(Supplementary Materials)

Ideal strength of two-dimensional stanene may reach or exceed Griffith strength estimate

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Table S1. Mechanical properties of stanene computed by adopting six different functionals.

		PBEsol (RRKJ)	PBEsol (PAW)	PW-LDA	HSE06	PBE0	B3LYP
Atoms/supercell		6	6	6	2	6	2
a_0 (Å)		4.587	4.580	4.484	4.665	4.484	4.483
δ (Å)		0.837	0.848	0.769	0.860	0.748	0.727
Bond length (Å)		2.773	2.776	2.701	2.827	2.695	2.689
Bond angle		111.346º	111.128º	112.238º	111.178º	112.603º	112.967º
UTS (N/m)	Armchair	3.656	3.718	4.076	2.919	3.821	3.622
	Zigzag	4.084	4.097	4.520	3.380	4.224	3.930
	Biaxial	3.318	3.361	3.670	3.318	3.333	3.186
UTS (GPa)	Armchair	11.216	11.405	12.502	8.953	11.720	11.110
	Zigzag	12.527	12.567	13.866	10.369	12.957	12.054
	Biaxial	10.178	10.311	11.258	10.178	10.223	9.773
ε_{UTS}^{True}	Armchair	0.215	0.199	0.199	0.199	0.191	0.182
	Zigzag	0.315	0.285	0.300	0.270	0.247	0.262
	Biaxial	0.191	0.182	0.166	0.191	0.157	0.157
ε_{UTS}^{Eng}	Armchair	0.240*	0.220	0.220	0.220	0.210	0.200
	Zigzag	0.370	0.330	0.350	0.310	0.280	0.300
	Biaxial	0.210	0.200	0.181	0.210	0.170	0.170
Poisson ratio ν		0.456	0.369	0.465	0.425	0.474	0.408
E (N/m)	Armchair	24.448‡	26.600	29.865	21.842	26.470	30.880
	Zigzag	23.897	26.685	29.637	21.637	27.670	30.620
E/UTS ratio	Armchair	6.687	7.154	7.328	7.483	6.928	8.526
	Zigzag	5.852	6.514	6.556	6.401	6.550	7.792

**Consider elongation of a specimen from an initial length L_0 to a final length L and denote the stretch ratio ($\frac{L_0}{L}$) as λ. The engineering, true, and Lagrangian strain can be expressed, respectively, as $\varepsilon^{True} = ln\,\lambda$, $\varepsilon^{Eng} = \lambda - 1$, and $\eta^{Lag} = \frac{1}{2}(\lambda^2 - 1)$.*

‡*Our Young's Modulus computed by suing the PEBsol functional implemented in Quantum ESPRESSO matches extremely well with another group's result (24.46117 N/m) with different DFT software*[1].

Table S2. Non-zero second and higher-order elastic constants (in Voigt notation and unit N/m) computed by adopting the six exchange-correlational (XC) functionals.

XC functional (method)	Second-order	Third-order	Fourth-order	Fifth-order
PBEsol (RRKJ)	C_{11} = 30.87	C_{111} = -191.79	C_{1111} = 186.06	C_{11111} = 5213.8
	C_{12} = 14.08	C_{112} = -136.76	C_{1112} = 2053.8	C_{11112} = -18823
	C_{22} = 30.41	C_{222} = -195.37	C_{1122} = -1822.5	C_{11122} = 18452
			C_{2222} = 100.94	C_{12222} = 916.99
				C_{22222} = 8260.8
PBEsol (PAW)	C_{11} = 29.80	C_{111} = -135.66	C_{1111} = -1099.6	C_{11111} = 17937
	C_{12} = 9.765	C_{112} = -32.13	C_{1112} = 63.32	C_{11112} = -1863.4
	C_{22} = 30.62	C_{222} = -182.80	C_{1122} = 1794.1	C_{11122} = -2513.2
			C_{2222} = -463.62	C_{12222} = 474.7
				C_{22222} = 15743
PW-LDA (MT)	C_{11} = 38.55	C_{111} = -347.24	C_{1111} = 2686.2	C_{11111} = -15198
	C_{12} = 18.297	C_{112} = -232.50	C_{1112} = 3035.3	C_{11112} = -20797
	C_{22} = 38.37	C_{222} = -377.62	C_{1122} = -3357.6	C_{11122} = 12033
			C_{2222} = 3084.1	C_{12222} = -16596
				C_{22222} = -14809
HSE06 (GHHT)	C_{11} = 26.64	C_{111} = -186.64	C_{1111} = 597.15	C_{11111} = -173.32
	C_{12} = 11.306	C_{112} = -78.37	C_{1112} = 484.47	C_{11112} = -2206.2
	C_{22} = 26.47	C_{222} = -226.93	C_{1122} = 172.39	C_{11122} = -3804.1
			C_{2222} = 1590	C_{12222} = -7560.6
				C_{22222} = -7188.7
PBE0 (MT)	C_{11} = 34.02	C_{111} = -278.59	C_{1111} = 1175.8	C_{11111} = -653.09
	C_{12} = 16.027	C_{112} = -251.68	C_{1112} = 3337.6	C_{11112} = -29272
	C_{22} = 34.87	C_{222} = -287.28	C_{1122} = -4882.2	C_{11122} = 28258
			C_{2222} = 608.02	C_{12222} = -1721.6
				C_{22222} = 9730.1
B3LYP (MT)	C_{11} = 37.05	C_{111} = -305.08	C_{1111} = 1411.8	C_{11111} = -4319.5
	C_{12} = 15.119	C_{112} = -123.33	C_{1112} = 812.42	C_{11112} = -1967.7
	C_{22} = 36.83	C_{222} = -331.66	C_{1122} = 1283	C_{11122} = -8760.9
			C_{2222} = 1710.9	C_{12222} = -13248
				C_{22222} = -1519.4

