Supporting Information

Structure-Property Relationships in TMD Materials AB_2 (A = Nb, Ta; B = S, Se, Te): Assessing Exchange-Correlation Functionals

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Non-Spin orbit Coupling (NSOC) Case:

Table S1: Details of the geometry optimization for all the 06 systems are tabulated below for LDA XC functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
LDA	NbS_2	2H	3.284	3.368	11.408	12.624	2.457	2.495	78.954	77.575	3.200	3.732
		1T	3.301	3.403	5.671	6.202	2.460	2.489	95.704	93.767	3.192	3.707
	$NbSe_2$	2H	3.404	3.499	12.103	13.413	2.580	2.622	80.750	79.201	3.345	3.924
		1T	3.412	3.518	6.037	6.528	2.583	2.614	97.308	95.431	3.339	3.820
	$NbTe_2$	2H	14.343	15.067	9.204	9.607	2.803	2.841	79.655	81.262	3.387	3.732
		1T	3.622	3.720	6.556	7.148	2.771	2.814	98.387	97.247	3.591	4.116
	TaS_2	2H	3.267	3.320	11.594	12.300	2.445	2.488	79.037	79.234	3.281	3.540
		1T	3.293	3.360	5.714	5.900	2.445	2.436	95.319	92.837	3.254	3.530
	$TaSe_2$	2H	3.389	3.476	12.231	13.418	2.568	2.607	80.762	79.354	3.405	3.930
		1T	3.407	3.509	6.087	6.599	2.568	2.599	96.888	95.058	3.410	3.910
	$TaTe_2$	2H	14.438	15.235	9.328	9.651	2.797	2.833	81.514	81.158	3.489	3.814
		1T	3.618	3.740	6.626	6.732	2.761	2.599	98.027	97.636	3.679	3.886

Table S2: Details of the geometry optimization for all the 06 systems are tabulated below for PBE XC functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
PBE	NbS_2	2H	3.356	3.368	13.667	12.624	2.492	2.495	77.926	77.575	4.169	3.732
		1T	3.382	3.403	6.666	6.202	2.493	2.489	94.592	93.767	4.064	3.707
	$NbSe_2$	2H	3.481	3.499	13.728	13.413	2.622	2.622	79.932	79.201	4.027	3.924
		1T	3.492	3.518	6.802	6.528	2.623	2.614	96.518	95.431	3.994	3.820
	$NbTe_2$	2H	15.184	15.067	9.628	9.607	2.852	2.841	81.201	81.262	3.712	3.732
		1T	3.683	3.720	7.360	7.148	2.818	2.814	98.376	97.247	4.235	4.116
	TaS_2	2H	3.336	3.320	13.820	12.300	2.479	2.488	78.049	79.234	4.246	3.540
		1T	3.369	3.360	6.712	5.900	2.478	2.436	94.345	92.837	4.128	3.530
	$TaSe_2$	2H	3.466	3.476	14.249	13.418	2.609	2.607	79.854	79.354	4.285	3.930
		1T	3.491	3.509	6.918	6.599	2.608	2.599	95.962	95.058	4.133	3.910
	$TaTe_2$	2H	15.354	15.235	9.686	9.651	2.844	2.833	81.001	81.158	3.911	3.814
		1T	3.685	3.740	7.380	6.732	2.806	2.599	97.883	97.636	4.301	3.886

Table S3: Details of the geometry optimization for all the 06 systems are tabulated below for PBESol XC functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
PBESol	NbS_2	2H	3.306	3.368	11.854	12.624	2.469	2.495	78.764	77.575	3.387	3.732
		1T	3.324	3.403	5.846	6.202	2.471	2.489	95.505	93.767	3.337	3.707
	$NbSe_2$	2H	3.425	3.499	12.355	13.413	2.594	2.622	80.686	79.201	3.448	3.924
		1T	3.432	3.518	6.185	6.528	2.597	2.614	97.273	95.431	3.453	3.820
	$NbTe_2$	2H	14.848	15.067	9.402	9.607	2.825	2.841	81.417	81.262	3.547	3.732
		1T	3.640	3.720	6.667	7.148	2.787	2.814	98.466	97.247	3.667	4.116
	TaS_2	2H	3.292	3.320	12.161	12.300	2.458	2.488	78.741	79.234	3.519	3.540
		1T	3.317	3.360	5.923	5.900	2.459	2.436	95.135	92.837	3.425	3.530
	$TaSe_2$	2H	3.413	3.476	12.623	13.418	2.584	2.607	80.617	79.354	3.560	3.930
		1T	3.429	3.509	6.256	6.599	2.583	2.599	96.813	95.058	3.543	3.910
	$TaTe_2$	2H	15.235	15.235	9.651	9.651	2.833	2.833	81.185	81.158	3.905	3.814
		1T	3.646	3.740	6.882	6.732	2.773	2.599	98.667	97.636	3.865	3.886

Table S4: Details of the geometry optimization for all the 06 systems are tabulated below for SCAN XC functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
SCAN	NbS_2	2H	3.363	3.368	12.735	12.624	2.490	2.495	77.526	77.575	3.785	3.732
		1T	3.385	3.403	6.047	6.202	2.490	2.489	94.351	93.767	3.548	3.707
	$NbSe_2$	2H	3.478	3.499	13.134	13.413	2.609	2.622	79.350	79.201	3.807	3.924
		1T	3.506	3.518	6.378	6.528	2.613	2.614	95.734	95.431	3.680	3.820
	$NbTe_2$	2H	15.067	15.067	9.607	9.607	2.841	2.841	81.773	81.262	3.836	3.732
		1T	3.656	3.720	7.170	7.148	2.794	2.814	98.299	97.247	4.092	4.116
	TaS_2	2H	3.319	3.320	12.161	12.300	2.464	2.488	77.921	79.234	3.543	3.540
		1T	3.359	3.360	5.993	5.900	2.463	2.436	93.996	92.837	3.536	3.530
	$TaSe_2$	2H	3.445	3.476	13.224	13.418	2.585	2.607	79.376	79.354	3.861	3.930
		1T	3.482	3.509	6.640	6.599	2.583	2.599	95.262	95.058	3.946	3.910

	$TaTe_2$	2H	14.974	15.235	9.462	9.651	2.772	2.833	81.251	81.158	3.854	3.814
		1T	3.655	3.740	7.243	6.732	2.771	2.599	97.558	97.636	4.226	3.886

Table S5: Details of the geometry optimization for all the 06 systems are tabulated below for optB88-vdW vdW-DF functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
optB88-vdW	NbS_2	2H	3.358	3.368	12.054	12.624	2.497	2.495	78.169	77.575	3.470	3.732
		1T	3.386	3.403	5.939	6.202	2.498	2.489	94.678	93.767	3.438	3.707
	$NbSe_2$	2H	3.486	3.499	12.732	13.413	2.628	2.622	80.043	79.201	3.597	3.924
		1T	3.505	3.518	6.306	6.528	2.628	2.614	96.360	95.431	3.578	3.820
	$NbTe_2$	2H	14.961	15.067	9.556	9.607	2.856	2.841	80.884	81.262	3.625	3.732
		1T	3.720	3.720	6.874	7.148	2.824	2.814	97.607	97.247	3.860	4.116
	TaS_2	2H	3.339	3.320	12.175	12.300	2.485	2.488	78.272	79.234	3.525	3.540
		1T	3.376	3.360	5.964	5.900	2.483	2.436	94.374	92.837	3.482	3.530
	$TaSe_2$	2H	3.471	3.476	12.856	13.418	2.615	2.607	79.991	79.354	3.661	3.930
		1T	3.501	3.509	6.327	6.599	2.614	2.599	95.903	95.058	3.628	3.910
	$TaTe_2$	2H	14.953	15.235	9.538	9.651	2.846	2.833	80.335	81.158	3.750	3.814
		1T	3.720	3.740	6.917	6.732	2.809	2.599	97.154	97.636	3.938	3.886

Table S6: Details of the geometry optimization for all the 06 systems are tabulated below for optPBE-vdW vdW-DF functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
optPBE-vdW	NbS_2	2H	3.371	3.368	12.352	12.624	2.504	2.495	77.986	77.575	3.597	3.732
		1T	3.398	3.403	6.072	6.202	2.505	2.489	94.592	93.767	3.548	3.707
	$NbSe_2$	2H	3.500	3.499	13.009	13.413	2.636	2.622	79.880	79.201	3.717	3.924
		1T	3.519	3.518	6.456	6.528	2.636	2.614	96.240	95.431	3.703	3.820
	$NbTe_2$	2H	15.171	15.067	9.650	9.607	2.703	2.841	81.664	81.262	3.823	3.732
		1T	3.727	3.720	7.059	7.148	2.832	2.814	97.722	97.247	4.002	4.116
	TaS_2	2H	3.350	3.320	12.456	12.300	2.491	2.488	78.150	79.234	3.646	3.540
		1T	3.389	3.360	6.105	5.900	2.489	2.436	94.226	92.837	3.603	3.530
	$TaSe_2$	2H	3.483	3.476	13.141	13.418	2.623	2.607	79.893	79.354	3.777	3.930
		1T	3.514	3.509	6.478	6.599	2.621	2.599	95.799	95.058	3.755	3.910
	$TaTe_2$	2H	15.192	15.235	9.641	9.651	2.856	2.833	81.412	81.158	3.840	3.814
		1T	3.729	3.740	7.074	6.732	2.818	2.599	97.195	97.636	4.065	3.886

Table S7: Details of the geometry optimization for all the 06 systems are tabulated below for vdW-DF2 vdW-DF functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
vdW-DF2	NbS_2	2H	3.454	3.368	12.548	12.624	2.546	2.495	76.920	77.575	3.684	3.732
		1T	3.510	3.403	6.135	6.202	2.546	2.489	92.875	93.767	3.662	3.707
	$NbSe_2$	2H	3.604	3.499	13.362	13.413	2.690	2.622	78.670	79.201	3.870	3.924
		1T	3.644	3.518	6.556	6.528	2.689	2.614	94.675	95.431	3.836	3.820
	$NbTe_2$	2H	14.861	15.067	9.464	9.607	2.845	2.841	81.722	81.262	3.670	3.732
		1T	3.880	3.720	7.205	7.148	2.891	2.814	95.421	97.247	4.184	4.116
	TaS_2	2H	3.426	3.320	12.632	12.300	2.530	2.488	77.168	79.234	3.725	3.540
		1T	3.487	3.360	6.163	5.900	2.528	2.436	92.786	92.837	3.701	3.530

	$TaSe_2$	2H	3.580	3.476	13.443	13.418	2.674	2.607	78.789	79.354	3.917	3.930
		1T	3.637	3.509	6.562	6.599	2.672	2.599	94.329	95.058	3.876	3.910
	$TaTe_2$	2H	15.617	15.235	9.970	9.651	2.742	2.833	81.321	81.158	4.003	3.814
		1T	3.888	3.740	7.217	6.732	2.688	2.599	98.002	97.636	3.789	3.886

Table S8: Details of the geometry optimization for all the 06 systems are tabulated below for rev-vdW-DF2 vdW-DF functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
rev-vdW-DF2	NbS_2	2H	3.333	3.368	11.884	12.624	2.487	2.495	78.615	77.575	3.392	3.732
		1T	3.356	3.403	5.866	6.202	2.488	2.489	95.173	93.767	3.359	3.707
	$NbSe_2$	2H	3.457	3.499	12.512	13.413	2.615	2.622	80.501	79.201	3.502	3.924
		1T	3.470	3.518	6.225	6.528	2.616	2.614	96.913	95.431	3.491	3.820
	$NbTe_2$	2H	14.861	15.067	9.464	9.607	2.844	2.841	81.728	81.262	3.670	3.732
		1T	3.681	3.720	6.766	7.148	2.809	2.814	98.118	97.247	3.752	4.116
	TaS_2	2H	3.315	3.320	12.018	12.300	2.475	2.488	78.719	79.234	3.450	3.540
		1T	3.347	3.360	5.901	5.900	2.473	2.436	94.849	92.837	3.411	3.530
	$TaSe_2$	2H	3.441	3.476	12.661	13.418	2.601	2.607	80.378	79.354	3.576	3.930
		1T	3.467	3.509	6.257	6.599	2.602	2.599	96.471	95.058	3.549	3.910
	$TaTe_2$	2H	14.793	15.235	9.435	9.651	2.834	2.833	81.008	81.158	3.562	3.814
		1T	3.677	3.740	6.845	6.732	2.799	2.599	97.825	97.636	3.849	3.886

Table S9: Details of the geometry optimization for all the 06 systems are tabulated below for SCAN+rVV10 vdW-DF functional.

