Supplementary Materials for

Strain Engineering of the Electronic and Transport Properties of Monolayer Tellurenyne

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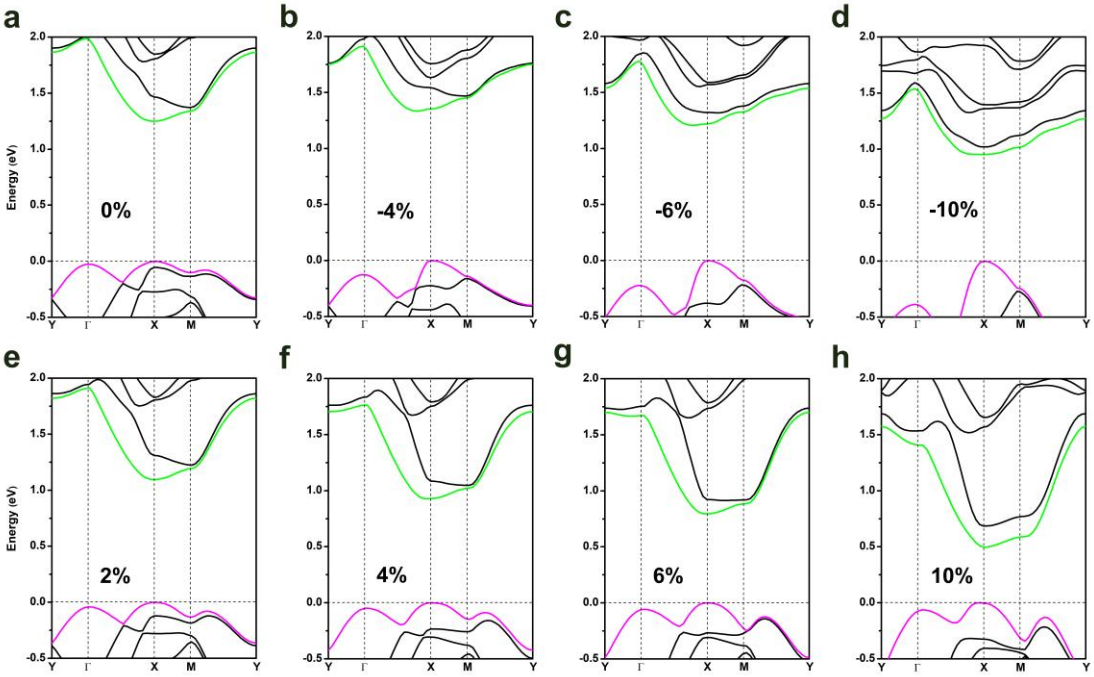

Figure S1. Representative band structures of tellurenyne (PBE results) under the uniaxial strain along the chain direction. (a) represents no strain. (b) to (d) represent the compression strain. (e) to (h) represent the tension strain.

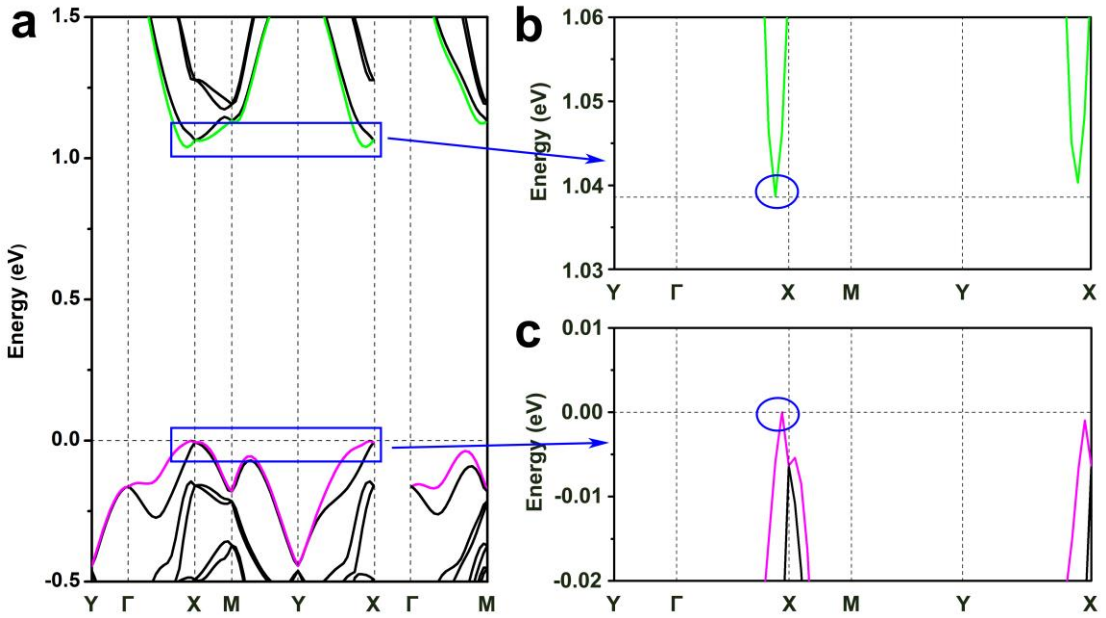

Figure S2. Band structures of tellurenyne (PBE-SOC results) under no strain. (a) represents total band structure. (b) represents local band structure around the CBM. (c) represents the local band structure around the VBM.

