Supplementary Information (SI) for New Journal of Chemistry.

Supporting Information

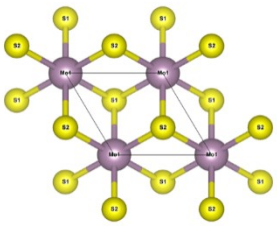
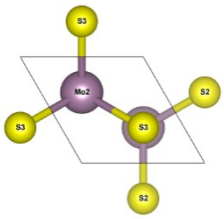
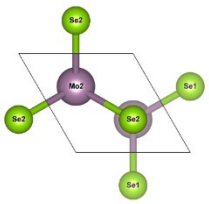
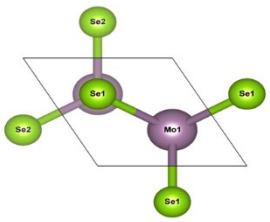
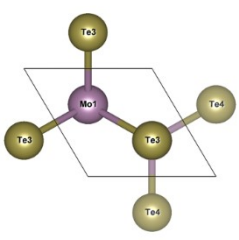
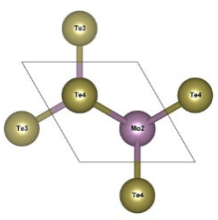
Structural Characterization and Functional Assessment of Exchange-Correlation Functionals in van der Waals TMDs AB_2 (A = Mo, W; B = S, Se, Te)

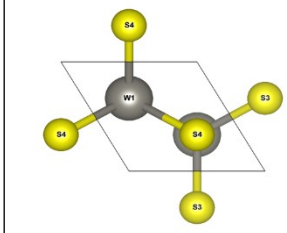
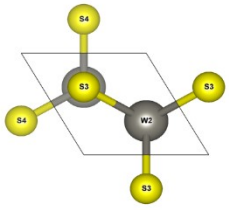
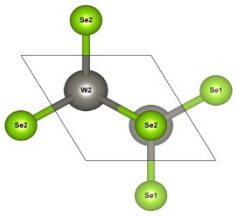
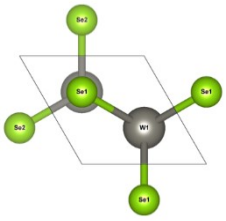
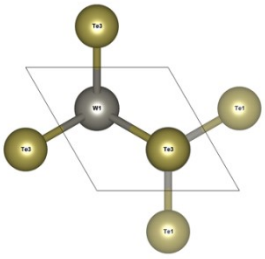
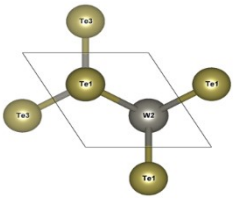
Sushant Kumar Behera, Praveen C Ramamurthy*

Organic Nano Electronic Group, Department of Materials Engineering, Indian Institute of Science, Bangalore -560012, India.

*Email: *onegroupb203@gmail.com*

Table S1: This table shows the 06 TMDs materials with their structure, space group information that are considered for the simulation.

Group	System	Phases					
		1T			2H		
		Space group	No. of atoms per unit cell	Structure	Space group	No. of atoms per unit cell	Structure
I	MoS_2	$P\bar{3}m1$ (164)	3		$P6_3/mmc$ (194)	6	
	$MoSe_2$	$P\bar{3}m1$ (164)	6		$P6_3/mmc$ (194)	6	
	$MoTe_2$	$P\bar{3}m1$ (164)	6		$P6_3/mmc$ (194)	6	

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	MoS_2	2H	3.124	3.192	12.058	13.378	2.383	2.417	81.622	80.641	3.437	4.009
		1T	3.132	3.199	5.829	6.493	2.400	2.434	98.530	97.851	3.228	3.800
	$MoSe_2$	2H	3.249	3.322	12.741	13.542	2.505	2.533	83.005	81.585	3.580	3.956
		1T	3.247	3.321	21.780	22.893	2.502	2.531	83.010	81.557	12.248	12.952
	$MoTe_2$	2H	3.471	3.565	13.743	14.647	2.691	2.727	83.727	82.002	3.843	4.273
		1T	3.468	3.560	23.057	24.811	2.687	2.724	83.762	82.090	12.757	13.866
	WS_2	2H	3.125	3.184	12.159	12.978	2.387	2.411	81.786	80.630	3.463	3.838
		1T	3.124	3.183	22.442	23.668	2.387	2.410	81.776	80.618	3.455	3.848
	WSe_2	2H	3.249	3.319	12.823	13.737	2.510	2.537	83.282	81.863	3.602	4.029
		1T	3.305	3.317	23.982	24.068	2.467	2.536	81.266	81.912	14.588	14.062
	WTe_2	2H	3.473	3.561	13.825	14.847	2.697	2.728	83.951	82.199	3.865	4.352
		1T	3.167	3.560	24.217	24.728	2.192	2.729	81.585	82.177	12.994	13.858
II	WS_2	$P\bar{3}m1$ (164)	6				$P6_3/mmc$ (194)	6				
	WSe_2	$P\bar{3}m1$ (164)	6				$P6_3/mmc$ (194)	6				
	WTe_2	$P\bar{3}m1$ (164)	6				$P6_3/mmc$ (194)	6				

Details of the geometry optimization for all the 06 systems are tabulated below for 09 XC functional (04 functional+05 vdW-DFs).

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

Table S3: 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	MoS_2	2H	3.183	3.192	14.736	13.378	2.413	2.417	80.769	80.641	4.631	4.009
		1T	3.278	3.199	6.002	6.493	2.890	2.434	98.121	97.851	3.887	3.800
	$MoSe_2$	2H	3.318	3.322	15.087	13.542	2.540	2.533	82.110	81.585	4.627	3.956
		1T	3.318	3.321	24.866	22.893	2.540	2.531	82.111	81.557	14.141	12.952
	$MoTe_2$	2H	3.731	3.565	14.886	14.647	2.810	2.727	82.510	82.002	4.030	4.273
		1T	3.550	3.560	25.160	24.811	2.731	2.724	82.756	82.090	14.043	13.866
	WS_2	2H	3.182	3.184	14.508	12.978	2.416	2.411	81.012	80.630	4.507	3.838
		1T	3.182	3.183	26.194	23.668	2.418	2.410	81.086	80.618	4.619	3.848
	WSe_2	2H	3.316	3.319	15.184	13.737	2.545	2.537	82.425	81.863	4.655	4.029
		1T	3.316	3.317	25.913	24.068	2.545	2.536	82.446	81.912	15.226	14.062
	WTe_2	2H	3.553	3.561	15.382	14.847	2.736	2.728	82.894	82.199	4.552	4.352
		1T	3.554	3.560	24.906	24.728	2.737	2.729	82.853	82.177	13.944	13.858

Table S4: 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	MoS_2	2H	3.141	3.192	12.598	13.378	2.393	2.417	81.447	80.641	3.661	4.009
		1T	3.124	3.199	6.231	6.493	2.411	2.434	99.271	97.851	3.525	3.800
	$MoSe_2$	2H	3.269	3.322	13.122	13.542	2.517	2.533	82.848	81.585	3.738	3.956
		1T	3.268	3.321	22.280	22.893	2.515	2.531	82.854	81.557	12.549	12.952
	$MoTe_2$	2H	3.421	3.565	14.552	14.647	2.801	2.727	81.972	82.002	4.007	4.273
		1T	3.489	3.560	23.377	24.811	2.702	2.724	83.654	82.090	12.946	13.866
	WS_2	2H	3.142	3.184	12.709	12.978	2.397	2.411	81.666	80.630	3.689	3.838
		1T	3.142	3.183	23.201	23.668	2.398	2.410	81.658	80.618	3.674	3.848
	WSe_2	2H	3.268	3.319	13.223	13.737	2.522	2.537	83.168	81.863	3.768	4.029
		1T	3.315	3.317	24.122	24.068	2.547	2.536	81.998	81.912	14.251	14.062
	WTe_2	2H	3.558	3.561	14.488	14.847	2.732	2.728	82.355	82.199	4.421	4.352
		1T	3.491	3.560	23.665	24.728	2.711	2.729	83.880	82.177	13.164	13.858

Table S5: 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	MoS_2	2H	3.168	3.192	13.154	13.378	2.404	2.417	80.916	80.641	3.911	4.009
		1T	3.203	3.199	6.370	6.493	2.420	2.434	97.122	97.851	3.737	3.800
	$MoSe_2$	2H	3.301	3.322	13.328	13.542	2.525	2.533	81.995	81.585	3.854	3.956
		1T	3.300	3.321	22.642	22.893	2.523	2.531	82.020	81.557	12.782	12.952
	$MoTe_2$	2H	3.514	3.565	14.593	14.647	2.708	2.727	82.956	82.002	4.228	4.273
		1T	3.513	3.560	24.296	24.811	2.706	2.724	82.958	82.090	13.568	13.866
	WS_2	2H	3.157	3.184	12.760	12.978	2.398	2.411	81.085	80.630	3.736	3.838
		1T	3.157	3.183	24.210	23.668	2.397	2.410	81.008	80.618	3.982	3.848
	WSe_2	2H	3.290	3.319	13.828	13.737	2.519	2.537	82.145	81.863	4.072	4.029
		1T	3.455	3.317	24.420	24.068	2.664	2.536	82.078	81.912	14.428	14.062
	WTe_2	2H	3.510	3.561	14.606	14.847	2.704	2.728	82.959	82.199	4.236	4.352
		1T	3.398	3.560	25.021	24.728	2.748	2.729	83.649	82.177	13.962	13.858

