

Supporting information

First-principles study on the structural properties of 2D MXene SnSiGeN₄ and its electronic properties under the effect of strain and external electric field

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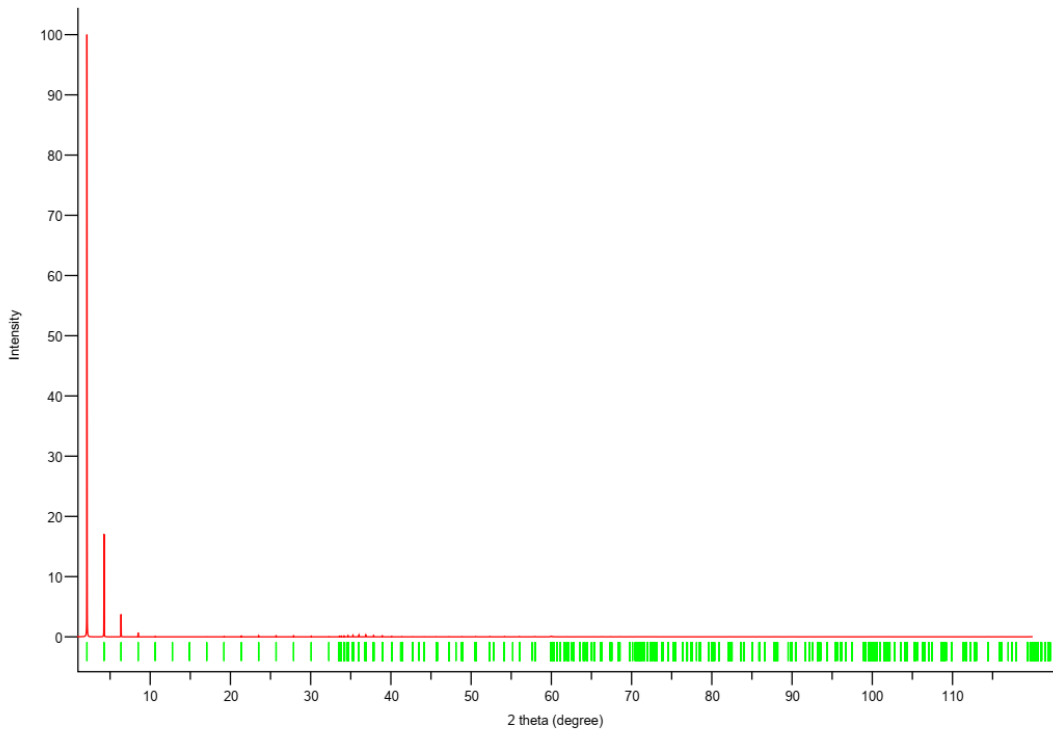


Figure S1. The theoretical X-ray diffraction pattern of layered SnSiGeN₄.

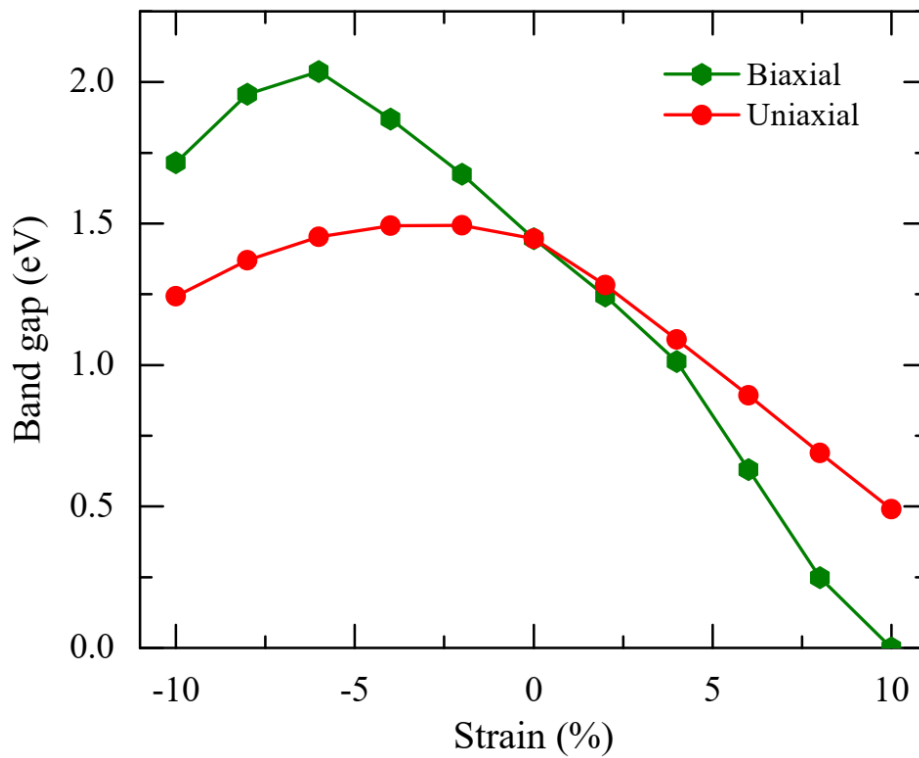


Figure S2. Band gap of SnSiGeN₄ monolayer as a function of biaxial and uniaxial strains.

Table S1. Calculated Bader charges of Si, Sn, Ge, and N atoms of SnSiGeN₄ under biaxial strains. The minus sign indicates electron loss from the neutral atom.

Atom	-10 %	-8%	-6%	-4%	-2%	0%	2%	4%	6%	8%	10%
Si	-2.356	-2.158	-2.132	-2.108	-2.083	-1.936	-1.917	-1.889	-1.914	-1.931	-3.952
Sn	-2.030	-2.035	-1.995	-1.959	-1.930	-1.900	-1.867	-1.827	-1.785	-1.750	-1.843
Ge	-1.581	-1.644	-1.629	-1.626	-1.595	-1.577	-1.549	-1.552	-1.532	-1.502	-1.755
N1	1.409	1.440	1.408	1.382	1.364	1.341	1.316	1.288	1.268	1.244	1.370
N2	1.193	1.214	1.205	1.209	1.181	1.167	1.143	1.155	1.133	1.109	1.297
N3	1.825	1.567	1.542	1.521	1.494	1.343	1.327	1.297	1.321	1.332	2.879
N4	1.540	1.616	1.601	1.582	1.569	1.561	1.546	1.529	1.509	1.499	2.003

Table S2. Calculated Bader charges of Si, Sn, Ge, and N atoms of SnSiGeN₄ under uniaxial strains. The minus sign indicates electron loss from the neutral atom.

Atom	-10 %	-8%	-6%	-4%	-2%	0%	2%	4%	6%	8%	10%
Si	-2.097	-2.029	-2.023	-2.023	-2.003	-1.936	-1.974	-1.984	-1.973	-1.985	-2.366
Sn	-2.011	-1.945	-1.946	-1.930	-1.914	-1.900	-1.879	-1.869	-1.853	-1.828	-1.820
Ge	-1.643	-1.595	-1.618	-1.598	-1.591	-1.577	-1.581	-1.557	-1.538	-1.531	-1.622
N1	1.412	1.383	1.372	1.360	1.350	1.341	1.329	1.320	1.307	1.295	1.272
N2	1.228	1.173	1.204	1.186	1.180	1.167	1.174	1.151	1.137	1.131	1.241
N3	1.456	1.435	1.432	1.430	1.409	1.343	1.383	1.395	1.384	1.401	1.699
N4	1.653	1.579	1.580	1.575	1.570	1.561	1.547	1.545	1.536	1.517	1.596