Supplementary Information for:

Monolayer β-Tellurene: A promising p-type Thermoelectric Material via First-Principles Calculations

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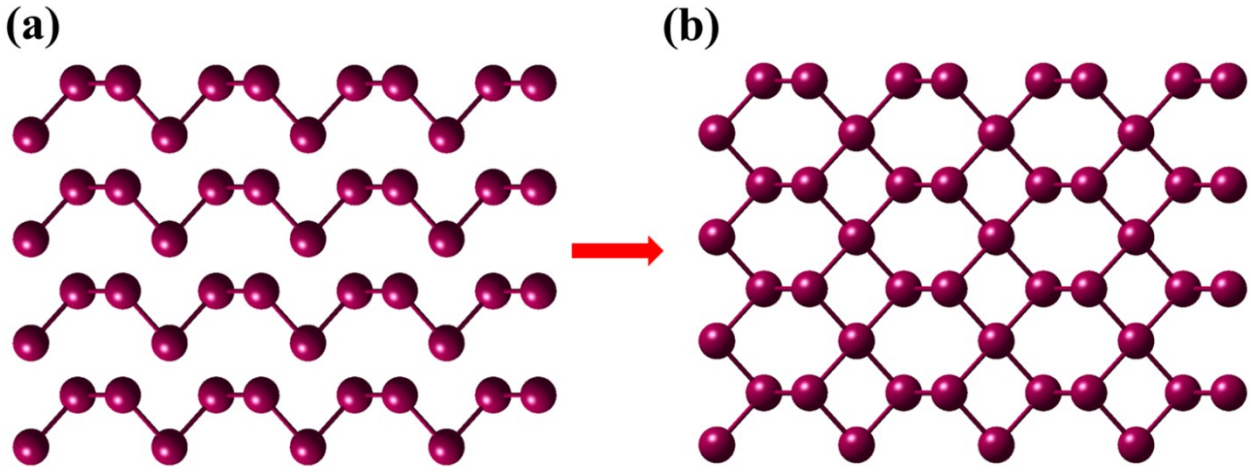
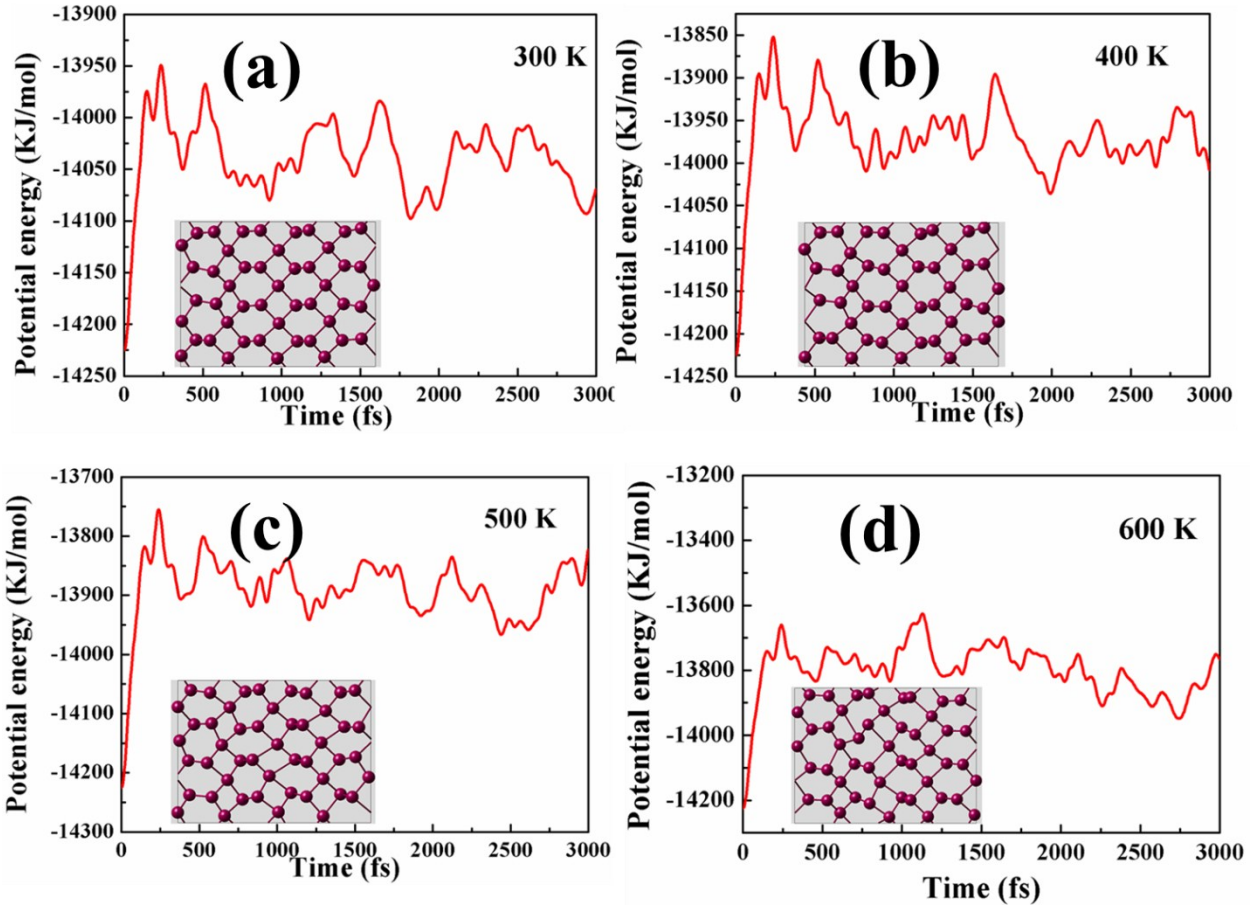