Table S6: 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	MoS_2	2H	3.219	3.192	12.877	13.378	2.554	2.417	80.021	80.641	3.998	4.009
		1T	3.221	3.199	6.057	6.493	2.438	2.434	97.329	97.851	3.447	3.800
	$MoSe_2$	2H	3.330	3.322	13.166	13.542	2.551	2.533	82.194	81.585	3.756	3.956
		1T	3.327	3.321	22.436	22.893	2.549	2.531	82.242	81.557	12.649	12.952
	$MoTe_2$	2H	3.568	3.565	14.233	14.647	2.742	2.727	82.618	82.002	4.057	4.273
		1T	3.564	3.560	23.751	24.811	2.740	2.724	82.701	82.090	13.175	13.866
	WS_2	2H	3.191	3.184	12.528	12.978	2.425	2.411	81.131	80.630	3.613	3.838
		1T	3.190	3.183	22.883	23.668	2.424	2.410	81.154	80.618	3.618	3.848
	WSe_2	2H	3.328	3.319	13.227	13.737	2.555	2.537	82.502	81.863	3.770	4.029
		1T	3.325	3.317	23.495	24.068	2.553	2.536	82.551	81.912	13.650	14.062
	WTe_2	2H	3.512	3.561	14.224	14.847	2.790	2.728	82.466	82.199	4.044	4.352
		1T	3.567	3.560	23.921	24.728	2.747	2.729	82.834	82.177	13.311	13.858

Table S7: 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	MoS_2	2H	3.202	3.192	12.744	13.378	2.427	2.417	80.787	80.641	3.717	4.009
		1T	3.226	3.199	6.235	6.493	2.443	2.434	97.380	97.851	3.592	3.800
	$MoSe_2$	2H	3.341	3.322	13.442	13.542	2.557	2.533	82.044	81.585	3.878	3.956
		1T	3.339	3.321	23.099	22.893	2.555	2.531	82.055	81.557	13.050	12.952
	$MoTe_2$	2H	3.502	3.565	14.332	14.647	2.769	2.727	82.003	82.002	4.054	4.273
		1T	3.577	3.560	24.096	24.811	2.749	2.724	82.555	82.090	13.383	13.866
	WS_2	2H	3.200	3.184	12.791	12.978	2.430	2.411	81.012	80.630	3.728	3.838
		1T	3.198	3.183	23.407	23.668	2.429	2.410	81.058	80.618	3.728	3.848
	WSe_2	2H	3.338	3.319	13.505	13.737	2.561	2.537	82.383	81.863	3.889	4.029
		1T	3.317	3.317	24.068	24.068	2.534	2.536	81.932	81.912	14.061	14.062
	WTe_2	2H	3.558	3.561	14.690	14.847	2.774	2.728	81.803	82.199	4.554	4.352
		1T	3.579	3.560	24.282	24.728	2.752	2.729	82.696	82.177	13.541	13.858

Table S8: 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	MoS_2	2H	3.218	3.192	13.012	13.378	2.505	2.417	80.811	80.641	4.078	4.009
		1T	3.353	3.199	6.192	6.493	2.486	2.434	95.192	97.851	3.631	3.800
	$MoSe_2$	2H	3.443	3.322	13.726	13.542	2.611	2.533	80.847	81.585	4.004	3.956
		1T	3.440	3.321	23.219	22.893	2.609	2.531	80.914	81.557	13.109	12.952
	$MoTe_2$	2H	3.452	3.565	14.076	14.647	2.665	2.727	82.303	82.002	3.997	4.273
		1T	3.708	3.560	24.627	24.811	2.813	2.724	80.943	82.090	13.708	13.866
	WS_2	2H	3.278	3.184	12.916	12.978	2.470	2.411	79.980	80.630	3.785	3.838
		1T	3.276	3.183	23.588	23.668	2.469	2.410	80.001	80.618	3.788	3.848
	WSe_2	2H	3.436	3.319	13.725	13.737	2.613	2.537	81.177	81.863	3.991	4.029
		1T	3.434	3.317	24.307	24.068	2.612	2.536	81.219	81.912	14.175	14.062
	WTe_2	2H	3.711	3.561	15.002	14.847	2.816	2.728	81.909	82.199	4.403	4.352
		1T	3.709	3.560	24.779	24.728	2.815	2.729	81.971	82.177	13.844	13.858

Table S9: 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	MoS_2	2H	3.210	3.192	12.775	13.378	2.610	2.417	81.809	80.641	3.765	4.009
		1T	3.177	3.199	6.037	6.493	2.428	2.434	98.269	97.851	3.394	3.800
	$MoSe_2$	2H	3.300	3.322	13.021	13.542	2.538	2.533	82.695	81.585	3.688	3.956
		1T	3.298	3.321	22.201	22.893	2.536	2.531	82.706	81.557	12.488	12.952
	$MoTe_2$	2H	3.531	3.565	14.005	14.647	2.728	2.727	83.299	82.002	3.964	4.273
		1T	3.527	3.560	23.507	24.811	2.724	2.724	83.329	82.090	13.019	13.866
	WS_2	2H	3.167	3.184	12.414	12.978	2.415	2.411	81.578	80.630	3.556	3.838
		1T	3.166	3.183	22.834	23.668	2.415	2.410	81.577	80.618	3.560	3.848
	WSe_2	2H	3.298	3.319	13.087	13.737	2.543	2.537	83.032	81.863	3.701	4.029
		1T	3.297	3.317	23.324	24.068	2.541	2.536	83.025	81.912	13.552	14.062
	WTe_2	2H	3.531	3.561	14.104	14.847	2.733	2.728	83.525	82.199	3.974	4.352
		1T	3.323	3.560	24.199	24.728	2.443	2.729	82.458	82.177	13.221	13.858

Table S10: 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	MoS_2	2H	3.506	3.192	12.998	13.378	2.554	2.417	80.987	80.641	3.779	4.009
		1T	3.204	3.199	5.958	6.493	2.417	2.434	96.950	97.851	3.395	3.800
	$MoSe_2$	2H	3.292	3.322	13.118	13.542	2.522	2.533	82.213	81.585	3.758	3.956
		1T	3.291	3.321	20.722	22.893	2.522	2.531	82.23	81.557	11.056	12.952
	$MoTe_2$	2H	3.500	3.565	14.030	14.647	2.705	2.727	83.324	82.002	3.972	4.273
		1T	3.498	3.560	23.124	24.811	2.703	2.724	83.334	82.090	12.699	13.866
	WS_2	2H	3.148	3.184	12.646	12.978	2.394	2.411	81.245	80.630	3.684	3.838
		1T	3.149	3.183	24.039	23.668	2.394	2.410	81.172	80.618	3.933	3.848
	WSe_2	2H	3.278	3.319	13.144	13.737	2.517	2.537	82.512	81.863	3.761	4.029
		1T	3.278	3.317	22.594	24.068	2.517	2.536	82.505	81.912	12.881	14.062
	WTe_2	2H	3.494	3.561	14.043	14.847	2.702	2.728	83.423	82.199	3.973	4.352
		1T	3.226	3.560	24.641	24.728	2.965	2.729	82.571	82.177	13.993	13.858

Table S11: 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	MoS_2	-7.8897	-8.1642	0.2745
		$MoSe_2$	-7.5424	-7.5632	0.0208
		$MoTe_2$	-6.8752	-6.9017	0.0265
	II	WS_2	-8.7639	-8.7819	0.0180
		WSe_2	-8.0907	-8.1106	0.0199
		WTe_2	-7.3419	-7.3680	0.0261
PBE	I	MoS_2	-6.9893	-7.2679	0.2786
		$MoSe_2$	-6.6583	--6.6590	0.0007
		$MoTe_2$	-6.0125	-6.0148	0.0023
	II	WS_2	-7.9072	-7.9082	0.0010

