

Supplementary Material

First principles rationale of strain-induced modifications in hybrid double halide perovskite: optoelectronics and photovoltaic perspectives

Tanmoy Kalita^a, Manjet Rajak^a, and Dhruba Jyoti Kalita^{a*}

^aDepartment of Chemistry, Gauhati University

Electronic mail: dhrubajyoti.kalita@gauhati.ac.in

Table S1: Calculated lattice parameters and band gap (E_g) values of the reference perovskite material.

Compound	Functionals	Theoretical		Experimental	
		a=b=c(Å)	E_g (eV)	a=b=c(Å)	E_g (eV)
Cs ₂ AgBiCl ₆	LDA	10.616	1.6	10.777 ± 0.005	2.2
	PBE	11.089	1.8		
	PBEsol	10.824	1.7		
	PBE0	10.749	4.2		
	HSE06	10.889	2.7		

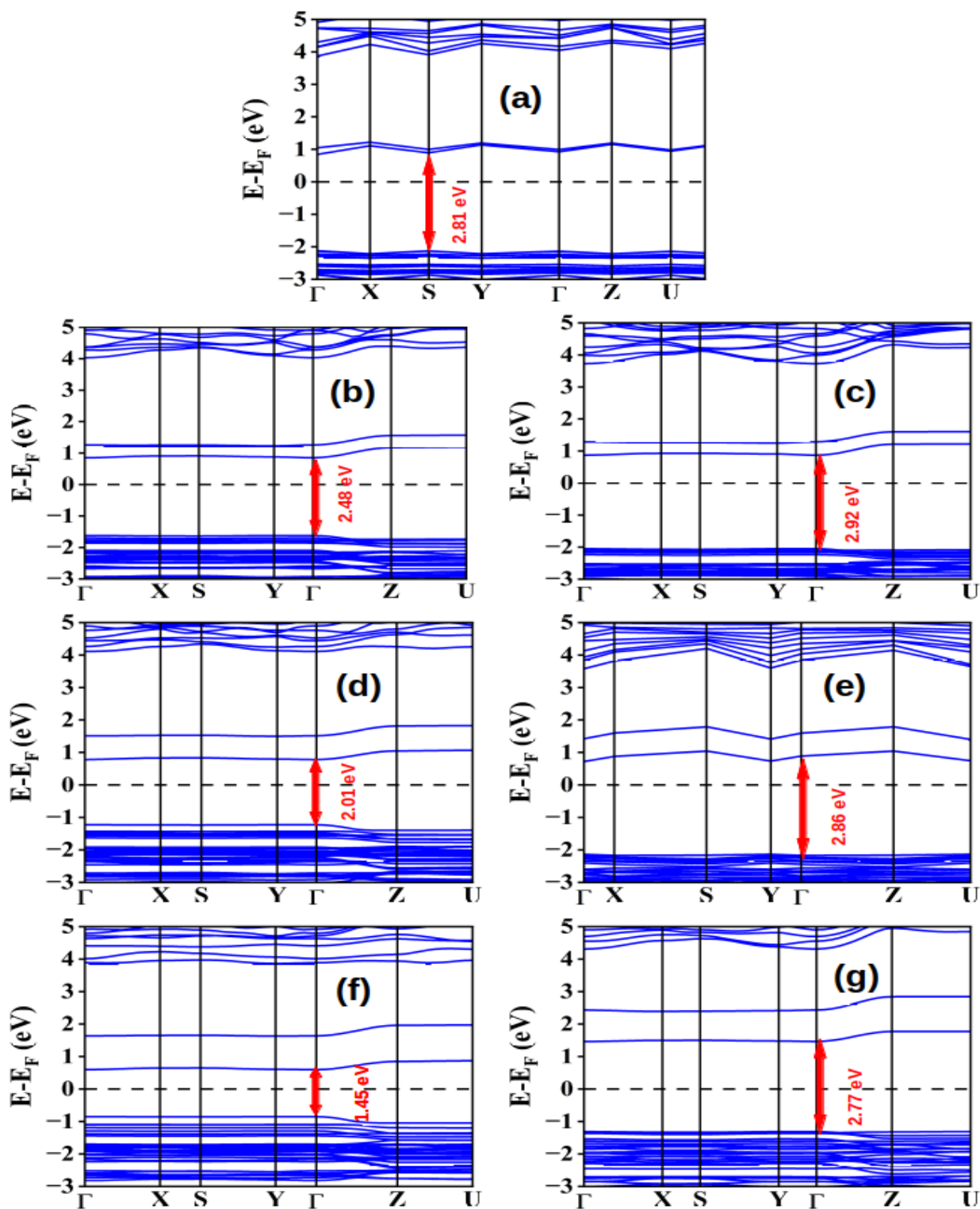


Fig. S1: Calculated band structures of $(\text{DMA})_2\text{SnCl}_6$ applying different percentile of strain: (a) 0%, (b,d,f) 2%, 4%, and 6% tensile strain, and (c, e, g) 2%, 4%, and 6% compressive strain, respectively.

Table S2: Coordinates of the optimized geometries of the studied compound under different percentile of strain employing PBE XC functional.

0% Strain

<u>Atoms</u>	<u>Coordinates (Å)</u>		
	<u>X</u>	<u>Y</u>	<u>Z</u>
Sn	0.0000000000	0.0000000000	-0.0000000000
Sn	3.7514610000	7.3467290000	3.6942970000
H	0.4930818244	9.8596474032	0.8981150399
H	7.0098391756	4.8338105968	6.4904779601
H	7.0098391756	4.8338105968	0.8981150399
H	0.4930818244	9.8596474032	6.4904779601
H	4.2445428244	12.1805395968	2.7961809601
H	3.2583781756	2.5129184032	4.5924120399
H	3.2583781756	2.5129184032	2.7961809601
H	4.2445428244	12.1805395968	4.5924120399
H	1.1117051946	1.4014529774	2.8711217970
H	6.3912158054	13.2920050226	4.5174712030
H	6.3912158054	13.2920050226	2.8711217970
H	1.1117051946	1.4014529774	4.5174712030
H	4.8631651946	5.9452760226	0.8231742030
H	2.6397558054	8.7481819774	6.5654187970
H	2.6397558054	8.7481819774	0.8231742030
H	4.8631651946	5.9452760226	6.5654187970
H	1.1558939393	3.8367270687	2.8019854144
H	6.3470270607	10.8567309313	4.5866075856
H	6.3470270607	10.8567309313	2.8019854144
H	1.1558939393	3.8367270687	4.5866075856
H	4.9073539393	3.5100019313	0.8923115856
H	2.5955670607	11.1834560687	6.4962814144
H	2.5955670607	11.1834560687	0.8923115856
H	4.9073539393	3.5100019313	6.4962814144
H	0.2692688016	11.4975833562	3.6942970000
H	7.2336521984	3.1958746438	3.6942960000
H	4.0207298016	10.5426036438	0.0000000000

H	3.4821911984	4.1508543562	0.0000000000
H	0.4460664103	8.3089935062	0.0000000000
H	7.0568545897	6.3844644938	0.0000000000
H	4.1975264103	13.7311934938	3.6942970000
H	3.3053945897	0.9622645062	3.6942970000
C	0.8179975747	3.3006456895	3.6942970000
C	6.6849234253	11.3928123105	3.6942960000
C	4.5694575747	4.0460833105	-0.0000000000
C	2.9334634253	10.6473746895	0.0000000000
C	0.8254279026	9.3322347754	-0.0000000000
C	6.6774930974	5.3612232246	-0.0000000000
C	4.5768879026	12.7079522246	3.6942970000
C	2.9260330974	1.9855057754	3.6942970000
N	1.4359505948	1.9420523189	3.6942970000
N	6.0669704052	12.7514056811	3.6942960000
N	5.1874105948	5.4046766811	-0.0000000000
N	2.3155104052	9.2887813189	0.0000000000
Cl	1.4441173133	13.7551015705	1.7688095689
Cl	6.0588036867	0.9383564295	5.6197834311
Cl	6.0588036867	0.9383564295	1.7688095689
Cl	1.4441173133	13.7551015705	5.6197834311
Cl	5.1955783133	8.2850854295	1.9254864311
Cl	2.3073426867	6.4083725705	5.4631065689
Cl	2.3073426867	6.4083725705	1.9254864311
Cl	5.1955783133	8.2850854295	5.4631065689
Cl	1.3311816796	2.0859672310	-0.0000000000
Cl	6.1717393204	12.6074907690	-0.0000000000
Cl	5.0826426796	5.2607617690	3.6942970000
Cl	2.4202783204	9.4326962310	3.6942970000

2% Tensile Strain

Along x-axis

Sn	-0.0660400610	-0.0013482125	0.0000000000
Sn	3.7514347410	7.3467445262	3.6942970000
H	0.4919499453	9.8560607105	0.8979174068