Fig. S1 Structural reconstruction (a) before optimization, (b) after optimization of monolayer β-Tellurene.



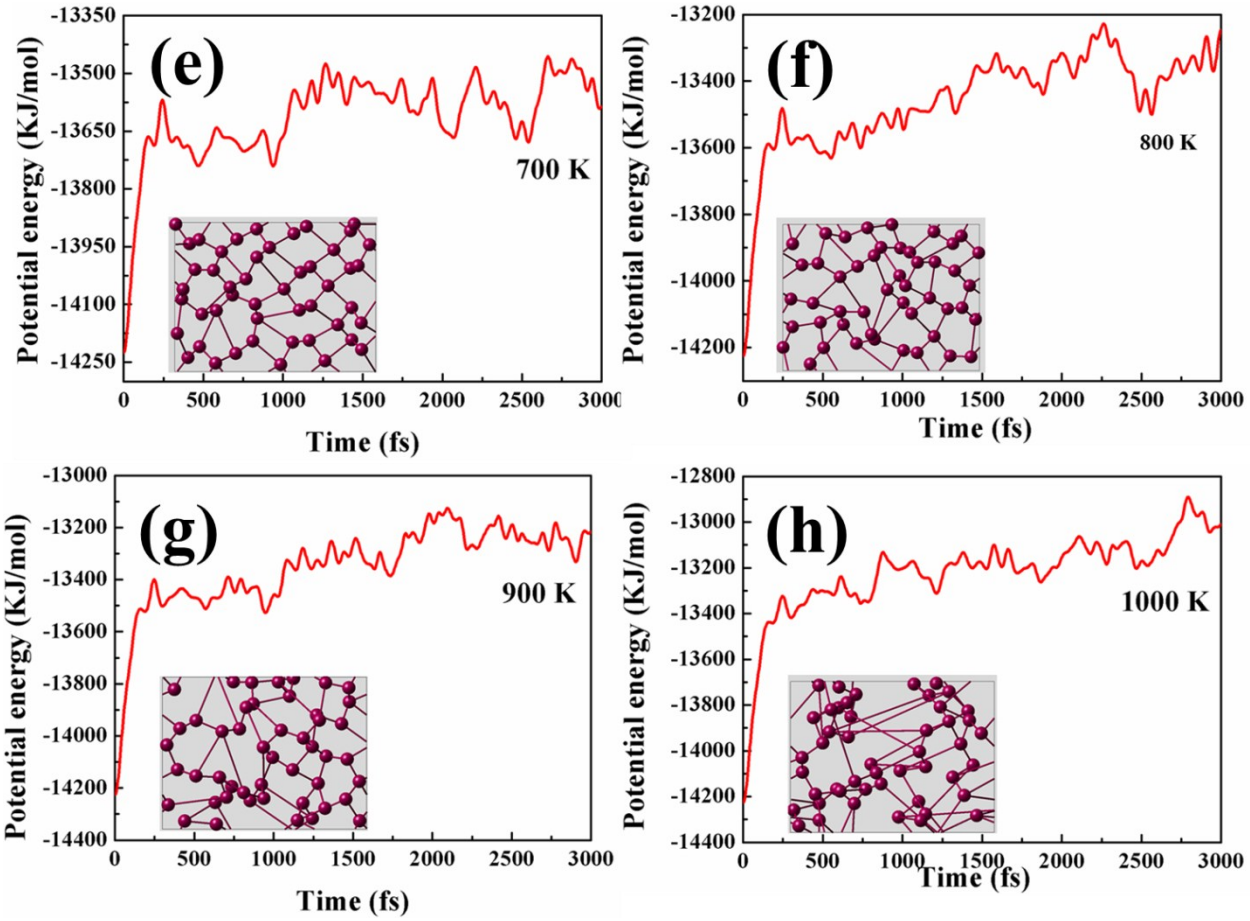


Fig. S2 Potential energy fluctuation AIMD simulations of monolayer β-Tellurene at different temperatures, namely (a) 300 K, (b) 400 K, (c) 500 K, (d) 600 K, (e) 700 K, (f) 800 K, (g) 900 K and (h) 1000 K. The insets show the snapshots of atomic configuration from the top view of monolayer β-Tellurene at the end of AIMD simulations.

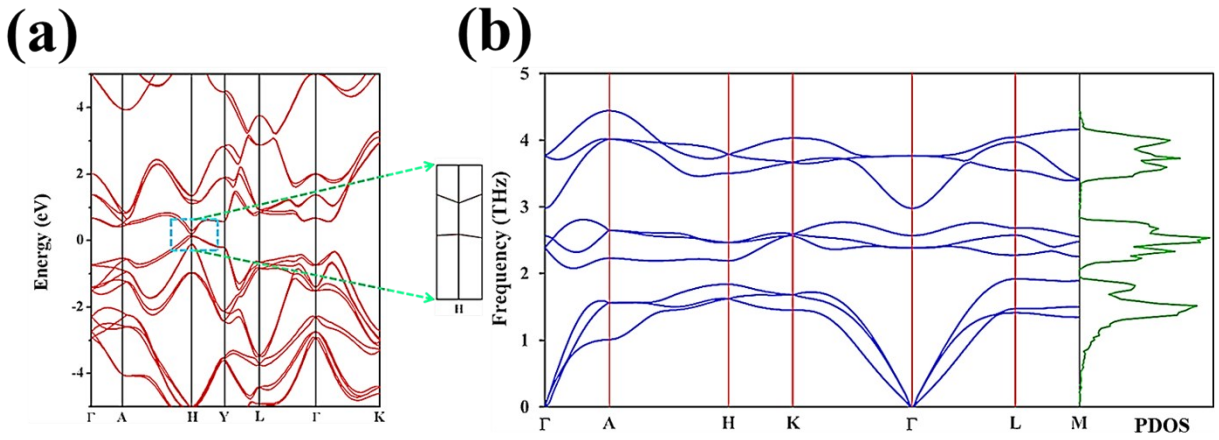


Fig. S3 (a) Electronic band structure (E_g = 0.32 eV) extracted from HSE06 functional, (b) Phonon spectrum of bulk Tellerium.

