.10	2100	119	1260	72	900	51	700	40

3L

Carrier type	Direction	C_{2D} (J/m^2)	E_1 (eV)	m^* (m_0)	T = 300K		T = 500K		T = 700K		T = 900K	
					μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)
hole	Armchair	17.2	5.7	0.41	140	33	84	20	60	14	47	11
	Zigzag	28.9	7.7	0.10	378	31	227	18	162	13	126	10
electron	Armchair	17.2	4.1	0.28	406	65	243	39	174	28	135	22
	Zigzag	28.9	8.2	0.13	371	27	223	16	15	12	124	9

4L

Carrier type	Direction	C_{2D} (J/m^2)	E_1 (eV)	m^* (m_0)	T = 300K		T = 500K		T = 700K		T = 900K	
					μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)
hole	Armchair	14.0	1.4	2.40	35	31	21	18	15	13	12	10
	Zigzag	27.0	4.3	3.50	5	6	3	4	2	3	2	2
electron	Armchair	14.0	3.6	0.22	741	58	444	35	31	25	247	19
	Zigzag	27.0	4.7	0.22	719	57	431	34	308	24	240	19

5L

Carrier type	Direction	C_{2D} (J/m^2)	E_1 (eV)	m^* (m_0)	T = 300K		T = 500K		T = 700K		T = 900K	
					μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)
hole	Armchair	14.6	1.6	1.18	48	32	29	19	21	14	16	11
	Zigzag	27.1	4.4	2.6	6	8	3	5	2	3	2	3
electron	Armchair	14.6	3.7	0.24	406	55	244	33	174	24	135	18
	Zigzag	27.1	5.4	0.22	396	49	237	30	169	21	132	16

6L

Carrier type	Direction	C_{2D} (J/m^2)	E_1 (eV)	m^* (m_0)	T = 300K		T = 500K		T = 700K		T = 900K	
					μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)	μ ($cm^2V^{-1}s^{-1}$)	τ (fs)
hole	Armchair	14.4	1.9	1.10	41	26	25	15	18	11	14	9
	Zigzag	27.1	4.5	3.30	5	9	3	5	2	4	2	3
electron	Armchair	14.4	3.9	0.22	392	49	235	29	168	21	131	16
	Zigzag	27.1	6.2	0.26	240	35	144	21	103	15	80	12