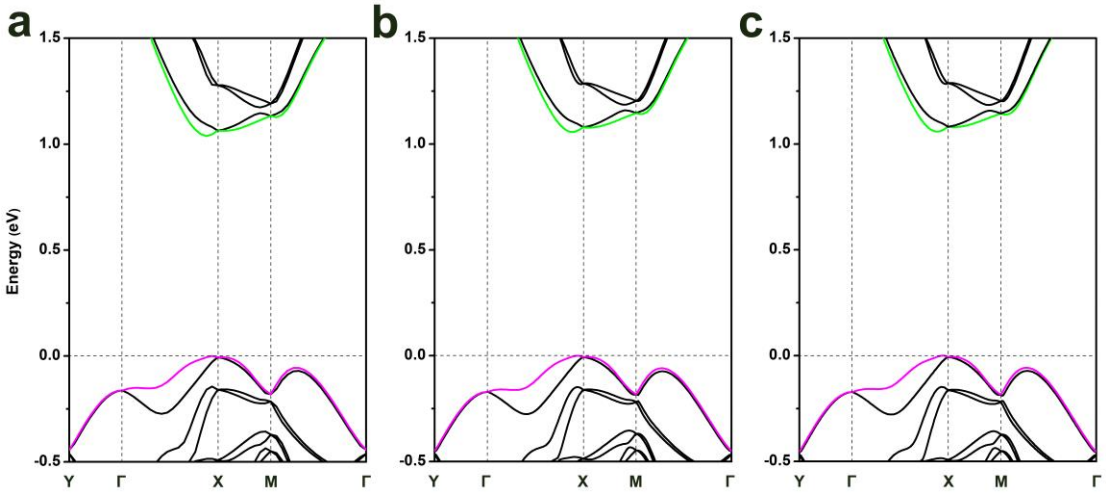

Figure S3. Band structures of tellurenyne (PBE-SOC results) under no strain with (a) norm-conserving pseudopotentials (NP) in CASTEP code,[1] (b) projector augmented-wave (PAW) method in VASP code,[2, 3] (c) all-electron (AE) in FHI-aims code.[4]

Table S1. Band gap in eV, Rashba parameter α_R in eV Å, Rashba energy E_R in meV, momentum offset Δk_R in Å^{-1} of the original tellurenyne (without strain) calculated with different methods.

		CBM			VBM		
	Band gap	α_R	E_R	Δk_R	α_R	E_R	Δk_R
NP	1.04	1.66	25.23	0.06	0.42	6.33	0.03
PAW	1.06	1.87	22.20	0.07	0.37	6.30	0.03
AE	1.06	1.85	25.33	0.06	0.39	6.69	0.03