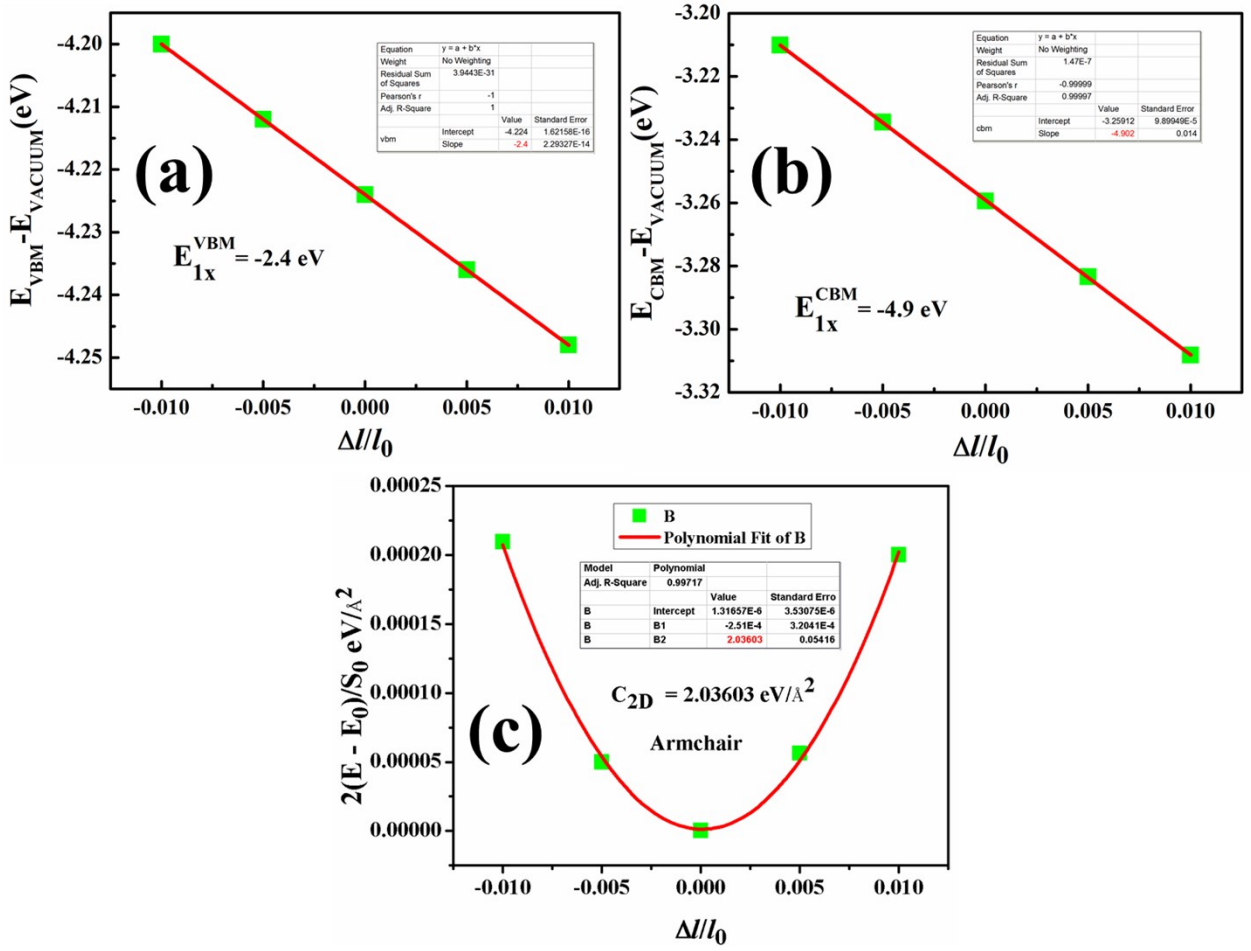


Fig. S4 Deformation potential constants and elastic modulus along armchair (x-direction) of monolayer β-Tellurene, (a) VBM linear fitting for deformation potential, (b) CBM linear fitting for deformation potential and (c) Parabolic fitting for elastic modulus, with strain ranging from -1% ~ 1% with a step of 0.5%.