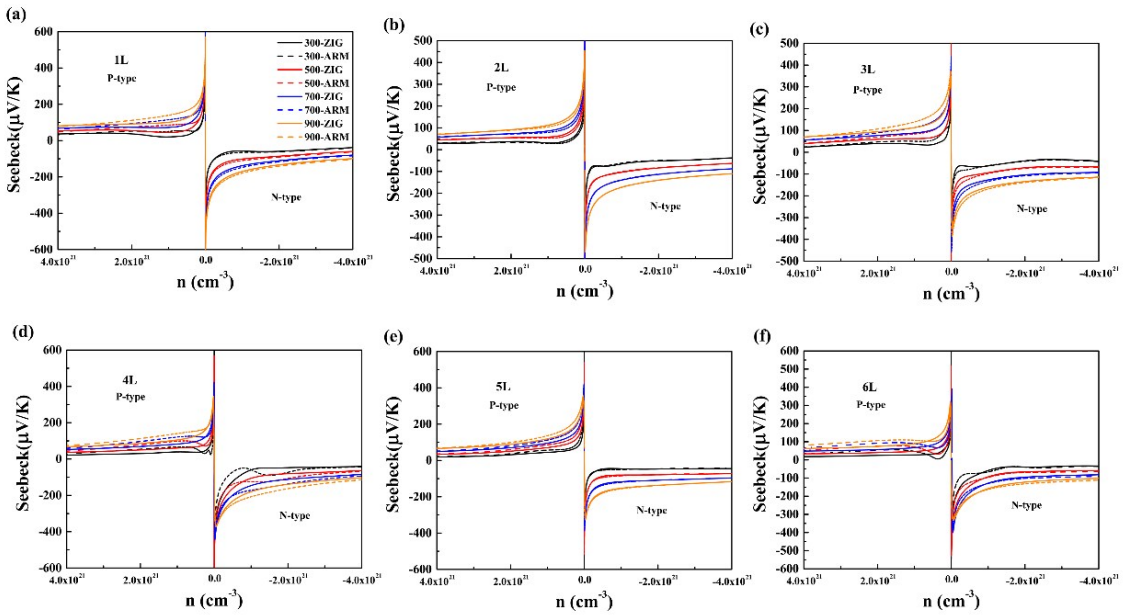


Figure S6. Seebeck coefficient (S) of monolayer (1 L) and few-layer (2 L, 3 L, 4 L, 5 L and 6 L) of SnTe in the armchair (broken line) and zigzag (solid line) directions, (a)-(f) at 300 K (black), 500 K (red), 700 K (blue) and 900 K (orange).

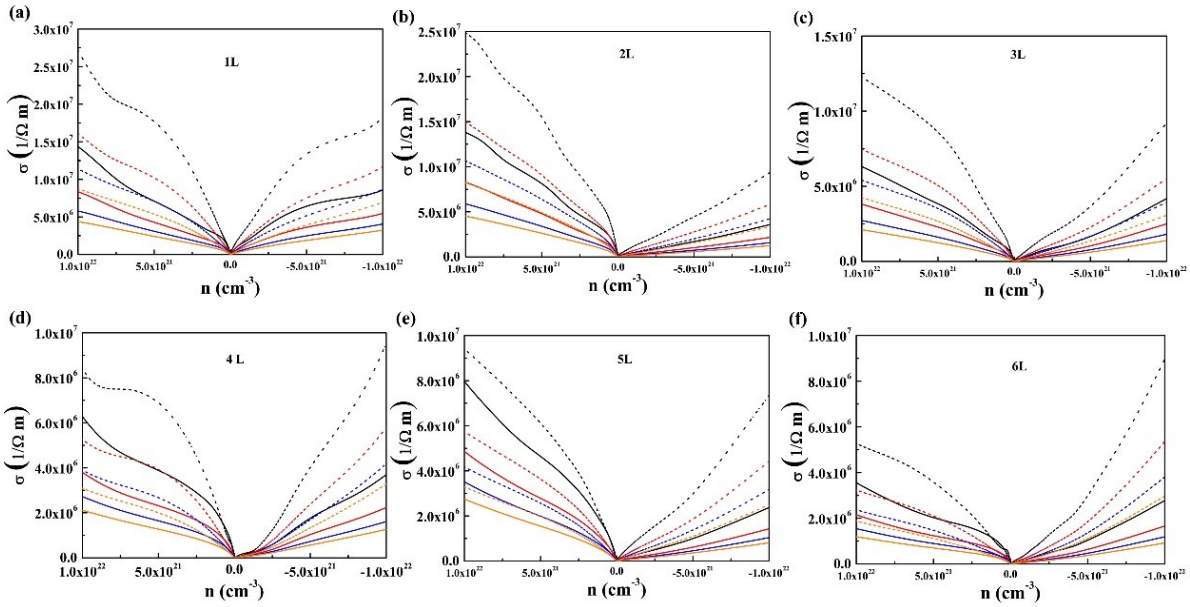


Figure. S7. Electrical conductivity (σ) of monolayer (1 L) and few-layer (2 L, 3 L, 4 L, 5 L and 6 L) of SnTe in the armchair (broken line) and zigzag (solid line) directions, (a)-(f) at 300 K (black), 500 K (red), 700 K (blue) and 900 K (orange).

