Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

2D-Double Transition Metal MXenes for Spintronics Applications: Surface Functionalization Induced Ferromagnetic Half-Metallic Complexes

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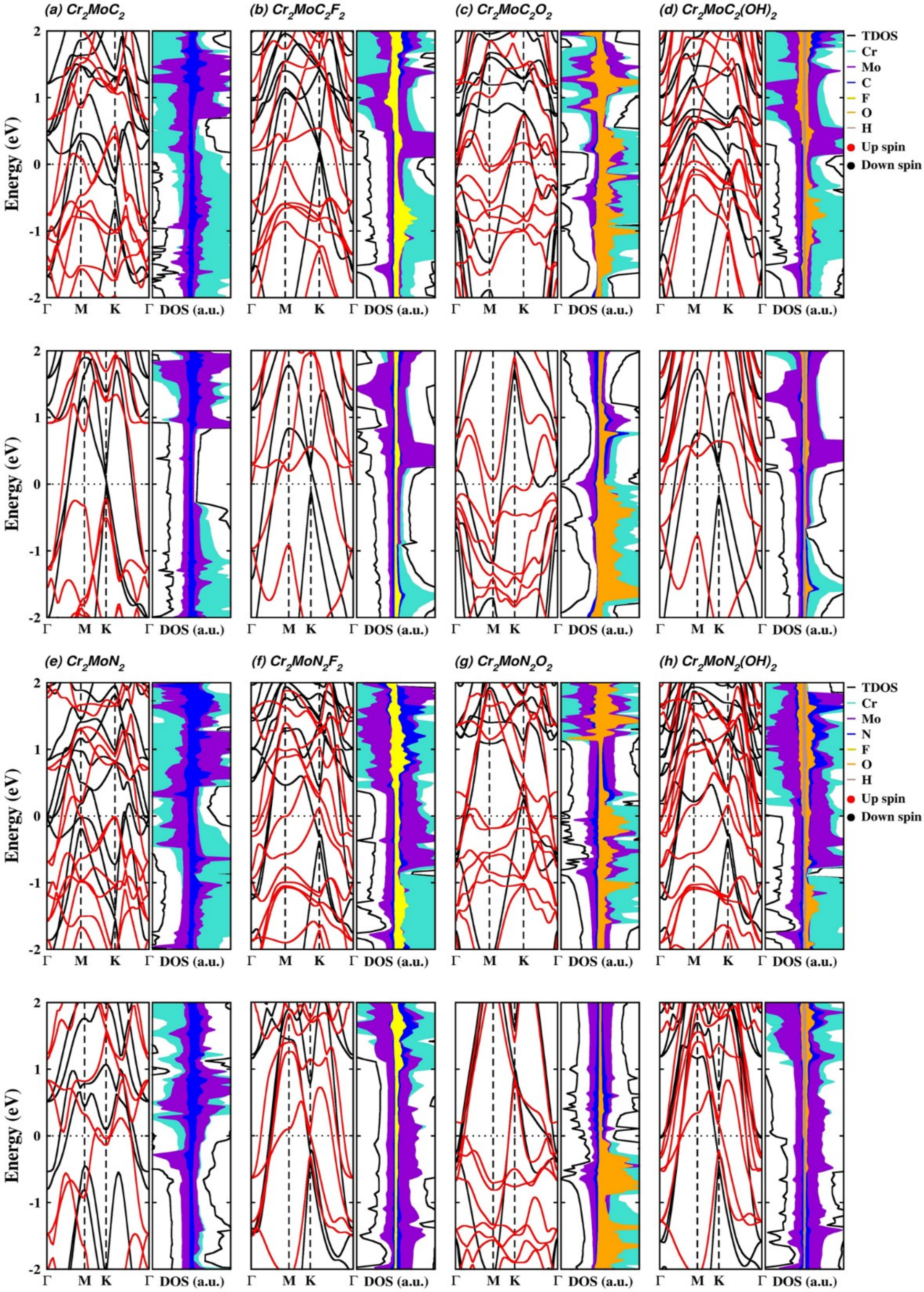

