Table S1 Fractional coordinates for all atoms of I-III structures.

atom	I			II			III		
S	0.167798	0.083986	0.27163	0.089529	0.04475	0.27173	0.252469	0.126194	0.27069
	0.165237	0.082694	0.382339	0.087926	0.043951	0.382697	0.253503	0.126708	0.381632
	0.417528	0.083535	0.272921	0.338651	0.044513	0.272079	0.503666	0.126274	0.270989
	0.415556	0.083213	0.384006	0.338962	0.044231	0.383138	0.502179	0.126777	0.381905
	0.665845	0.083527	0.272926	0.588509	0.044999	0.271389	0.753372	0.126428	0.271788
	0.667493	0.083238	0.384008	0.589134	0.043631	0.382277	0.752774	0.126678	0.382887
	0.916013	0.083986	0.271632	0.839432	0.045283	0.271011	1.002257	0.126352	0.27149
	0.917297	0.082703	0.382336	0.837998	0.043273	0.381816	1.003962	0.126657	0.382572
	0.167411	0.33499	0.272347	0.089054	0.294817	0.271813	0.252839	0.377126	0.271347
	0.165675	0.331537	0.383276	0.088496	0.29389	0.382818	0.2534	0.375666	0.382326
	0.417514	0.334163	0.272924	0.338655	0.294099	0.272076	0.503665	0.377324	0.270995
	0.415555	0.332489	0.384008	0.338969	0.294713	0.383134	0.502183	0.375327	0.381915
	0.66661	0.33339	0.273494	0.588696	0.294327	0.271993	0.753865	0.376906	0.271746
	0.666605	0.333395	0.38469	0.588932	0.294458	0.383036	0.752192	0.376066	0.382796
	0.916474	0.334156	0.272927	0.839087	0.295065	0.271723	1.003076	0.376758	0.27209
	0.916762	0.332507	0.384008	0.838489	0.293611	0.382708	1.003292	0.376347	0.383191
	0.167019	0.583579	0.273047	0.088554	0.544263	0.271894	0.253123	0.626533	0.272
	0.166182	0.583182	0.384172	0.089053	0.544514	0.38291	0.253281	0.626621	0.383108
	0.416416	0.583586	0.273054	0.337943	0.543738	0.271564	0.503402	0.627179	0.27169
	0.416821	0.58318	0.384179	0.339776	0.545139	0.382507	0.502823	0.625756	0.382788
	0.665838	0.582487	0.272924	0.588518	0.54349	0.271387	0.753358	0.626881	0.271786
	0.667511	0.584445	0.384008	0.589132	0.545474	0.382275	0.752772	0.626045	0.382884
	0.916466	0.582473	0.272921	0.839086	0.543994	0.271723	1.003066	0.626269	0.272084
	0.916788	0.584445	0.384006	0.838483	0.544854	0.382708	1.003289	0.626908	0.383187