PBESol		WSe_2	-7.2247	-7.2252	0.0005
		WTe_2	-6.4949	-6.4974	0.0025
	I	MoS_2	-18.6625	-18.9551	0.2926
		$MoSe_2$	-25.6873	-25.6962	0.0089
		$MoTe_2$	-36.7242	-36.7364	0.0122
	II	WS_2	-30.5459	-30.5540	0.0081
		WSe_2	-37.2012	-37.2099	0.0087
		WTe_2	-48.1406	-48.1528	0.0122
SCAN	I	MoS_2	-18.6625	-18.9551	0.2926
		$MoSe_2$	-25.6873	-25.6962	0.0089
		$MoTe_2$	-36.7242	-36.7364	0.0122
	II	WS_2	-30.5459	-30.5540	0.0081
		WSe_2	-37.2010	-37.2099	0.0089
		WTe_2	-48.1406	-48.1528	0.0122
optB88-vdW	I	MoS_2	-5.1351	-5.3994	0.2643
		$MoSe_2$	-4.6545	-4.6946	0.0401
		$MoTe_2$	-3.7995	-3.8447	0.0452
	II	WS_2	-6.0246	-6.0627	0.0381
		WSe_2	-5.2459	-5.2861	0.0402
		WTe_2	-4.3123	-4.3576	0.0453
optPBE-vdW	I	MoS_2	-4.9774	-5.2435	0.2661
		$MoSe_2$	-4.4947	-4.5303	0.0356
		$MoTe_2$	-3.6417	-3.6812	0.0395
	II	WS_2	-5.8835	-5.9182	0.0347
		WSe_2	-5.0966	-5.1322	0.0356
		WTe_2	-4.1637	-4.2034	0.0397
vdW-DF2	I	MoS_2	-4.5613	-4.8015	0.2402
		$MoSe_2$	-4.0355	-4.0671	0.0316
		$MoTe_2$	-3.1872	-3.2213	0.0341
	II	WS_2	-5.3948	-5.4257	0.0309
		WSe_2	-4.5826	-4.6143	0.0317
		WTe_2	-3.6589	-3.6871	0.0282
rev-vdW-DF2	I	MoS_2	-5.4962	-5.7657	0.2695
		$MoSe_2$	-5.0331	-5.0702	0.0371
		$MoTe_2$	-4.1986	-4.2422	0.0436
	II	WS_2	-6.4082	-6.4431	0.0349
		WSe_2	-5.6389	-5.6761	0.0372
		WTe_2	-4.7241	-4.7678	0.0437
SCAN+rVV10	I	MoS_2	-18.5763	-18.8713	0.2950
		$MoSe_2$	-25.5722	-25.6034	0.0312
		$MoTe_2$	-36.5923	-36.6297	0.0374
	II	WS_2	-30.4357	-30.4687	0.0330
		WSe_2	-37.0886	-37.1197	0.0311
		WTe_2	-48.0154	-48.0155	0.0001

Electronic Band structures:

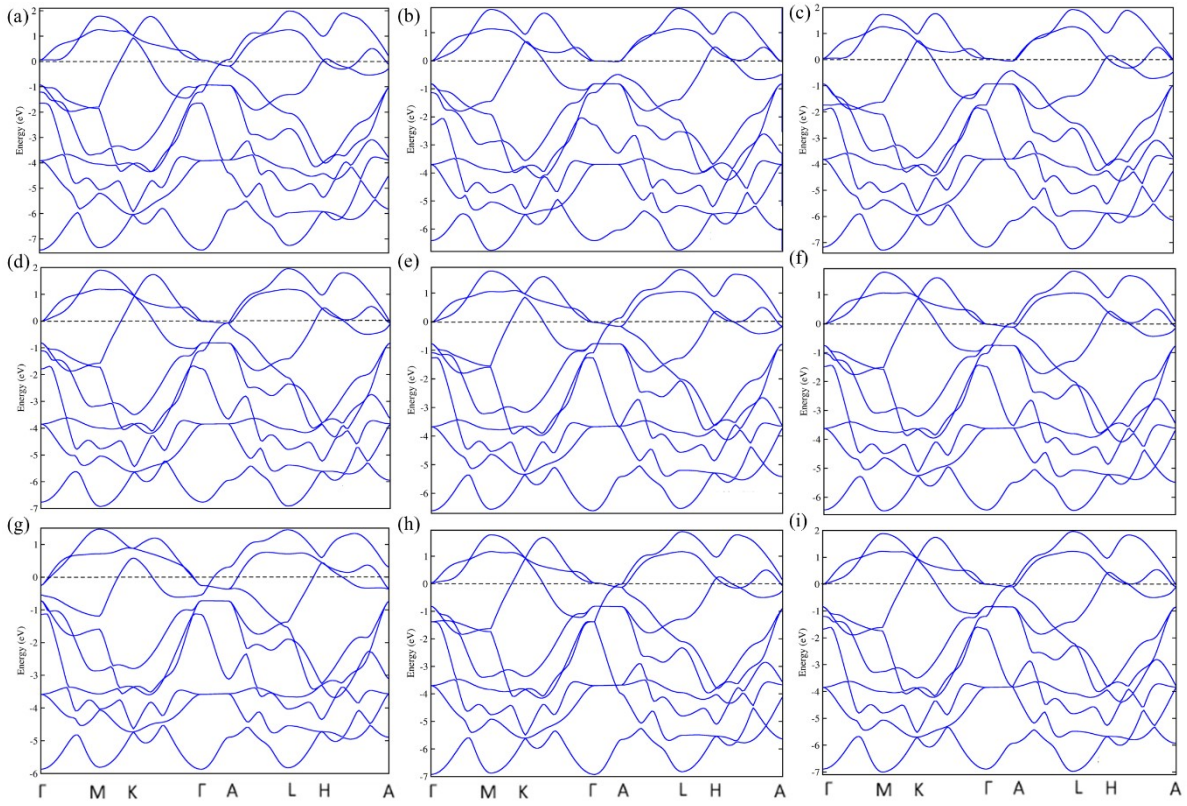


Figure S1: Band structures of 1T phase of MoS_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

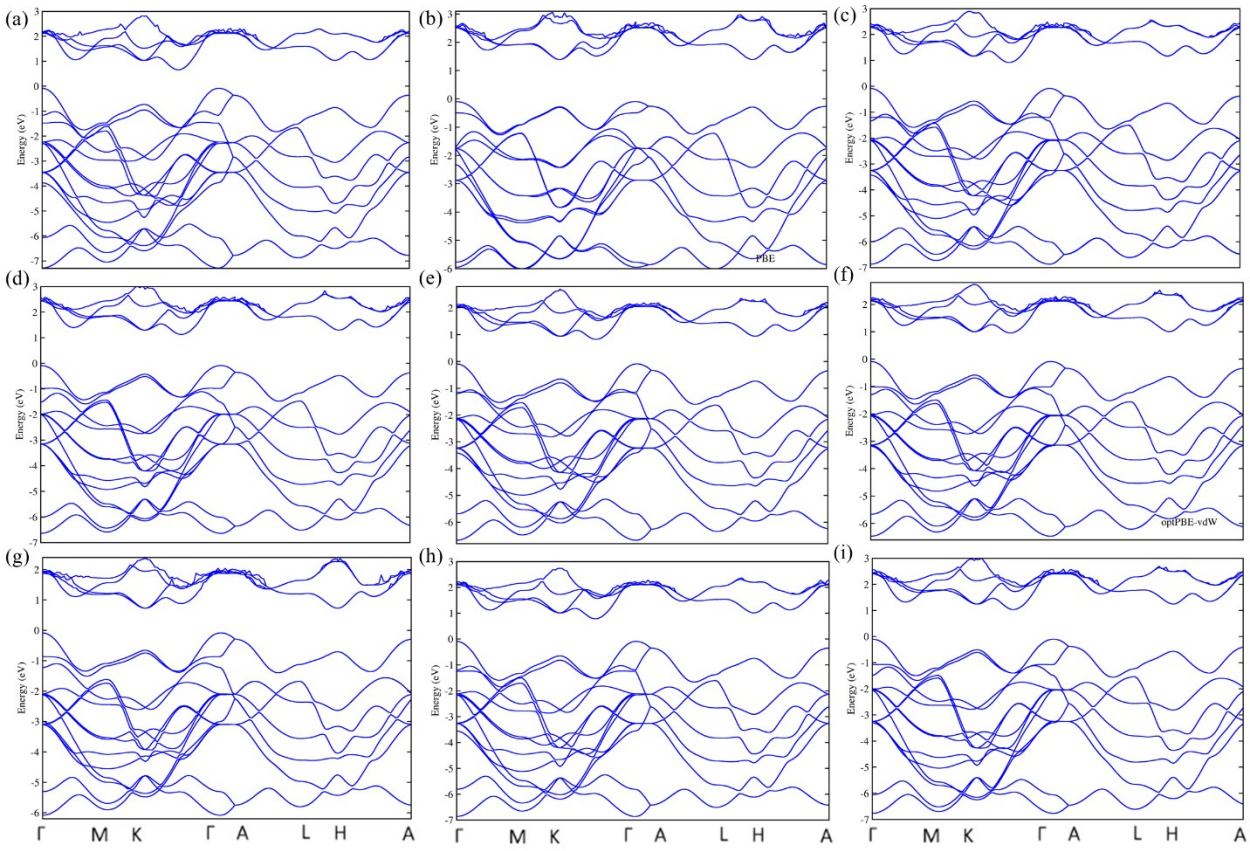


Figure S2: Band structures of 2H phase of MoS_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