H	7.0111644319	4.8374310740	6.4906394916
H	7.0111644319	4.8374310740	0.8979535084
H	0.4919499453	9.8560607105	6.4906755932
H	4.2594888341	12.1780094153	2.7971484390
H	3.2432069635	2.5155719446	4.5915950348
H	3.2432069635	2.5155719446	2.7969979652
H	4.2594888341	12.1780094153	4.5914445610
H	1.1021878984	1.3978582939	2.8703479100
H	6.4002642909	13.2968569095	4.5183311463
H	6.4002642909	13.2968569095	2.8702618537
H	1.1021878984	1.3978582939	4.5182450900
H	4.8621178496	5.9453510086	0.8236816199
H	2.6407855192	8.7479222155	6.5649474572
H	2.6407855192	8.7479222155	0.8236455428
H	4.8621178496	5.9453510086	6.5649113801
H	1.1283780149	3.8318705143	2.8030551091
H	6.3746918663	10.8624347755	4.5855217424
H	6.3746918663	10.8624347755	2.8030712576
H	1.1283780149	3.8318705143	4.5855378909
H	4.9039966157	3.5122536260	0.8926056012
H	2.5991604536	11.1811998986	6.4961749066
H	2.5991604536	11.1811998986	0.8924180934
H	4.9039966157	3.5122536260	6.4959873988
H	0.1419646374	11.5204311460	3.6942970000
H	7.3611223399	3.1740059011	3.6942960000
H	4.0243204416	10.5378674562	0.0000000000
H	3.4787869830	4.1550375070	0.0000000000
H	0.4489334133	8.3040330175	0.0000000000
H	7.0539884497	6.3892951051	0.0000000000
H	4.2075372552	13.7290585159	3.6942970000
H	3.2942436408	0.9643219106	3.6942970000
C	0.7944093640	3.2922272983	3.6942970000
C	6.7086089669	11.4020906714	3.6942960000
C	4.5664068379	4.0480614387	0.0000000000
C	2.9366336101	10.6451552761	0.0000000000

C	0.8257189610	9.3287822864	0.0000000000
C	6.6771989091	5.3646435173	0.0000000000
C	4.5910020512	12.7068995002	3.6942970000
C	2.9117911220	1.9868550760	3.6942970000
N	1.4224777244	1.9391467682	3.6942970000
N	6.0804680398	12.7552418752	3.6942960000
N	5.1864336325	5.4056963407	0.0000000000
N	2.3165368761	9.2875273893	0.0000000000
Cl	1.3858090510	13.7548337676	1.7692173460
Cl	6.1406912851	0.9379739280	5.6160223296
Cl	6.1406912851	0.9379739280	1.7725706704
Cl	1.3858090510	13.7548337676	5.6193756540
Cl	5.2015334796	8.2884992254	1.9270026945
Cl	2.3010250329	6.4049830856	5.4616354836
Cl	2.3010250329	6.4049830856	1.9269575164
Cl	5.2015334796	8.2884992254	5.4615903055
Cl	1.2649756625	2.0908255479	0.0000000000
Cl	6.2585362544	12.5990648001	0.0000000000
Cl	5.0836894125	5.2571679865	3.6942970000
Cl	2.4191666703	9.4364995685	3.6942970000

2% Tensile Strain

Along y-axis

Sn	-0.7659885507	-0.2369092282	0.0000000000
Sn	3.7934031971	7.3372481865	3.6942970000
H	0.7842985008	9.9709517367	0.9021862689
H	6.7701550736	4.7324342819	6.4893720150
H	6.7701550736	4.7324342819	0.8992209850
H	0.7842985008	9.9709517367	6.4864067311
H	4.1759307374	13.2804271118	2.8009140411
H	3.1653718553	1.8707720158	4.5911768849
H	3.1653718553	1.8707720158	2.7974161151
H	4.1759307374	13.2804271118	4.5876789589
H	0.7250667882	1.5240734662	2.8752287573
H	6.6634387032	13.2515473455	4.4989847166

H	6.6634387032	13.2515473455	2.8896082834
H	0.7250667882	1.5240734662	4.5133642427
H	4.6041390265	5.8176742887	0.8247035283
H	2.7740289558	8.6131189937	6.5650326523
H	2.7740289558	8.6131189937	0.8235603477
H	4.6041390265	5.8176742887	6.5638894717
H	1.5165455594	3.8317099516	2.8043043073
H	5.4534778362	11.1446345471	4.5889022598
H	5.4534778362	11.1446345471	2.7996907402
H	1.5165455594	3.8317099516	4.5842886927
H	4.6498676029	3.3984311215	0.8921596926
H	3.0332169320	11.0288957470	6.4901314071
H	3.0332169320	11.0288957470	0.8984615929
H	4.6498676029	3.3984311215	6.4964333074
H	-0.4834411274	11.0698539489	3.6942970000
H	7.4842821178	3.6021215887	3.6942960000
H	4.3610744288	10.2041491000	0.0000000000
H	3.2265753852	4.0558922232	0.0000000000
H	0.5523043973	8.4335074019	0.0000000000
H	6.8010063047	6.2864302766	0.0000000000
H	4.8416907566	14.6898949948	3.6942970000
H	2.7306013048	0.3859257540	3.6942970000
C	1.0543577722	3.3931466485	3.6942970000
C	5.9974787519	11.4653164577	3.6942960000
C	4.3136451759	3.9352143773	0.0000000000
C	3.2995228110	10.4624178502	0.0000000000
C	1.0457063884	9.4090965774	0.0000000000
C	6.4339964964	5.2573035142	0.0000000000
C	4.7212262480	13.6026334131	3.6942970000
C	2.6772688540	1.4792902832	3.6942970000
N	1.2468913798	1.9091278569	3.6942970000
N	6.0699336306	12.9531109172	3.6942960000
N	4.9419474193	5.2887382306	0.0000000000
N	2.5193584069	9.1916492975	0.0000000000
Cl	1.3315155926	13.5524024832	2.4273003758

Cl	6.2574531657	1.4537588415	5.5697885354
Cl	6.2574531657	1.4537588415	1.8188044646
Cl	1.3315155926	13.5524024832	4.9612926242
Cl	5.2824073299	8.2413569098	1.9504297780
Cl	2.3221106842	6.4262669425	5.4863384731
Cl	2.3221106842	6.4262669425	1.9022545269
Cl	5.2824073299	8.2413569098	5.4381632220
Cl	1.7341913160	0.1369009661	0.0000000000
Cl	8.7922636521	13.5862204373	0.0000000000
Cl	4.9617337185	5.1808981852	3.6942970000
Cl	2.4641700775	9.4074621722	3.6942970000

2% Tensile Strain

Along z-axis

Sn	0.0000000000	0.0000000000	-0.0772074964
Sn	3.7514610000	7.3467290000	3.7318314742
H	0.5656837889	9.7948962058	0.8331280227
H	6.9146569363	4.9069927547	6.5709253053
H	6.9372372111	4.8985617942	0.8331280227
H	0.5882640637	9.7864652453	6.5709253053
H	4.3265480809	12.2437309065	2.8152032025
H	3.1728186557	2.4383430011	4.6127101310
H	3.1763729191	2.4497270935	2.8152032025
H	4.3301023443	12.2551149989	4.6127101310
H	1.0343491055	1.3259534832	2.8828014003
H	6.4676888746	13.3756699411	4.5317652258
H	6.4685718945	13.3675045168	2.8828014003
H	1.0352321254	1.3177880589	4.5317652258
H	4.7936578320	6.0096877644	0.7960018220
H	2.7234539498	8.6505183906	6.6845567110
H	2.7092631680	8.6837702356	0.7960018220
H	4.7794670502	6.0429396094	6.6845567110
H	1.0457636397	3.7617306719	2.8258473498
H	6.4639846399	10.9453650997	4.6138065354
H	6.4571573603	10.9317273281	2.8258473498
H	1.0389363601	3.7480929003	4.6138065354

H	4.7777262805	3.5827378947	0.8271569151
H	2.6954955795	11.0900257126	6.5747247820
H	2.7251947195	11.1107201053	0.8271569151
H	4.8074254205	3.6034322874	6.5747247820
H	0.3711893663	11.6002423477	3.7107221613
H	7.1317316337	3.0932156523	3.7107211613
H	4.1222505949	10.4393093829	-0.0848929902
H	3.3806704051	4.2541486171	-0.0848929902
H	0.5299558549	8.2428819924	-0.0611436648
H	6.9729651451	6.4505760076	-0.0611436648
H	4.2819750374	13.7990259421	3.7057486680
H	3.2209459626	0.8944320579	3.7057486680
C	0.7145515147	3.2159793217	3.7146727435
C	6.7883694853	11.4774786783	3.7146717435
C	4.4659010105	4.1318210293	-0.0662463439
C	3.0370199895	10.5616369707	-0.0662463439
C	0.9099549957	9.2656729853	-0.0593704859
C	6.5929660043	5.4277850147	-0.0593704859
C	4.6611249892	12.7754434478	3.7101414547
C	2.8417960108	1.9180145522	3.7101414547
N	1.3518186664	1.8663877000	3.7092494679
N	6.1511023336	12.8270703000	3.7092484679
N	5.1032346365	5.4810541192	-0.0416527618
N	2.3996863635	9.2124038808	-0.0416527618
Cl	1.4646785879	13.7754694536	1.6977510435
Cl	6.0326147952	0.9040025476	5.6797899221
Cl	6.0382424121	0.9179885464	1.6977510435
Cl	1.4703062048	13.7894554524	5.6797899221
Cl	5.2197411125	8.2583600672	1.9570427463
Cl	2.2864212123	6.4388758255	5.5137136947
Cl	2.2831798875	6.4350979328	1.9570427463
Cl	5.2164997877	8.2545821745	5.5137136947
Cl	1.2769235791	2.1146882830	-0.0849659332
Cl	6.2259974209	12.5787697170	-0.0849659332
Cl	5.0343021410	5.2341321670	3.7251753859