Table S3. Indifferent results obtained through 2-atom supercell simulation (for phonon) and 6-atom supercell simulation (for stress-strain response) with the implementation of LDA.

		Phonon calculation (DFPT)	Stress-strain calculation
Functional		LDA	LDA
k-grid		21×21×1	11×11×3
Atoms/supercell		2	6
a_0 (Å)		4.483	4.484
δ (Å)		0.771	0.769
Bond length (Å)		2.701	2.701
Bond angle		113.187°	112.238°
UTS (N/m)	Armchair	4.107	4.076
	Zigzag	4.508	4.520
	Biaxial	3.690	3.670

Figure S1. Demonstration of the negligible effect of spin-orbit coupling in mechanical property calculations in stanene (2atoms/supercell, LDA functional incorporated).

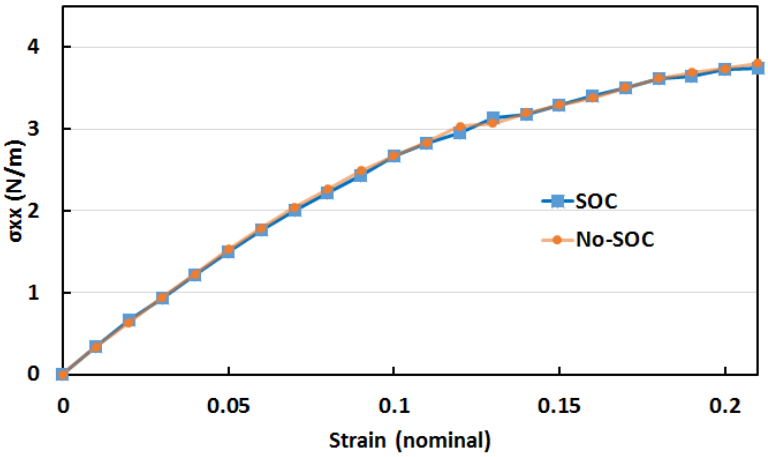


Figure S2. The sensitivity of Young's modulus fitting on a true stress-true strain curve. The two fitted curves are almost identical but yield slightly different E_{fitted}. The choice of DFT data point (A vs. B) as the choice of onset point of nonlinearity has an appreciable influence on determining elastic constants. To eliminate this ambiguity, E was determined from elastic constants fitted to PK2 stress - Lagrangian strain curve.

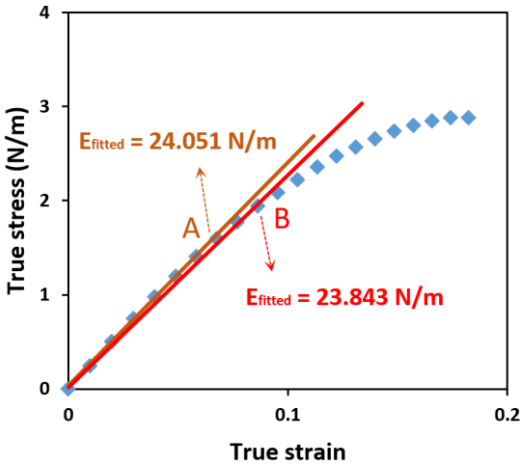


Figure S3. (a) Phonon dispersion and density of states for stanene at the undeformed state. (b) The reciprocal space and first Brillouin zone with high symmetrical points associated with the phonon calculations. The present dispersion shows excellent agreement with the previous phonon calculations for stanene using either DFPT[2,3] or the small displacement method[4].