Fig. S1: Electronic spin-polarized band structures along with projected density of states (PDOS) of pristine Cr_2MoX_2 and functionalized $Cr_2MoX_2T_2$ (where X = C/N, and T = –F/–OH/=O) MXenes. Top row (PBE) and 2nd row (HSE06) for pristine and functionalized Cr_2MoC_2 systems [(a)-(d)]. 3rd row (PBE), and bottom row (HSE06) for pristine and functionalized Cr_2MoN_2 systems [(e)-(h)]. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

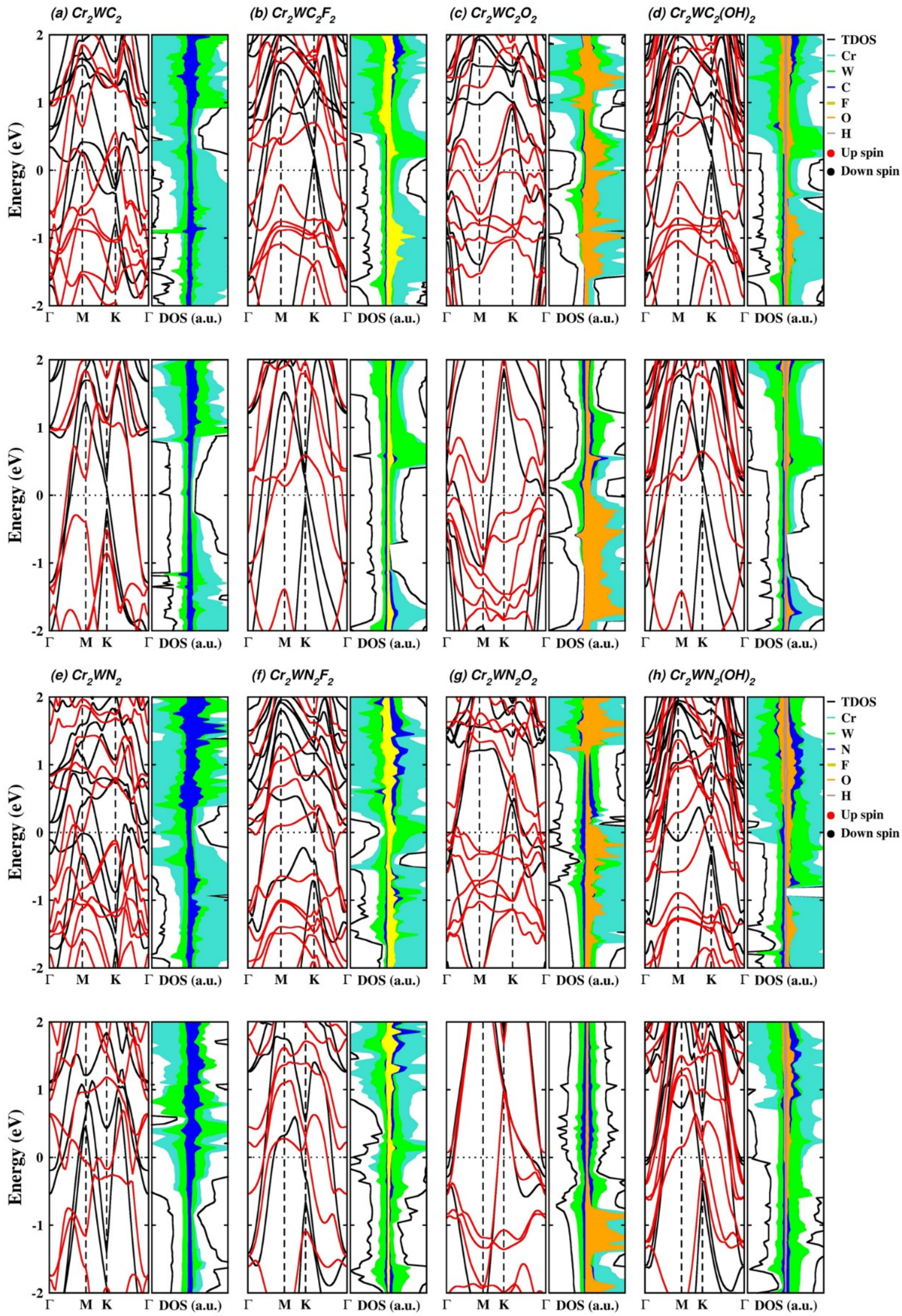

Fig. S2: Electronic spin-polarized band structures and projected density of states (PDOS) of pristine Cr_2WX_2 and functionalized $Cr_2WX_2T_2$ (where X = C/N, and T = –F/–OH/=O) MXenes. Top row (PBE) and 2nd row (HSE06) for pristine and functionalized Cr_2WC_2 systems [(a)-(d)]. 3rd row (PBE), and bottom row (HSE06) for pristine and functionalized Cr_2WN_2 systems [(e)-(h)]. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