Functional	System	Phase	a(Å)		c(Å)		A-B (Å)		Angle (^{0})		vdW gap (Å)	
			Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.	Cal.	Expt.
SCAN+rVV10	NbS_2	2H	3.348	3.368	11.945	12.624	2.481	2.495	77.663	77.575	3.452	3.732
		1T	3.361	3.403	6.070	6.202	2.490	2.489	95.117	93.767	3.529	3.707
	$NbSe_2$	2H	3.463	3.499	12.592	13.413	2.606	2.622	79.810	79.201	3.565	3.924
		1T	3.486	3.518	6.295	6.528	2.608	2.614	96.149	95.431	3.593	3.820
	$NbTe_2$	2H	15.067	15.067	9.607	9.607	2.842	2.841	81.728	81.262	3.835	3.732
		1T	3.649	3.720	6.893	7.148	2.792	2.814	98.411	97.247	3.854	4.116
	TaS_2	2H	3.311	3.320	12.095	12.300	2.461	2.488	78.071	79.234	3.513	3.540
		1T	3.348	3.360	5.960	5.900	2.458	2.436	94.174	92.837	3.503	3.530
	$TaSe_2$	2H	3.430	3.476	12.606	13.418	2.584	2.607	79.914	79.354	3.583	3.930
		1T	3.461	3.509	6.299	6.599	2.581	2.599	95.814	95.058	3.630	3.910
	$TaTe_2$	2H	15.067	15.235	9.578	9.651	2.843	2.833	81.003	81.158	3.859	3.814
		1T	3.635	3.740	6.904	6.732	2.774	2.599	97.954	97.636	3.901	3.886

Table S10: Details of the energy values and the 1T-2H difference for all the 06 systems for 09 XC functional (04 functional+05 vdW-DFs).

Functional	Serial	System	1T (eV/atom)	2H (eV/atom)	1T-2H (eV/atom)
LDA	I	NbS_2	-7.9093	-7.9451	0.0358
		$NbSe_2$	-7.3420	-7.3750	0.0330
		NbTe2	-6.7006	-6.7463	0.0457
	II	TaS_2	-8.5216	-8.5450	0.0234
		$TaSe_2$	-7.8872	-7.9107	0.0235

PBE		$TaTe_2$	-7.1591	-7.2150	0.0559
	I	NbS_2	-7.1010	-7.1355	0.0345
		$NbSe_2$	-6.5158	-6.5466	0.0308
		NbTe2	-5.8838	-5.9206	0.0368
	II	TaS_2	-7.7320	-7.7537	0.0217
		$TaSe_2$	-7.0778	-7.1000	0.0222
		$TaTe_2$	-6.3604	-6.4013	0.0409
PBESol	I	NbS_2	-7.5761	-7.6120	0.0359
		$NbSe_2$	-7.0159	-7.0482	0.0323
		NbTe2	-6.3976	-6.4431	0.0455
	II	TaS_2	-8.2058	-8.2298	0.0240
		$TaSe_2$	-7.5774	-7.6003	0.0229
		$TaTe_2$	-6.8728	-6.3965	-0.4763
SCAN	I	NbS_2	-18.5616	-18.5951	0.0335
		$NbSe_2$	-25.3056	-25.3389	0.0333
		NbTe2	-36.3233	-36.3661	0.0428
	II	TaS_2	-29.7512	-29.7739	0.0227
		$TaSe_2$	-36.4291	-36.4575	0.0284
		$TaTe_2$	-47.3592	-47.4125	0.0533
optB88-vdW	I	NbS_2	-5.2066	-5.2365	0.0299
		$NbSe_2$	-4.5201	-4.5466	0.0265
		NbTe2	-3.6728	-3.7087	0.0359
	II	TaS_2	-5.9236	-5.9401	0.0165
		$TaSe_2$	-5.1703	-5.1879	0.0176
		$TaTe_2$	-4.2432	-4.2843	0.0411
optPBE-vdW	I	NbS_2	-5.0613	-5.0904	0.0291
		$NbSe_2$	-4.3643	-4.3916	0.0273
		NbTe2	-3.5169	-3.5519	0.0350
	II	TaS_2	-5.7871	-5.8043	0.0172
		$TaSe_2$	-5.0243	-5.0428	0.0185
		$TaTe_2$	-4.0969	-4.1363	0.0394
vdW-DF2	I	NbS_2	-4.7365	-4.7513	0.0148
		$NbSe_2$	-3.9996	-4.0176	0.0180
		NbTe2	-3.1393	-4.0890	0.9497
	II	TaS_2	-5.4015	-5.4050	0.0035
		$TaSe_2$	-4.5996	-4.6077	0.0081
		$TaTe_2$	-3.6684	-3.6943	0.0259
rev-vdW-DF2	I	NbS_2	-5.5384	-5.5706	0.0322
		$NbSe_2$	-4.8663	-4.8958	0.0295
		NbTe2	-4.0477	-4.0890	0.0413
	II	TaS_2	-6.2621	-6.2830	0.0209
		$TaSe_2$	-5.5235	-5.5445	0.0210
		$TaTe_2$	-4.6222	-4.6708	0.0558
SCAN+rVV10	I	NbS_2	-18.4604	-18.6592	0.1988
		$NbSe_2$	-25.1990	-25.2352	0.0362
		NbTe2	-36.2079	-36.2526	0.0447
	II	TaS_2	-29.6609	-29.6856	0.0247
		$TaSe_2$	-36.3306	-36.3581	0.0275

		$TaTe_2$	-47.2474	-47.3052	0.0578

Electronic Band structures:

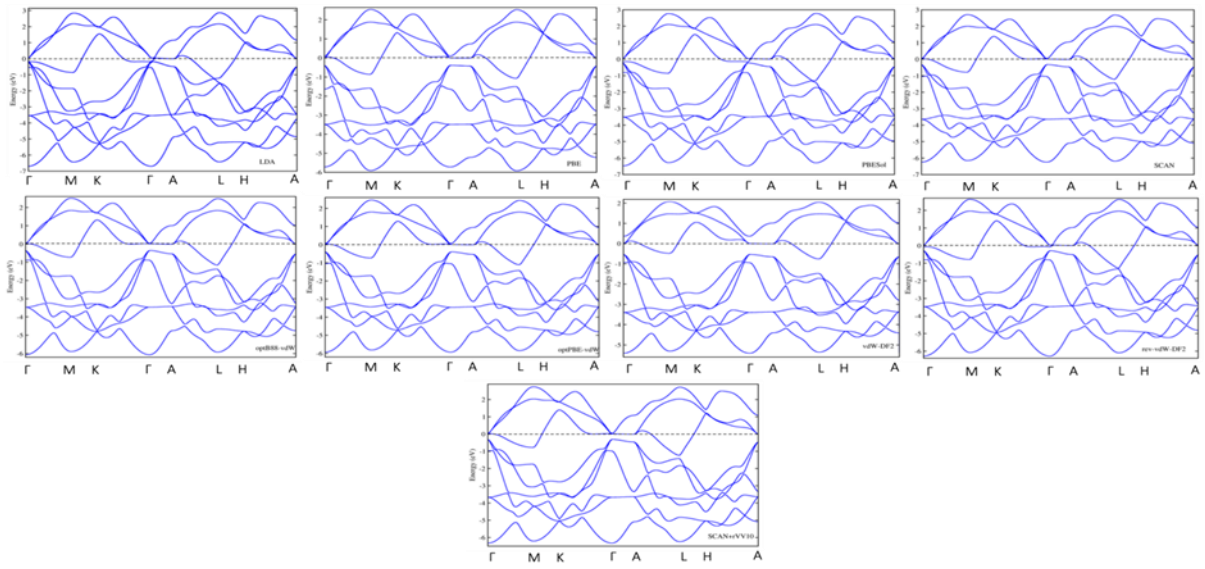

Figure S1: Band structures of 1T phase of NbS_2 for all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right).

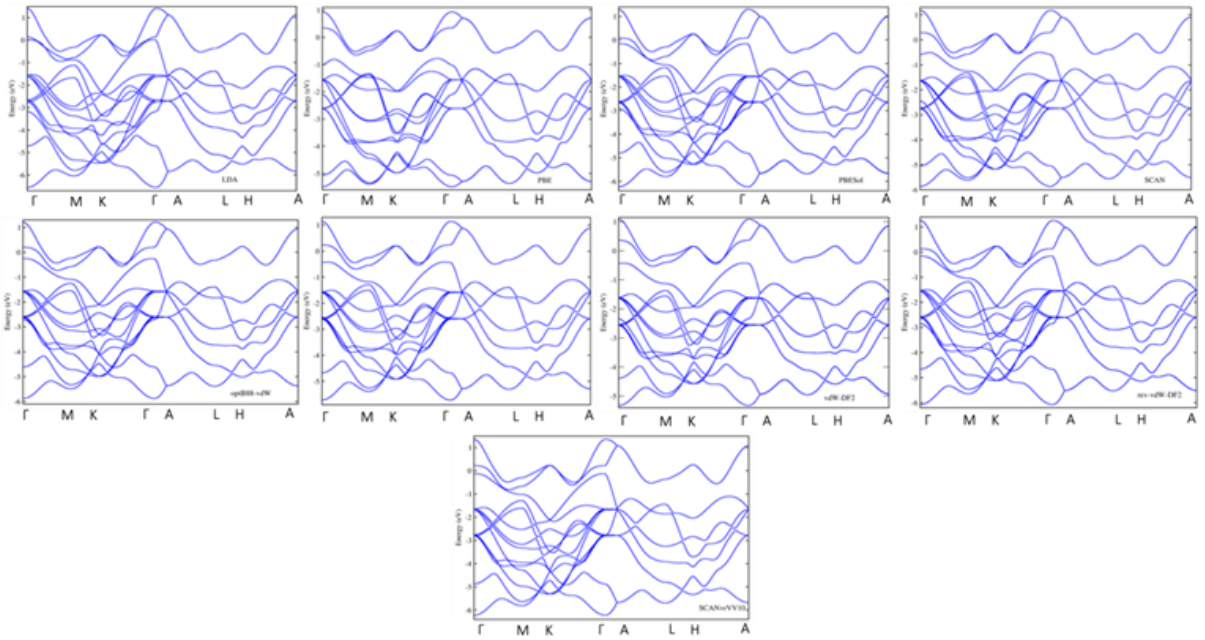

Figure S2: Band structures of 2H phase of NbS_2 for all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right).

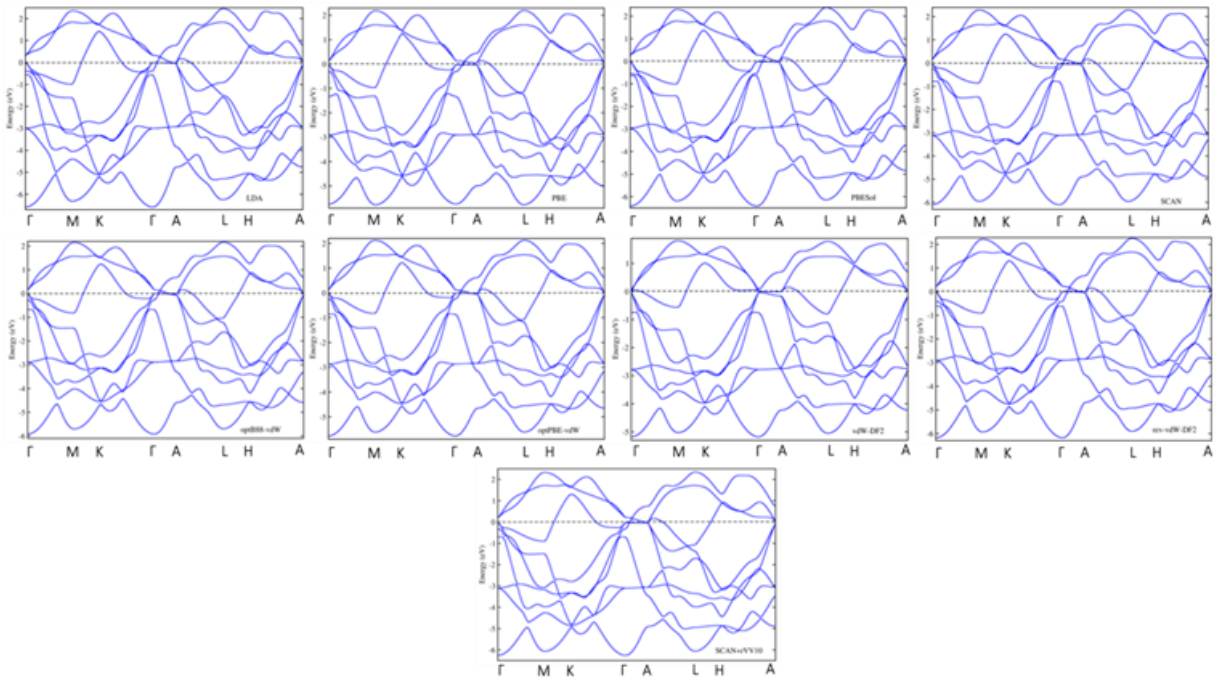

Figure S3: Band structures of 1T phase of $NbSe_2$ for all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right).