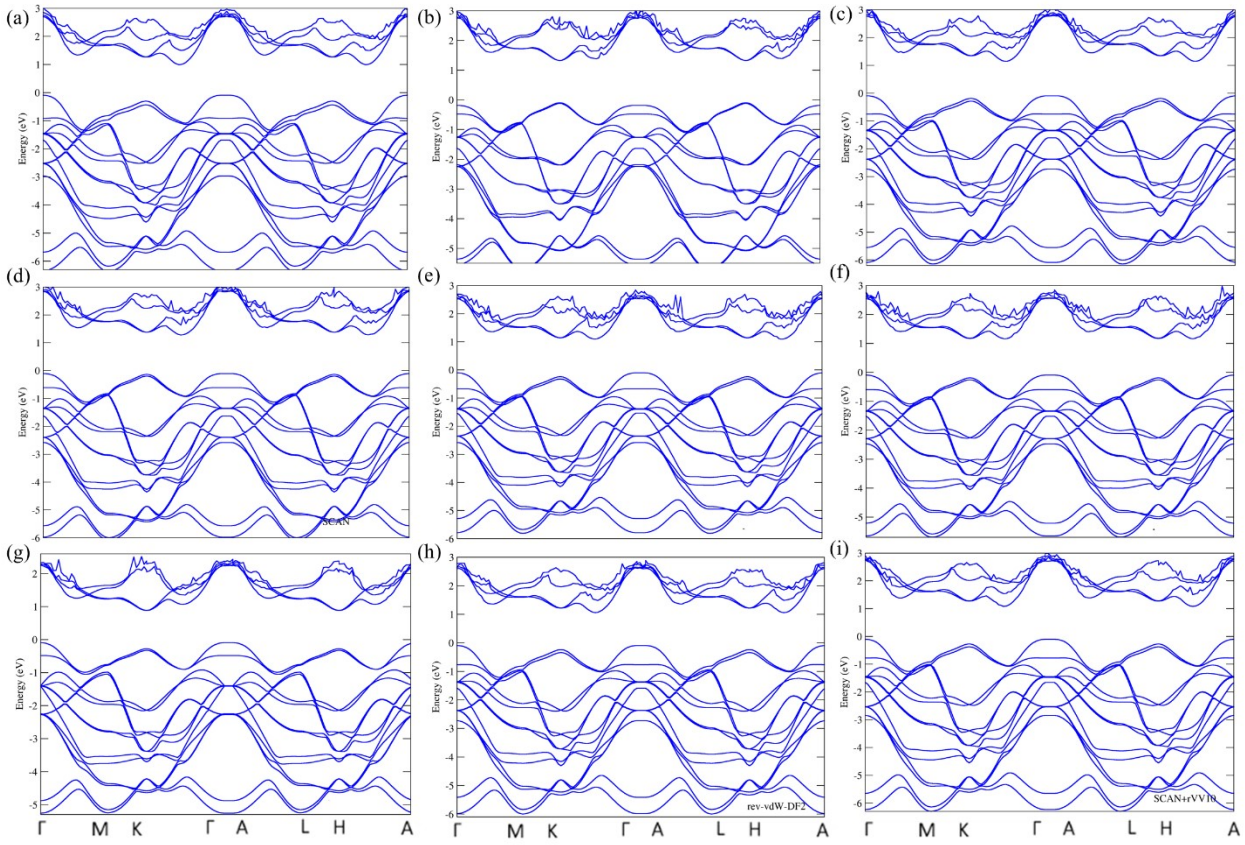


Figure S3: Band structures of 1T phase of $MoSe_2$ for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

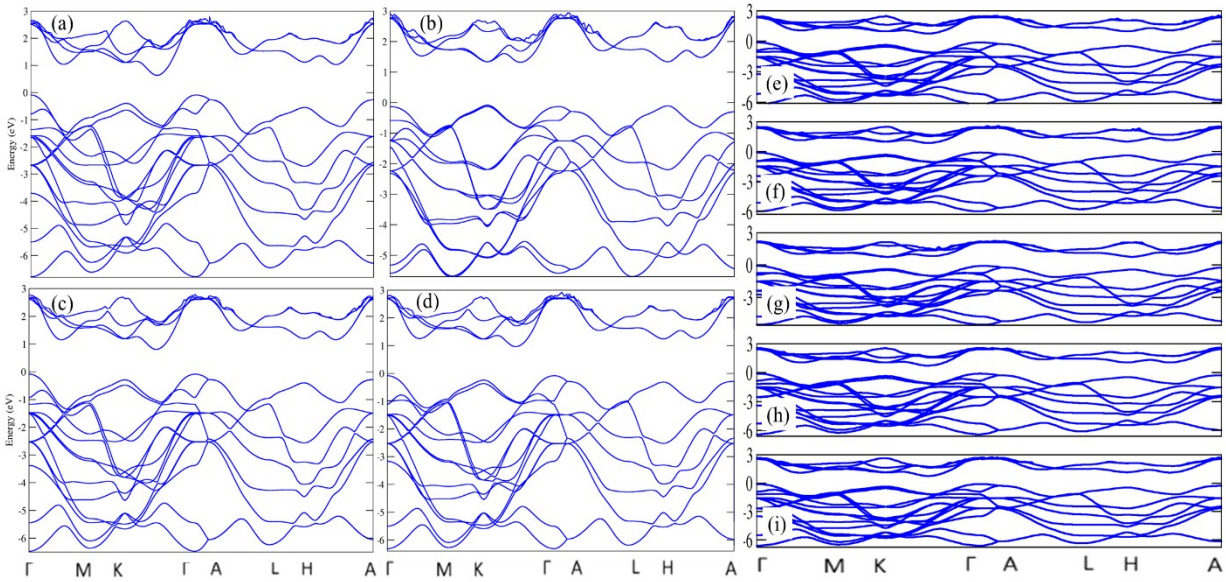


Figure S4: Band structures of 2H phase of $MoSe_2$ for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

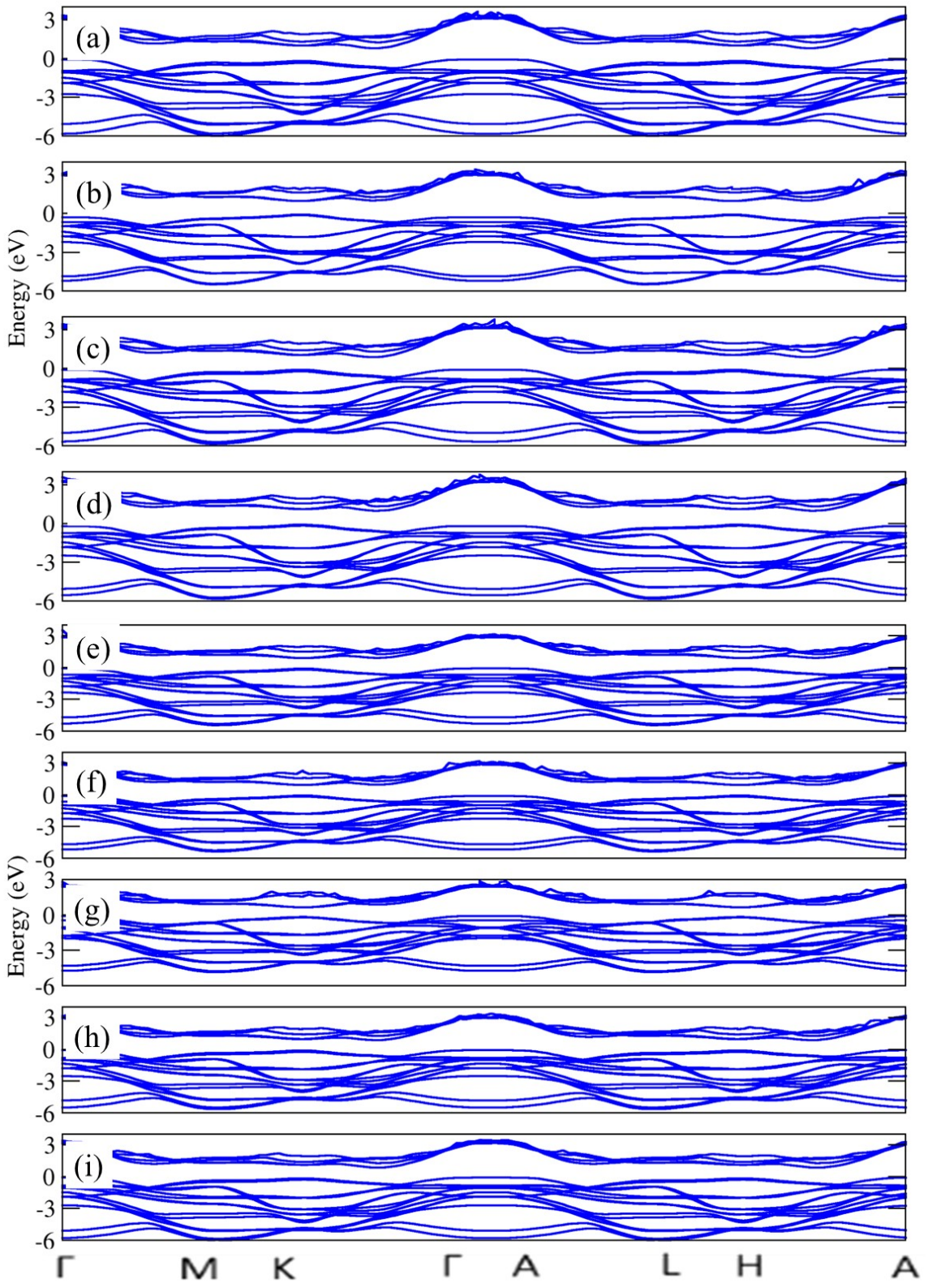


Figure S5: Band structures of 1T phase of $MoTe_2$ for all 09 XC functional ((a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