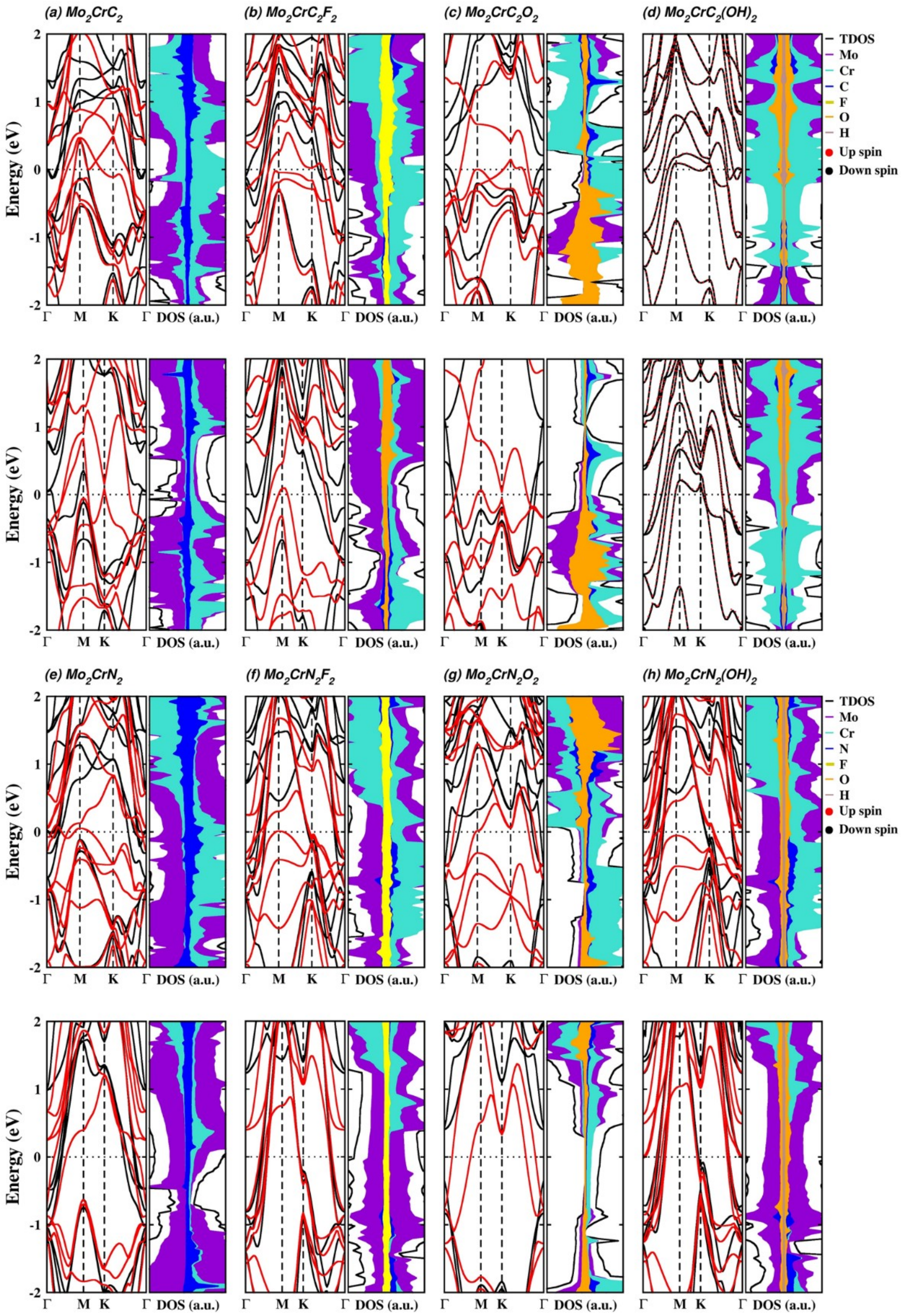

Fig. S3: Electronic spin-polarized band structures and projected density of states (PDOS) of pristine Mo_2CrX_2 and functionalized $Mo_2CrX_2T_2$ (where X = C/N, and T = –F/–OH/=O) MXenes. Top row (PBE) and 2nd row (HSE06) for pristine and functionalized Mo_2CrC_2 systems [(a)-(d)]. 3rd row (PBE), and bottom row (HSE06) for pristine and functionalized Mo_2CrN_2 systems [(e)-(h)]. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