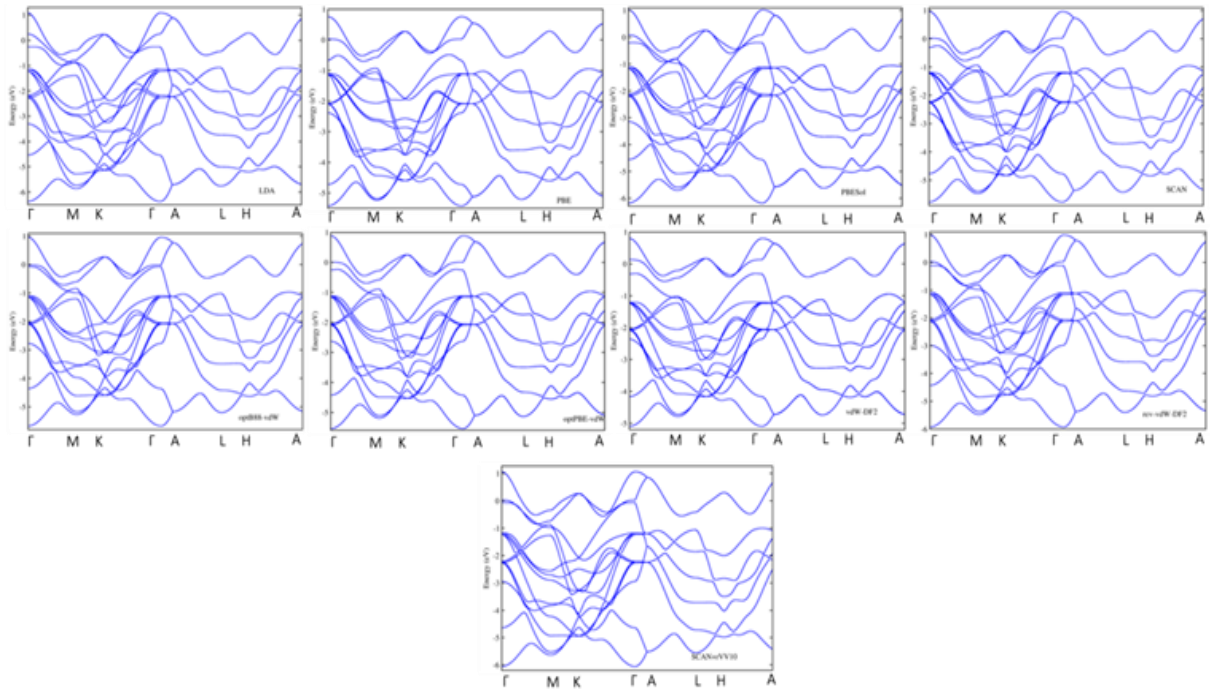

Figure S4: Band structures of 2H phase of $NbSe_2$ for all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; below column form for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

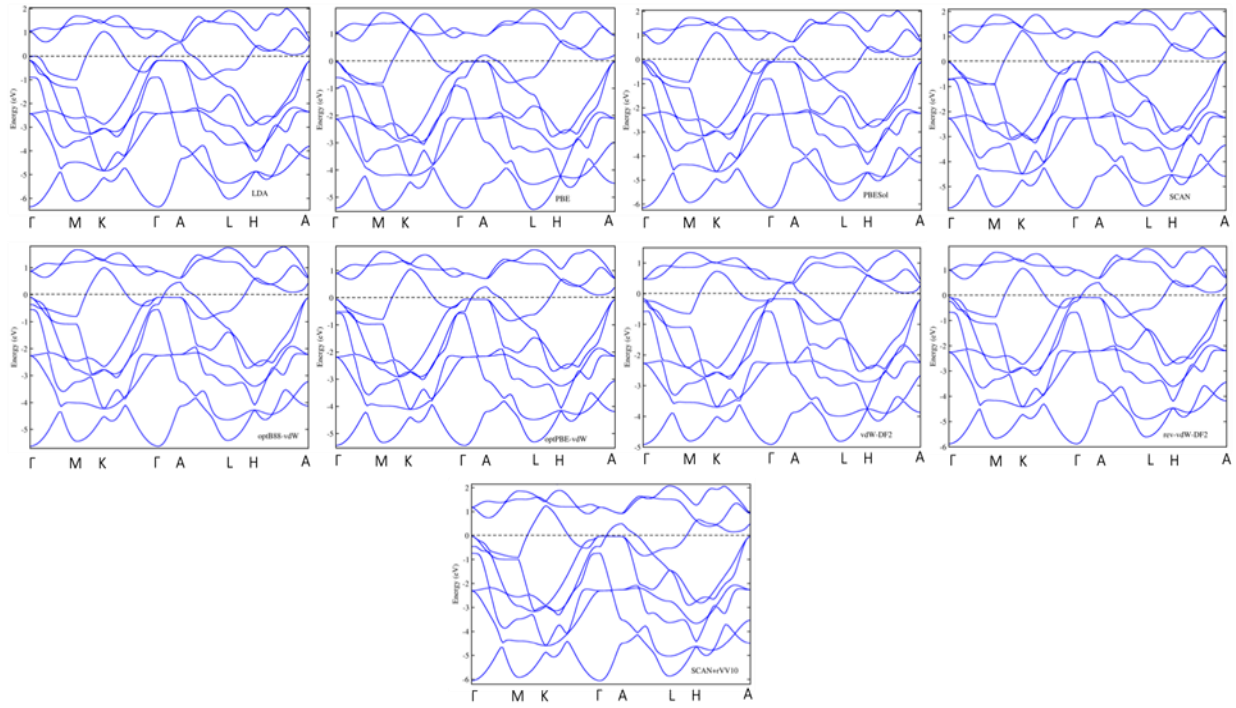

Figure S5: Band structures of 1T phase of $NbTe_2$ for all 09 XC functional (left column for LDA, PBE, PBESol, SCAN from top to bottom; right column for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

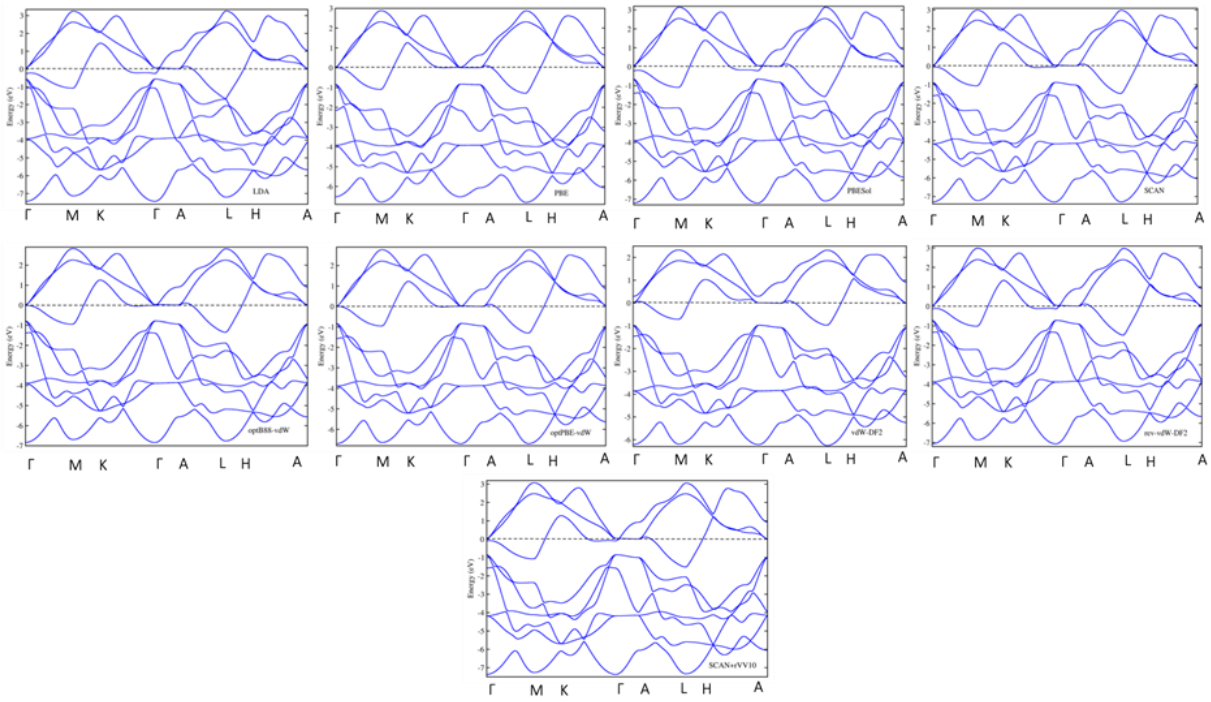

Figure S6: Band structures of 1T phase of TaS_2 for all 09 XC functional (left column for LDA, PBE, PBESol, SCAN from top to bottom; right column for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

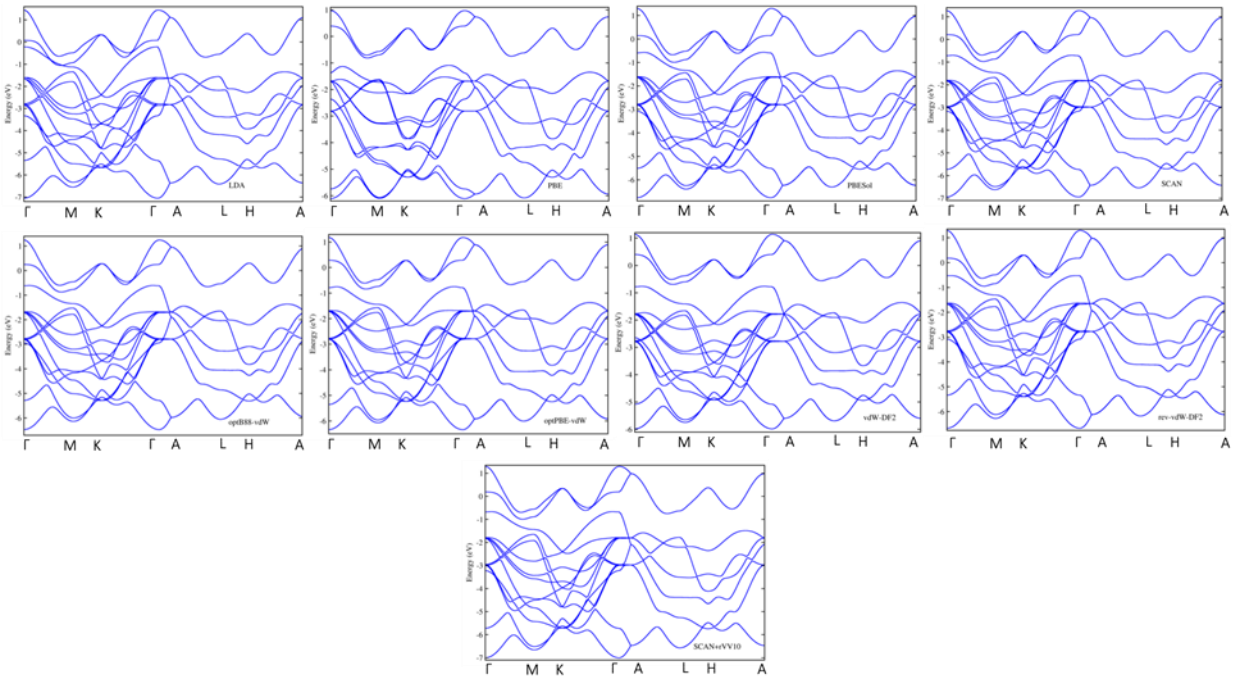

Figure S7: Band structures of 2H phase of TaS_2 for all 09 XC functional (left column for LDA, PBE, PBESol, SCAN from top to bottom; right column for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

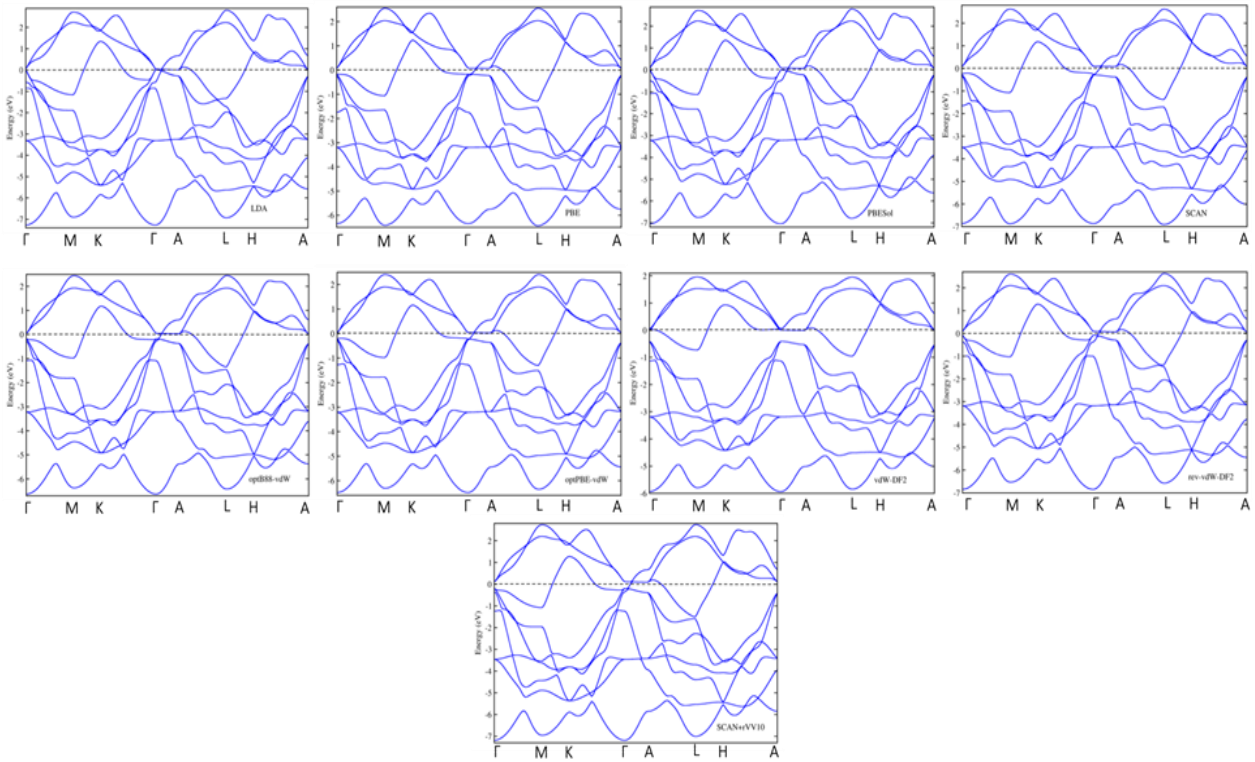

Figure S8: Band structures of 1T phase of $TaSe_2$ for all 09 XC functional (left column for LDA, PBE, PBESol, SCAN from top to bottom; right column for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