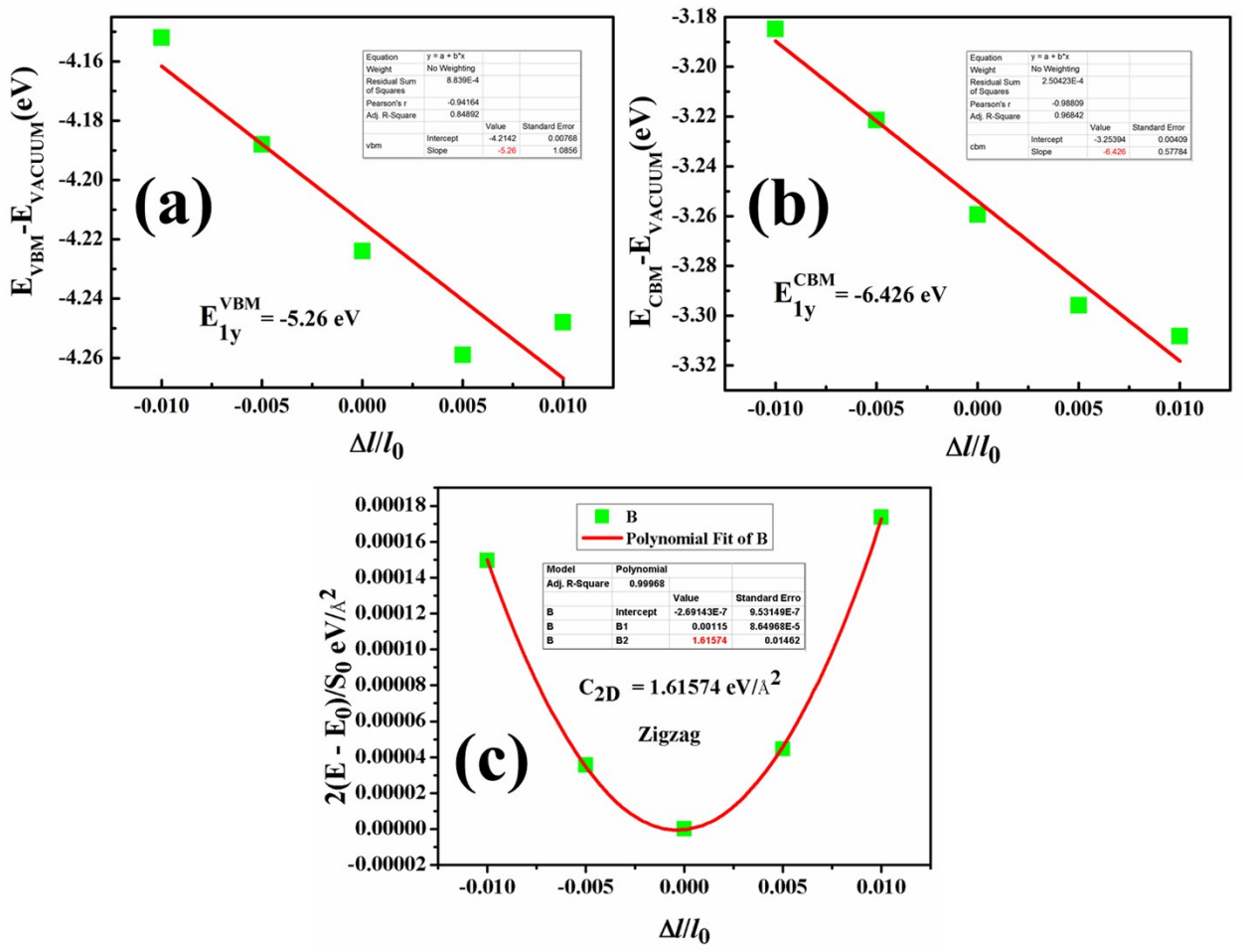


Fig. S5 Deformation potential constants and elastic modulus along zigzag (y-direction) of monolayer β-Tellurene, (a) VBM linear fitting for deformation potential, (b) CBM linear fitting for deformation potential and (c) Parabolic fitting for elastic modulus, with strain ranging from -1% ~ 1% with a step of 0.5%.

Table S1. Carrier type, hole (h) and electron (e), two-dimensional elastic constant, C_{2D}, (Jm^{-2}) Deformation potential constant E_1 (eV) effective mass (m^*), and carrier mobility μ ($cm^2\ V^{-1}\ s^{-1}$), and relaxation time τ (fs) at temperature 300 K, 400 K, 500 K ,600 K, and 700 K.

Carrier type	Direction	C_{2D}	E_1	m^* (m_0)	T=300K		T=400K		T=500K		T=600K		T=700K	
					μ	τ	μ	τ	μ	τ	μ	τ	μ	τ
h	Armchair	32.6	-2.4	0.37	1343	283	1007	212	806	170	671	141	576	121
	Zigzag	25.9	-5.26	0.16	514	47	385	35	308	28	257	23	220	20
e	Armchair	32.6	-4.9	0.82	81	38	61	28	49	23	41	19	35	16
	Zigzag	25.9	-6.43	0.23	134	18	101	13	80	11	67	9	57	8