	0.167413	0.832586	0.272336	0.08905	0.794205	0.271815	0.252841	0.87565	0.27134
	0.165695	0.834305	0.383258	0.088485	0.794577	0.38282	0.253406	0.87766	0.382329
	0.416421	0.83298	0.273047	0.337941	0.794178	0.271567	0.503414	0.876164	0.271689
	0.416819	0.833818	0.384172	0.339768	0.794603	0.382511	0.502826	0.877012	0.382788
	0.66501	0.832589	0.272347	0.588274	0.79413	0.270743	0.75287	0.876408	0.271822
	0.668463	0.834326	0.383276	0.589438	0.794704	0.381494	0.753342	0.876641	0.382942
	0.916015	0.832202	0.27163	0.839437	0.794133	0.271009	1.002256	0.87585	0.271488
	0.917307	0.834764	0.382339	0.83799	0.794706	0.381818	1.00396	0.87724	0.38257
Se	0.223366	0.111787	0.509563	0.222244	0.111416	0.509622	0.224636	0.11232	0.510963
	0.222658	0.111405	0.690216	0.222129	0.111052	0.693174	0.224696	0.112337	0.694387
	0.55643	0.111108	0.509379	0.554537	0.111402	0.509643	0.554297	0.10893	0.508607
	0.555765	0.111082	0.690258	0.555425	0.111059	0.693174	0.554657	0.109509	0.691704
	0.888856	0.111143	0.509597	0.888578	0.11115	0.509817	0.887568	0.112133	0.510939
	0.889018	0.110982	0.690235	0.888575	0.110797	0.690259	0.887706	0.112386	0.689095
	0.222623	0.44548	0.509411	0.221157	0.44417	0.509625	0.221239	0.442598	0.508138
	0.222315	0.444589	0.690277	0.222137	0.444419	0.693189	0.2246	0.449276	0.694444
	0.555843	0.444155	0.509406	0.554365	0.443481	0.50969	0.554629	0.445834	0.508746
	0.555571	0.444429	0.690256	0.555444	0.444381	0.693178	0.554721	0.445152	0.691694

	0.888891	0.443569	0.509379	0.887673	0.443965	0.509602	0.891105	0.445926	0.508299
	0.888918	0.444234	0.690258	0.888778	0.444404	0.6932	0.88941	0.444717	0.691697
	0.222351	0.777646	0.509451	0.221008	0.777524	0.509667	0.220969	0.778589	0.508307
	0.222043	0.777956	0.690271	0.222127	0.777754	0.693188	0.224614	0.775332	0.694449
	0.55452	0.777376	0.509411	0.554169	0.776904	0.509797	0.550408	0.775095	0.510807
	0.55541	0.777684	0.690277	0.555424	0.777708	0.693153	0.550535	0.775275	0.6944
	0.888213	0.776634	0.509563	0.888121	0.776477	0.509726	0.887501	0.775306	0.510891