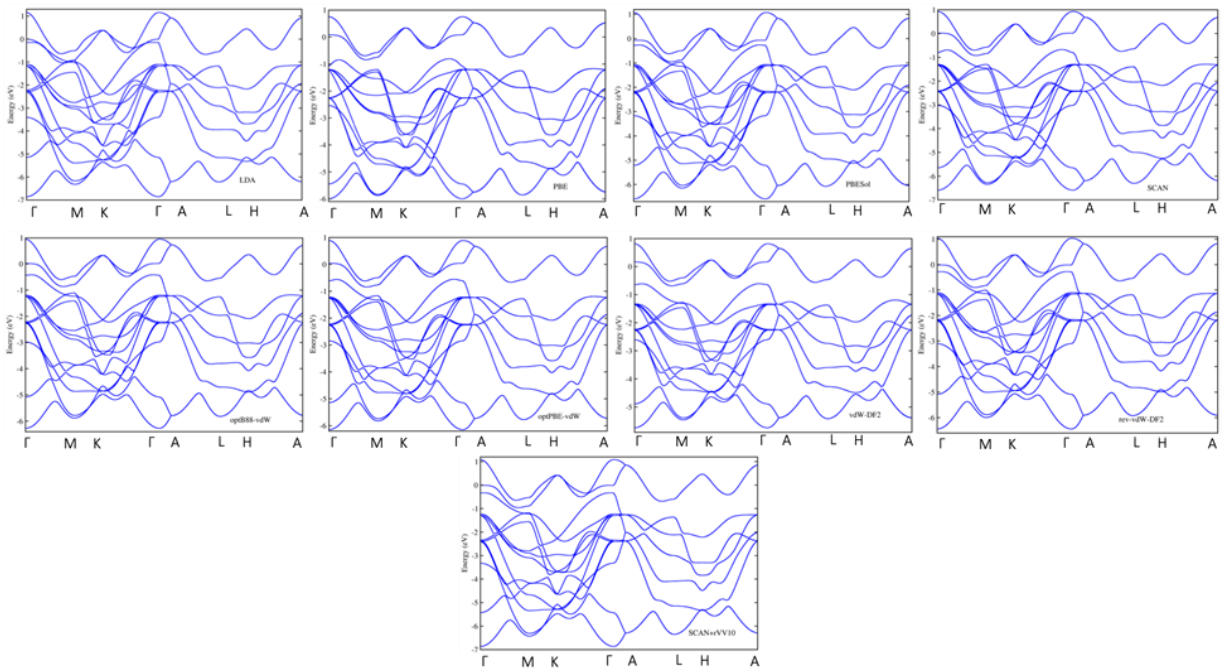

Figure S9: Band structures of 2H phase of $TaSe_2$ for all 09 XC functional (left column for LDA, PBE, PBESol, SCAN from top to bottom; right column for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

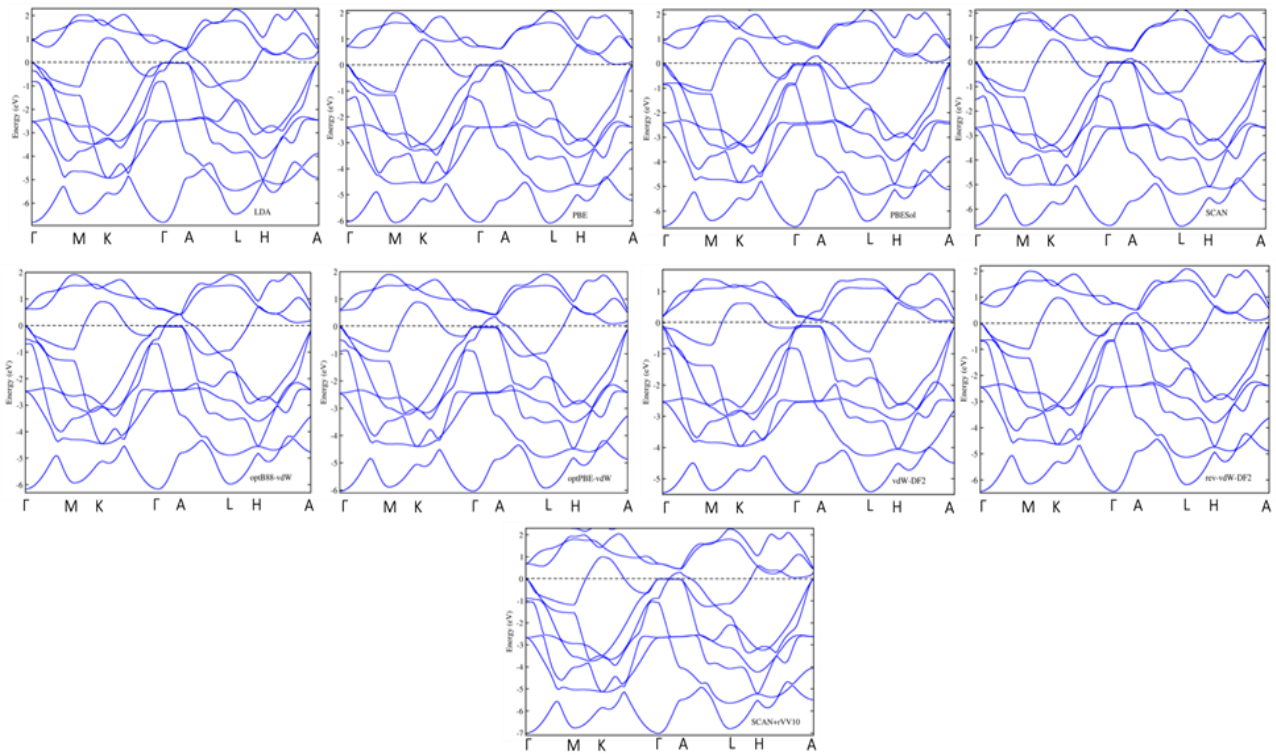

Figure S10: Band structures of 1T phase of $TaTe_2$ for all 09 XC functional (left column for LDA, PBE, PBESol, SCAN from top to bottom; right column for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from top to bottom).

Phonon response plot

For the phonon calculations, we consider 2*2*3 supercell for the 3 atom unit cells (total 36 atoms) in a few 1T phases of the system. Similarly, 2*2*2 supercell has been taken for the 6-atom unit cell (total 48 atoms) and 1*3*1 supercell for the 18-atom unit cell (total 54 atoms). In this way, it is obtained 18 displacements for 1T phase and 9 displacements for 2H phase for 3 atom unit cells, giving 36 displacements for both 1T and 2H phases of 6 atom unit cells and 108 displacements for the 2H phase of an 18-atom unit cell. In this way, it is a tedious calculation for phonons, which is still going on for NSOC cases. Some of the phonon plots are shown below

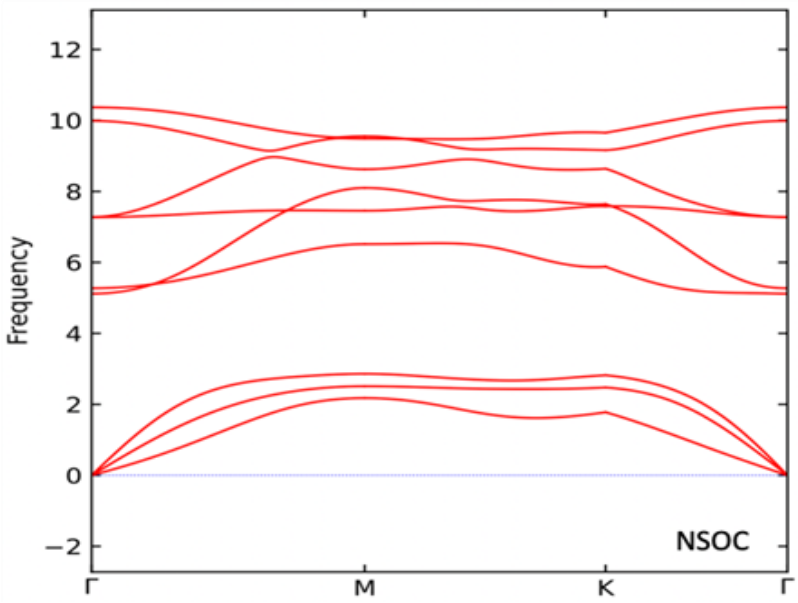

Figure S11: Phonon dispersion plot for 1T phase of TaS_2 for vdW-DF2 van der Waals XC functional in absence of SOC.

Fermi surface plots

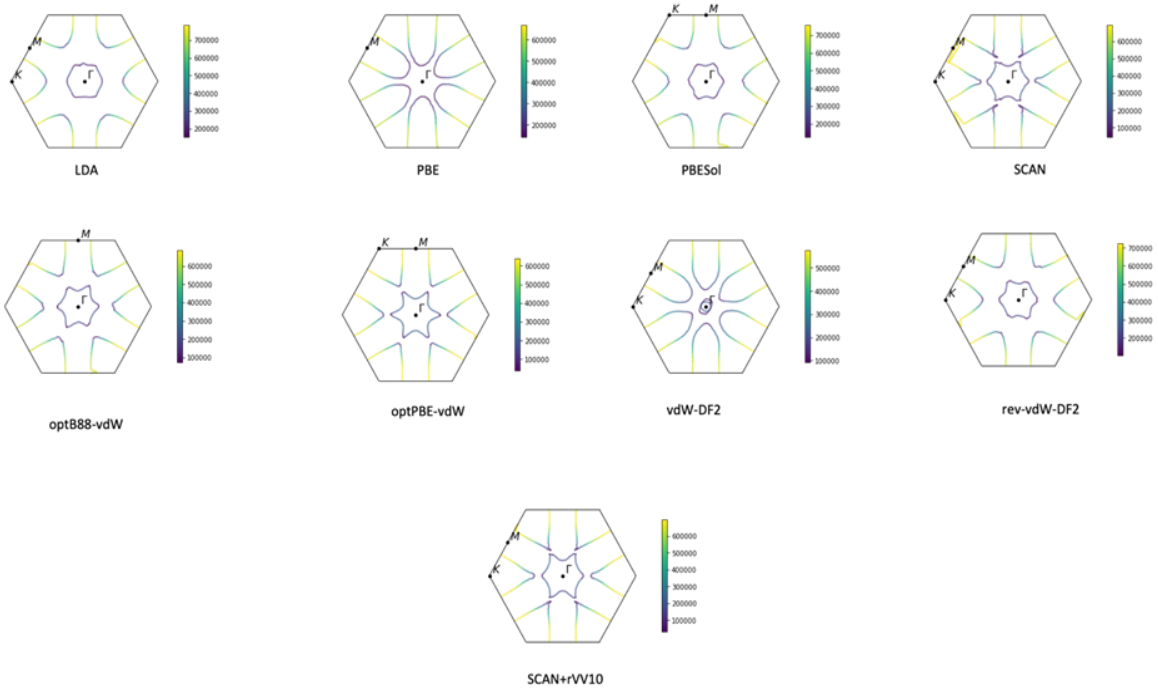

Figure S12: Fermi surface plots for 1T phase of NbS_2 all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