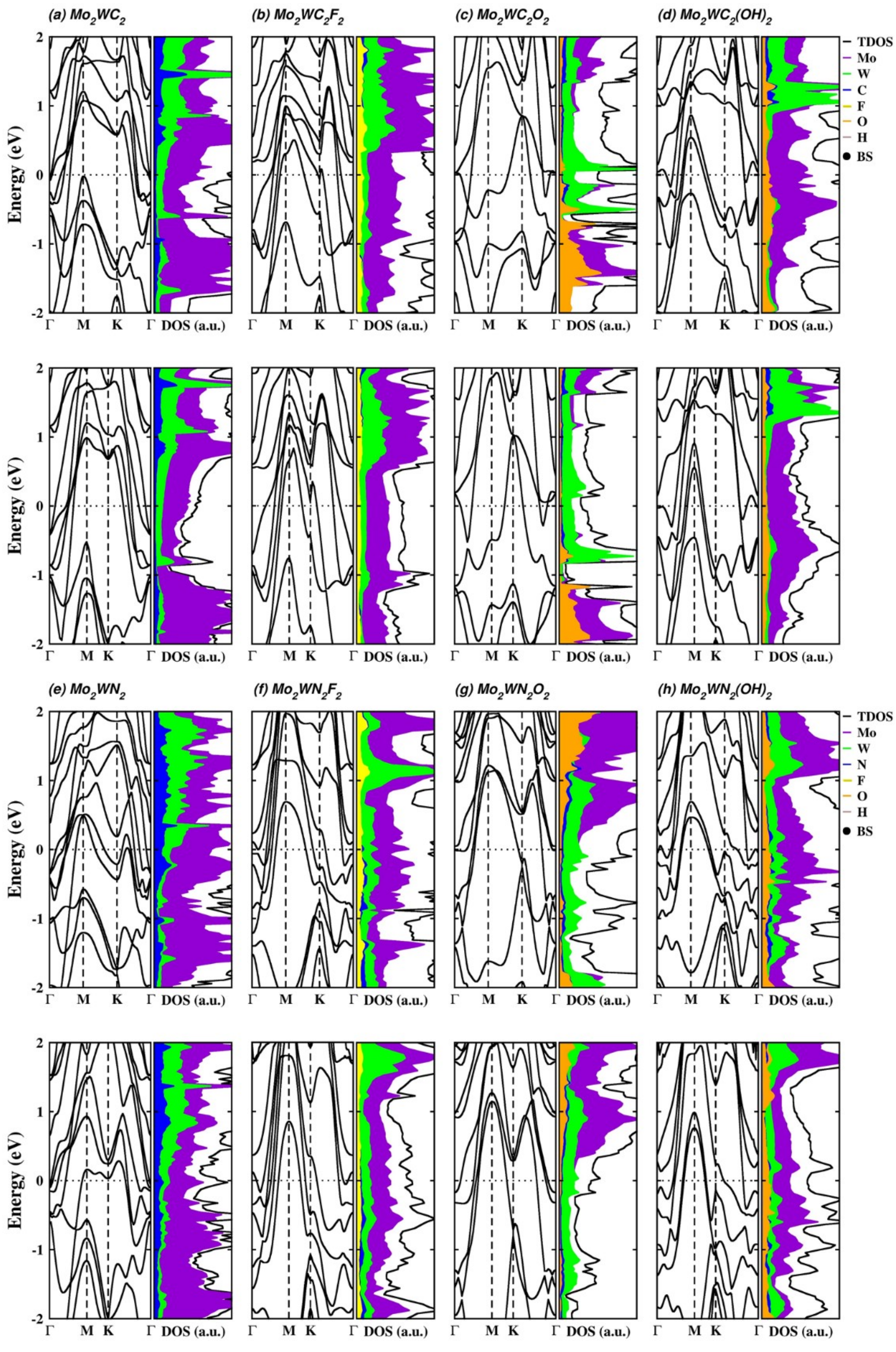

Fig. S4: Electronic spin-polarized band structures and projected density of states (PDOS) of pristine Mo_2WX_2 and functionalized $Mo_2WX_2T_2$ (where X = C/N, and T = –F/–OH/=O) MXenes. Top row (PBE) and 2nd row (HSE06) for pristine and functionalized Mo_2WC_2 systems [(a)-(d)]. 3rd row (PBE), and bottom row (HSE06) for pristine and functionalized Mo_2WN_2 systems [(e)-(h)]. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