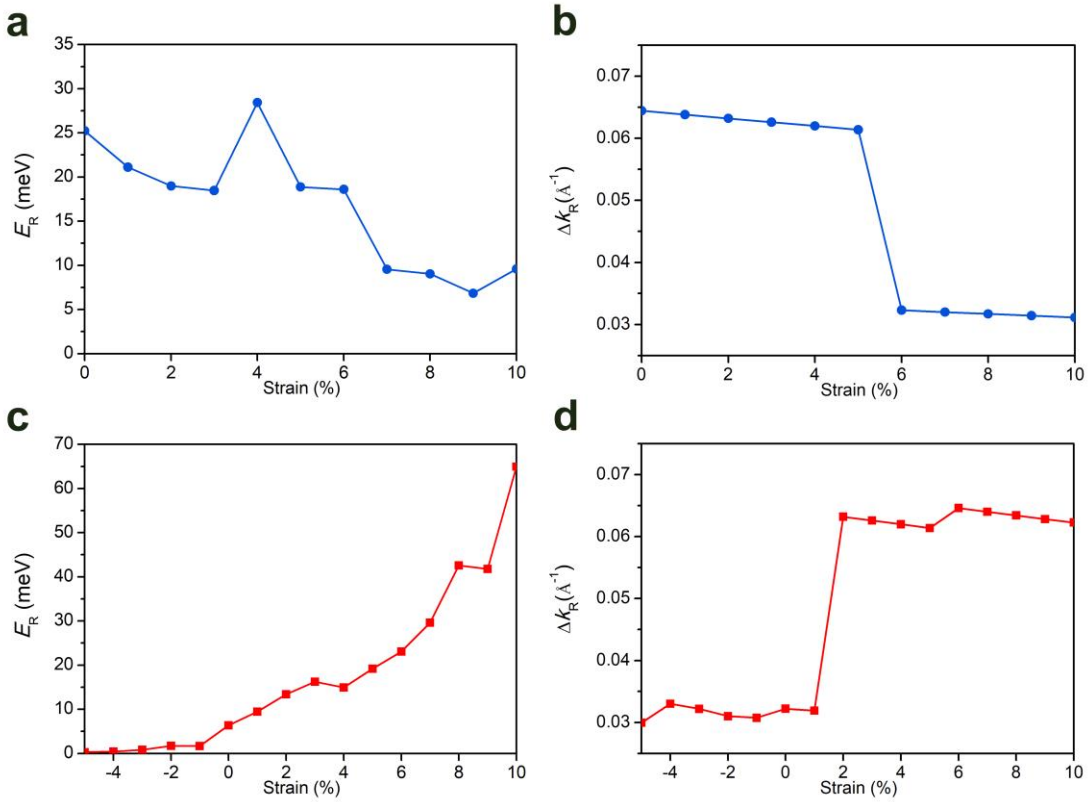

Figure S4. Rashba parameters of tellurenyne under the uniaxial strain along the chain direction. (a) and (b) Rashba energy E_R and momentum offset Δk_R in CBM. (c) and (d) Rashba energy E_R and momentum offset Δk_R in VBM.

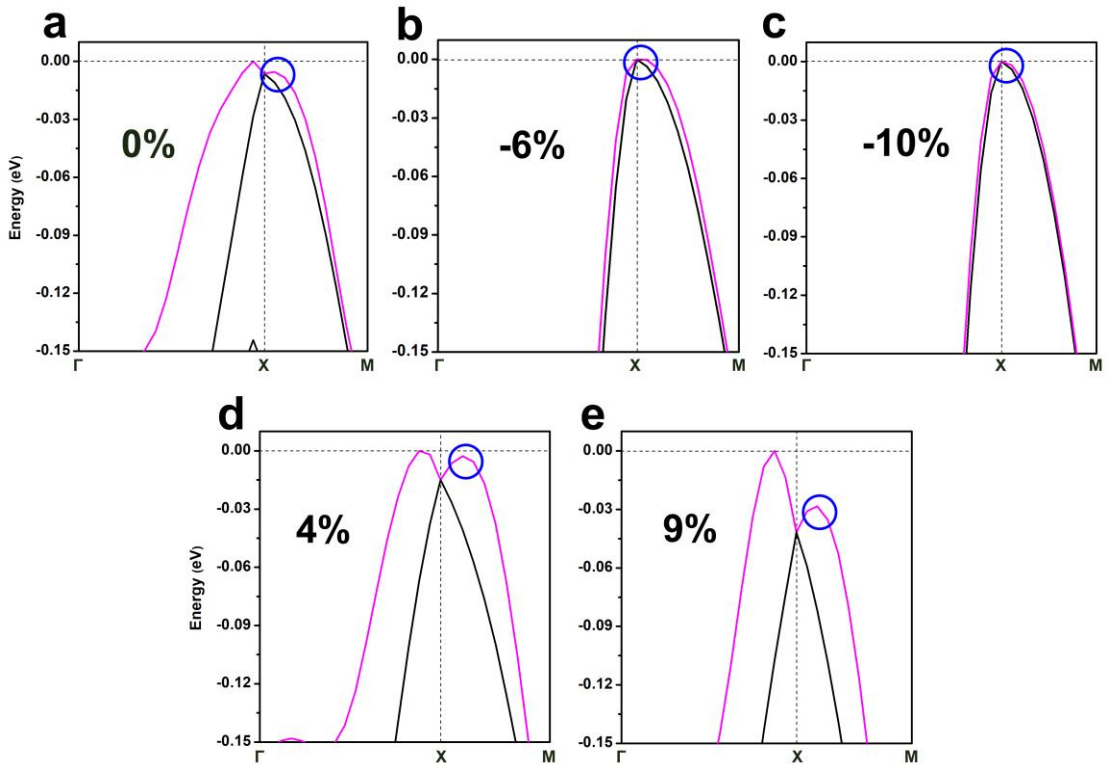

Figure S5. Local band structures of tellurenyne (PBE-SOC results) under the strain along the chain direction. (a) represents no strain, (b) and (c) represent the 6% and 10% compression strain, (d) and (e) represent 4% and 9% tension strain, respectively. The blue circles represent the local valence band edge along the y direction.

Table S2. Effective electron (hole) mass m^* (m_0) and electron (hole) mobility μ (10^3 cm^2/V s) of the phase VI of tellurenyne under the uniaxial strain along the chain direction (m_0 is the mass of the free electron). P represents the compression strain, Free represents no strain and T represents the tension strain.