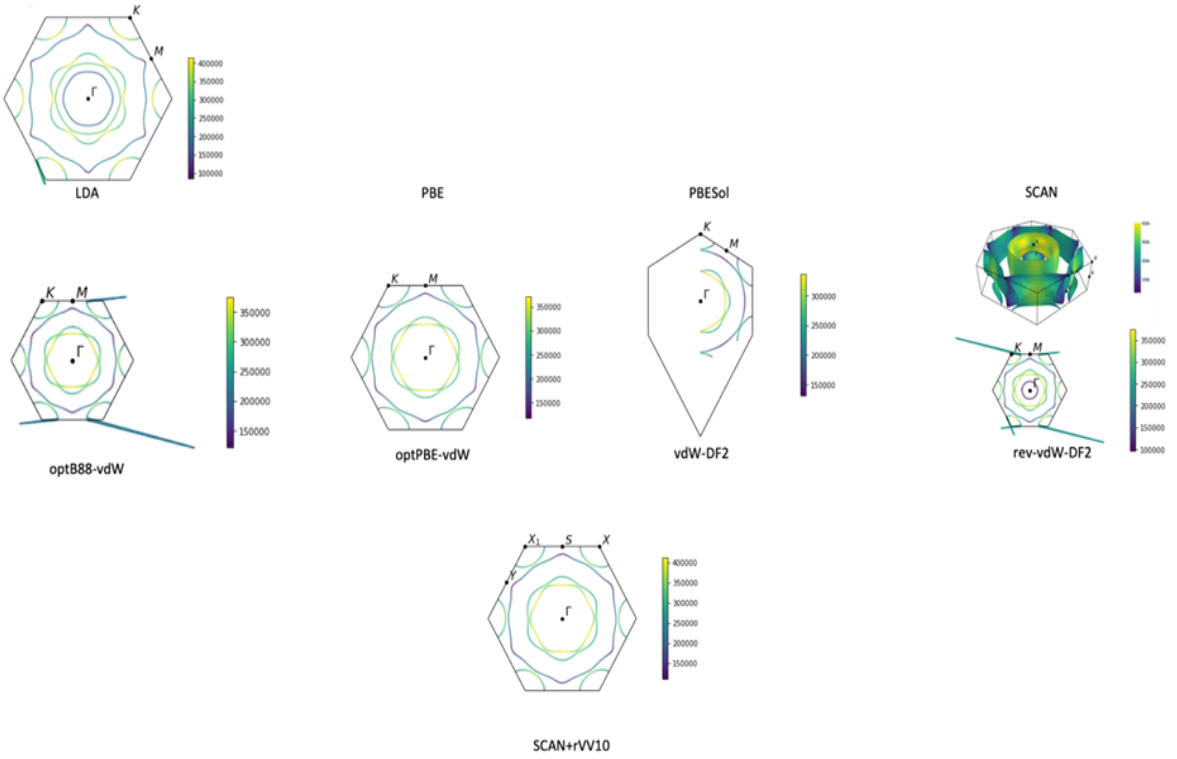

Figure S13: Fermi surface plots for 2H phase of NbS_2 all 09 XC functional in absence of SOC.

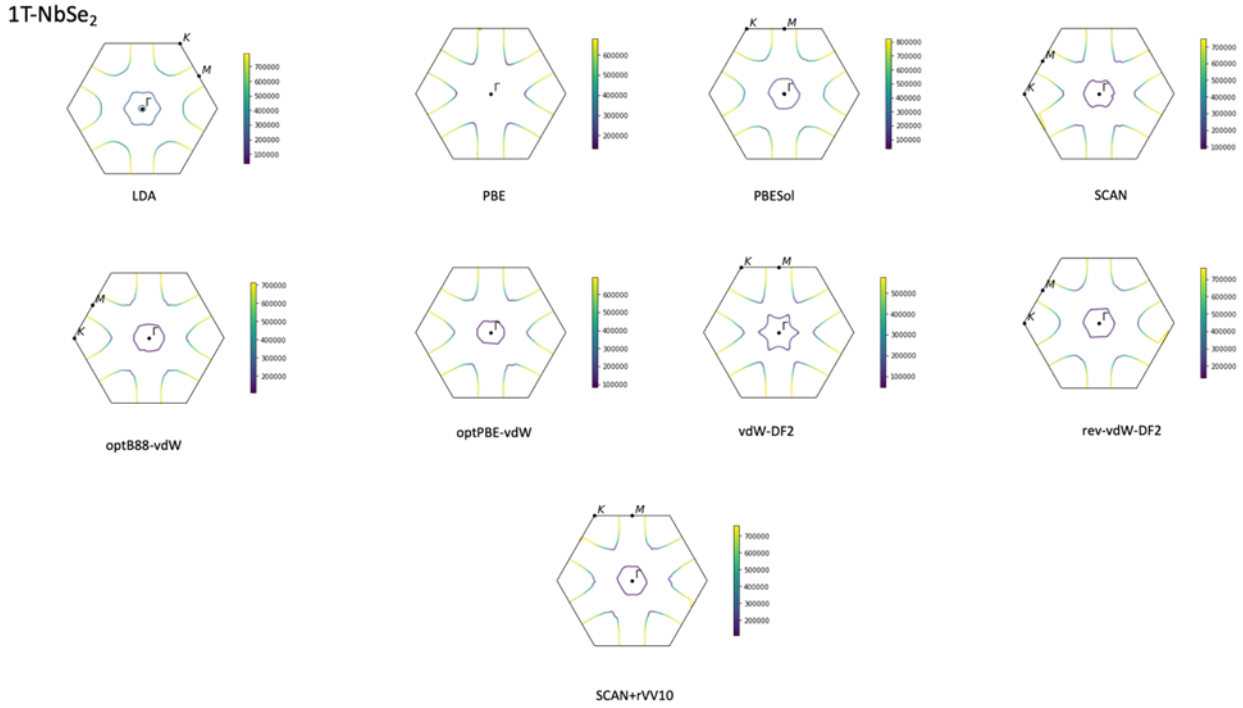

Figure S14: Fermi surface plots for 1T phase of $NbSe_2$ all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

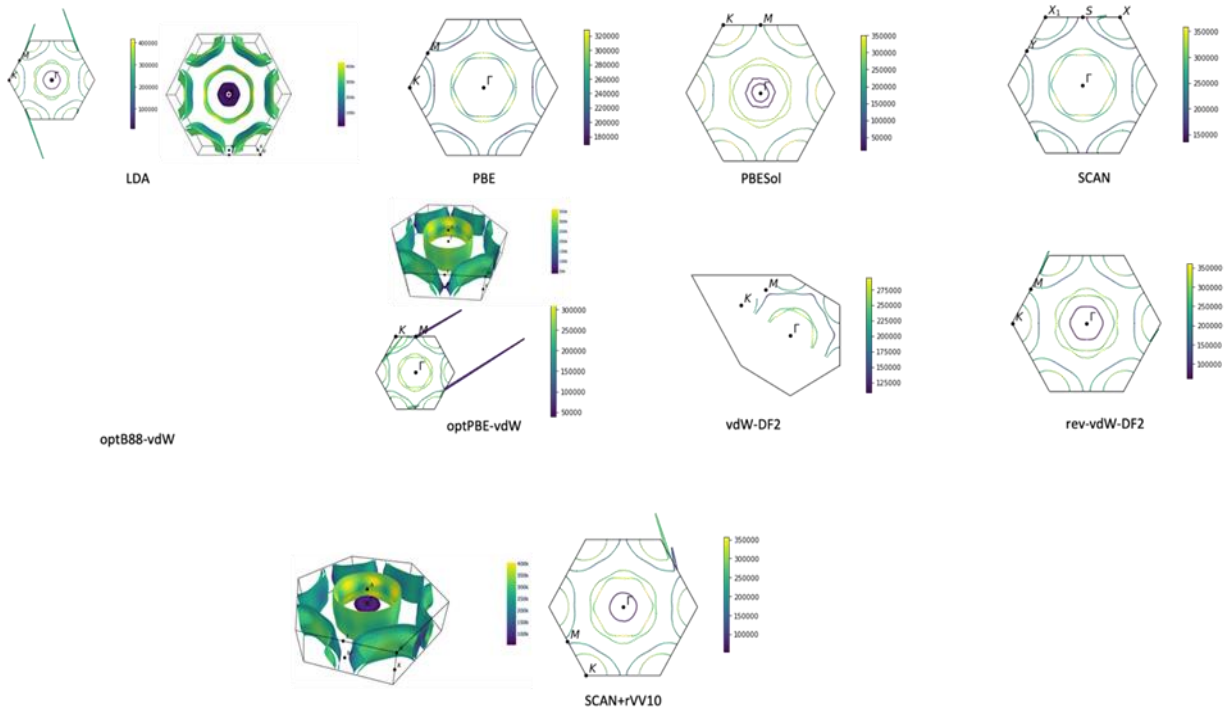

Figure S15: Fermi surface plots for 2H phase of $NbSe_2$ all 09 XC functional in absence of SOC.

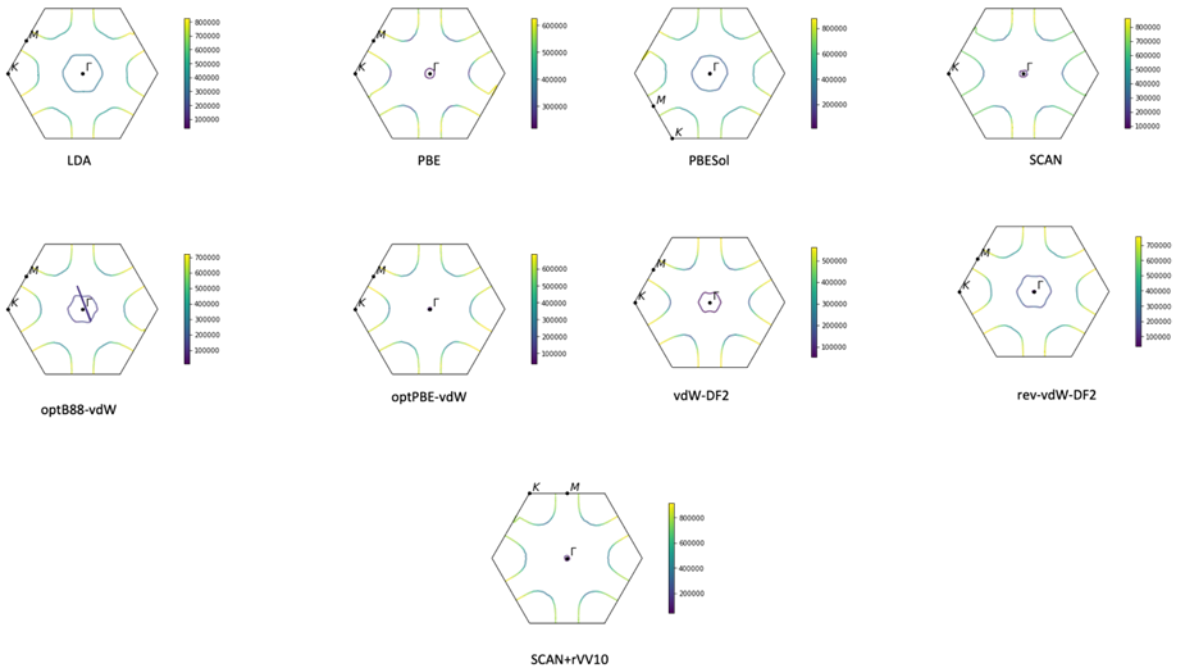

Figure S16: Fermi surface plots for 1T phase of $NbTe_2$ all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

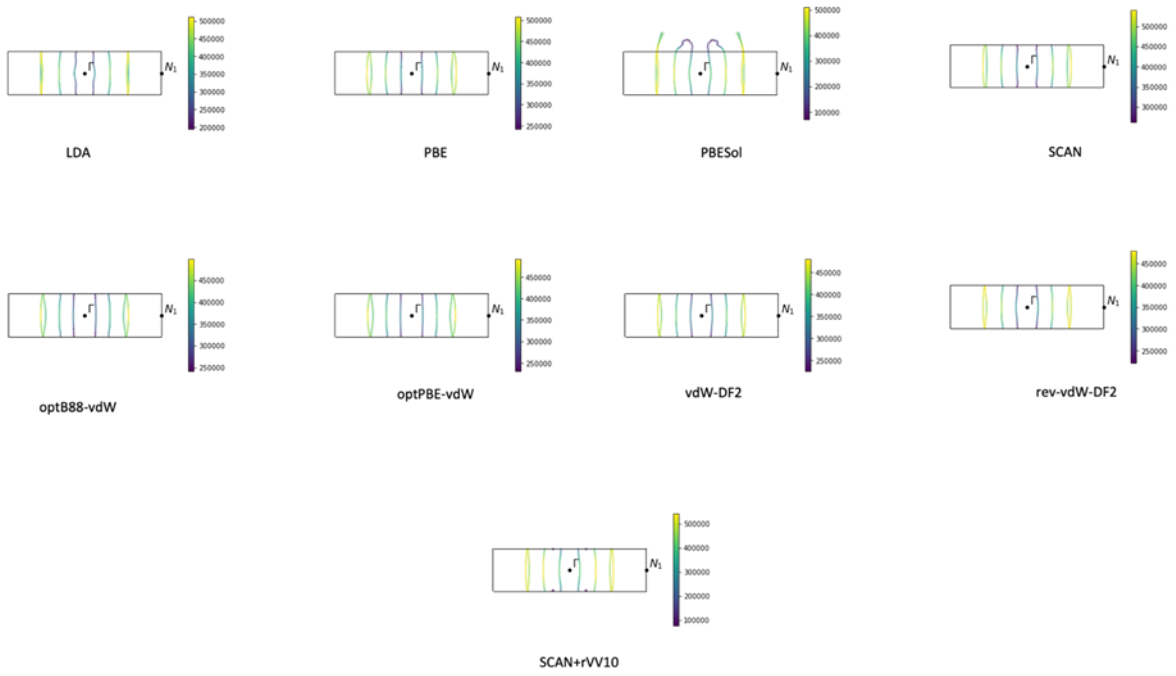

Figure S17: Fermi surface plots for 2H phase of $NbTe_2$ all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