	0.888594	0.777342	0.690216	0.888801	0.777715	0.693166	0.887711	0.775316	0.694406
Mo	0.08328	0.166727	0.326903	0.005385	0.127682	0.326981	0.169708	0.20977	0.326528
	0.333271	0.166717	0.327941	0.255412	0.127695	0.327659	0.419587	0.209757	0.326057
	0.583267	0.166708	0.328921	0.50544	0.12769	0.327446	0.669678	0.209824	0.327031
	0.833277	0.166723	0.327943	0.755424	0.127679	0.32675	0.91977	0.209841	0.327453
	0.083274	0.416714	0.328392	0.00542	0.377693	0.327418	0.169854	0.45986	0.327481
	0.333265	0.416713	0.328393	0.255426	0.377716	0.327441	0.41976	0.45981	0.326782
	0.583265	0.416736	0.32892	0.505444	0.377732	0.327441	0.669677	0.459793	0.327034
	0.833292	0.416733	0.328922	0.755441	0.377712	0.327432	0.919788	0.459871	0.327712
	0.08328	0.666727	0.328381	0.005416	0.627707	0.327419	0.169849	0.709937	0.327474
	0.333278	0.666721	0.328811	0.255433	0.627706	0.327212	0.419854	0.709897	0.327468
	0.583288	0.666735	0.328394	0.505439	0.62774	0.32652	0.669762	0.709834	0.327416
	0.833283	0.666729	0.327941	0.755427	0.627733	0.32675	0.919762	0.709872	0.327448
	0.083281	0.91672	0.326899	0.00538	0.877685	0.326982	0.16971	0.959864	0.326527
	0.333273	0.916721	0.328381	0.255419	0.877686	0.327445	0.41976	0.959883	0.326776
	0.583287	0.916727	0.328392	0.505436	0.877681	0.326522	0.66977	0.959875	0.327417
	0.833274	0.91672	0.326903	0.755397	0.877693	0.326002	0.919754	0.959848	0.327181
In	0.000235	0.999765	0.649784	0.000791	0.998815	0.65112	0.001586	0.998267	0.652493
	0.000278	0.999722	0.549569	-0.00011	0.999296	0.550357	0.000258	0.999574	0.551214
	0.333646	1.000083	0.649718	0.333088	0.999872	0.651803	0.331329	0.99702	0.652243
	0.334224	1.00026	0.549606	0.332567	0.99992	0.550803	0.333643	0.998673	0.551213
	0.666704	0.999741	0.649803	0.664347	0.998894	0.65118	0.662368	0.995377	0.651047
	0.666748	0.999623	0.549752	0.665379	0.999648	0.550415	0.663716	0.998196	0.550664
	0.000258	0.333296	0.649803	0.000722	0.335225	0.651281	0.004527	0.337922	0.650976
	0.000376	0.333252	0.549752	-0.00073	0.333469	0.55061	0.001341	0.335694	0.550396