	Electron				Hole			
Strain	m^*_x	m^*_y	μ_x	μ_y	m^*_x	m^*_y	μ_x	μ_y
P-10%	0.43	1.24	0.042	0.048	0.32	1.37	22.709	0.124
P-9%	0.41	1.42	0.043	0.041	0.29	1.44	24.553	0.119
P-8%	0.37	1.45	0.048	0.041	0.27	1.45	27.243	0.121
P-7%	0.32	1.52	0.059	0.041	0.27	1.64	26.468	0.102
P-6%	0.37	1.43	0.050	0.042	0.26	1.70	26.771	0.098
P-5%	0.35	1.68	0.049	0.034	0.26	1.17	33.186	0.172
P-4%	0.35	1.68	0.050	0.034	0.27	1.15	31.588	0.174
P-3%	0.29	1.75	0.064	0.035	0.26	1.06	35.298	0.201
P-2%	0.27	1.80	0.071	0.035	0.27	1.16	32.035	0.174
P-1%	0.31	1.68	0.061	0.037	0.47	1.23	13.301	0.120
Free	0.29	1.63	0.067	0.039	0.57	1.10	10.329	0.127
T-1%	0.27	1.59	0.075	0.042	0.58	1.06	10.486	0.135
T-2%	0.25	1.50	0.086	0.047	0.54	0.69	14.422	0.264
T-3%	0.24	1.71	0.086	0.040	0.51	0.63	16.487	0.310
T-4%	0.23	1.64	0.097	0.044	0.38	0.59	26.175	0.399
T-5%	0.21	1.57	0.108	0.049	0.37	0.51	29.314	0.502
T-6%	0.27	1.58	0.074	0.042	0.28	0.46	46.104	0.669
T-7%	0.30	1.59	0.064	0.040	0.22	0.55	60.165	0.577
T-8%	0.29	1.26	0.077	0.058	0.18	0.46	91.909	0.840
T-9%	0.29	1.32	0.073	0.053	0.20	0.36	88.322	1.135
T-10%	0.25	1.36	0.089	0.055	0.16	0.44	113.336	0.949

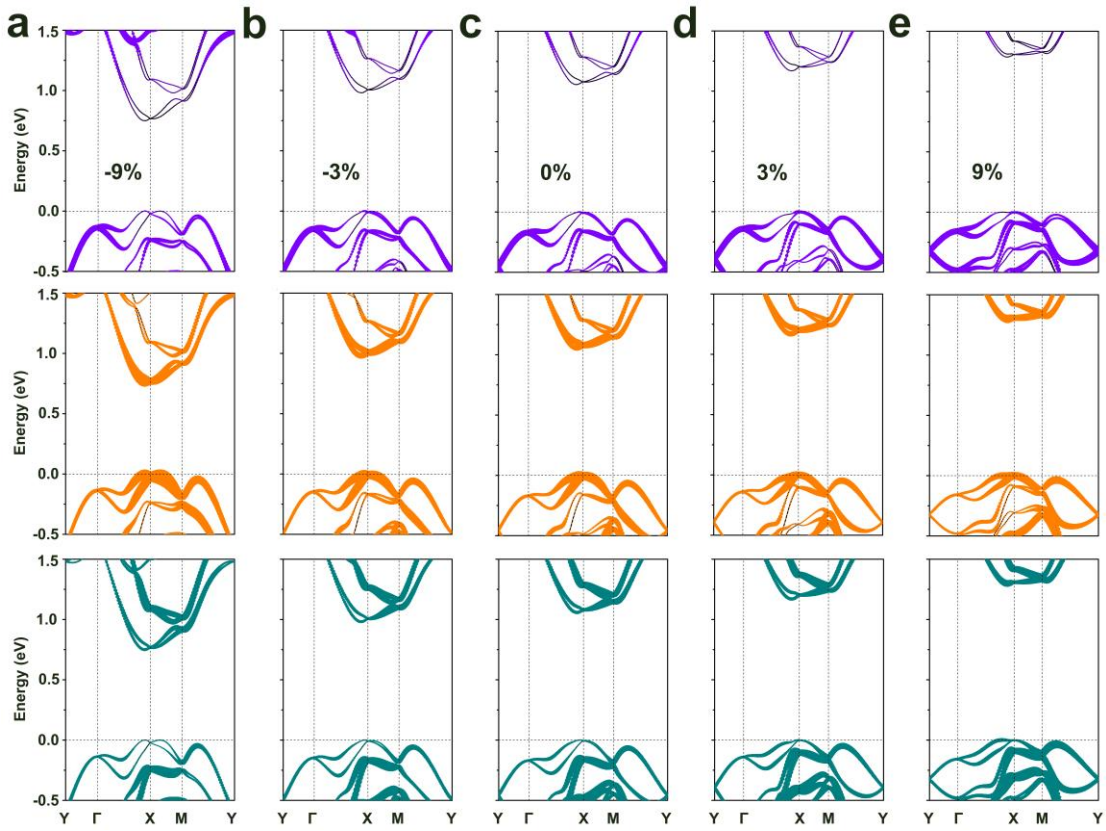

Figure S6. Orbital-projected band structures of tellurenyne under the effect of strain along the y direction. (a) and (b) represent the compression strain. (c) represents no strain. (d) and (e) represent the tension strain. The violet above, orange middle and dark cyan below represent the p_x, p_y and p_z orbitals, respectively. The size of circles represents the weights of the corresponding orbitals.