Cl	2.4686188590	9.4593258330	3.7251753859
----	--------------	--------------	--------------

4% Tensile Strain

Along x-axis

Sn	-0.1381908969	-0.0048774892	0.0000000000
Sn	3.7535877844	7.3457947084	3.6942970000
H	0.5308639880	9.7867278665	0.8988710498
H	6.9754583496	4.9044612209	6.4897151721
H	6.9754583496	4.9044612209	0.8988778279
H	0.5308639880	9.7867278665	6.4897219502
H	4.3669143643	12.2223661874	2.7954370413
H	3.1382806478	2.4721606288	4.5933632769
H	3.1382806478	2.4721606288	2.7952297231
H	4.3669143643	12.2223661874	4.5931559587
H	1.0296863163	1.3010313780	2.8721126867
H	6.4720364612	13.4005009354	4.5164598381
H	6.4720364612	13.4005009354	2.8721331619
H	1.0296863163	1.3010313780	4.5164803133
H	4.8209197699	5.9984735887	0.8234187663
H	2.6849910977	8.6918337568	6.5652440442
H	2.6849910977	8.6918337568	0.8233489558
H	4.8209197699	5.9984735887	6.5651742337
H	0.9697286100	3.7412816089	2.8002547786
H	6.5402363684	10.9597017118	4.5884584434
H	6.5402363684	10.9597017118	2.8001345566
H	0.9697286100	3.7412816089	4.5883382214
H	4.8604494797	3.5664063338	0.8944741680
H	2.6464966795	11.1241907131	6.4942549888
H	2.6464966795	11.1241907131	0.8943380112
H	4.8604494797	3.5664063338	6.4941188320
H	0.1305424166	11.6630771096	3.6942970000
H	7.3772178160	3.0418085879	3.6942960000
H	4.0681008913	10.4777709448	0.0000000000
H	3.4386186292	4.2120626964	0.0000000000
H	0.5036257411	8.2345161313	0.0000000000

H	7.0022446052	6.4566011651	0.0000000000
H	4.2899634294	13.7707160317	3.6942970000
H	3.2119771728	0.9235888247	3.6942970000
C	0.6566934997	3.1937282932	3.6942970000
C	6.8515180251	11.5080125291	3.6942960000
C	4.5261091018	4.1008229478	0.0000000000
C	2.9806585615	10.5894523271	0.0000000000
C	0.8690620722	9.2637488550	0.0000000000
C	6.6370552039	5.4272967342	0.0000000000
C	4.6893852328	12.7544651766	3.6942970000
C	2.8150516526	1.9409207476	3.6942970000
N	1.3271393257	1.8604998587	3.6942970000
N	6.1771015105	12.8392153927	3.6942960000
N	5.1461186245	5.4580117850	0.0000000000
N	2.3600363506	9.2325169318	0.0000000000
Cl	1.3604494234	13.8113585370	1.7620507326
Cl	6.1635238352	0.8758901400	5.6294943053
Cl	6.1635238352	0.8758901400	1.7590986947
Cl	1.3604494234	13.8113585370	5.6265422674
Cl	5.2178508980	8.2758057383	1.9324692135
Cl	2.2888819461	6.4150100008	5.4563508343
Cl	2.2888819461	6.4150100008	1.9322421657
Cl	5.2178508980	8.2758057383	5.4561237865
Cl	1.0951596414	2.1407234642	0.0000000000
Cl	6.4247657757	12.5477451070	0.0000000000
Cl	5.0615718860	5.2410376465	3.6942970000
Cl	2.4445984768	9.4498958001	3.6942970000

4% Tensile Strain

Along y-axis

Sn	-0.1684900969	-0.2954706457	0.0000000000
Sn	3.7564431201	7.3716634640	3.6942970000
H	0.5242960048	9.8036452894	0.9001739405
H	6.9793342888	4.8948617838	6.4884843520

H	6.9793342888	4.8948617838	0.9001086480
H	0.5242960048	9.8036452894	6.4884190595
H	4.4640109715	12.5541011303	2.7942330619
H	3.0473242939	2.1506462115	4.5940577618
H	3.0473242939	2.1506462115	2.7945352382
H	4.4640109715	12.5541011303	4.5943599381
H	0.8769617808	1.0865075404	2.8703622956
H	6.6317026760	13.6203527069	4.5183638984
H	6.6317026760	13.6203527069	2.8702291016
H	0.8769617808	1.0865075404	4.5182307044
H	4.7923461979	5.9262687146	0.8240122139
H	2.7065593456	8.7641339371	6.5650427504
H	2.7065593456	8.7641339371	0.8235502496
H	4.7923461979	5.9262687146	6.5645807861
H	0.9346229796	3.5182840840	2.7983037270
H	6.5792506822	11.1892598244	4.5907197949
H	6.5792506822	11.1892598244	2.7978732051
H	0.9346229796	3.5182840840	4.5902892730
H	4.8979995541	3.4987069707	0.8956397724
H	2.6138654945	11.1934987206	6.4926695961
H	2.6138654945	11.1934987206	0.8959234039
H	4.8979995541	3.4987069707	6.4929532276
H	0.1497456327	11.8299070771	3.6942970000
H	7.3625701723	2.8799081720	3.6942960000
H	4.0475617809	10.5798467716	0.0000000000
H	3.4607171852	4.1051052121	0.0000000000
H	0.5361770333	8.2526098928	0.0000000000
H	6.9647631831	6.4461073392	0.0000000000
H	4.4617492041	14.1065661651	3.6942970000
H	3.0473210575	0.5976875482	3.6942970000
C	0.5994740586	2.9866415495	3.6942970000
C	6.9131512160	11.7209822660	3.6942960000
C	4.5513784817	4.0235664450	0.0000000000
C	2.9574844846	10.6671339031	0.0000000000
C	0.8755124576	9.2909032637	0.0000000000

C	6.6272959514	5.4071579237	0.0000000000
C	4.8101114709	13.0708411607	3.6942970000
C	2.7003249069	1.6338427313	3.6942970000
N	1.2080762347	1.6234177740	3.6942970000
N	6.3020723291	13.0829299570	3.6942960000
N	5.1348092543	5.3980467247	0.0000000000
N	2.3675850455	9.2958080972	0.0000000000
Cl	1.3028577265	14.0648011449	1.7630816837
Cl	6.2106522559	0.6262108690	5.6278051323
Cl	6.2106522559	0.6262108690	1.7607878677
Cl	1.3028577265	14.0648011449	5.6255113163
Cl	5.2183666944	8.2977493211	1.9293301011
Cl	2.2934827684	6.4389991618	5.4570340839
Cl	2.2934827684	6.4389991618	1.9315589161
Cl	5.2183666944	8.2977493211	5.4592628989
Cl	1.1223673604	1.8229742452	0.0000000000
Cl	6.3913915952	12.8698617239	0.0000000000
Cl	5.0547427562	5.2542164781	3.6942970000
Cl	2.4516456953	9.4852429394	3.6942970000

4% Tensile Strain

Along z-axis

Sn	-0.1561260713	-0.0080599962	-0.1394743156
Sn	3.7532923280	7.3455271384	3.7549324263
H	0.5458447032	9.7537376560	0.7743956623
H	6.9267771422	4.9575902502	6.6629109919
H	6.9623186048	4.9410770923	0.7747360125
H	0.5811273358	9.7364804518	6.6628652877
H	4.3965496699	12.2442634395	2.8244833384
H	3.1086191380	2.4287415949	4.6222694202
H	3.1048706786	2.4499973507	2.8258375999
H	4.3927380300	12.2673447363	4.6210348202
H	1.0032100282	1.2558349724	2.8917566933
H	6.4895689641	13.4632438672	4.5363540579
H	6.4934337503	13.4453554294	2.8877770600

H	1.0067494664	1.2426836274	4.5404327025
H	4.8019205575	6.0088952116	0.7658798399
H	2.7295829001	8.6160186267	6.8000729803
H	2.7039805622	8.6803268993	0.7656876415
H	4.7758841787	6.0730679083	6.7999325770
H	0.9430095552	3.7011198641	2.8451703479
H	6.5754223609	11.0240116268	4.6343124926
H	6.5652117416	10.9992337995	2.8464200799
H	0.9308806172	3.6817064617	4.6331682561
H	4.8049620616	3.5893372594	0.7635556973
H	2.6625369502	11.0623244414	6.6608389851
H	2.7057419444	11.0999499557	0.7637641149
H	4.8475541116	3.6276665955	6.6603029702
H	0.1141963022	11.7135409432	3.7229594982
H	7.3908494258	2.9940229054	3.7236826142
H	4.1038572670	10.4319681675	-0.1516193252
H	3.4055228149	4.2547348573	-0.1514058505
H	0.5366193001	8.1921168747	-0.1102935158
H	6.9676397683	6.5020818216	-0.1103940942
H	4.3026692984	13.8018936297	3.7022718439
H	3.1946423234	0.8925647585	3.7048388188
C	0.6231059966	3.1435023910	3.7311103159
C	6.8823923952	11.5604377669	3.7309507672
C	4.4925532822	4.1438248530	-0.1265559472
C	3.0170448674	10.5450266502	-0.1264358568
C	0.9022991879	9.2212881533	-0.1118437341
C	6.6043970684	5.4721107264	-0.1118383910
C	4.7138150643	12.7908265938	3.7163494444
C	2.7866835094	1.9047647122	3.7183492975
N	1.2981633127	1.8105811472	3.7197756769
N	6.2018580703	12.8903809506	3.7168207181
N	5.1127182024	5.5019341191	-0.0844804068
N	2.3940459679	9.1880785465	-0.0846234690
Cl	1.3596822703	13.8500946447	1.6427845713
Cl	6.1787833968	0.8239112154	5.7534696474