	0.333487	0.333715	0.649699	0.333086	0.333237	0.651782	0.331337	0.334371	0.65213
	0.333768	0.334137	0.549623	0.332289	0.333224	0.550803	0.333636	0.335017	0.551098
	0.666701	0.333299	0.649769	0.6665	0.333283	0.65176	0.666083	0.333048	0.650603
	0.666901	0.333097	0.549686	0.665743	0.332987	0.550824	0.667067	0.333502	0.549179
	-8.4E-05	0.666353	0.649718	-0.00025	0.666426	0.651829	0.002642	0.668318	0.652194
	-0.00026	0.665775	0.549606	-0.00097	0.665761	0.550882	0.001044	0.666216	0.551091
	0.333138	0.666862	0.649833	0.332966	0.66649	0.651805	0.332811	0.666317	0.650551
	0.333071	0.666929	0.549887	0.331925	0.666312	0.550798	0.327323	0.663639	0.549931
	0.666284	0.666513	0.649699	0.666435	0.666443	0.651748	0.66594	0.668712	0.652126
	0.665862	0.666231	0.549623	0.66557	0.665772	0.55071	0.664528	0.666167	0.551226

Table S2 Fractional coordinates for all atoms of IV-VI structures.

atom	IV			V			VI		
S	0.174469	0.086561	0.27168	0.184097	0.122587	0.272297	0.253876	0.053167	0.271604
	0.173036	0.086521	0.382759	0.182804	0.123162	0.383317	0.252079	0.051043	0.382347
	0.423352	0.086538	0.271836	0.432599	0.122578	0.272358	0.504146	0.052614	0.272652
	0.424341	0.086529	0.382921	0.434473	0.123208	0.383396	0.501733	0.051642	0.383678
	0.673245	0.086725	0.270922	0.682419	0.122392	0.271347	0.752777	0.052377	0.273164
	0.674628	0.08643	0.381892	0.684741	0.12347	0.382107	0.753321	0.052014	0.384305
	0.92442	0.086742	0.270758	0.933993	0.122428	0.271276	1.002424	0.05286	0.272128
	0.923173	0.086391	0.381697	0.932904	0.123435	0.382014	1.003769	0.051447	0.383007
	0.174532	0.337145	0.271622	0.184626	0.373534	0.272062	0.253549	0.303455	0.272589
	0.17288	0.335843	0.382662	0.182131	0.372074	0.382993	0.252507	0.300816	0.38362
	0.423889	0.336618	0.272203	0.433559	0.373081	0.2728	0.503736	0.303092	0.272801
	0.423668	0.336488	0.383308	0.433379	0.372654	0.383931	0.502232	0.301169	0.383878
	0.673566	0.336963	0.271801	0.682911	0.373468	0.272123	0.753068	0.302124	0.273351
	0.674071	0.336037	0.382863	0.684125	0.372214	0.383068	0.75301	0.302303	0.384517