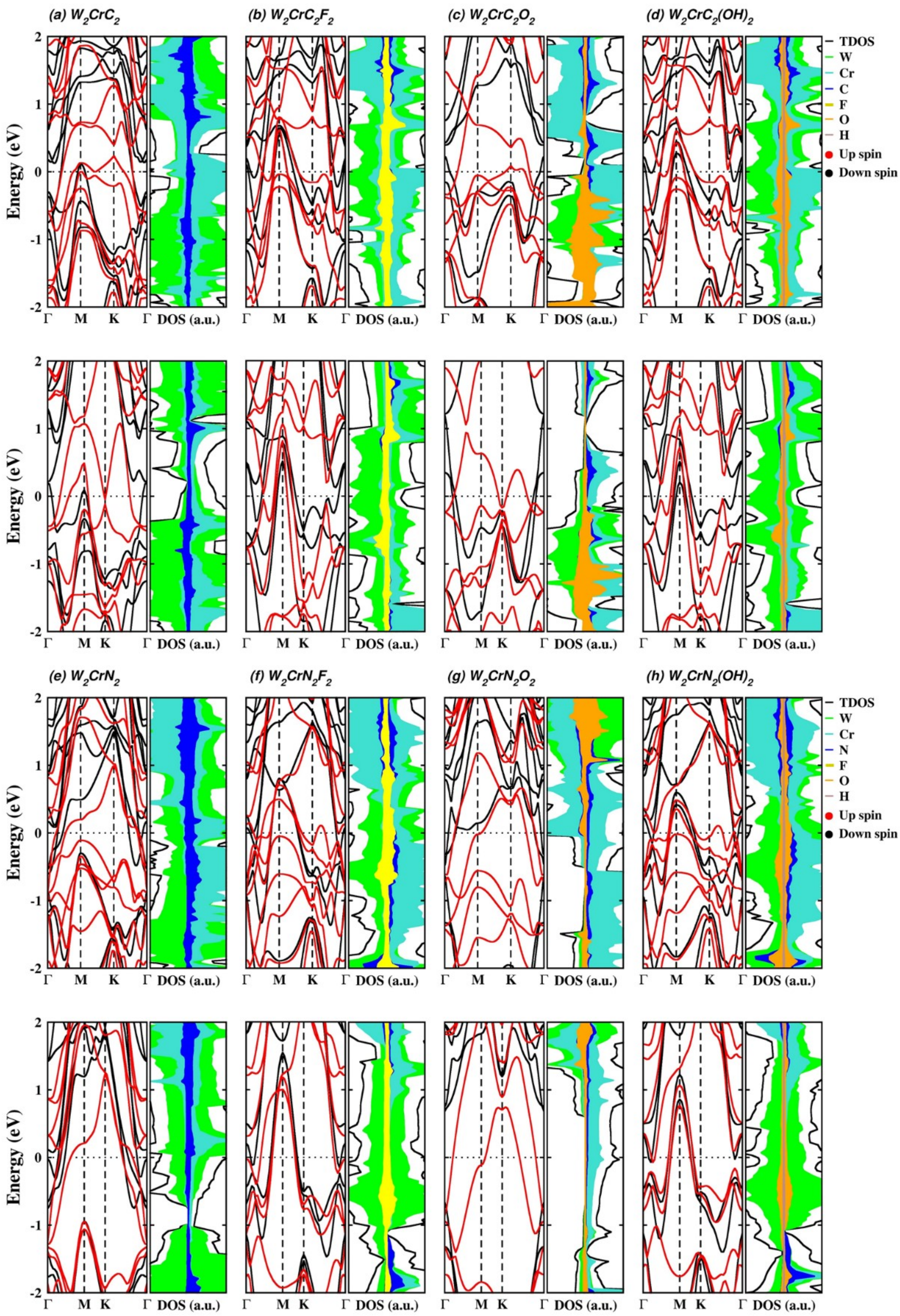

Fig. S5: Electronic spin-polarized band structures and projected density of states (PDOS) of pristine W_2CrX_2 and functionalized $W_2CrX_2T_2$ (where X = C/N, and T = –F/–OH/=O) MXenes. Top row (PBE) and 2nd row (HSE06) for pristine and functionalized W_2CrC_2 systems [(a)-(d)]. 3rd row (PBE), and bottom row (HSE06) for pristine and functionalized W_2CrN_2 systems [(e)-(h)]. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