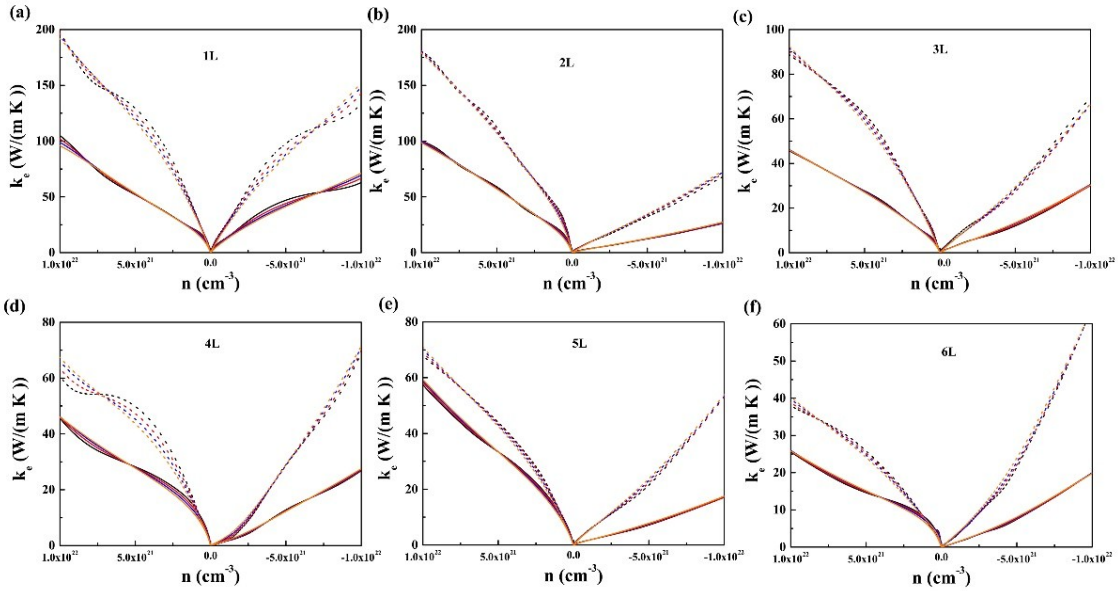


Figure S8. Electrical thermal conductivity of monolayer (1 L) and few-layer (2 L, 3 L, 4 L, 5 L and 6 L) of SnTe in the armchair (broken line) and zigzag (solid line) directions, (a)-(f) at 300K (black), 500K (red), 700K (blue) and 900K (orange).

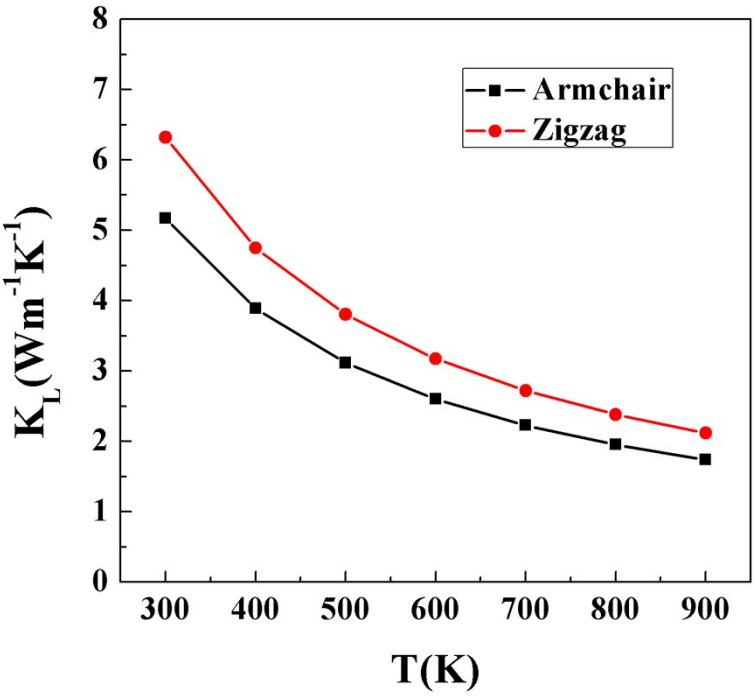


Figure S9. The calculated directional lattice thermal conductivity of monolayer SnTe at various temperatures. [1]

Table S2 The calculated directional lattice thermal conductivity values of monolayer SnTe at 300K, 500K, 700K and 900K, respectively.