	0.924226	0.337545	0.271208	0.934012	0.373979	0.271362	1.00288	0.302435	0.273145
	0.923315	0.33534	0.382186	0.932869	0.371586	0.38213	1.003235	0.301949	0.384287
	0.173887	0.586921	0.271824	0.184045	0.623797	0.272366	0.253436	0.551882	0.272877
	0.173686	0.586171	0.382934	0.182837	0.621828	0.3834	0.252695	0.552524	0.383986
	0.423478	0.586199	0.271894	0.433495	0.622816	0.272793	0.502926	0.552293	0.273044
	0.4242	0.587064	0.382983	0.433464	0.622962	0.383918	0.503207	0.552083	0.384167
	0.673638	0.586071	0.271902	0.683269	0.622773	0.272786	0.752098	0.551461	0.272767
	0.674004	0.587204	0.382976	0.683729	0.623026	0.383911	0.754145	0.553057	0.383835
	0.924024	0.586768	0.271837	0.933792	0.623744	0.272361	1.002645	0.551082	0.2726
	0.923543	0.586313	0.382949	0.93316	0.621903	0.383397	1.003586	0.553514	0.383614
	0.173802	0.836338	0.271872	0.183495	0.872847	0.2726	0.253762	0.801544	0.271891
	0.173785	0.836767	0.382982	0.183506	0.87289	0.383683	0.252248	0.802905	0.382719
	0.422938	0.836121	0.271525	0.432529	0.872293	0.272351	0.503361	0.801849	0.272897
	0.424945	0.83716	0.382556	0.434568	0.873572	0.383379	0.502717	0.802515	0.384008
	0.673349	0.83581	0.271033	0.682833	0.871729	0.272033	0.751775	0.801724	0.272577
	0.674531	0.837622	0.382011	0.684303	0.874274	0.382951	0.75446	0.80272	0.383601
	0.924226	0.836009	0.271383	0.9338	0.872261	0.272282	1.002131	0.801436	0.271572
	0.923376	0.837242	0.382434	0.933212	0.87359	0.383297	1.004158	0.803104	0.382307
Se	0.299458	0.09971	0.510847	0.29297	0.097934	0.509469	0.292689	0.098546	0.509575
	0.29966	0.099738	0.694419	0.29618	0.099519	0.691898	0.292671	0.098208	0.690259
	0.625239	0.099774	0.510923	0.625545	0.098178	0.509698	0.626196	0.098483	0.509384
	0.629442	0.096771	0.691733	0.626707	0.097935	0.690225	0.62594	0.098341	0.690285
	0.962437	0.099524	0.510977	0.959665	0.097517	0.509677	0.958736	0.098576	0.509473
	0.962538	0.099725	0.68908	0.959746	0.097892	0.690287	0.959251	0.098306	0.690278