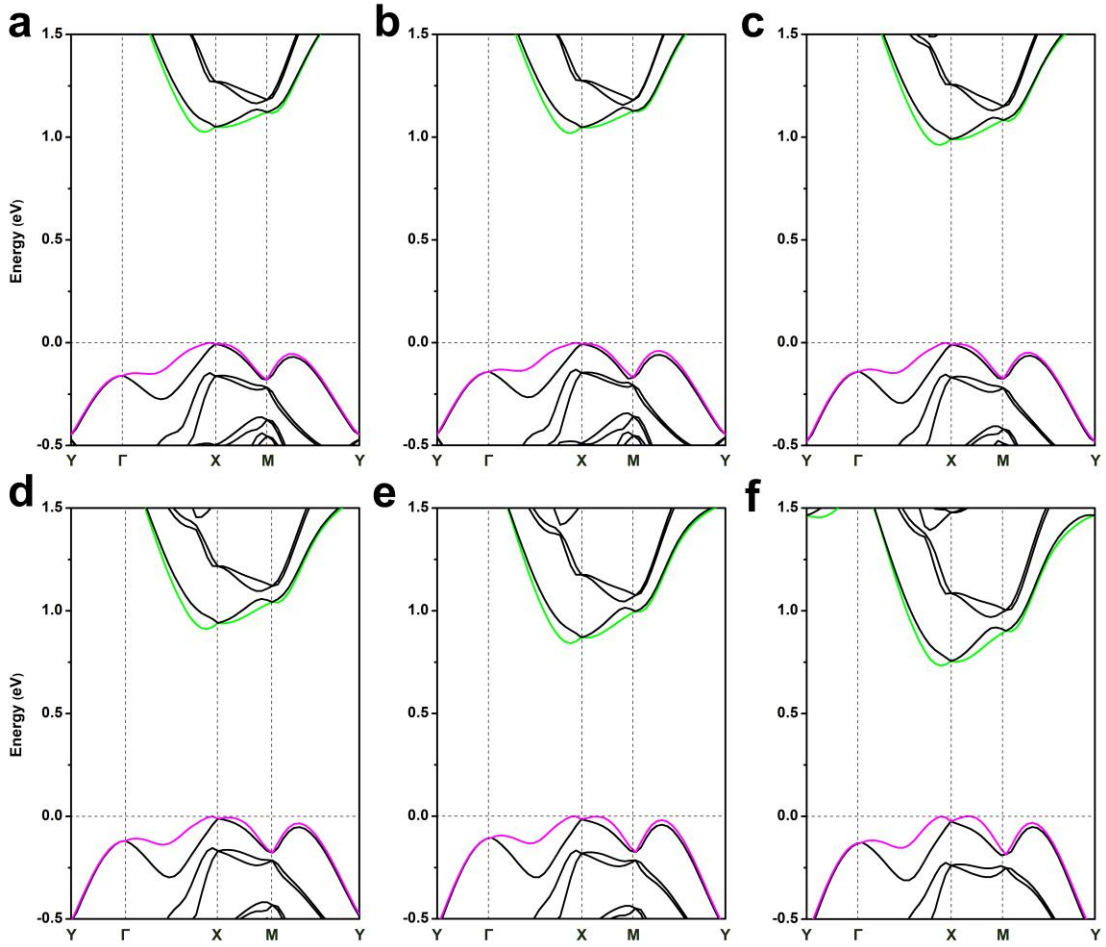

Figure S7. Band structures of tellurenyne (PBE-SOC results) under the compression strain along the y direction. (a) to (f) represent the 0.5%, 1%, 3%, 5%, 7%, 9% compression strain, respectively.