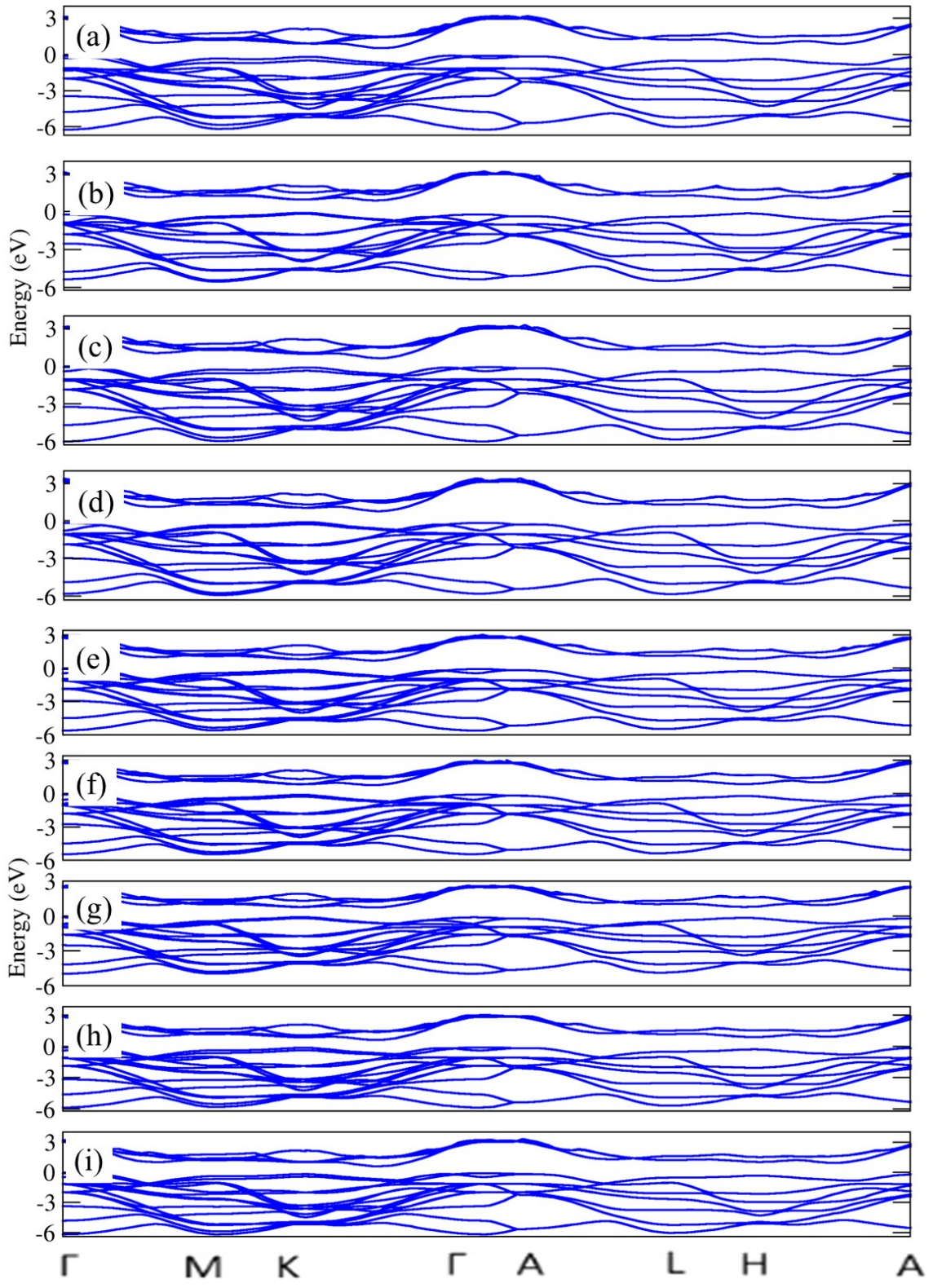


Figure S6: Band structures of 2H phase of $MoTe_2$ for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

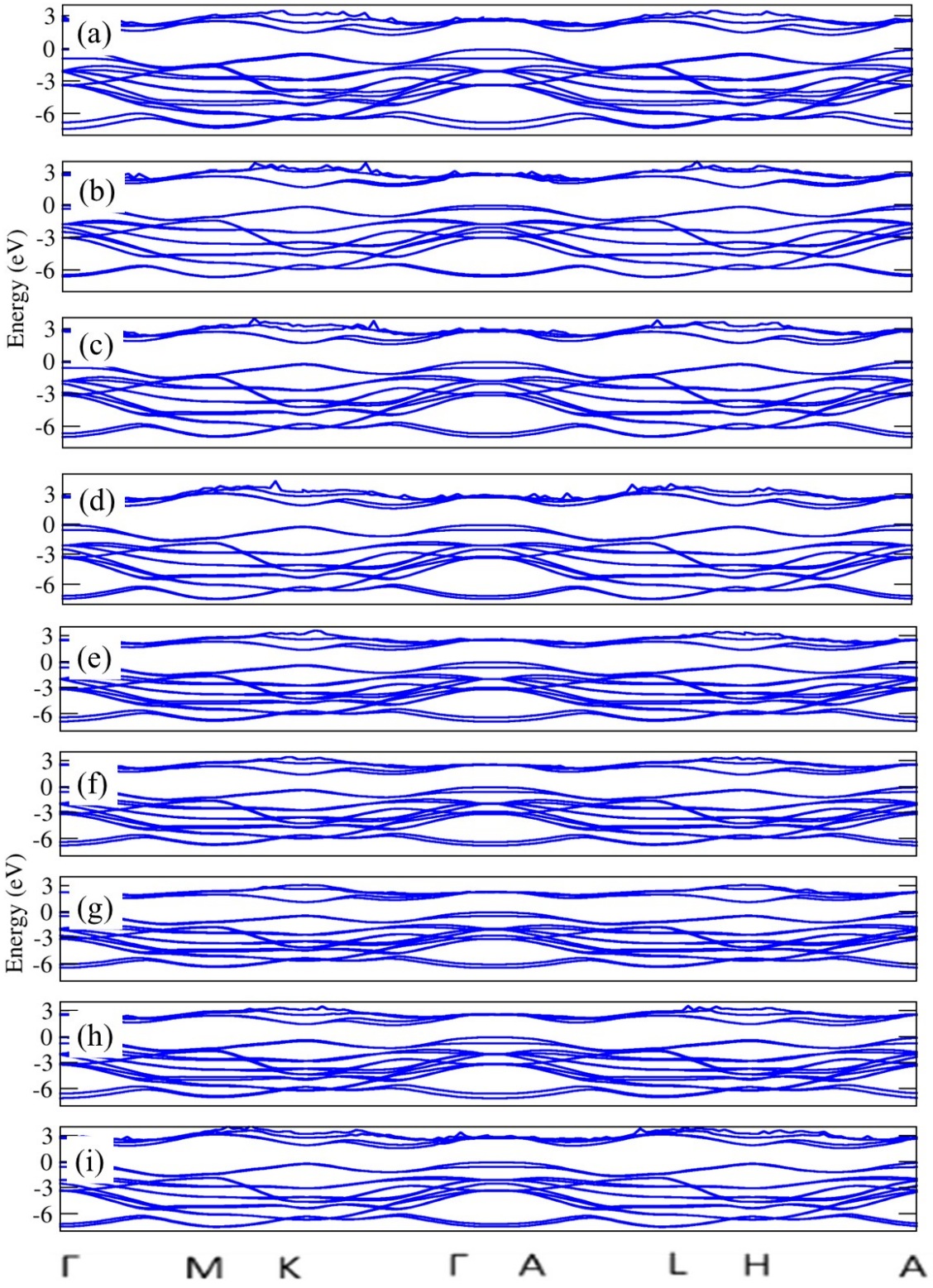


Figure S7: Band structures of 1T phase of WS_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