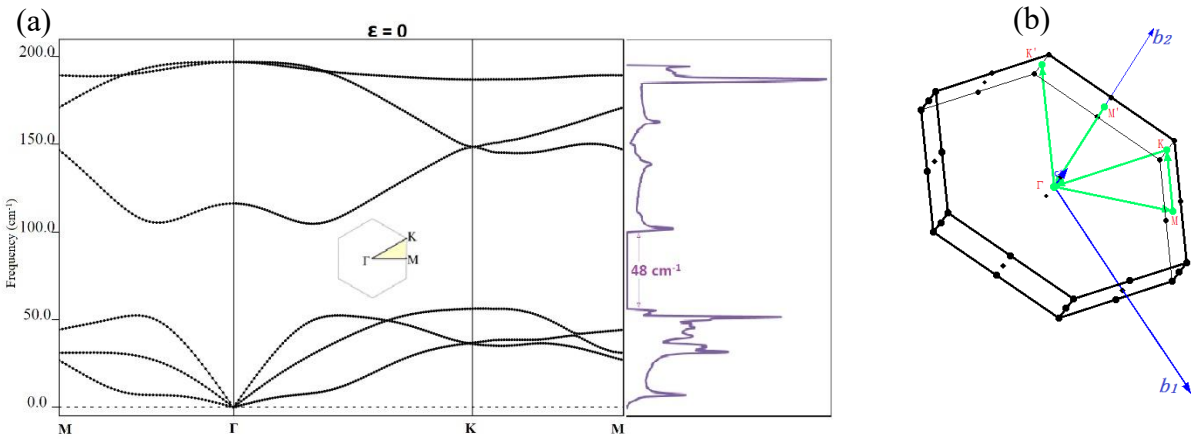
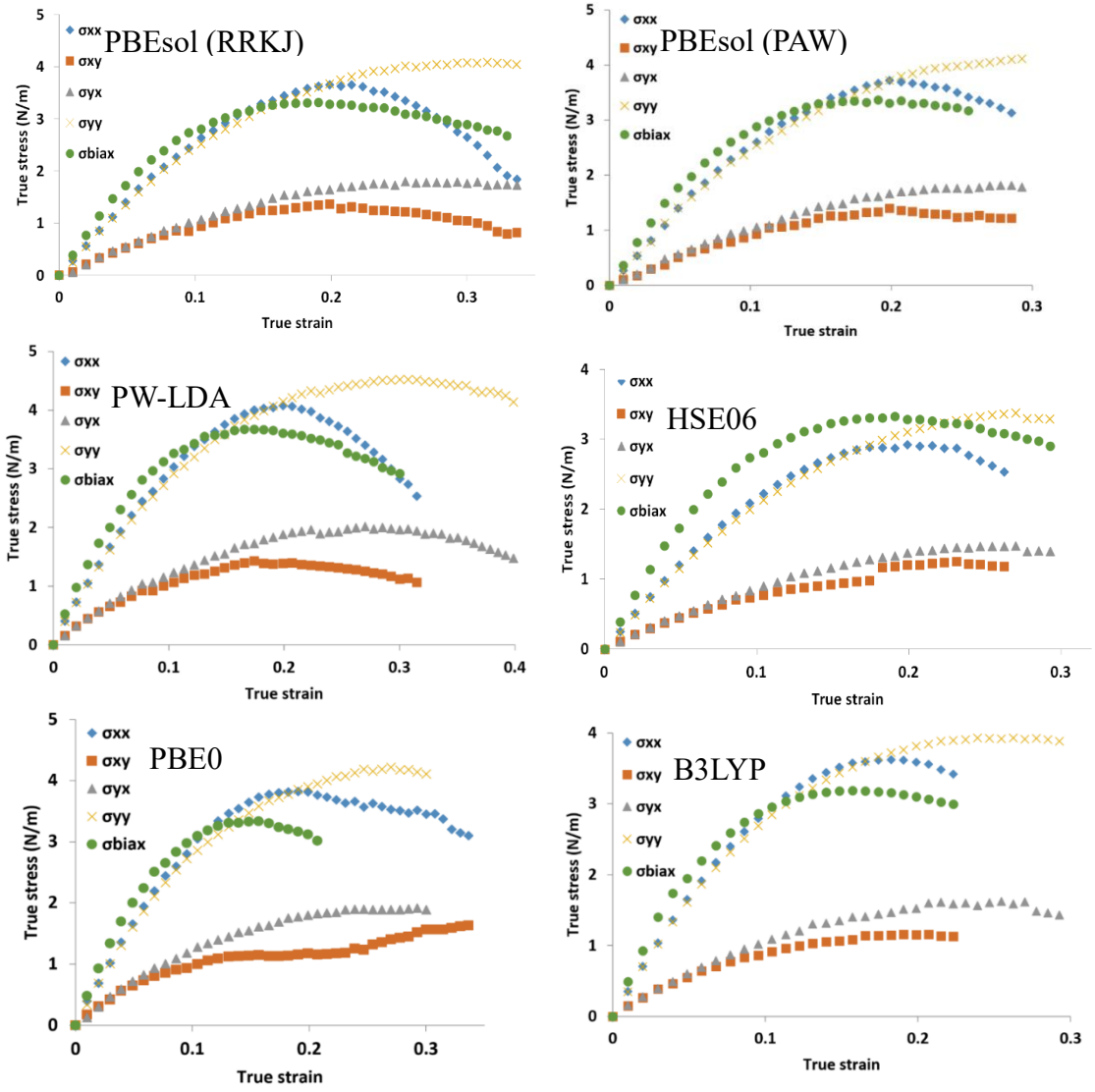


Figure S4. The computed stress-strain response of stanene by using the PBEsol (RRKJ), PBEsol (PAW), PW-LDA, HSE06, PBE0, and B3LYP functional, respectively.



Movie S1. *(Online)* Charge density in the horizontal middle plane passing through the buckled stanene at different strain values under uniaxial armchair, zigzag, and equibiaxial tension is shown.

References

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