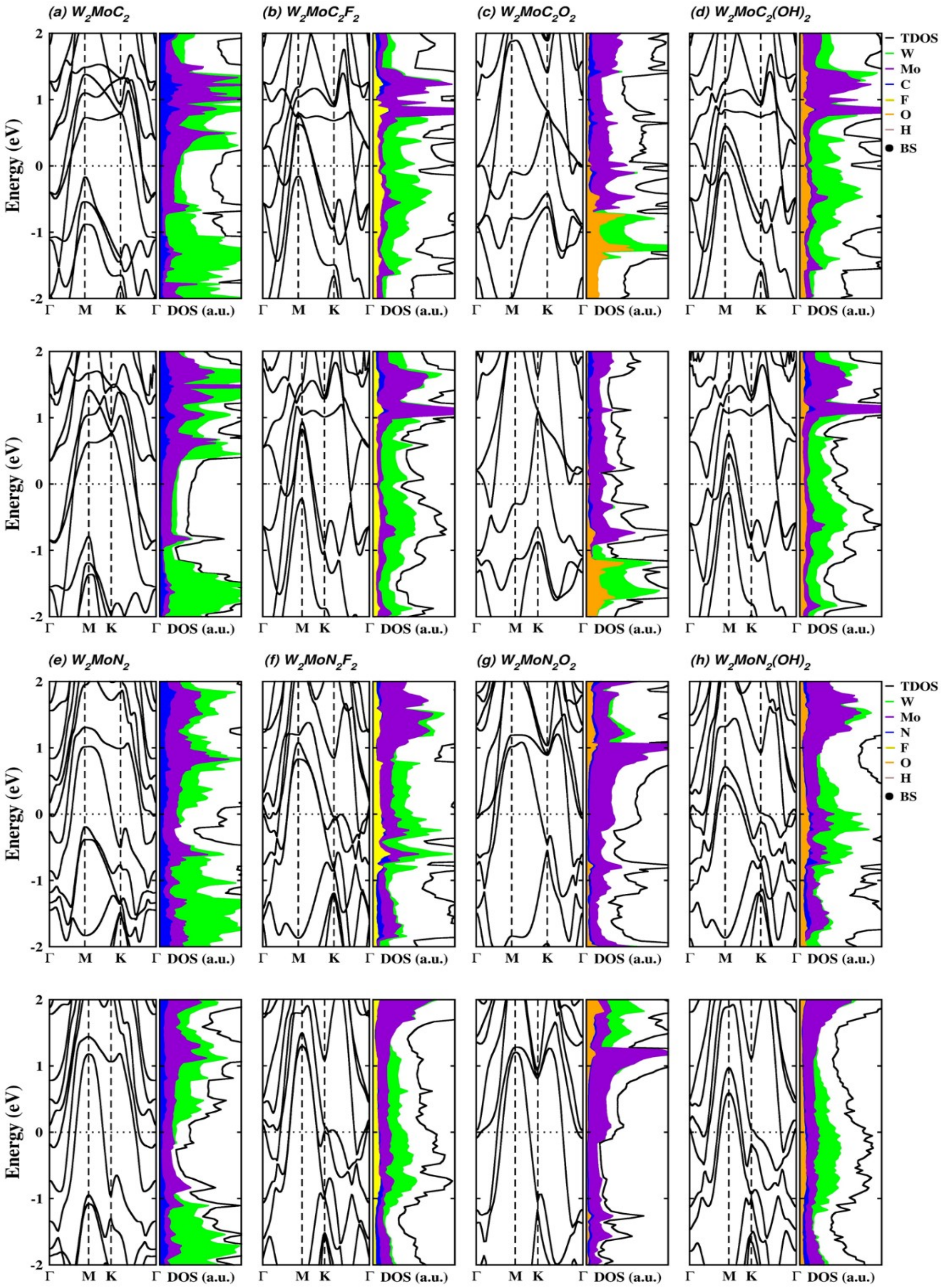

Fig. S6: Electronic spin-polarized band structures and projected density of states (PDOS) of pristine W_2MoX_2 and functionalized $W_2MoX_2T_2$ (where X = C/N, and T = –F/–OH/=O) MXenes. Top row (PBE) and 2[nd] row (HSE06) for pristine and functionalized W_2MoC_2 systems [(a)-(d)]. 3[rd] row (PBE), and bottom row (HSE06) for pristine and functionalized W_2MoN_2 systems [(e)-(h)]. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