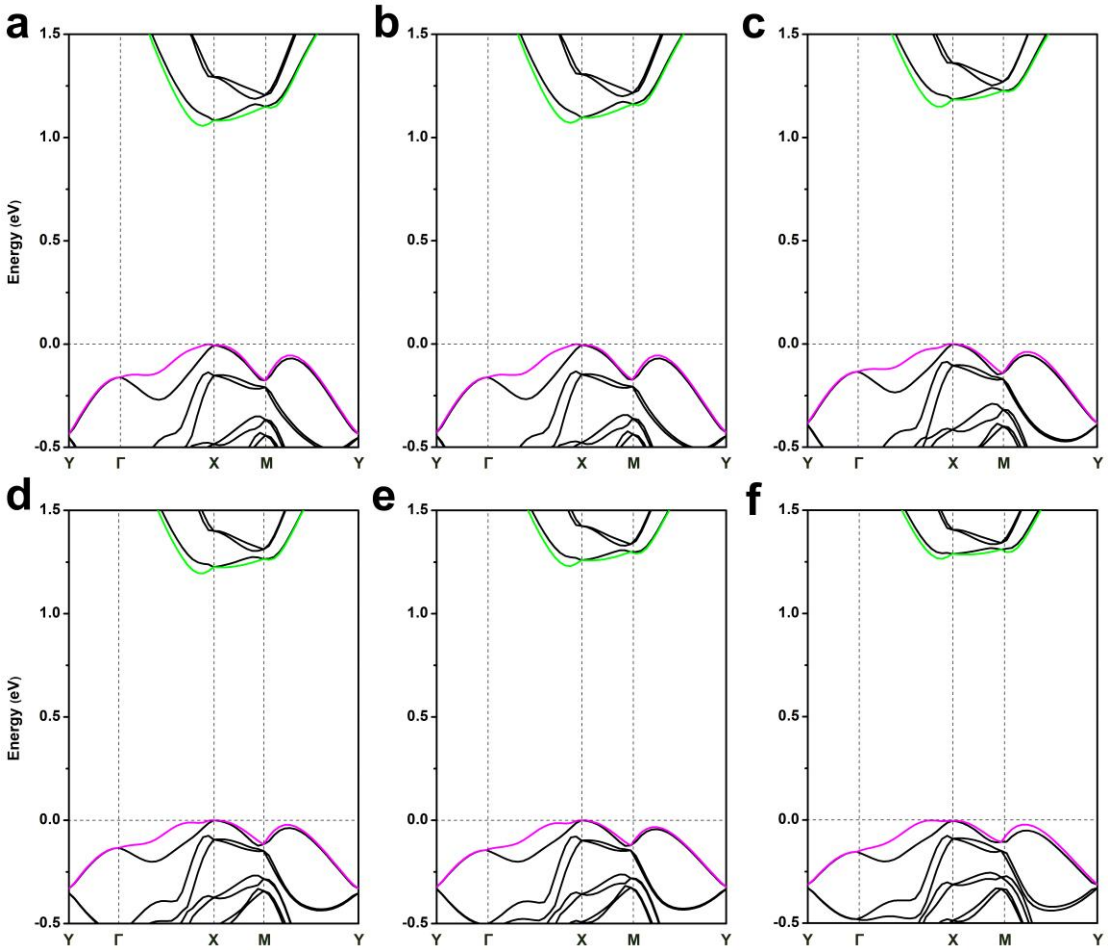

Figure S8. Band structures of tellurenyne (PBE-SOC results) under the tension strain along the y direction. (a) to (f) represent the 0.5%, 1%, 3%, 5%, 7%, 9% tension strain, respectively.