$K_L(Wm^{-1}K^{-1})$	T = 300K	T = 500K	T = 700K	T = 900K
Armchair	5.17	3.12	2.23	1.74
Zigzag	6.32	3.80	2.72	2.12

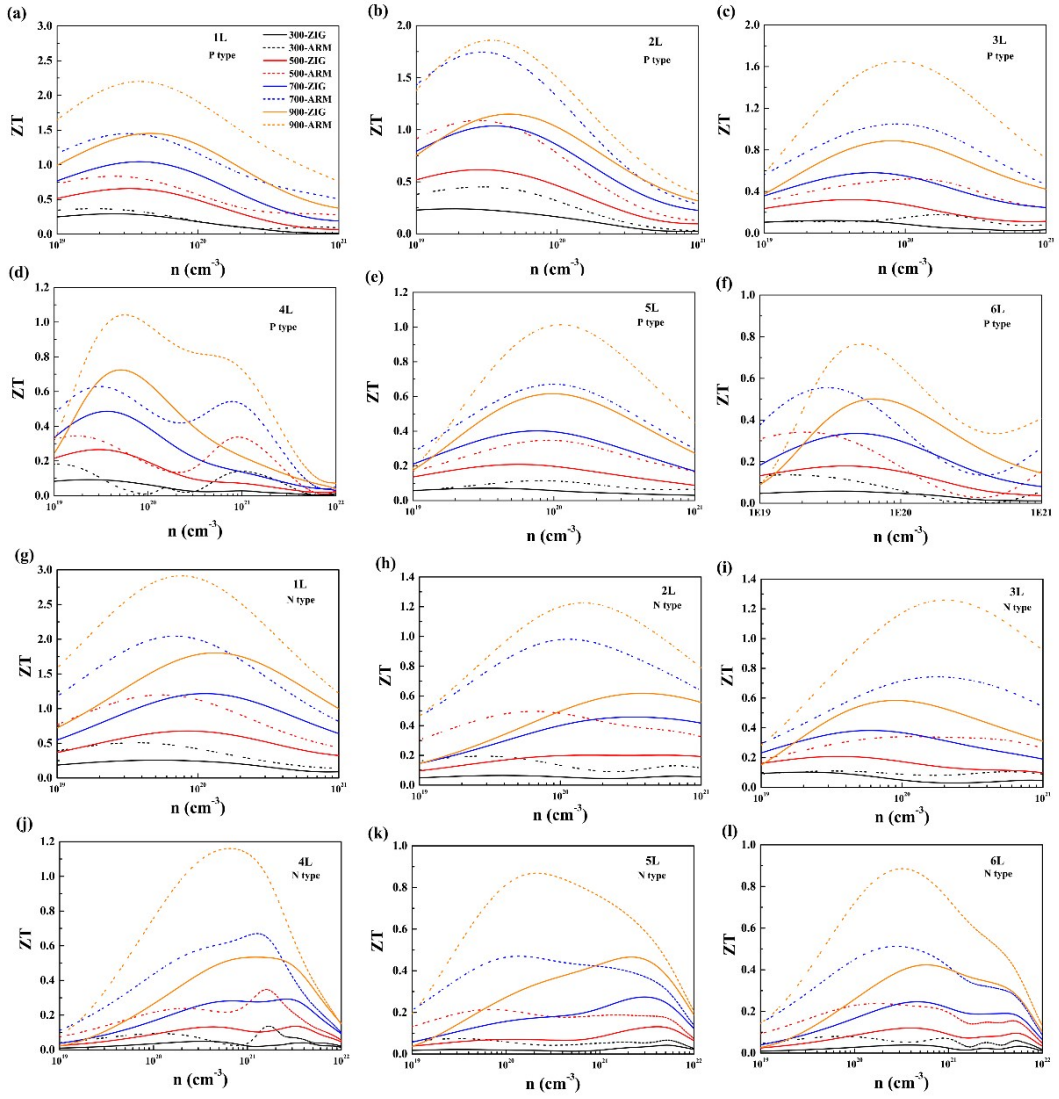


Figure S10. Thermoelectric figure-of-merit (ZT) of monolayer (1 L) and few-layer (2 L, 3 L, 4 L, 5 L and 6 L) of SnTe in the armchair (broken line) and zigzag (solid line) directions, at 300 K (black), 500 K (red), 700 K (blue) and 900 K (orange) for *n*-type (a)-(f) and *p*-type (g)-(l).

Reference

1. Y. Li, M. N. Wu, T. Ding, K. Ma, F. S. Liu, W. Q. Ao and J. Q. Li, *Appl. Phys. Lett.*, 2019, **114**, 5.