Cl	6.1770171596	0.8416684474	1.6341772238
Cl	1.3634588307	13.8540583193	5.7654373257
Cl	5.2203839118	8.2603683337	1.9709003812
Cl	2.2929008519	6.4387453010	5.5531025276
Cl	2.2865132392	6.4292275486	1.9705534866
Cl	5.2141780755	8.2508540205	5.5524572818
Cl	1.0169924588	2.1668500053	-0.1451131196
Cl	6.5164106412	12.5148559521	-0.1402526059
Cl	5.0372480013	5.2342645713	3.7443869383
Cl	2.4689454287	9.4554978119	3.7444061975

6% Tensile Strain

Along x-axis

Sn	-0.2067671538	-0.0065284755	0.0000000000
Sn	3.7570879783	7.3463339251	3.6942970000
H	0.5160259087	9.7829520981	0.8987942934
H	6.9882822601	4.9090346527	6.4897445211
H	6.9882822601	4.9090346527	0.8988484789
H	0.5160259087	9.7829520981	6.4897987066
H	4.3774415682	12.2175349375	2.7956603940
H	3.1295707357	2.4802594149	4.5933020945
H	3.1295707357	2.4802594149	2.7952909055
H	4.3774415682	12.2175349375	4.5929326060
H	1.0345562620	1.2846015877	2.8723656936
H	6.4703959759	13.4183743357	4.5162604746
H	6.4703959759	13.4183743357	2.8723325254
H	1.0345562620	1.2846015877	4.5162273064
H	4.8270775830	5.9910766333	0.8235026446
H	2.6753613674	8.6972470118	6.5651836051
H	2.6753613674	8.6972470118	0.8234093949
H	4.8270775830	5.9910766333	6.5650903554
H	0.9467677822	3.7276096989	2.8000782614
H	6.5648961013	10.9746989609	4.5885911595
H	6.5648961013	10.9746989609	2.8000018405
H	0.9467677822	3.7276096989	4.5885147386

H	4.8778398103	3.5596825436	0.8948055290
H	2.6298200241	11.1294025967	6.4940198987
H	2.6298200241	11.1294025967	0.8945731013
H	4.8778398103	3.5596825436	6.4937874710
H	-0.0019245432	11.6920178362	3.6942970000
H	7.5120570857	3.0128365586	3.6942960000
H	4.0530536422	10.4862253010	0.0000000000
H	3.4533335282	4.1995148675	0.0000000000
H	0.4968766847	8.2295163365	0.0000000000
H	7.0055824940	6.4623519369	0.0000000000
H	4.2887589913	13.7654875375	3.6942970000
H	3.2175331920	0.9320623202	3.6942970000
C	0.6398990044	3.1768603244	3.6942970000
C	6.8706655266	11.5259701200	3.6942960000
C	4.5415032689	4.0924375166	0.0000000000
C	2.9651028507	10.5956474215	0.0000000000
C	0.8566529475	9.2610835598	0.0000000000
C	6.6470551698	5.4304132707	0.0000000000
C	4.6966202958	12.7523586466	3.6942970000
C	2.8109302256	1.9457416532	3.6942970000
N	1.3237808613	1.8504490906	3.6942970000
N	6.1835730590	12.8507680543	3.6942960000
N	5.1554608484	5.4526071234	0.0000000000
N	2.3483317720	9.2366459389	0.0000000000
Cl	1.3090952257	13.8320104555	1.7600546184
Cl	6.2265190568	0.8520913295	5.6325613779
Cl	6.2265190568	0.8520913295	1.7560316221
Cl	1.3090952257	13.8320104555	5.6285383816
Cl	5.2188648347	8.2798093743	1.9324160963
Cl	2.2938421852	6.4114771524	5.4562566667
Cl	2.2938421852	6.4114771524	1.9323363333
Cl	5.2188648347	8.2798093743	5.4561769037
Cl	0.9963540656	2.1560811905	0.0000000000
Cl	6.5366971442	12.5294886379	0.0000000000
Cl	5.0725808703	5.2448702324	3.6942970000

Cl	2.4397358279	9.4465865086	3.6942970000
----	--------------	--------------	--------------

6% Tensile Strain

Along y-axis

Sn	0.0093771871	-0.4285553435	0.0000000000
Sn	3.7562905790	7.3536160455	3.6942970000
H	0.7852169198	9.6704817850	0.9022588674
H	6.7118830233	5.0469396687	6.4862230341
H	6.7118830233	5.0469396687	0.9023699659
H	0.7852169198	9.6704817850	6.4863341326
H	4.5397716588	12.9647931719	2.7928861212
H	2.9620940975	1.7463870904	4.5968316094
H	2.9620940975	1.7463870904	2.7917613906
H	4.5397716588	12.9647931719	4.5957068788
H	0.5507970944	1.3743210039	2.8715433274
H	6.9528939655	13.3310461772	4.5169034476
H	6.9528939655	13.3310461772	2.8716895524
H	0.5507970944	1.3743210039	4.5170496726
H	4.3843159347	5.7536328175	0.8215971496
H	3.1064221477	8.9449111487	6.5662741587
H	3.1064221477	8.9449111487	0.8223188413
H	4.3843159347	5.7536328175	6.5669958504
H	1.3204426671	3.6798148338	2.8016403837
H	6.1671367967	11.0290685930	4.5859902622
H	6.1671367967	11.0290685930	2.8026027378
H	1.3204426671	3.6798148338	4.5869526163
H	4.8193077425	3.3686273384	0.8947452304
H	2.6900159221	11.3322895380	6.4938770396
H	2.6900159221	11.3322895380	0.8947159604
H	4.8193077425	3.3686273384	6.4938477696
H	0.2068882079	11.2295578189	3.6942970000
H	7.2837911341	3.4685111832	3.6942960000
H	4.1844733079	10.8935338080	0.0000000000
H	3.3217830990	3.7958540430	0.0000000000
H	1.0017274422	8.1373471781	0.0000000000

H	6.4818307435	6.5777492357	0.0000000000
H	4.9874221333	14.4463727813	3.6942970000
H	2.5159961100	0.2654802789	3.6942970000
C	0.8537027935	3.2529749442	3.6942970000
C	6.6386902749	11.4528188969	3.6942960000
C	4.4144117764	3.8515180536	0.0000000000
C	3.0916484270	10.8464953347	0.0000000000
C	1.1994030389	9.2117084048	0.0000000000
C	6.2938097596	5.5020575348	0.0000000000
C	5.0205792311	13.3544523924	3.6942970000
C	2.4827217858	1.3574056000	3.6942970000
N	1.0515461569	1.7765039077	3.6942970000
N	6.4509022955	12.9309301912	3.6942960000
N	4.8183055711	5.2878784550	0.0000000000
N	2.6769263212	9.4132017451	0.0000000000
Cl	1.3307222928	13.9842069391	1.7489125675
Cl	6.1928172457	0.7370865066	5.6429626239
Cl	6.1928172457	0.7370865066	1.7456303761
Cl	1.3307222928	13.9842069391	5.6396804325
Cl	5.1662344275	8.3778800513	1.9355419684
Cl	2.3444610348	6.3379371010	5.4562196384
Cl	2.3444610348	6.3379371010	1.9323733616
Cl	5.1662344275	8.3778800513	5.4530510316
Cl	1.5833682003	1.4681739087	0.0000000000
Cl	5.9396640715	13.2470765564	0.0000000000
Cl	5.1556448686	5.3191834657	3.6942970000
Cl	2.3632785420	9.3928590511	3.6942970000

6% Tensile Strain

Along z-axis

Sn	0.0000000000	0.0000000000	-0.1923719586
Sn	3.7514610000	7.3467290000	3.7788371452
H	0.6507860131	9.7888487530	0.7086723543
H	6.8444674599	4.9920346668	6.7455818603
H	6.8521349869	4.9046092470	0.7086723543