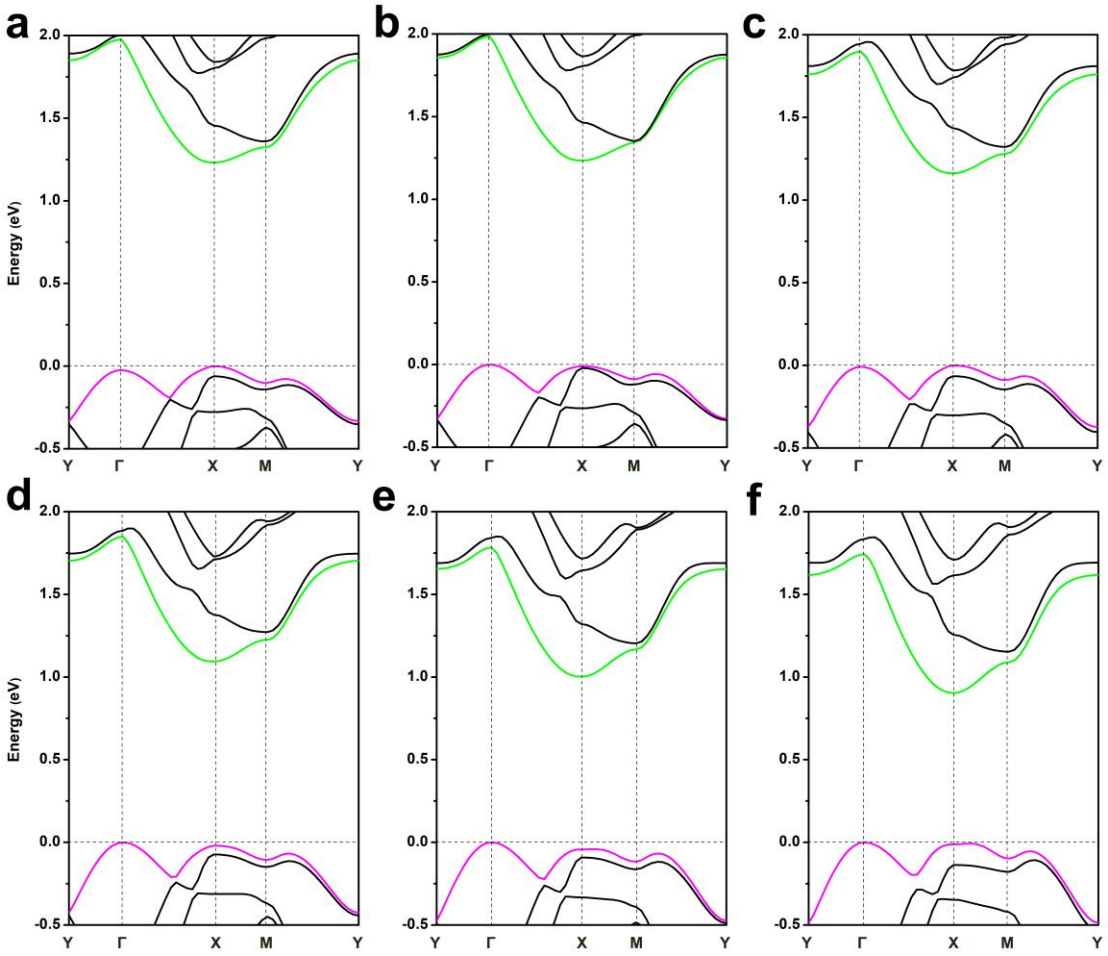

Figure S9. Band structures of tellurenyne (PBE results) under the compression strain along the y direction. (a) to (f) represent the 0.5%, 1%, 3%, 5%, 7%, 9% compression strain, respectively.

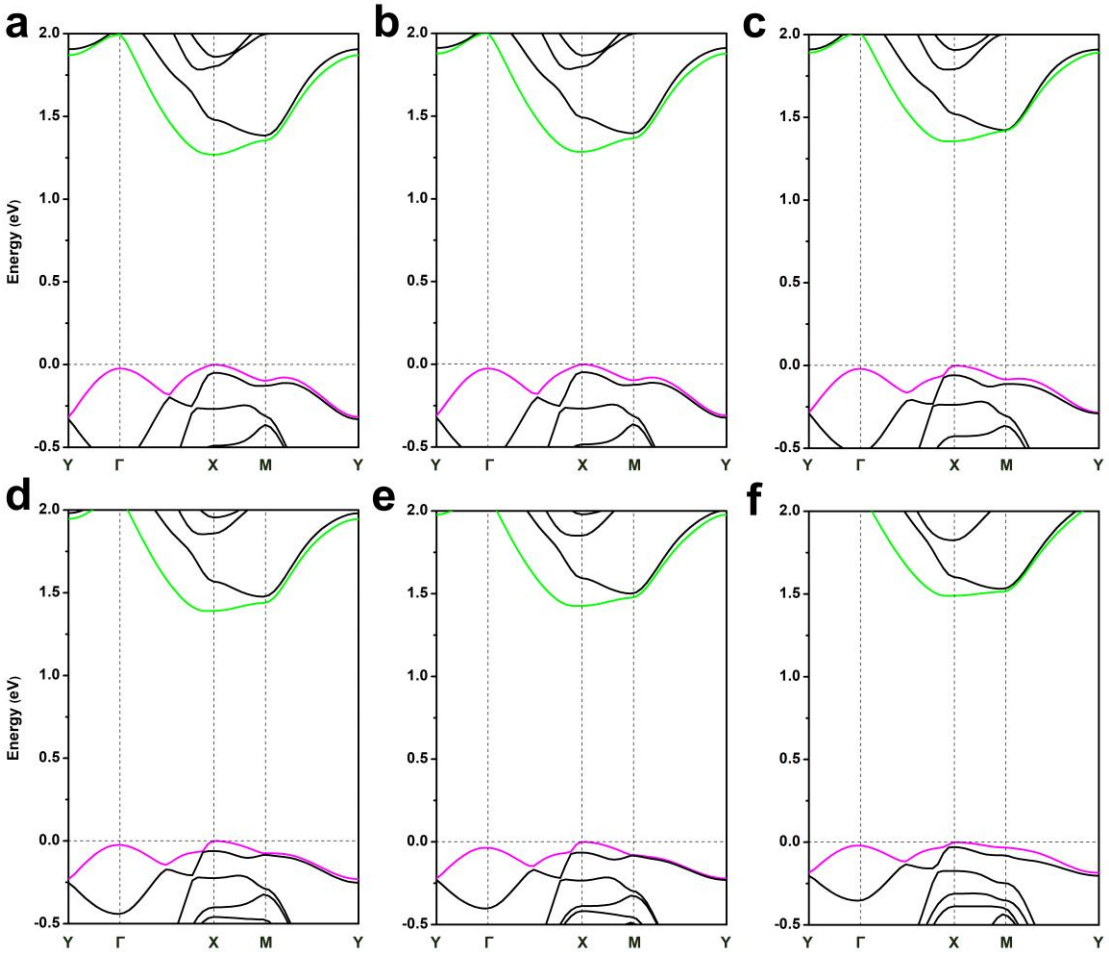

Figure S10. Band structures of tellurenyne (PBE results) under the tension strain along the y direction. (a) to (f) represent the 0.5%, 1%, 3%, 5%, 7%, 9% tension strain, respectively.