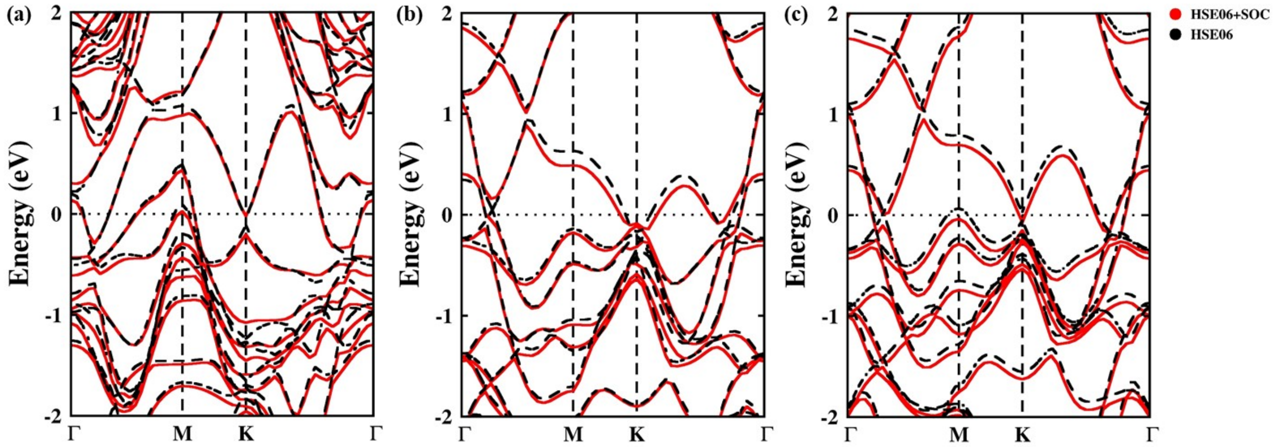

Fig. S7: Electronic band structures for (a) W_2CrC_2 (b) $W_2CrC_2O_2$ and (c) $Mo_2CrC_2O_2$ systems with (HSE06+SOC) and without (HSE06) spin orbit coupling effect. The red and dashed black bands are representing with and without spin orbit coupling effect electronic bands structure, respectively. The Fermi energy is shifted to zero and indicated by the horizontal dashed black line.