Table S2. The values of seebeck coefficient (**μ**V/k), power factor (μW/K^2) and the ZT in both armchair and zigzag for *p*-type doping, at 300 K, 400 K, 500 K, 600 K and 700 K.

Temperature (K)	Seebeck coefficient (**μ**V/k)		Power factor (μW/K^2)		ZT	
	Armchair	Zigzag	Armchair	Zigzag	Armchair	Zigzag
300	104.74	81.96	26706	3627	0.54	0.17
400	120.76	96.35	25968	4054	1.0	0.27
500	132.57	112.35	26497	4385	1.7	0.44
600	146.79	126.73	23111	3995	2.3	0.64
700	153.71	139.42	23580	3862	2.9	0.84

Table S3. The values of seebeck coefficient (μV/k), power factor ($\mu W/K^2$) and the ZT in both armchair and zigzag for *n*-type doping, at 300 K, 400 K, 500 K, 600 K and 700 K.

Temperature (K)	Seebeck coefficient (μV/k)		Power factor ($\mu W/K^2$)		ZT	
	Armchair	Zigzag	Armchair	Zigzag	Armchair	Zigzag
300	130.35	160.48	11568.13	2615.27	0.1	0.12
400	167.66	175.78	11126.87	2247.53	0.29	0.19
500	222.60	183.86	9926.06	1993.90	0.41	0.26
600	270.99	232.79	8736.88	1735.30	0.53	0.32
700	296.84	229.32	8285.74	1649.85	0.65	0.39