	0.296121	0.429946	0.508097	0.293045	0.43136	0.509573	0.29288	0.43182	0.509385
	0.295842	0.429322	0.691806	0.293345	0.431262	0.690305	0.292704	0.431499	0.690304
	0.629414	0.433563	0.508333	0.626359	0.431438	0.509528	0.626045	0.431817	0.509394
	0.629395	0.43272	0.691942	0.628748	0.431007	0.6914	0.626076	0.431473	0.690292
	0.960529	0.430748	0.508338	0.959565	0.432091	0.509615	0.959471	0.431579	0.509407

	0.964491	0.432218	0.691794	0.962925	0.432907	0.691886	0.959243	0.431507	0.690269
	0.295571	0.765966	0.508265	0.29294	0.764679	0.50948	0.292965	0.764599	0.509517
	0.299524	0.76255	0.694472	0.298193	0.767139	0.692397	0.292489	0.765023	0.690273
	0.625296	0.76263	0.510861	0.625767	0.763291	0.50951	0.625671	0.765067	0.509408
	0.625403	0.762621	0.694389	0.628688	0.764128	0.691328	0.625855	0.765058	0.690307
	0.962531	0.762778	0.510902	0.959831	0.764517	0.509547	0.958724	0.764863	0.509593
	0.962715	0.762791	0.694395	0.963178	0.766273	0.691924	0.959168	0.764978	0.690261
Mo	0.090428	0.169856	0.326791	0.100155	0.206241	0.32718	0.169705	0.135562	0.32734
	0.340453	0.169844	0.327612	0.350165	0.206269	0.328162	0.419664	0.135528	0.327749
	0.590515	0.16984	0.327044	0.600172	0.20627	0.327286	0.669651	0.13554	0.328832
	0.840506	0.169861	0.326172	0.850173	0.206257	0.326222	0.919691	0.135545	0.328457
	0.090439	0.419874	0.327093	0.100165	0.456267	0.327278	0.169703	0.385551	0.328558
	0.340436	0.419913	0.32762	0.350145	0.456265	0.328251	0.419681	0.385539	0.328461
	0.590495	0.419908	0.327702	0.600176	0.456273	0.328277	0.669671	0.385563	0.328717
	0.840495	0.419868	0.327194	0.850177	0.456273	0.327304	0.919711	0.385583	0.328797
	0.090457	0.669881	0.327535	0.100168	0.706251	0.328085	0.169716	0.635541	0.327911
	0.340488	0.669939	0.32739	0.350178	0.706274	0.328189	0.419699	0.635543	0.32865
	0.590523	0.670007	0.327177	0.600198	0.706311	0.328238	0.669713	0.635562	0.328436
	0.840507	0.669942	0.32733	0.850177	0.70628	0.328143	0.919721	0.635578	0.327681
	0.090455	0.919883	0.327239	0.100169	0.956258	0.327992	0.169704	0.885548	0.326646