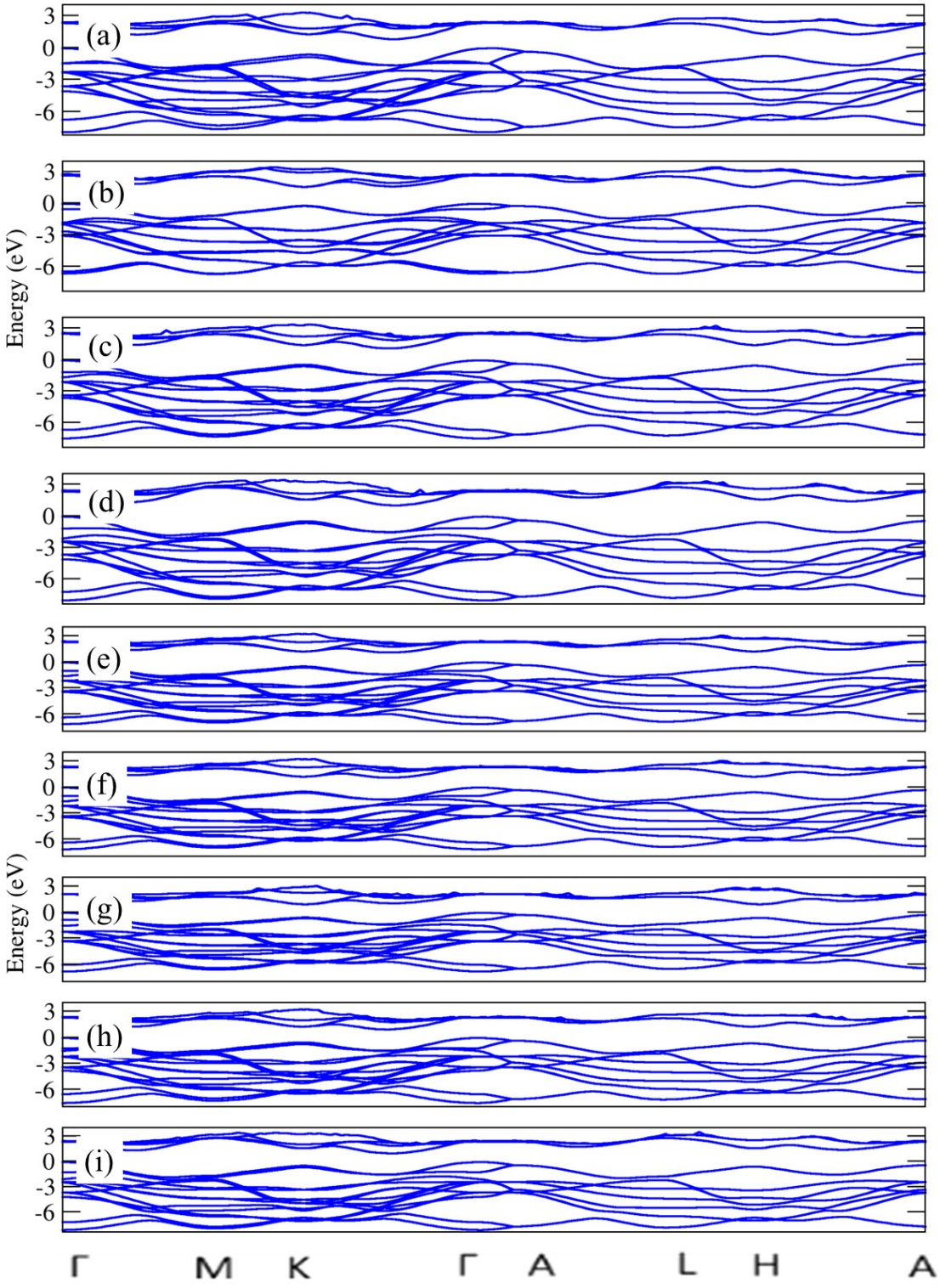


Figure S8: Band structures of 2H phase of WS_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

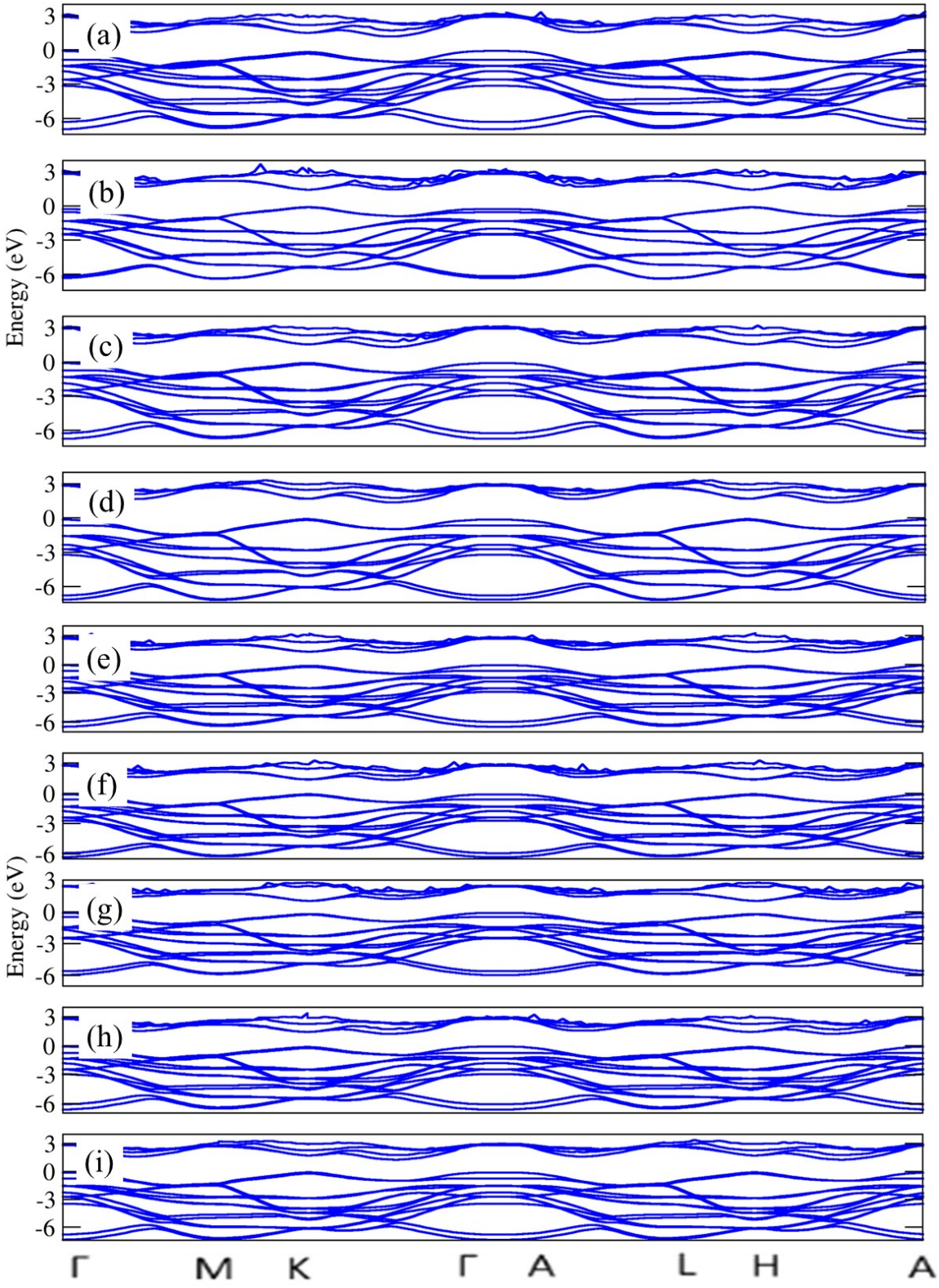


Figure S9: Band structures of 1T phase of WSe_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