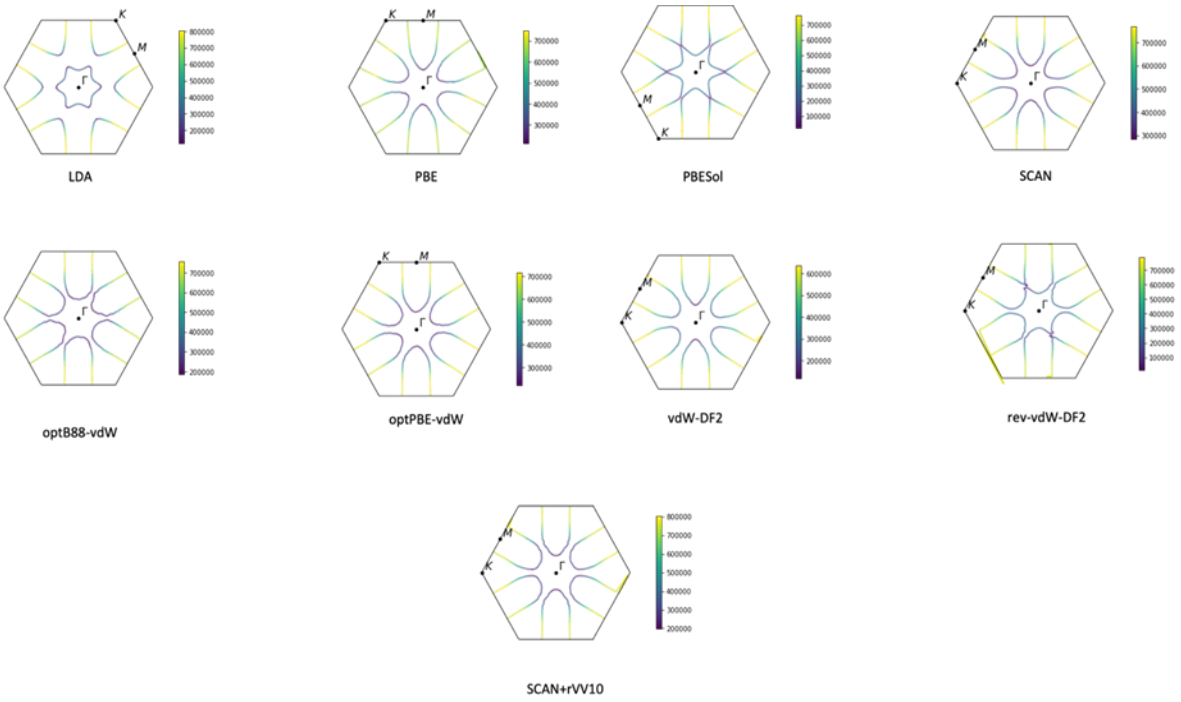

Figure S18: Fermi surface plots for 1T phase of TaS_2 all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

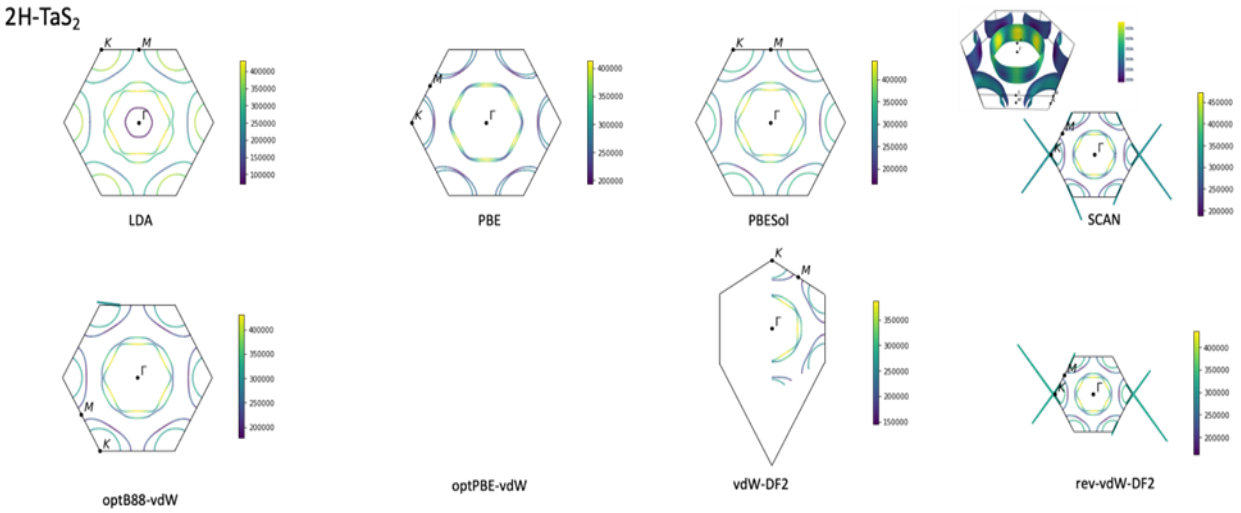

Figure S19: Fermi surface plots for 2H phase of TaS_2 all 09 XC functional in absence of SOC.

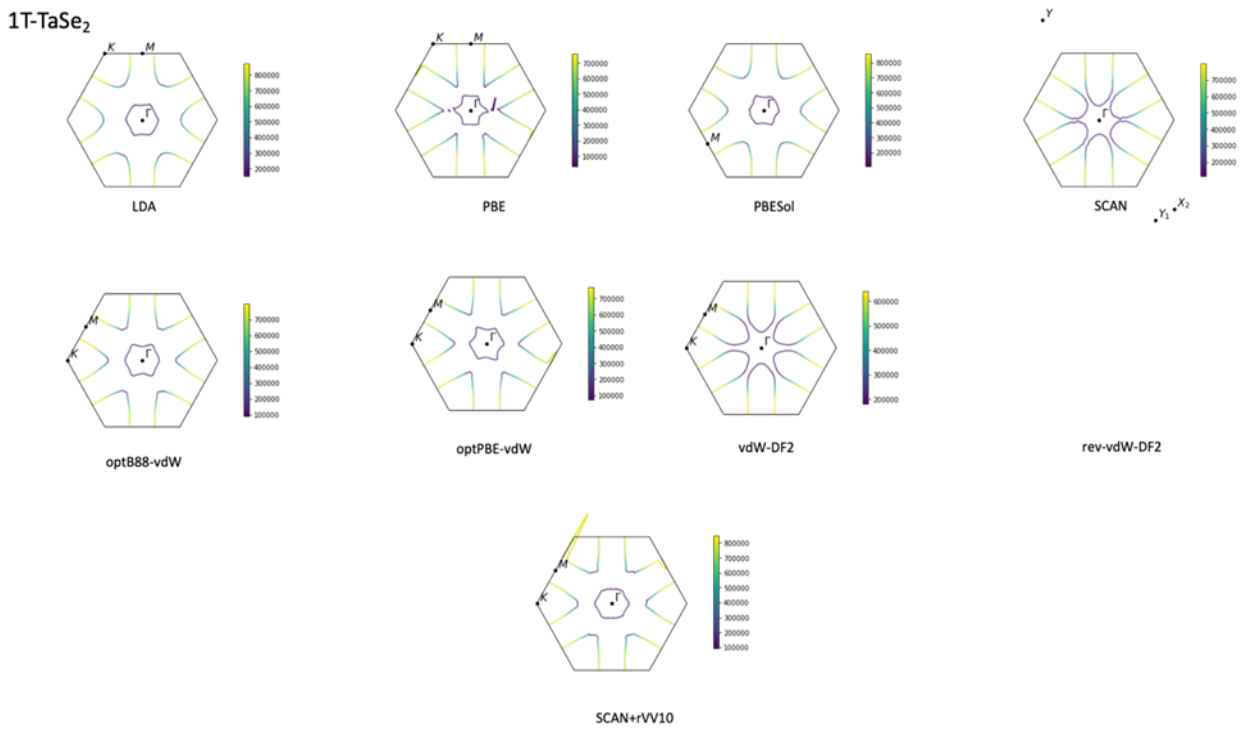

Figure S20: Fermi surface plots for 1T phase of $TaSe_2$ all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

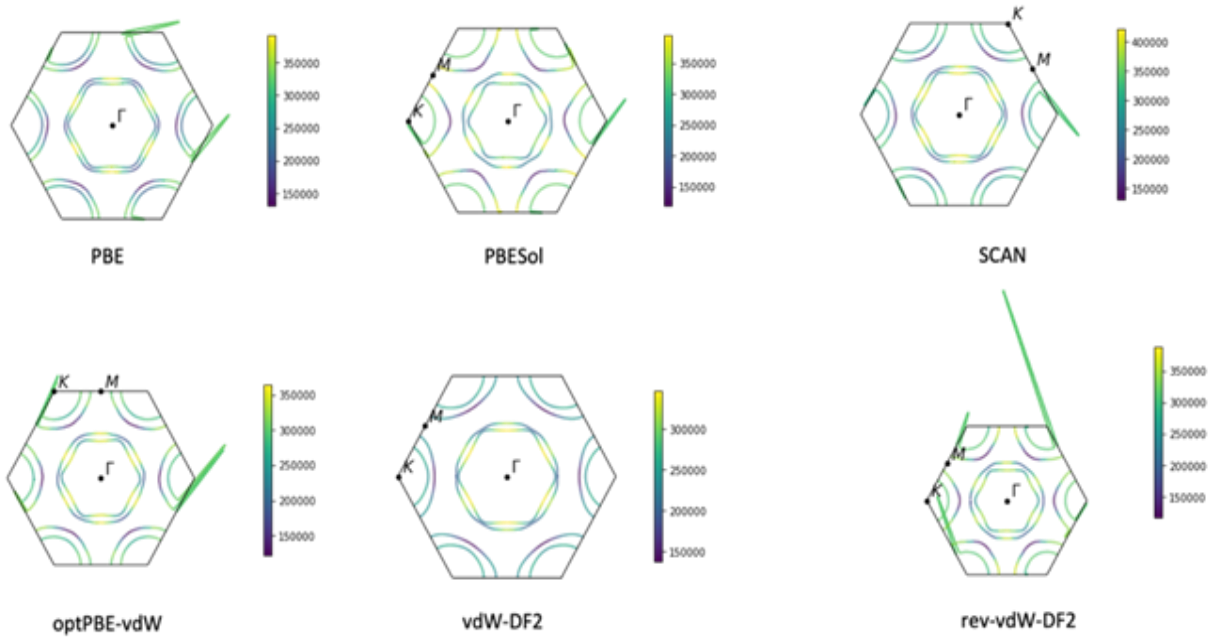

Figure S21: Fermi surface plots for 2H phase of $TaSe_2$ all 09 XC functional in absence of SOC.

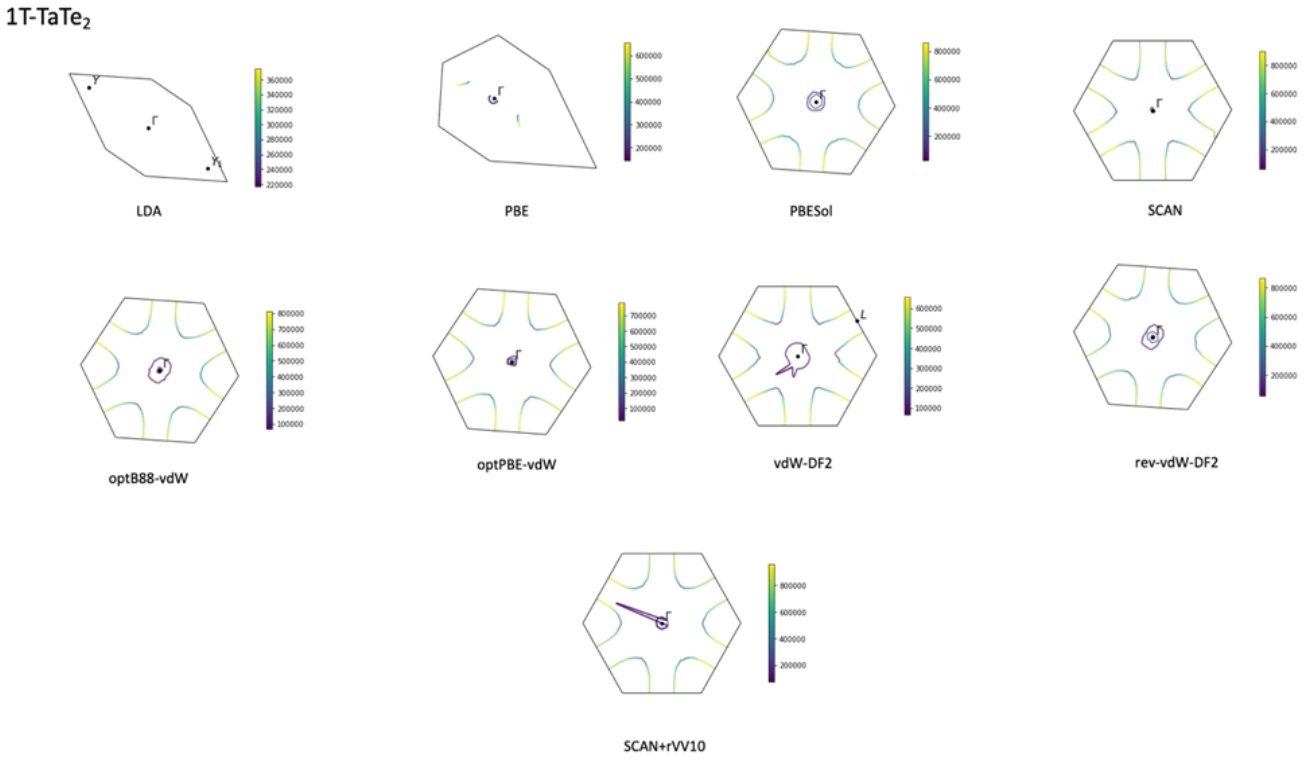

Figure S22: Fermi surface plots for 1T phase of $TaTe_2$ all 09 XC functional (top level for LDA, PBE, PBESol, SCAN from left to right; bottom level for optB88-vdW, optPBE-vdW, vdW-DF2, rev-vdW-DF2 and SCAN+rVV10 from left to right) in absence of SOC.