H	0.6584535401	9.7014233332	6.7455818603
H	4.4116586251	12.2857579778	2.8359392256
H	3.0927365172	2.3882826608	4.6329406876
H	3.0912623749	2.4077000222	2.8359392256
H	4.4101844828	12.3051753392	4.6329406876
H	0.9544390211	1.2757233323	2.9005652765
H	6.5502801801	13.4335642092	4.5540102870
H	6.5484819789	13.4177346677	2.9005652765
H	0.9526408199	1.2598937908	4.5540102870
H	4.7147983771	6.0595788577	0.6881217985
H	2.7935346974	8.5937995637	6.8667293692
H	2.7881226229	8.6338791423	0.6881217985
H	4.7093863026	6.0996584363	6.8667293692
H	0.9521579451	3.7126405126	2.8594760743
H	6.5541103122	11.0063797416	4.6481199985
H	6.5507630549	10.9808174874	2.8594760743
H	0.9488106878	3.6870782584	4.6481199985
H	4.7052418407	3.6203699830	0.6899741524
H	2.8175939467	11.0189084298	6.7346810547
H	2.7976791593	11.0730880170	0.6899741524
H	4.6853270533	3.6745495702	6.7346810547
H	0.4585182570	11.6622438640	3.7450685416
H	7.0444027430	3.0312141360	3.7450675416
H	4.2121712533	10.3673626434	-0.1672142169
H	3.2907497467	4.3260953566	-0.1672142169
H	0.6041255384	8.1959496448	-0.1122113978
H	6.8987954616	6.4975083552	-0.1122113978
H	4.3591618361	13.8453849833	3.7185005794
H	3.1437591639	0.8480730167	3.7185005794
C	0.6263897934	3.1593110980	3.7457890673
C	6.8765312066	11.5341469020	3.7457880673
C	4.3749876485	4.1905899464	-0.1836518384
C	3.1279333515	10.5028680536	-0.1836518384
C	0.9858781333	9.2178838611	-0.1616734731
C	6.5170428667	5.4755741389	-0.1616734731

C	4.7421924989	12.8232732088	3.7294622365
C	2.7607285011	1.8701847912	3.7294622365
N	1.2699845820	1.8112010047	3.7321014518
N	6.2329364180	12.8822569953	3.7321004518
N	5.0260934470	5.5352584862	-0.1524372839
N	2.4768275530	9.1581995138	-0.1524372839
Cl	1.4736578250	13.8021122503	1.6064242505
Cl	6.0561486486	0.9205857125	5.8302154698
Cl	6.0292631750	0.8913457497	1.6064242505
Cl	1.4467723514	13.7728722875	5.8302154698
Cl	5.2038730577	8.2568892312	1.9726589892
Cl	2.2830800085	6.4468075417	5.5786614452
Cl	2.2990479423	6.4365687688	1.9726589892
Cl	5.2198409915	8.2466504583	5.5786614452
Cl	1.2688484397	2.1144678761	-0.1970541962
Cl	6.2340725603	12.5789901239	-0.1970541962
Cl	5.0140492973	5.2307742296	3.7789901430
Cl	2.4888717027	9.4626837704	3.7789901430

2% Compressive Strain

Along x-axis

Sn	0.0752905443	0.0030858300	0.0000000000
Sn	3.7504839699	7.3468168034	3.6942970000
H	0.6069839313	9.8236621752	0.8990389116
H	6.8943941942	4.8717791492	6.4895468303
H	6.8943941942	4.8717791492	0.8990461697
H	0.6069839313	9.8236621752	6.4895540884
H	4.2924808566	12.2378886039	2.7940961350
H	3.2069752615	2.4548600446	4.5944756636
H	3.2069752615	2.4548600446	2.7941173364
H	4.2924808566	12.2378886039	4.5944968650
H	1.0513125599	1.3644433549	2.8718233370
H	6.4508997071	13.3232986888	4.5169305424
H	6.4508997071	13.3232986888	2.8716624576
H	1.0513125599	1.3644433549	4.5167696630

H	4.7631997016	6.0081524205	0.8230974107
H	2.7383255011	8.6874833159	6.5655122404
H	2.7383255011	8.6874833159	0.8230807596
H	4.7631997016	6.0081524205	6.5654955893
H	1.0802336072	3.7936513443	2.8010629055
H	6.4161643723	10.8943383735	4.5874530698
H	6.4161643723	10.8943383735	2.8011399302
H	1.0802336072	3.7936513443	4.5875300945
H	4.7568207883	3.5766374522	0.8936743808
H	2.7442752690	11.1189514440	6.4948910117
H	2.7442752690	11.1189514440	0.8937019883
H	4.7568207883	3.5766374522	6.4949186192
H	0.4805470344	11.5510171304	3.6942970000
H	7.0176214342	3.1336215912	3.6942960000
H	4.1527492021	10.4464675319	0.0000000000
H	3.3484448785	4.2495852350	0.0000000000
H	0.5458551059	8.2756476302	0.0000000000
H	6.9555668310	6.4198274126	0.0000000000
H	4.2710241773	13.7854317715	3.6942970000
H	3.2320637039	0.9075381462	3.6942970000
C	0.7506192981	3.2551742868	3.6942970000
C	6.7470008180	11.4321145450	3.6942960000
C	4.4328065557	4.1180371520	0.0000000000
C	3.0684111193	10.5776242709	0.0000000000
C	0.9346207168	9.2954231552	0.0000000000
C	6.5668060719	5.4000639096	0.0000000000
C	4.6328203873	12.7561066148	3.6942970000
C	2.8677293696	1.9361569563	3.6942970000
N	1.3789299090	1.9032321181	3.6942970000
N	6.1218466641	12.7856550883	3.6942960000
N	5.0786610321	5.4620013117	0.0000000000
N	2.4227270632	9.2335973555	0.0000000000
Cl	1.5249937926	13.7537363983	1.7641094220
Cl	5.9720754158	0.9435909119	5.6280117299
Cl	5.9720754158	0.9435909119	1.7605812701

Cl	1.5249937926	13.7537363983	5.6244835780
Cl	5.2199518780	8.2618041249	1.9308863437
Cl	2.2806173159	6.4328383222	5.4576185742
Cl	2.2806173159	6.4328383222	1.9309744258
Cl	5.2199518780	8.2618041249	5.4577066563
Cl	1.3797789160	2.1026788999	0.0000000000
Cl	6.1197537753	12.5976538750	0.0000000000
Cl	5.0272525042	5.2315780190	3.6942970000
Cl	2.4744296132	9.4631841107	3.6942970000

2% Compressive Strain

Along y-axis

Sn	0.0023022004	0.1586819021	0.0000000000
Sn	3.7516057448	7.3420978126	3.6942970000
H	0.5562244310	9.8006182412	0.8986470551
H	6.9495727074	4.8886150162	6.4903156490
H	6.9495727074	4.8886150162	0.8982773510
H	0.5562244310	9.8006182412	6.4899459449
H	4.2870985584	12.0582156358	2.7965116989
H	3.2130192245	2.6251340555	4.5921218227
H	3.2130192245	2.6251340555	2.7964711773
H	4.2870985584	12.0582156358	4.5920813011
H	1.0859823382	1.4724135085	2.8720377746
H	6.4127942378	13.2139338380	4.5166958991
H	6.4127942378	13.2139338380	2.8718971009
H	1.0859823382	1.4724135085	4.5165552254
H	4.8220086232	6.0290106317	0.8231562360
H	2.6804542745	8.6533223317	6.5657740700
H	2.6804542745	8.6533223317	0.8228189300
H	4.8220086232	6.0290106317	6.5654367640
H	1.0678970579	3.9062742061	2.8013132611
H	6.4313302329	10.7800367270	4.5870088624
H	6.4313302329	10.7800367270	2.8015841376
H	1.0678970579	3.9062742061	4.5872797389

H	4.8122103756	3.5954189506	0.8928851752
H	2.6972268274	11.0871993166	6.4952109806
H	2.6972268274	11.0871993166	0.8933820194
H	4.8122103756	3.5954189506	6.4957078248
H	0.3336663583	11.4645948961	3.6942970000
H	7.1662404341	3.2220368669	3.6942960000
H	4.1037752085	10.4100778640	0.0000000000
H	3.4029953508	4.2694028681	0.0000000000
H	0.4904582785	8.2517320612	0.0000000000
H	7.0106706171	6.4385401064	0.0000000000
H	4.2087287286	13.6060724336	3.6942970000
H	3.2874144712	1.0774627170	3.6942970000
C	0.7463990898	3.3619093654	3.6942970000
C	6.7533611903	11.3247603637	3.6942960000
C	4.4872413453	4.1376529130	0.0000000000
C	3.0198664526	10.5444955621	0.0000000000
C	0.8818366369	9.2705202719	0.0000000000
C	6.6224007781	5.4182640179	0.0000000000
C	4.6106984851	12.5913279881	3.6942970000
C	2.8879758616	2.0933448580	3.6942970000
N	1.3994711464	2.0210901899	3.6942970000
N	6.0994032045	12.6657145953	3.6942960000
N	5.1342415336	5.4809365222	0.0000000000
N	2.3698386510	9.2026967649	0.0000000000
Cl	1.4572760039	13.6179191326	1.7642333545
Cl	6.0507434637	1.0962175885	5.6251283167
Cl	6.0507434637	1.0962175885	1.7634646833
Cl	1.4572760039	13.6179191326	5.6243596455
Cl	5.2158641152	8.2648072221	1.9286838749
Cl	2.2874334813	6.4173869368	5.4606100492
Cl	2.2874334813	6.4173869368	1.9279829508
Cl	5.2158641152	8.2648072221	5.4599091251
Cl	1.3311935209	2.2406614127	0.0000000000
Cl	6.1738543733	12.4741509688	0.0000000000
Cl	5.0541366100	5.2446935666	3.6942970000

Cl	2.4492008223	9.4375874339	3.6942970000
----	--------------	--------------	--------------