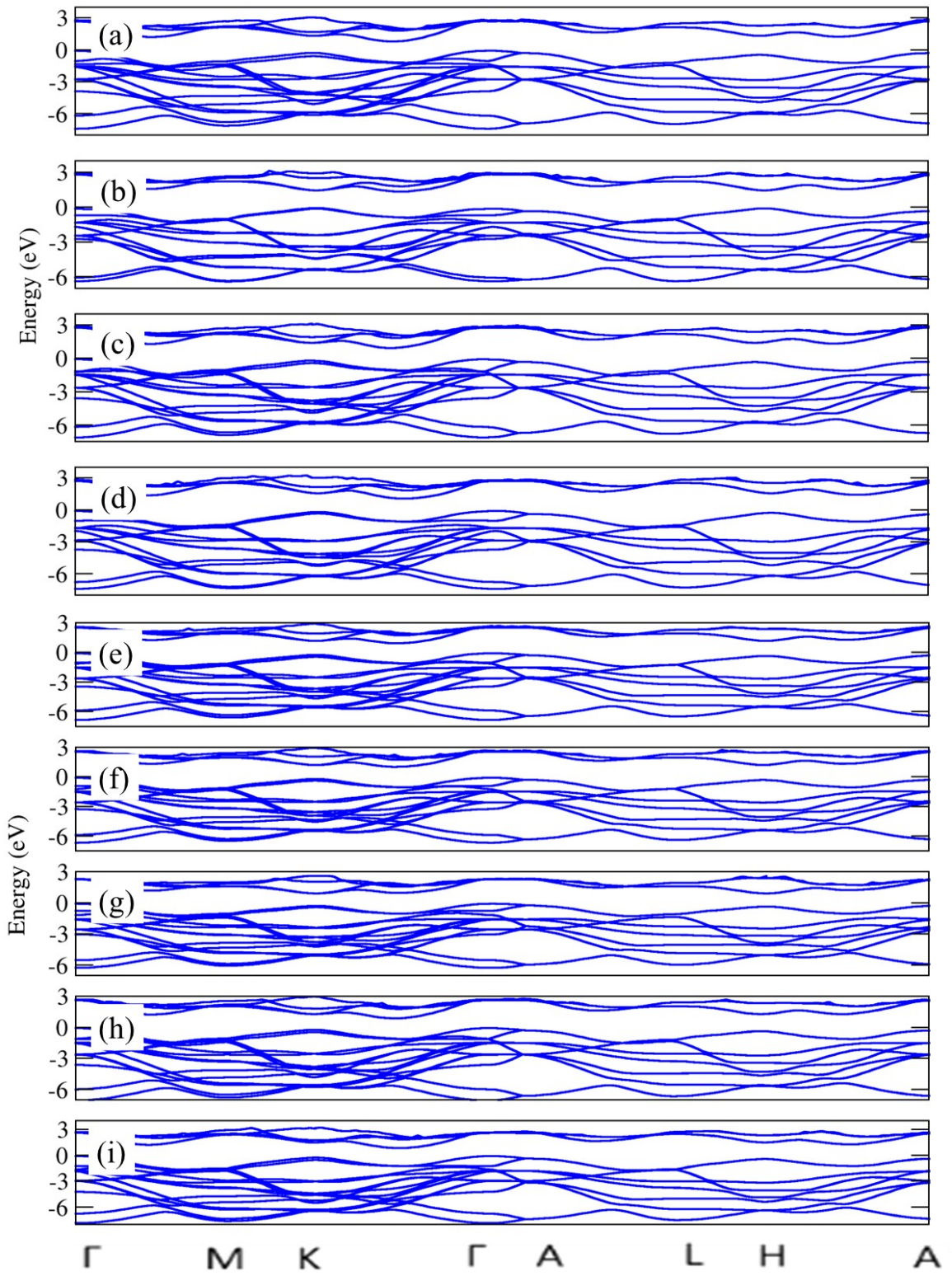


Figure S10: Band structures of 2H phase of WSe_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

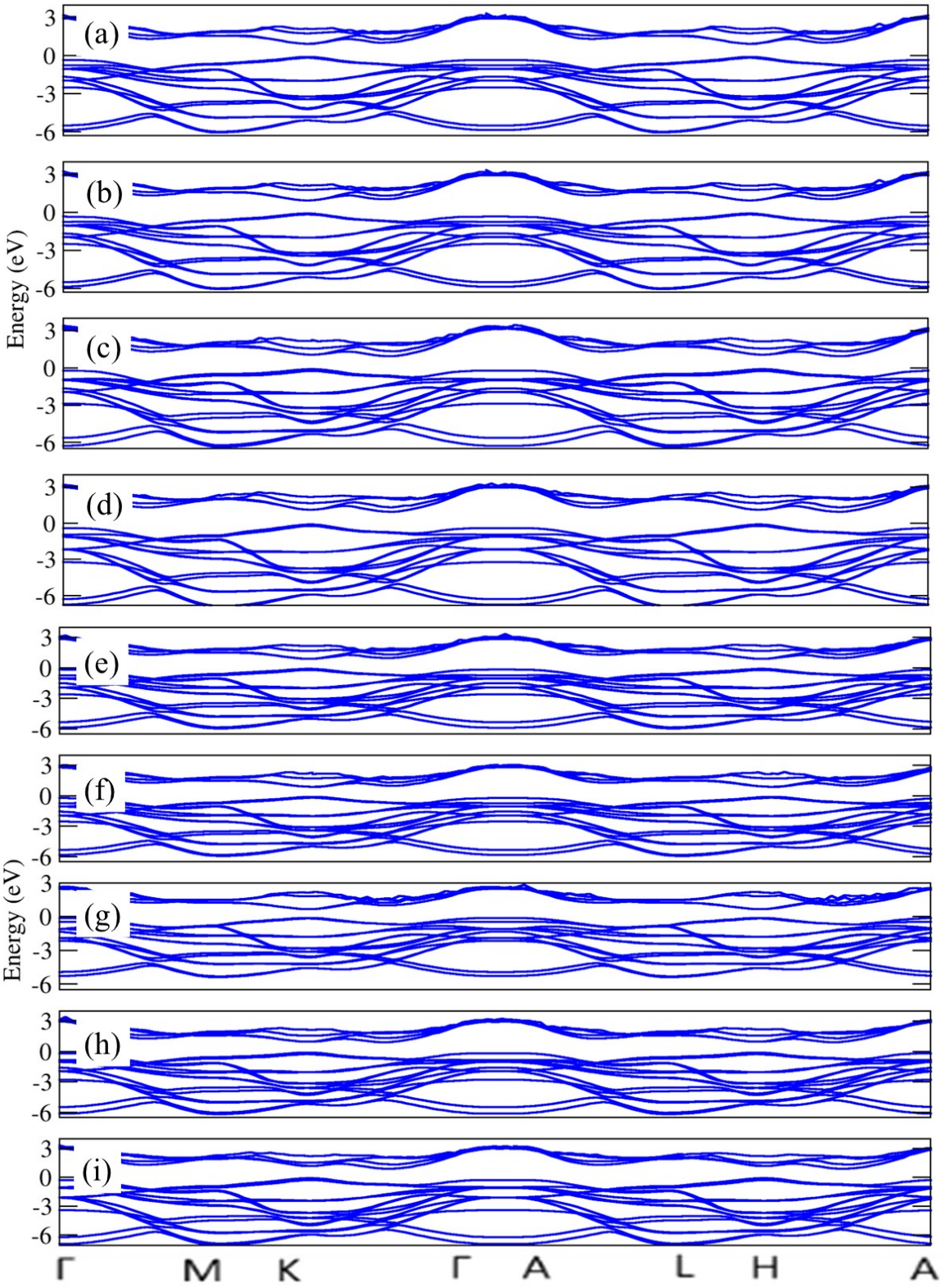


Figure S11: Band structures of 1T phase of WTe_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