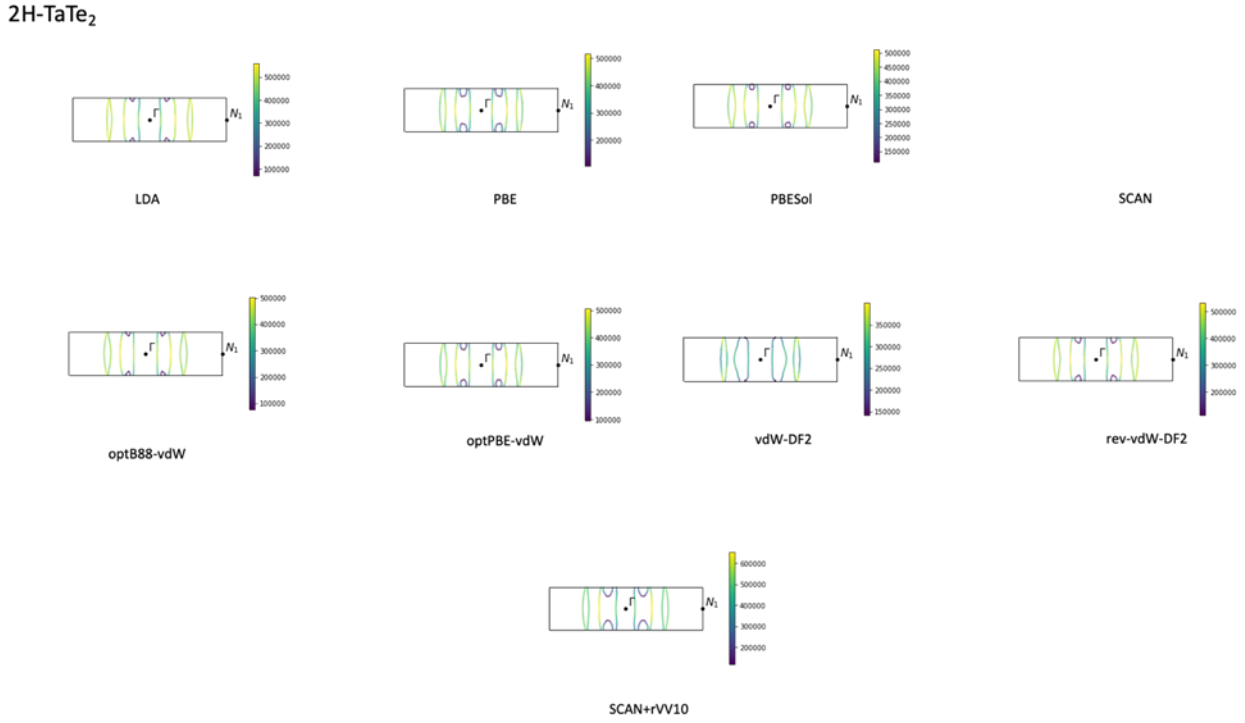

Figure S23: Fermi surface plots for 2H phase of $TaTe_2$ all 09 XC functional in absence of SOC.

Spin orbit Coupling (SOC) Case:

Similarly, the SOC optimization is complete for 1T phases of 6 systems which are shown below in tabular form.

Table S11: Details of the Energy comparison of SOC with NSOC (1T) geometry optimization for all the 06 systems are tabulated below for 04 XC and 05 vdW-DF functional in SOC case. Phase. It is noticed from the above table, the energy difference is in positive range, showing the energetic dynamic nature of SOC compared to NSOC case. The energy values are nearly same and higher in SOC case.

f_{XC}	Phase	System	NSOC (eV/atom)	SOC (eV/atom)	Difference (eV/atom)
LDA	1T	NbS_2	-7.9093	-7.9276	0.0183
		$NbSe_2$	-7.3420	-7.3755	0.0335
		$NbTe_2$	-6.7006	-6.7914	0.0908
		TaS_2	-8.5216	-8.5633	0.0417
		$TaSe_2$	-7.8872	-7.9464	0.0592
		$TaTe_2$	-7.1591	-7.2792	0.1201
PBE	1T	NbS_2	-7.1010	-7.1186	0.0176
		$NbSe_2$	-6.5158	-6.5480	0.0322
		$NbTe_2$	-5.8838	-5.9716	0.0878
		TaS_2	-7.7320	-7.7724	0.0404
		$TaSe_2$	-7.0778	-7.1352	0.0574
		$TaTe_2$	-6.3604	-6.4763	0.1159
PBESol	1T	NbS_2	-7.5761	-7.5938	0.0177
		$NbSe_2$	-7.0159	-7.0475	0.0316
		$NbTe_2$	-6.3976	-6.4850	0.0874
		TaS_2	-8.2058	-8.2464	0.0406
		$TaSe_2$	-7.5774	-7.6350	0.0576
		$TaTe_2$	-6.8728	-6.9880	0.1152
SCAN	1T	NbS_2	-18.5616	-18.5782	0.0166
		$NbSe_2$	-25.3056	-25.3360	0.0304
		$NbTe_2$	-36.3233	-36.4073	0.0840
		TaS_2	-29.7512	-29.7904	0.0392

		$TaSe_2$	-36.4291	-36.4842	0.0551
		$TaTe_2$	-47.3592	-47.4712	0.1120
optB88-vdW	1T	NbS_2	-5.2066	-6.3385	1.1319
		$NbSe_2$	-4.5201	-5.7501	1.2300
		$NbTe_2$	-3.6728	-5.1115	1.4387
		TaS_2	-5.9236	-6.9390	1.0154
		$TaSe_2$	-5.1703	-6.2839	1.1136
		$TaTe_2$	-4.2432	-5.5700	1.3268
optPBE-vdW	1T	NbS_2	-5.0613	-6.2161	1.1548
		$NbSe_2$	-4.3643	-5.6133	1.2490
		$NbTe_2$	-3.5169	-4.9766	1.4597
		TaS_2	-5.7871	-6.8193	1.0322
		$TaSe_2$	-5.0243	-6.1554	1.1311
		$TaTe_2$	-4.0969	-5.4439	1.3470
vdW-DF2	1T	NbS_2	-4.7365	-5.8835	1.1470
		$NbSe_2$	-3.9996	-5.2423	1.2427
		$NbTe_2$	-3.1393	-4.5963	1.4570
		TaS_2	-5.4015	-6.4328	1.0313
		$TaSe_2$	-4.5996	-5.7306	1.1310
		$TaTe_2$	-3.6684	-5.0212	1.3528
rev-vdW-DF2	1T	NbS_2	-5.5384	-6.5986	1.0602
		$NbSe_2$	-4.8663	-6.0089	1.1426
		$NbTe_2$	-4.0477	-5.3798	1.3321
		TaS_2	-6.2621	-7.2163	0.9542
		$TaSe_2$	-5.5235	-6.5648	1.0413
		$TaTe_2$	-4.6222	-5.8569	1.2347
SCAN+rVV10	1T	NbS_2	-18.4604	-18.5776	0.1172
		$NbSe_2$	-25.1990	-25.3360	0.1370
		$NbTe_2$	-36.2079	-36.4077	0.1998
		TaS_2	-29.6609	-29.7838	0.1229
		$TaSe_2$	-36.3306	-36.4762	0.1456
		$TaTe_2$	-47.2474	-47.4614	0.2140

The electronic band structures for the SOC cases are shown below;

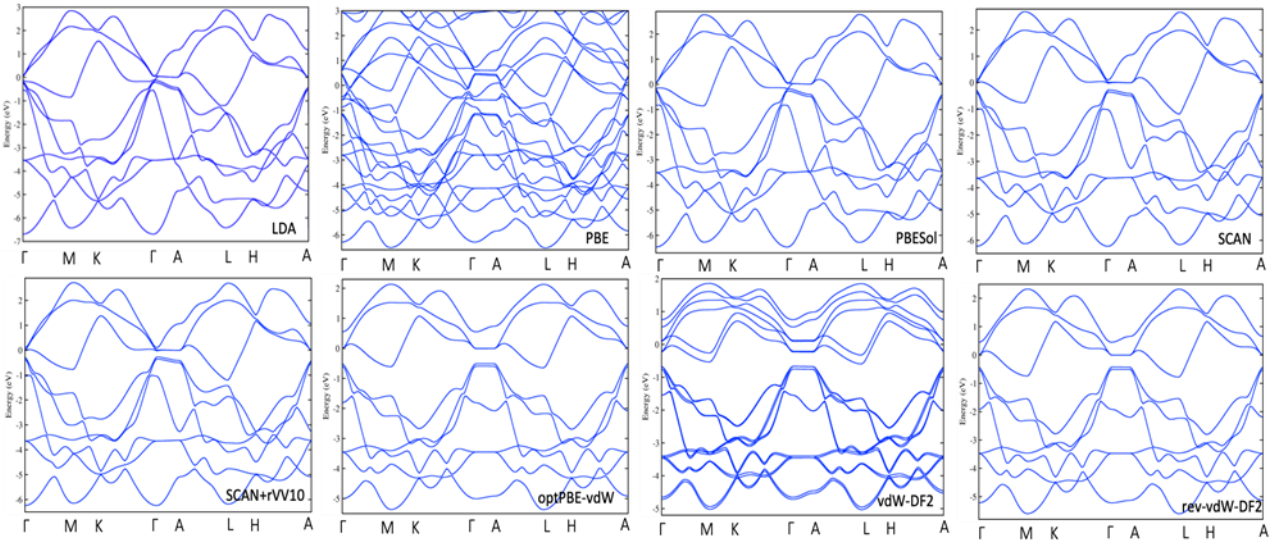

Figure S24: The electronic band structures of 1T-NbS_2 for the SOC cases.

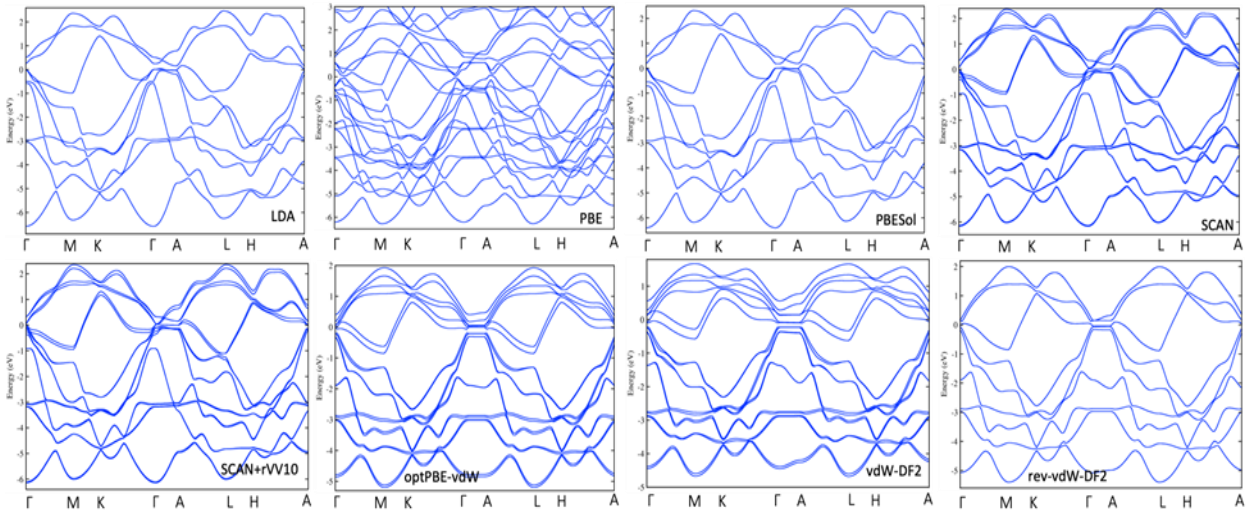

Figure S25: The electronic band structures of 1T-$NbSe_2$ for the SOC cases.