2% Compressive Strain

Along z-axis

Sn	0.0000000000	0.0000000000	0.0771966117
Sn	3.7514610000	7.3467290000	3.6621547032
H	0.5460373930	9.8312861335	0.9649137924
H	6.9778439663	4.8457123418	6.4093157842
H	6.9568836070	4.8621718665	0.9649137924
H	0.5250770337	9.8477456582	6.4093157842
H	4.2906405875	12.2069893392	2.7728177620
H	3.2205657935	2.4994826976	4.5705733330
H	3.2122804125	2.4864686608	2.7728177620
H	4.2823552065	12.1939753024	4.5705733330
H	1.0724615081	1.3733933301	2.8644733093
H	6.4287808370	13.3066101761	4.5090875694
H	6.4304594919	13.3200646699	2.8644733093
H	1.0741401630	1.3868478239	4.5090875694
H	4.8181540901	5.9808999805	0.8531337735
H	2.6726348648	8.7418862727	6.4489255982
H	2.6847669099	8.7125580195	0.8531337735
H	4.8302861352	5.9515717273	6.4489255982
H	1.0915460103	3.8019505116	2.7718946232
H	6.4043769398	10.8726268087	4.5587385428
H	6.4113749897	10.8915074884	2.7718946232
H	1.0985440602	3.8208311913	4.5587385428
H	4.8553390952	3.5473278059	0.9615568450
H	2.6647591021	11.1703424962	6.4165966513
H	2.6475819048	11.1461301941	0.9615568450
H	4.8381618979	3.5231155038	6.4165966513
H	0.3221762385	11.5384770024	3.6770774583
H	7.1807447615	3.1549809976	3.6770764583
H	4.0733358355	10.5015757220	0.0755199696
H	3.4295851645	4.1918822780	0.0755199696
H	0.4906970566	8.2899142533	0.0547807296

H	7.0122239434	6.4035437467	0.0547807296
H	4.2420902186	13.7498525366	3.6817233386
H	3.2608307814	0.9436054634	3.6817233386
C	0.7639694960	3.2737452325	3.6722507297
C	6.7389515040	11.4197127675	3.6722497297
C	4.5155405850	4.0733292303	0.0641858007
C	2.9873804150	10.6201287697	0.0641858007
C	0.8688439629	9.3139890515	0.0577130151
C	6.6340770371	5.3794689485	0.0577130151
C	4.6196646882	12.7256687187	3.6769838335
C	2.8832563118	1.9677892813	3.6769838335
N	1.3943317373	1.9228692461	3.6823307585
N	6.1085892627	12.7705887539	3.6823297585
N	5.1453155373	5.4243295966	0.0424935515
N	2.3576054627	9.2691284034	0.0424935515
Cl	1.4678247122	13.7727367145	1.8305276651
Cl	6.0404493186	0.9382289347	5.5710917134
Cl	6.0350962878	0.9207212855	1.8305276651
Cl	1.4624716814	13.7552290653	5.5710917134
Cl	5.2156567745	8.2764201762	1.9090279159
Cl	2.2821658349	6.4108231765	5.4063669309
Cl	2.2872642255	6.4170378238	1.9090279159
Cl	5.2207551651	8.2826348235	5.4063669309
Cl	1.3084058518	2.1050853384	0.0782786898
Cl	6.1945151482	12.5883726616	0.0782786898
Cl	5.0549465453	5.2417387413	3.6696191580
Cl	2.4479744547	9.4517192587	3.6696191580

4% Compressive Strain

Along x-axis

Sn	0.1657159239	0.0053454766	0.0000000000
Sn	3.7522340847	7.3458014088	3.6942970000
H	0.6390341339	9.8494013224	0.8986025375
H	6.8555352873	4.8465472792	6.4899676254
H	6.8555352873	4.8465472792	0.8986253746

H	0.6390341339	9.8494013224	6.4899904625
H	4.2543118691	12.2349861318	2.7947396582
H	3.2349879865	2.4584344364	4.5939899156
H	3.2349879865	2.4584344364	2.7946030844
H	4.2543118691	12.2349861318	4.5938533418
H	1.0709886088	1.3827451663	2.8723859518
H	6.4212587552	13.3021007062	4.5165152034
H	6.4212587552	13.3021007062	2.8720777966
H	1.0709886088	1.3827451663	4.5162070482
H	4.7398135141	6.0105164142	0.8230803116
H	2.7547677983	8.6857784488	6.5654667238
H	2.7547677983	8.6857784488	0.8231262762
H	4.7398135141	6.0105164142	6.5655126884
H	1.1182786700	3.8089371488	2.8004448669
H	6.3641849197	10.8746214949	4.5877461617
H	6.3641849197	10.8746214949	2.8008468383
H	1.1182786700	3.8089371488	4.5881481331
H	4.7174240001	3.5793365340	0.8933513621
H	2.7762779289	11.1174427822	6.4954182711
H	2.7762779289	11.1174427822	0.8931747289
H	4.7174240001	3.5793365340	6.4952416379
H	0.5846823636	11.5176955603	3.6942970000
H	6.9016536655	3.1584132866	3.6942960000
H	4.1819497438	10.4387013019	0.0000000000
H	3.3126699700	4.2593110361	0.0000000000
H	0.5523091614	8.3028282419	0.0000000000
H	6.9426266782	6.3930499547	0.0000000000
H	4.2428926906	13.7829850005	3.6942970000
H	3.2535757196	0.9109150378	3.6942970000
C	0.7853737361	3.2733501187	3.6942970000
C	6.7003919741	11.4092328653	3.6942960000
C	4.3957290466	4.1226107658	0.0000000000
C	3.0986260177	10.5742438449	0.0000000000
C	0.9583284440	9.3156488703	0.0000000000
C	6.5364647940	5.3804295233	0.0000000000

C	4.5981090547	12.7509672630	3.6942970000
C	2.8936136506	1.9409504291	3.6942970000
N	1.4055663908	1.9176468737	3.6942970000
N	6.0865196700	12.7681265581	3.6942960000
N	5.0505701283	5.4614929397	0.0000000000
N	2.4443955651	9.2349026245	0.0000000000
Cl	1.6075772266	13.7465890583	1.7641750352
Cl	5.9259507293	0.9541140823	5.6213421409
Cl	5.9259507293	0.9541140823	1.7672508591
Cl	1.6075772266	13.7465890583	5.6244179648
Cl	5.2273265409	8.2493526299	1.9315565403
Cl	2.2772776624	6.4443874403	5.4575394189
Cl	2.2772776624	6.4443874403	1.9310535811
Cl	5.2273265409	8.2493526299	5.4570364597
Cl	1.4775967883	2.0989580734	0.0000000000
Cl	6.0376577144	12.6168920582	0.0000000000
Cl	5.0060703292	5.2201110531	3.6942970000
Cl	2.4979344325	9.4723606816	3.6942970000

4% Compressive Strain

Along y-axis

Sn	-0.0049587870	0.2752873332	0.0000000000
Sn	3.7519114830	7.3430754704	3.6942970000
H	0.5767281322	9.8153154581	0.8969747191
H	6.9271203800	4.8734006083	6.4912853986
H	6.9271203800	4.8734006083	0.8973076014
H	0.5767281322	9.8153154581	6.4916182809
H	4.3219211398	11.9266111955	2.7971977140
H	3.1805535627	2.7624497902	4.5913610126
H	3.1805535627	2.7624497902	2.7972319874
H	4.3219211398	11.9266111955	4.5913952860
H	1.0761559290	1.5790280060	2.8707261950
H	6.4275532696	13.1081509614	4.5171538479
H	6.4275532696	13.1081509614	2.8714391521
H	1.0761559290	1.5790280060	4.5178668050

H	4.8367224879	6.0812814814	0.8227710777
H	2.6651108611	8.6041746194	6.5655454607
H	2.6651108611	8.6041746194	0.8230475393
H	4.8367224879	6.0812814814	6.5658219223
H	1.0238618773	4.0122320945	2.8025420770
H	6.4846600828	10.6750426608	4.5866036832
H	6.4846600828	10.6750426608	2.8019893168
H	1.0238618773	4.0122320945	4.5860509230
H	4.7507687099	3.6486879359	0.8927346937
H	2.7554927037	11.0364105852	6.4961499169
H	2.7554927037	11.0364105852	0.8924430831
H	4.7507687099	3.6486879359	6.4958583063
H	0.3775275808	11.3763473160	3.6942970000
H	7.1282714521	3.3149637204	3.6942960000
H	4.1419723307	10.3163658433	0.0000000000
H	3.3630596514	4.3660730217	0.0000000000
H	0.4644023815	8.2678445267	0.0000000000
H	7.0370371334	6.4208132572	0.0000000000
H	4.2304769791	13.4758926263	3.6942970000
H	3.2764489137	1.2134657380	3.6942970000
C	0.7071656871	3.4638137521	3.6942970000
C	6.7991657889	11.2236635025	3.6942960000
C	4.4422895111	4.2001091432	0.0000000000
C	3.0632172948	10.4840673480	0.0000000000
C	0.8873998111	9.2740983978	0.0000000000
C	6.6157765485	5.4138023241	0.0000000000
C	4.6394786000	12.4636618333	3.6942970000
C	2.8644367521	2.2244343741	3.6942970000
N	1.3777657484	2.1325300213	3.6942970000
N	6.1260581200	12.5533658518	3.6942960000
N	5.1306682540	5.5218834545	0.0000000000
N	2.3722518571	9.1636661726	0.0000000000
Cl	1.4624293552	13.4684609057	1.7677631912
Cl	6.0252915241	1.1922231178	5.6280626280
Cl	6.0252915241	1.1922231178	1.7605303720