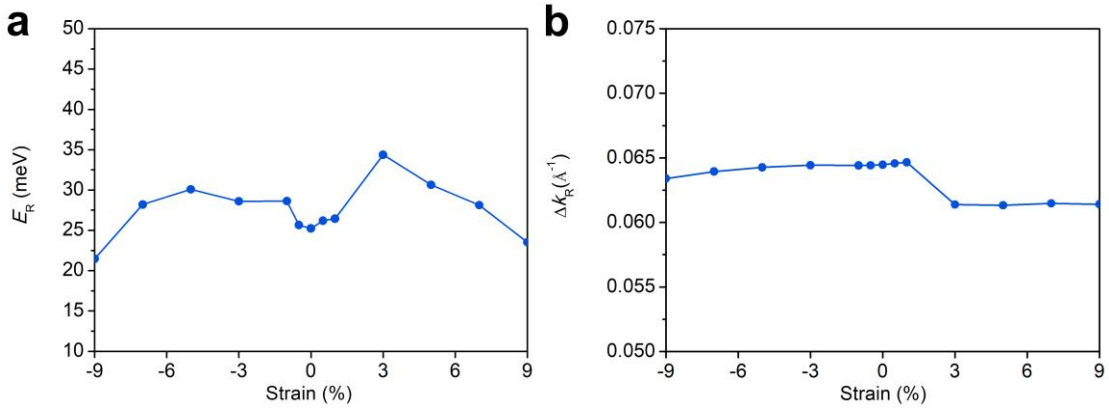

Figure S11. Rashba parameters of tellurenyne under the uniaxial strain along the y direction. (a) Rashba energy E_R and (b) momentum offset Δk_R in CBM.

Table S3. Effective electron (hole) mass m^* (m_0) and electron (hole) mobility μ (10^3 $cm^2/V\ s$) of the phase VI of tellurenyne under the uniaxial strain along the y direction (m_0 is the mass of the free electron). P represents the compression strain, Free represents no strain and T represents the tension strain.

	Electron				Hole			
Strain	m^*_x	m^*_y	μ_x	μ_y	m^*_x	m^*_y	μ_x	μ_y
P-9%	0.28	0.80	0.103	0.117	0.29	0.46	45.211	0.659
P-7%	0.29	0.94	0.088	0.089	0.33	0.65	30.360	0.369
P-5%	0.30	1.13	0.078	0.067	0.37	1.01	21.092	0.181
P-3%	0.30	1.29	0.073	0.055	0.41	1.51	14.437	0.093
P-1%	0.28	1.49	0.072	0.045	0.57	1.31	9.700	0.099
P-0.5%	0.29	1.57	0.069	0.042	0.55	1.15	10.637	0.121
T-0.5%	0.29	1.72	0.064	0.036	0.59	1.10	9.937	0.126
T-1%	0.30	1.78	0.062	0.034	0.60	1.08	9.822	0.129
T-3%	0.29	2.78	0.052	0.018	0.61	1.83	7.339	0.058
T-5%	0.31	2.76	0.047	0.017	0.90	2.26	3.649	0.035
T-7%	0.32	2.85	0.044	0.016	0.87	1.95	4.161	0.044
T-9%	0.34	3.93	0.034	0.010	1.02	1.65	3.541	0.052

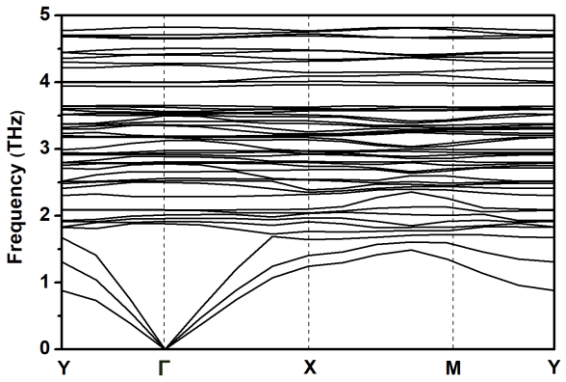

Figure S12. Phonon dispersion of tellurenyne under the 10% tension strain.

[1] M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark and M. C. Payne, *J. Phys.: Condens. Matter*, 2002, **14**, 2717-2744.

[2] P. E. Blöchl, *Phys. Rev. B*, 1994, **50**, 17953-17979.

[3] G. Kresse and D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758-1775.

[4] V. Blum, R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, and M. Scheffler, *Comput. Phys. Commun.*, 2009, **180**, 2175-2196.