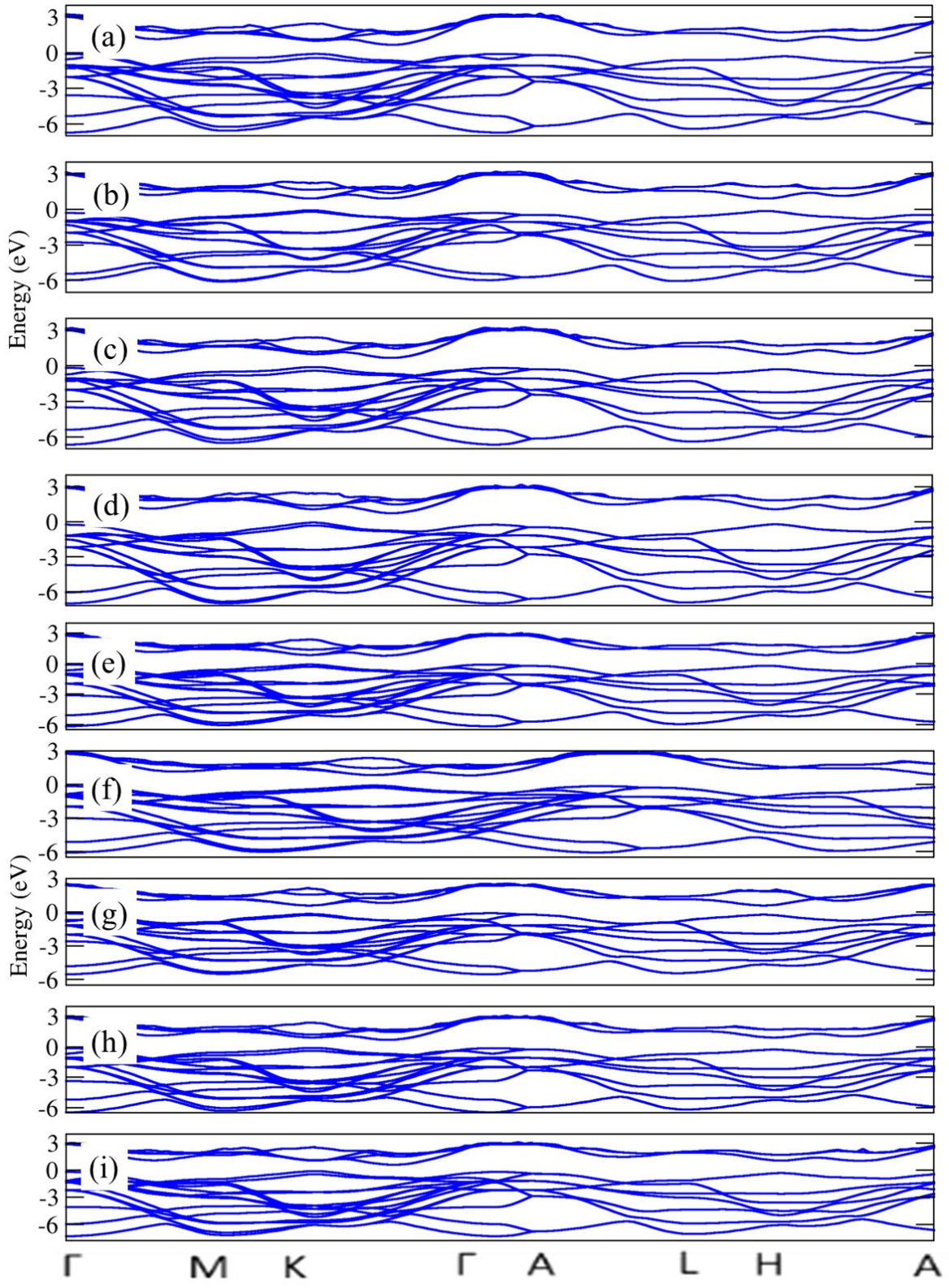


Figure S12: Band structures of 2H phase of WTe_2 for all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10.

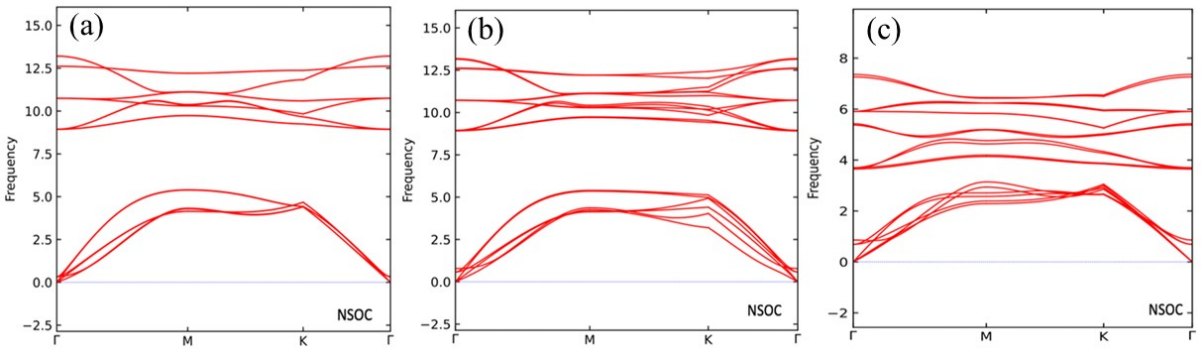


Figure S13: Phonon dispersion plot for 1T phase of WS_2 (a), 2H phase of WS_2 (b), and 2H phase of WTe_2 (c) for PBESol XC functional in absence of SOC.

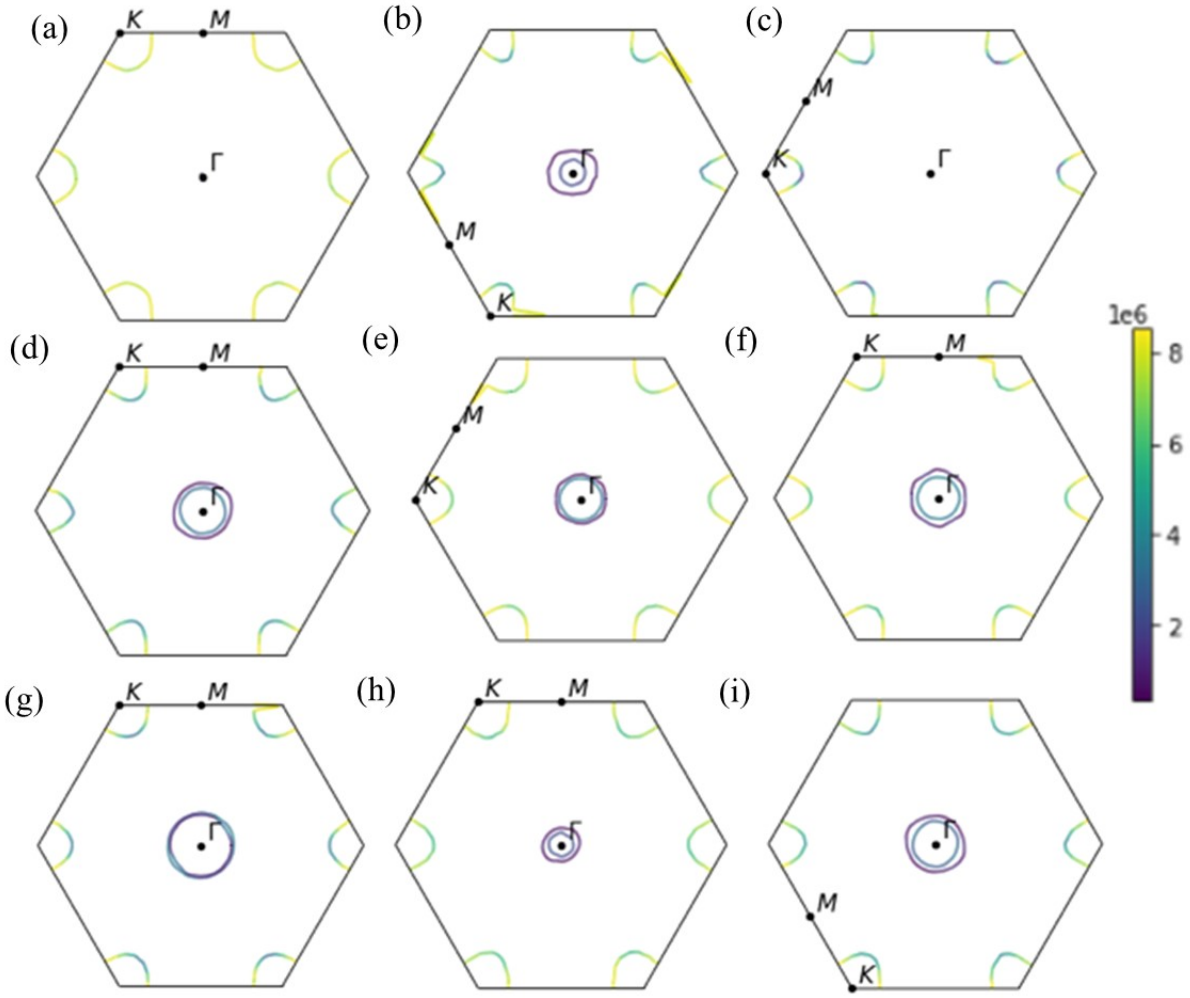


Figure S14: Fermi surface plots for 1T phase of MoS_2 all 09 XC functional (a) LDA, (b) PBE, (c) PBESol, (d) SCAN, (e) optB88-vdW, (f) optPBE-vdW, (g) vdW-DF2, (h) rev-vdW-DF2 and (i) SCAN+rVV10 in absence of SOC.

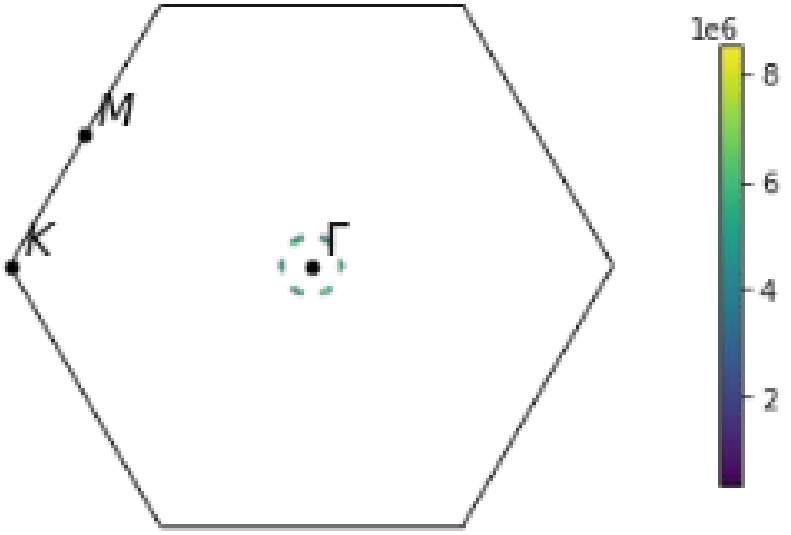


Figure S15: Fermi surface plots for 1T phase of WTe_2 for PBESol XC functional in absence of SOC.