Cl	1.4624293552	13.4684609057	5.6208298088
Cl	5.2202545462	8.2588582972	1.9291775747
Cl	2.2831355341	6.4264743343	5.4591179792
Cl	2.2831355341	6.4264743343	1.9294750208
Cl	5.2202545462	8.2588582972	5.4594154253
Cl	1.2940876101	2.3718970849	0.0000000000
Cl	6.2076089436	12.2788668613	0.0000000000
Cl	5.0529709548	5.2513318349	3.6942970000
Cl	2.4512382087	9.4346280873	3.6942970000

4% Compressive Strain

Along z-axis

Sn	0.0000000000	0.0000000000	0.1233163042
Sn	3.7514610000	7.3467290000	3.6530517249
H	0.4903611723	9.8166372033	1.0149052294
H	7.0040823757	4.8040823867	6.3116844225
H	7.0125598277	4.8768207967	1.0149052294
H	0.4988386243	9.8893756133	6.3116844225
H	4.2532662142	12.1877003318	2.7755319116
H	3.2612842404	2.5108077727	4.5734758268
H	3.2496547858	2.5057576682	2.7755319116
H	4.2416367596	12.1826502273	4.5734758268
H	1.1026047534	1.3965144537	2.8753201042
H	6.3888374922	13.2760119495	4.5189423530
H	6.4003162466	13.2969435463	2.8753201042
H	1.1140835078	1.4174460505	4.5189423530
H	4.8606746942	5.9446838510	0.9144350428
H	2.6408641878	8.7584822356	6.3646045482
H	2.6422463058	8.7487741490	0.9144350428
H	4.8620568122	5.9349757644	6.3646045482
H	1.1364042519	3.8275484574	2.7758537752
H	6.3656690856	10.8473467348	4.5619028409
H	6.3665167481	10.8659095426	2.7758537752
H	1.1372519144	3.8461112652	4.5619028409

H	4.8605012910	3.5206222225	1.0090155788
H	2.5919792284	11.1938657901	6.3174215104
H	2.6424197090	11.1728357775	1.0090155788
H	4.9109417716	3.4995922099	6.3174215104
H	0.2819308006	11.5110661368	3.6757094574
H	7.2209901994	3.1823918632	3.6757084574
H	4.0350028357	10.5303915909	0.0676797576
H	3.4679181643	4.1630664091	0.0676797576
H	0.4571968293	8.3060627480	0.0513960001
H	7.0457241707	6.3873952520	0.0513960001
H	4.2114419524	13.7344320428	3.6791057075
H	3.2914790476	0.9590259572	3.6791057075
C	0.8045313212	3.2993427702	3.6745523733
C	6.6983896788	11.3941152298	3.6745513733
C	4.5545121607	4.0478040729	0.1007738061
C	2.9484088393	10.6456539271	0.1007738061
C	0.8307594589	9.3308890264	0.0969808073
C	6.6721615411	5.3625689736	0.0969808073
C	4.5833649456	12.7082711922	3.6780881467
C	2.9195560544	1.9851868078	3.6780881467
N	1.4310827955	1.9477962589	3.6879879351
N	6.0718382045	12.7456617411	3.6879869351
N	5.1834883026	5.3984083672	0.0964400912
N	2.3194326974	9.2950496328	0.0964400912
Cl	1.4707729604	13.7409953181	1.8428886981
Cl	6.0457652983	0.9361522007	5.4741409214
Cl	6.0321480396	0.9524626819	1.8428886981
Cl	1.4571557017	13.7573057993	5.4741409214
Cl	5.2186672017	8.2878571601	1.9221532713
Cl	2.2901396707	6.4014212829	5.3907442710
Cl	2.2842537983	6.4056008399	1.9221532713
Cl	5.2127813293	8.2920367171	5.3907442710
Cl	1.3224768917	2.0993298205	0.1264177688
Cl	6.1804441083	12.5941281795	0.1264177688
Cl	5.0762630496	5.2519361427	3.6553383289

Cl	2.4266579504	9.4415218573	3.6553383289
----	--------------	--------------	--------------

6% Compressive Strain

Along x-axis

Sn	0.2500745066	0.0062397932	0.0000000000
Sn	3.7479910745	7.3458064623	3.6942970000
H	0.6834266419	9.8777756452	0.8981550078
H	6.8066153325	4.8230479104	6.4903942790
H	6.8066153325	4.8230479104	0.8981987210
H	0.6834266419	9.8777756452	6.4904379922
H	4.2107322520	12.2285663046	2.7947410976
H	3.2746422440	2.4657843148	4.5941208616
H	3.2746422440	2.4657843148	2.7944721384
H	4.2107322520	12.2285663046	4.5938519024
H	1.1061909285	1.3964739013	2.8724695829
H	6.3834844031	13.2848533763	4.5168320022
H	6.3834844031	13.2848533763	2.8717609978
H	1.1061909285	1.3964739013	4.5161234171
H	4.7001696430	6.0031583122	0.8231790786
H	2.7879096432	8.6938776003	6.5653845224
H	2.7879096432	8.6938776003	0.8232084776
H	4.7001696430	6.0031583122	6.5654139214
H	1.1688828989	3.8203631035	2.8017627569
H	6.3056099827	10.8593212647	4.5862893470
H	6.3056099827	10.8593212647	2.8023036530
H	1.1688828989	3.8203631035	4.5868302431
H	4.6755659633	3.5732130357	0.8927944310
H	2.8147872986	11.1241907999	6.4960029728
H	2.8147872986	11.1241907999	0.8925900272
H	4.6755659633	3.5732130357	6.4957985690
H	0.6804497569	11.4925146434	3.6942970000
H	6.7999017887	3.1758801866	3.6942960000
H	4.2199146613	10.4441041232	0.0000000000
H	3.2706476773	4.2532511713	0.0000000000
H	0.5748637844	8.3322948237	0.0000000000

H	6.9121594533	6.3684850004	0.0000000000
H	4.2032556106	13.7749067552	3.6942970000
H	3.2926997223	0.9195222275	3.6942970000
C	0.8335712746	3.2843773267	3.6942970000
C	6.6457613332	11.3934531766	3.6942960000
C	4.3532436146	4.1168269985	0.0000000000
C	3.1372347102	10.5803089946	0.0000000000
C	0.9950944428	9.3391230535	0.0000000000
C	6.4938872120	5.3608947538	0.0000000000
C	4.5557984347	12.7431344699	3.6942970000
C	2.9335528828	1.9490856525	3.6942970000
N	1.4473019100	1.9273166089	3.6942970000
N	6.0425193801	12.7556771246	3.6942960000
N	5.0099598753	5.4541436961	0.0000000000
N	2.4791377073	9.2434637177	0.0000000000
Cl	1.6827283181	13.7382977905	1.7638381100
Cl	5.8662556512	0.9634971985	5.6248570575
Cl	5.8662556512	0.9634971985	1.7637359425
Cl	1.6827283181	13.7382977905	5.6247548900
Cl	5.2228514741	8.2446611043	1.9315176041
Cl	2.2719870995	6.4489232903	5.4569729285
Cl	2.2719870995	6.4489232903	1.9316200715
Cl	5.2228514741	8.2446611043	5.4570753959
Cl	1.5661957842	2.0917725004	0.0000000000
Cl	5.9670393050	12.6250896666	0.0000000000
Cl	4.9912287235	5.2179700360	3.6942970000
Cl	2.5060848243	9.4759001316	3.6942970000

6% Compressive Strain

Along y-axis

Sn	-0.0056027309	0.4189163651	0.0000000000
Sn	3.7525717303	7.3388975719	3.6942970000
H	0.5830787748	9.8175605850	0.8966122131
H	6.9206649117	4.8681476460	6.4922442192
H	6.9206649117	4.8681476460	0.8963487808

H	0.5830787748	9.8175605850	6.4919807869
H	4.3360764741	11.8255946440	2.7967066043
H	3.1657647189	2.8607824872	4.5918263855
H	3.1657647189	2.8607824872	2.7967666145
H	4.3360764741	11.8255946440	4.5918863957
H	1.0544605268	1.6883539010	2.8716852039
H	6.4490051333	12.9942096390	4.5163147546
H	6.4490051333	12.9942096390	2.8722782454
H	1.0544605268	1.6883539010	4.5169077961
H	4.8616370960	6.1266004964	0.8224361230
H	2.6384933954	8.5530873949	6.5661999911
H	2.6384933954	8.5530873949	0.8223930089
H	4.8616370960	6.1266004964	6.5661568770
H	1.0136684195	4.1220219939	2.8034185367
H	6.4933671532	10.5616001859	4.5861536932
H	6.4933671532	10.5616001859	2.8024393068
H	1.0136684195	4.1220219939	4.5851744633
H	4.7159450082	3.6950929782	0.8921467286
H	2.7920633905	10.9847823734	6.4965459886
H	2.7920633905	10.9847823734	0.8920470114
H	4.7159450082	3.6950929782	6.4964462714
H	0.3894482384	11.2576105865	3.6942970000
H	7.1160480572	3.4278507195	3.6942960000
H	4.1584202103	10.2289398199	0.0000000000
H	3.3460807730	4.4455194860	0.0000000000
H	0.4337822330	8.2732361329	0.0000000000
H	7.0659866309	6.4135465596	0.0000000000
H	4.2580373661	13.3747700137	3.6942970000
H	3.2487778444	1.3105799084	3.6942970000
C	0.6947721384	3.5738280910	3.6942970000
C	6.8109940996	11.1088370897	3.6942960000
C	4.4204312947	4.2538708449	0.0000000000
C	3.0851209279	10.4245157608	0.0000000000
C	0.8810049441	9.2689213801	0.0000000000
C	6.6214367996	5.4164441425	0.0000000000