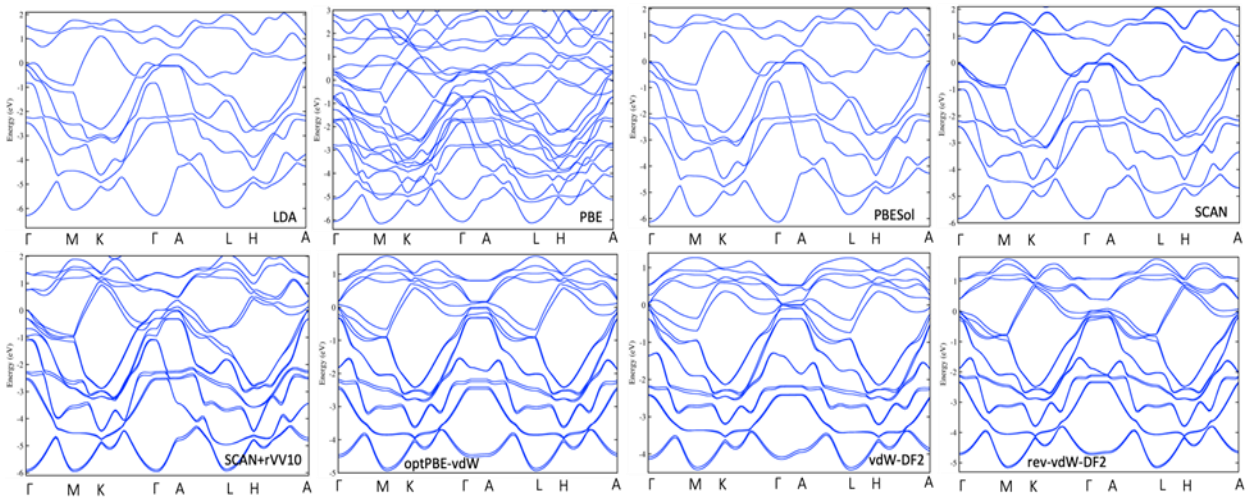

Figure S26: The electronic band structures of 1T-$NbTe_2$ for the SOC cases.

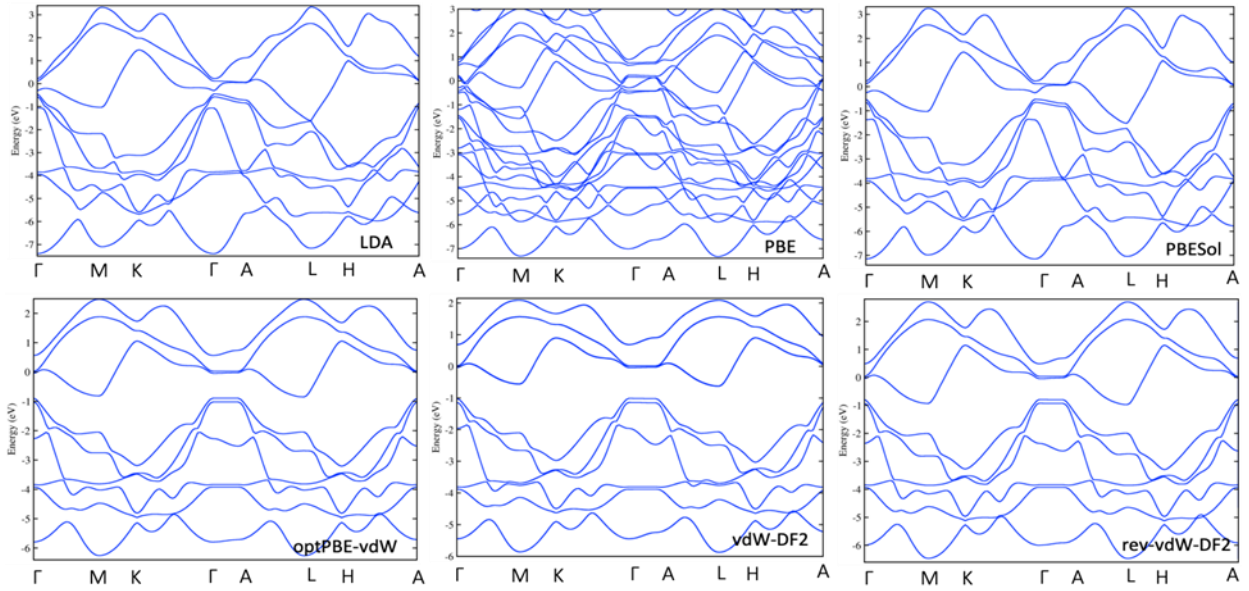

Figure S27: The electronic band structures of 1T-TaS_2 for the SOC cases.

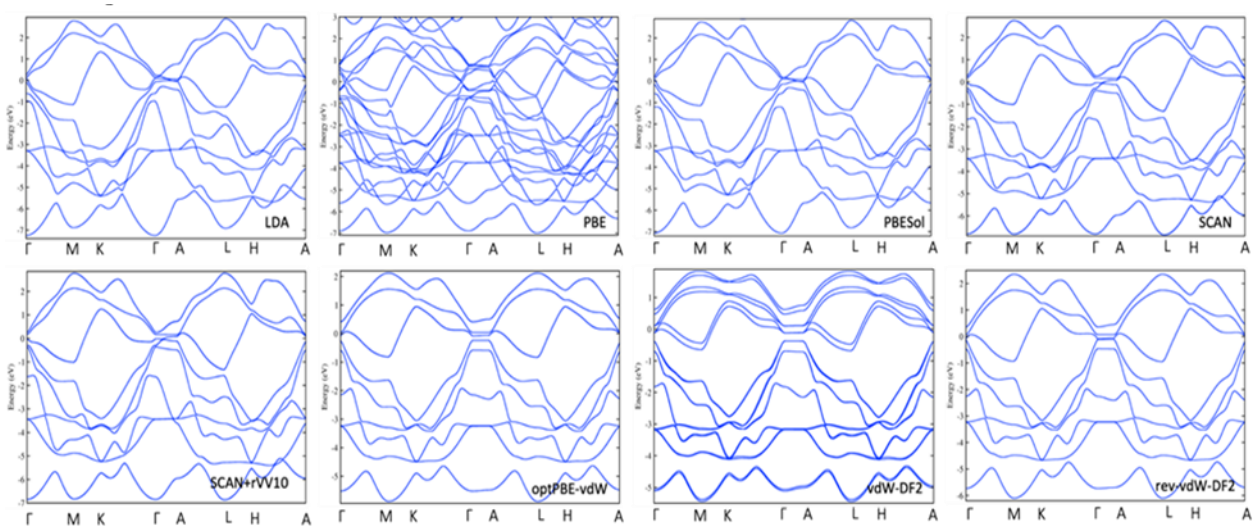

Figure S28: The electronic band structures of 1T-$TaSe_2$ for the SOC cases.

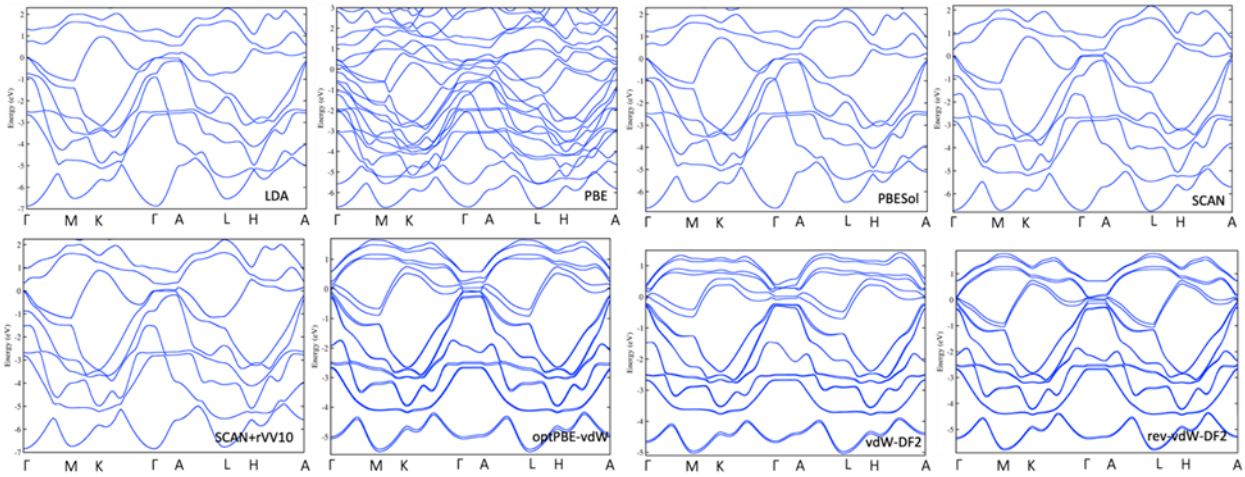

Figure S29: The electronic band structures of 1T-$TaTe_2$ for the SOC cases.

Here, the Fermi surfaces from both NSOC and SOC cases are compared. It is noticed that both cases, the surface is almost same, irrespective of case. As, Fermi surfaces of maximum systems are shown for NSOC cases, we skip to show them for SOC cases. One case of Fermi surface comparison in 2D plotter form for NbS_2 in 1T phase has been shown in Figure 5. Similarly, the bands and density of states plot in both SOC and NSOC cases are compared, it has been noticed that both are well matching with each other with very minor deviation. Here, one case of 1T-NbS_2 has been shown in Figure S31 (for band) and Figure 5 (c) for DOS plot.

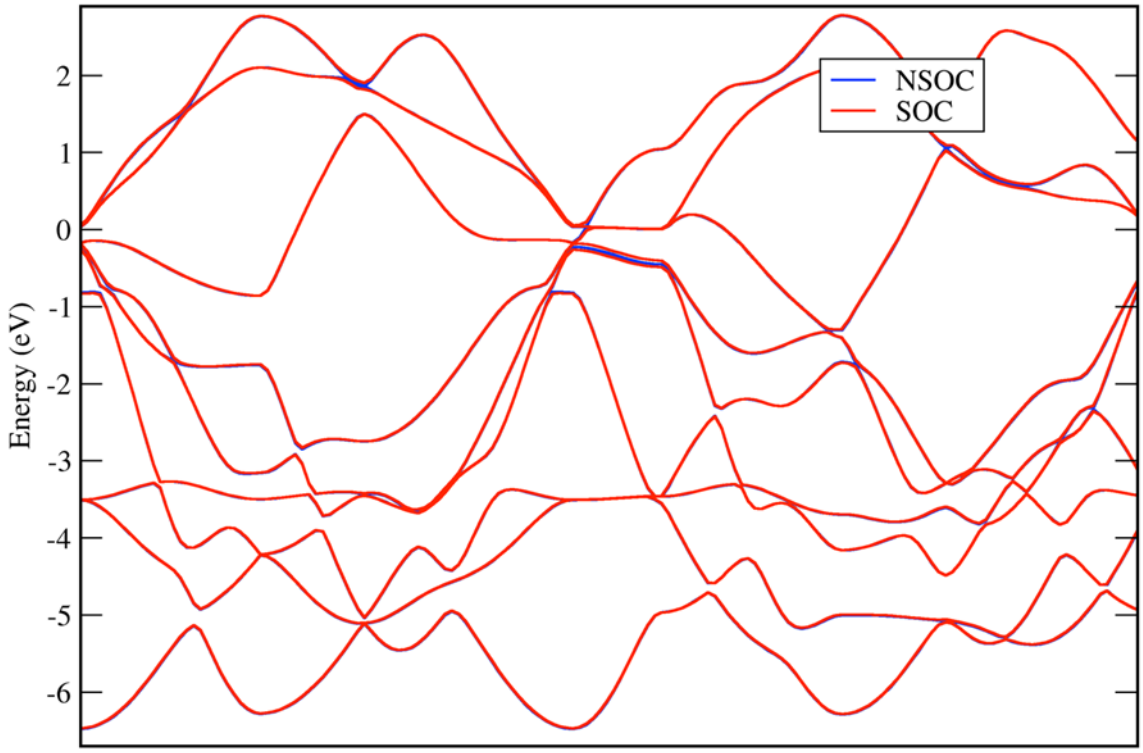

Figure S30: The band structure of 1T-NbS_2 for the both NSOC and SOC cases.

References:

[1] Patil, U.; Caffrey, N, M.; Composition dependence of the charge-driven phase transition in group-VI transition metal dichalcogenides. Physics Review B 100, 075424, 2019.

[2] Qu, Y.; et. al. Hydrogenation-controlled phase transition on two-dimensional transition metal dichalcogenides and their unique physical and catalytic properties. Scientific Reports, 6:34186, 2016.

[3] Shao, D., Luo, X., Lu, W. et al. Spin-orbit coupling enhanced superconductivity in Bi-rich compounds ABi3 (A = Sr and Ba). Sci Rep 6, 21484 (2016).