	0.340492	0.919877	0.327379	0.350183	0.956268	0.328062	0.419685	0.885514	0.327952
	0.590576	0.919959	0.326492	0.600183	0.956269	0.32724	0.669689	0.885543	0.328571
	0.840528	0.919951	0.326341	0.850182	0.95627	0.327198	0.919687	0.885545	0.327317
In	0.076677	0.985632	0.652396	0.074008	0.988073	0.650739	0.070389	0.987246	0.649809
	0.075358	0.987208	0.551133	0.071085	0.98674	0.550266	0.070015	0.987435	0.549688
	0.40567	0.983871	0.652658	0.40431	0.987056	0.650256	0.403828	0.987184	0.649757
	0.404585	0.984613	0.552091	0.403333	0.986552	0.550197	0.4039	0.98719	0.549644
	0.737157	0.982666	0.650965	0.737389	0.985367	0.65	0.737	0.987186	0.649802
	0.737287	0.986899	0.550414	0.736542	0.986028	0.549694	0.736747	0.987267	0.549751
	0.075587	0.323077	0.649858	0.070525	0.320277	0.650059	0.070572	0.320558	0.649798
	0.074772	0.323221	0.549627	0.070408	0.320339	0.54983	0.070577	0.320743	0.54972
	0.407832	0.319193	0.651113	0.406649	0.320701	0.650428	0.403875	0.320552	0.649792
	0.408995	0.322397	0.55055	0.404221	0.320186	0.550029	0.403973	0.320757	0.549728
	0.741004	0.321018	0.651358	0.740994	0.321513	0.650602	0.737088	0.320464	0.649715
	0.73962	0.323019	0.550585	0.737527	0.320575	0.550264	0.737251	0.320669	0.549618
	0.077755	0.655676	0.652028	0.075741	0.656209	0.651246	0.070238	0.653739	0.649801
	0.074801	0.652051	0.550796	0.071256	0.653986	0.550538	0.07037	0.653834	0.549682
	0.406383	0.651177	0.650885	0.406628	0.654659	0.650592	0.403634	0.653802	0.649886
	0.402329	0.651075	0.550089	0.403833	0.653522	0.550203	0.403835	0.653659	0.549857
	0.740809	0.655942	0.652158	0.741045	0.653703	0.650801	0.736775	0.653769	0.649865
	0.73935	0.653655	0.55118	0.737647	0.653294	0.550295	0.736587	0.653859	0.549792

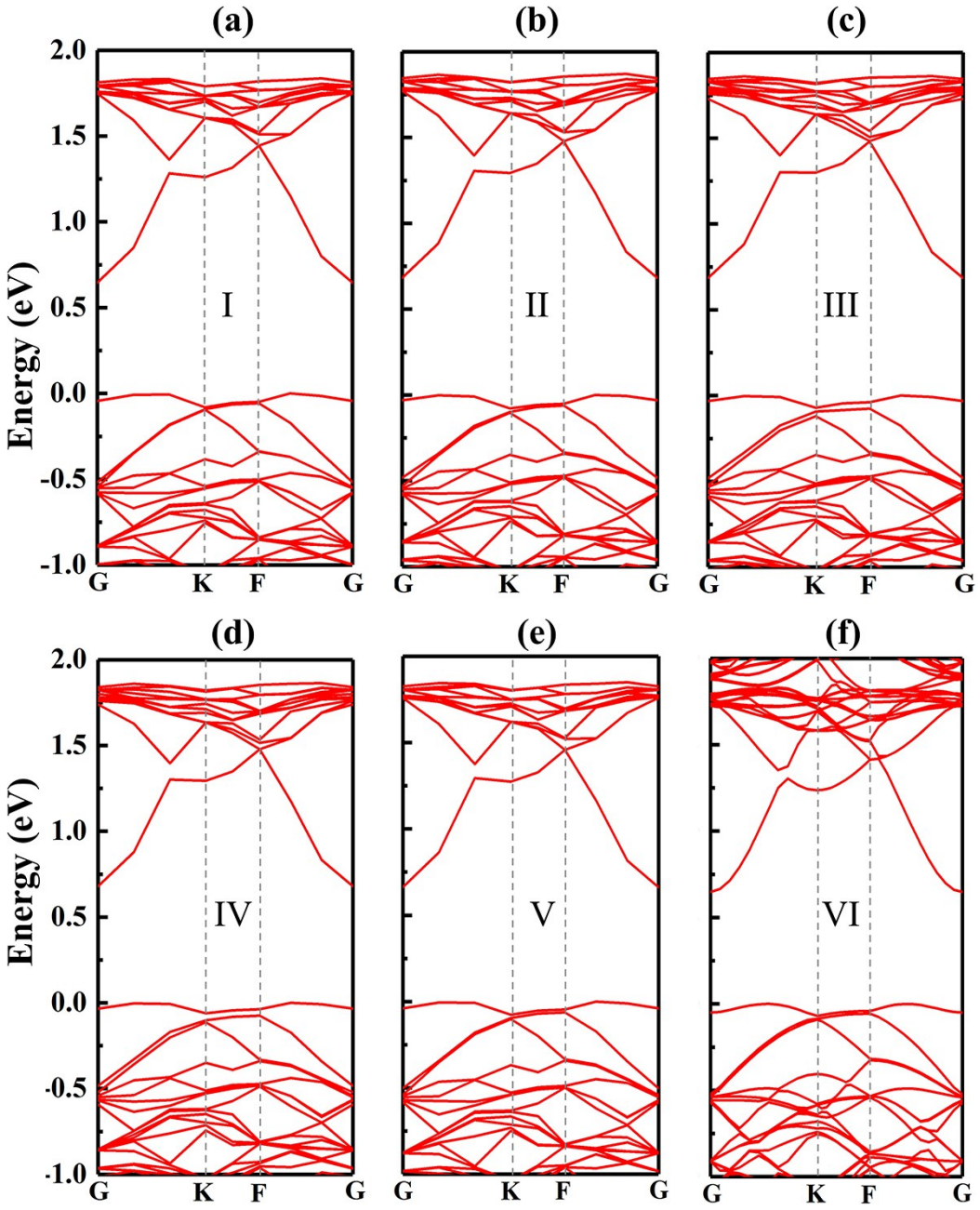

Fig. S1 Band structures of I-VI InSe/MoS_2 BL without strain.

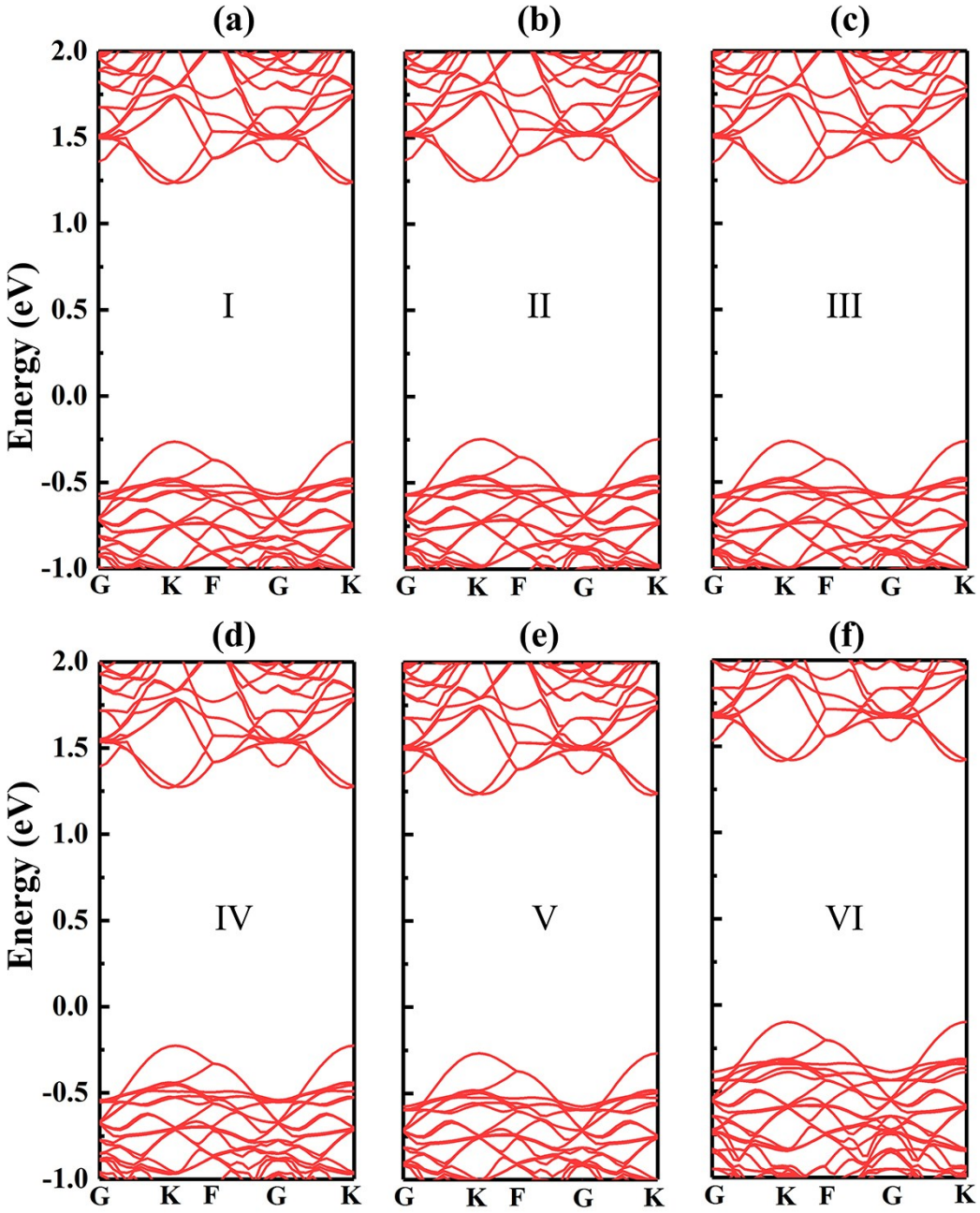

Fig. S2 Band structures of I-VI InSe/MoS_2 BL with 7% compressive strain.

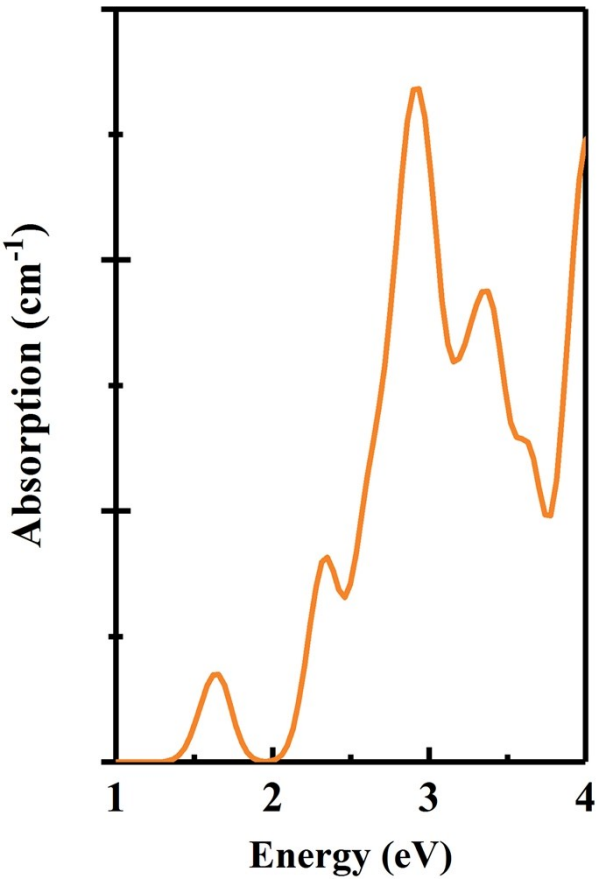

Fig. S3 Optical absorption spectra of MoS_2 monolayer as the function of energy.