C	4.6577011139	12.3593185353	3.6942970000
C	2.8464606408	2.3251283351	3.6942970000
N	1.3598140221	2.2410484751	3.6942970000
N	6.1441171037	12.4404158157	3.6942960000
N	5.1398033431	5.5581152896	0.0000000000
N	2.3618957698	9.1225167145	0.0000000000
Cl	1.4540836935	13.3058578958	1.7685067953
Cl	6.0342287848	1.3483194002	5.6275543717
Cl	6.0342287848	1.3483194002	1.7610386283
Cl	1.4540836935	13.3058578958	5.6200862047
Cl	5.2304798248	8.2432092748	1.9302440815
Cl	2.2748274766	6.4352760135	5.4585423752
Cl	2.2748274766	6.4352760135	1.9300506247
Cl	5.2304798248	8.2432092748	5.4583489185
Cl	1.3187956053	2.4918744121	0.0000000000
Cl	6.1865637066	12.1493737463	0.0000000000
Cl	5.0417972498	5.2485357780	3.6942970000
Cl	2.4633003236	9.4299476068	3.6942970000

6% Compressive Strain

Along z-axis

Sn	0.0000000000	0.0000000000	0.2003670869
Sn	3.7514610000	7.3467290000	3.6172155206
H	0.5103990166	9.8227110776	1.0843588251
H	7.0162654588	4.7786767241	6.2341300306
H	6.9925219834	4.8707469224	1.0843588251
H	0.4866555412	9.9147812759	6.2341300306
H	4.2597311430	12.1823565519	2.7488244751
H	3.2640982233	2.5339564071	4.5467780358
H	3.2431898570	2.5111014481	2.7488244751
H	4.2388227767	12.1595015929	4.5467780358
H	1.1023366255	1.3999571616	2.8701717720
H	6.3843703770	13.2537552376	4.5123142533
H	6.4005843745	13.2935008384	2.8701717720
H	1.1185506230	1.4397027624	4.5123142533

H	4.8561308343	5.9485132899	0.9429242412
H	2.6336085356	8.7850133400	6.2445597877
H	2.6467901657	8.7449447101	0.9429242412
H	4.8693124644	5.9084446600	6.2445597877
H	1.1320682779	3.8273090107	2.7437837579
H	6.3569008700	10.8264188146	4.5292446544
H	6.3708527221	10.8661489893	2.7437837579
H	1.1460201300	3.8670391854	4.5292446544
H	4.8803592911	3.5285156255	1.0796665651
H	2.6015235573	11.2193961447	6.2398970620
H	2.6225617089	11.1649423745	1.0796665651
H	4.9013974427	3.4740618553	6.2398970620
H	0.2804748395	11.4993657310	3.6610634865
H	7.2224461605	3.1940922690	3.6610624865
H	4.0304613118	10.5392549703	0.1516229601
H	3.4724596882	4.1542030297	0.1516229601
H	0.4550686891	8.3220737471	0.1066933119
H	7.0478523109	6.3713842529	0.1066933119
H	4.2101221900	13.7202464944	3.6667486070
H	3.2927988100	0.9732115056	3.6667486070
C	0.8060161143	3.3104443324	3.6510779121
C	6.6969048857	11.3830136676	3.6510769121
C	4.5585848218	4.0383206217	0.1670689831
C	2.9443361782	10.6551373783	0.1670689831
C	0.8316223697	9.3452289028	0.1551419897
C	6.6712986303	5.3482290972	0.1551419897
C	4.5834354936	12.6945852577	3.6584268473
C	2.9194855064	1.9988727423	3.6584268473
N	1.4322512726	1.9606125173	3.6753706070
N	6.0706697274	12.7328454827	3.6753696070
N	5.1841983641	5.3884048364	0.1367874123
N	2.3187226359	9.3050531636	0.1367874123
Cl	1.4706654360	13.7608482543	1.9200766893
Cl	6.0283687541	0.9490483513	5.4391559964
Cl	6.0322555640	0.9326097457	1.9200766893

Cl	1.4745522459	13.7444096487	5.4391559964
Cl	5.2303851158	8.2845300664	1.9035176186
Cl	2.2735142849	6.3890225677	5.3226642453
Cl	2.2725358842	6.4089279336	1.9035176186
Cl	5.2294067151	8.3044354323	5.3226642453
Cl	1.3235274487	2.1032956423	0.1948898526
Cl	6.1793935513	12.5901623577	0.1948898526
Cl	5.0680268965	5.2443286824	3.6259232167
Cl	2.4348941035	9.4491293176	3.6259232167

Table S3: Evolution of Sn–Cl bond lengths and Cl–Sn–Cl bond angles with applied strain.

Strain (%)	Sn–Cl bond length (Å)	cis-Cl–Sn–Cl angle (°)	trans-Cl–Sn–Cl angle (°)
0	2.4745	90.328	180
2 (Tensile)	2.4780	90.334	179.998
4 (Tensile)	2.4783	90.385	179.972
6 (Tensile)	2.4792	90.335	179.949
2 (Compressive)	2.4713	90.551	179.972
4 (Compressive)	2.4689	90.629	179.999
6 (Compressive)	2.4657	90.729	179.947

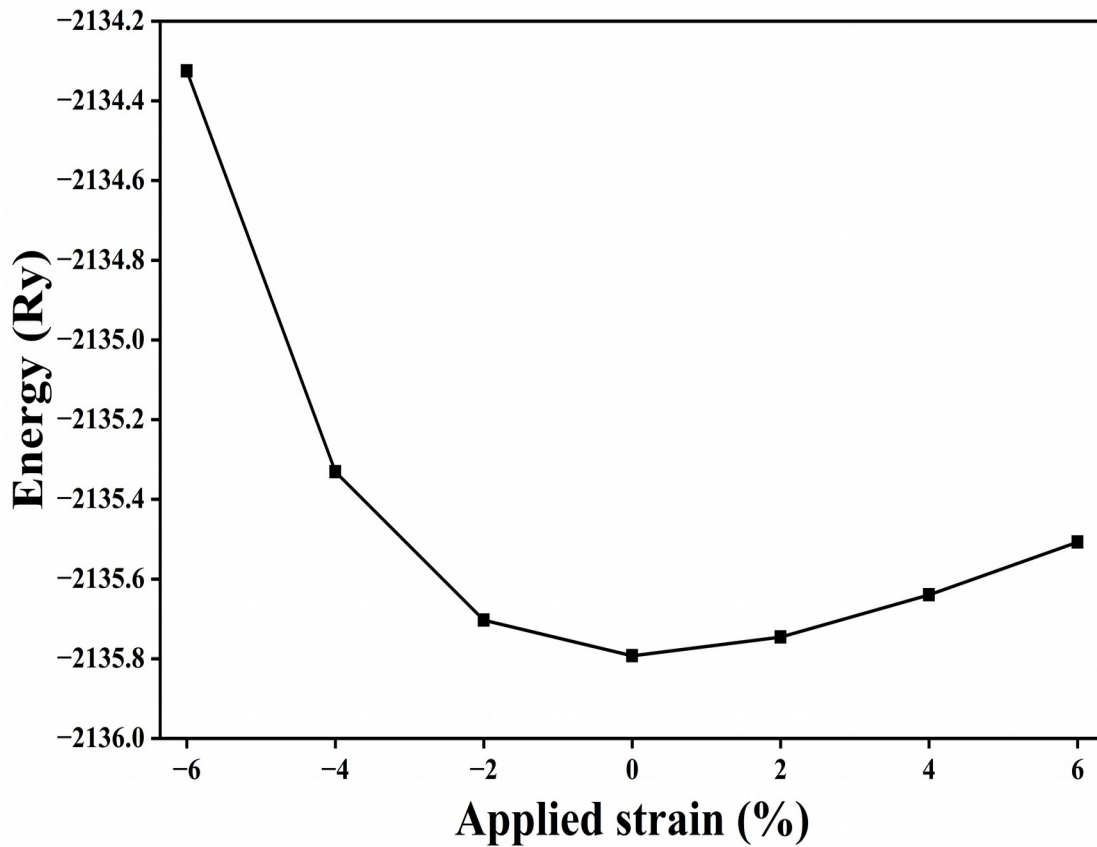


Fig. S2: Variation of total energy (in Ry) as a function of applied strain (-6% to +6%), showing a minimum near the equilibrium (0% strain) and an increase in energy under both compressive and tensile deformation, indicating structural stability around the unstrained configuration.