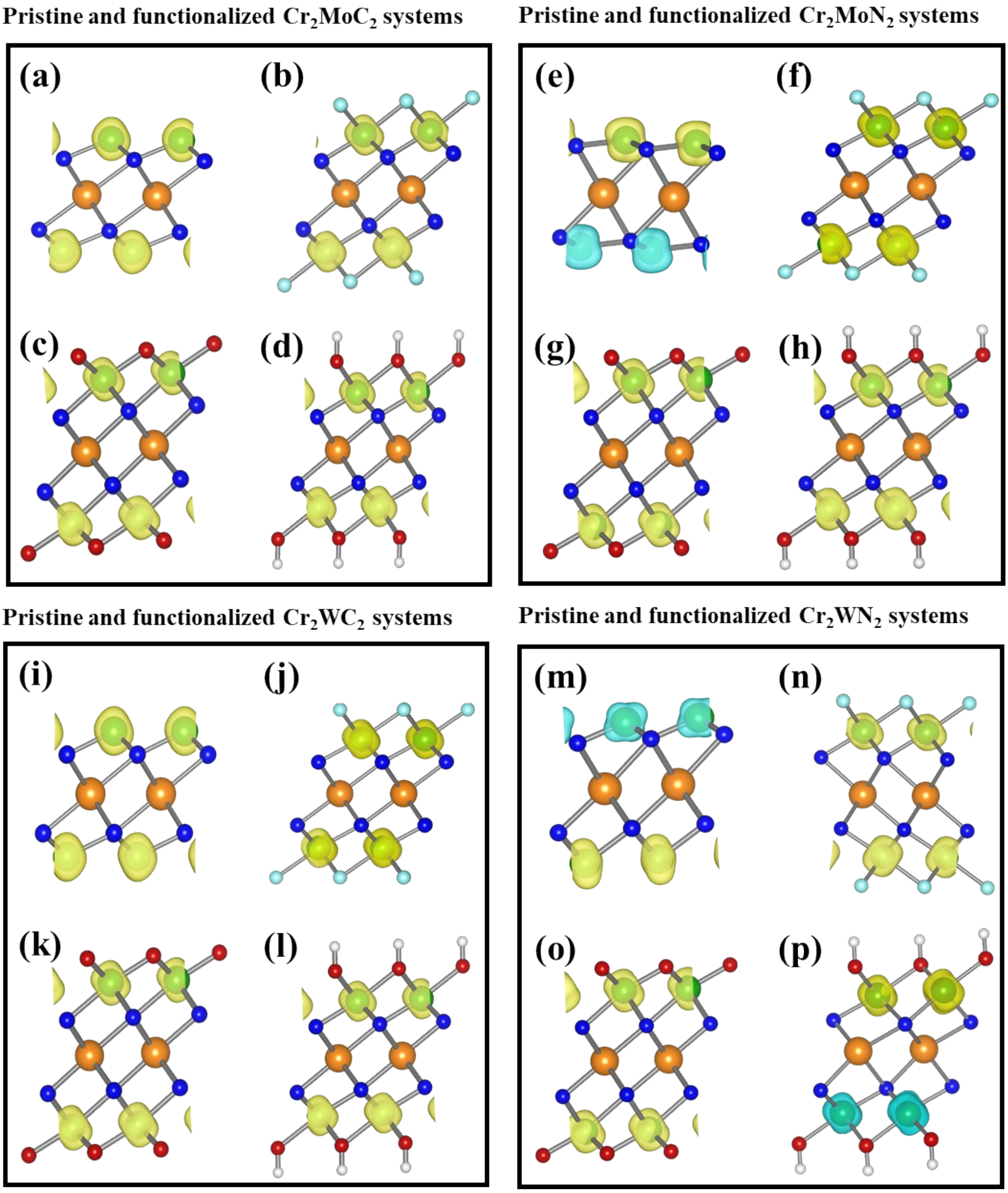

Fig. S8: Magnetic spin density distributions ($\Delta\rho = \rho\uparrow - \rho\downarrow$) side view for pristine $Cr_2M''X_2$ and functionalized $Cr_2M''X_2T_2$ (where M′′= Mo/W, X = C/N, and T = –F/–OH/=O) MXenes. Top panel [(a)-(h)] for (a) Cr_2MoC_2, (b) $Cr_2MoC_2F_2$, (c) $Cr_2MoC_2O_2$, (d) $Cr_2MoC_2(OH)_2$, (e) Cr_2MoN_2, (f) $Cr_2MoN_2F_2$, (g) $Cr_2MoN_2O_2$, (h) $Cr_2MoN_2(OH)_2$ MXenes. Bottom panel [(i)-(p)] for (i) Cr_2WC_2, (j) $Cr_2WC_2F_2$, (k) $Cr_2WC_2O_2$, (l) $Cr_2WC_2(OH)_2$, (m) Cr_2WN_2, (n) $Cr_2WN_2F_2$, (o) $Cr_2WN_2O_2$, and (p) $Cr_2WN_2(OH)_2$ MXenes. The yellow, and cyan isosurfaces indicate up and down spin densities, respectively.

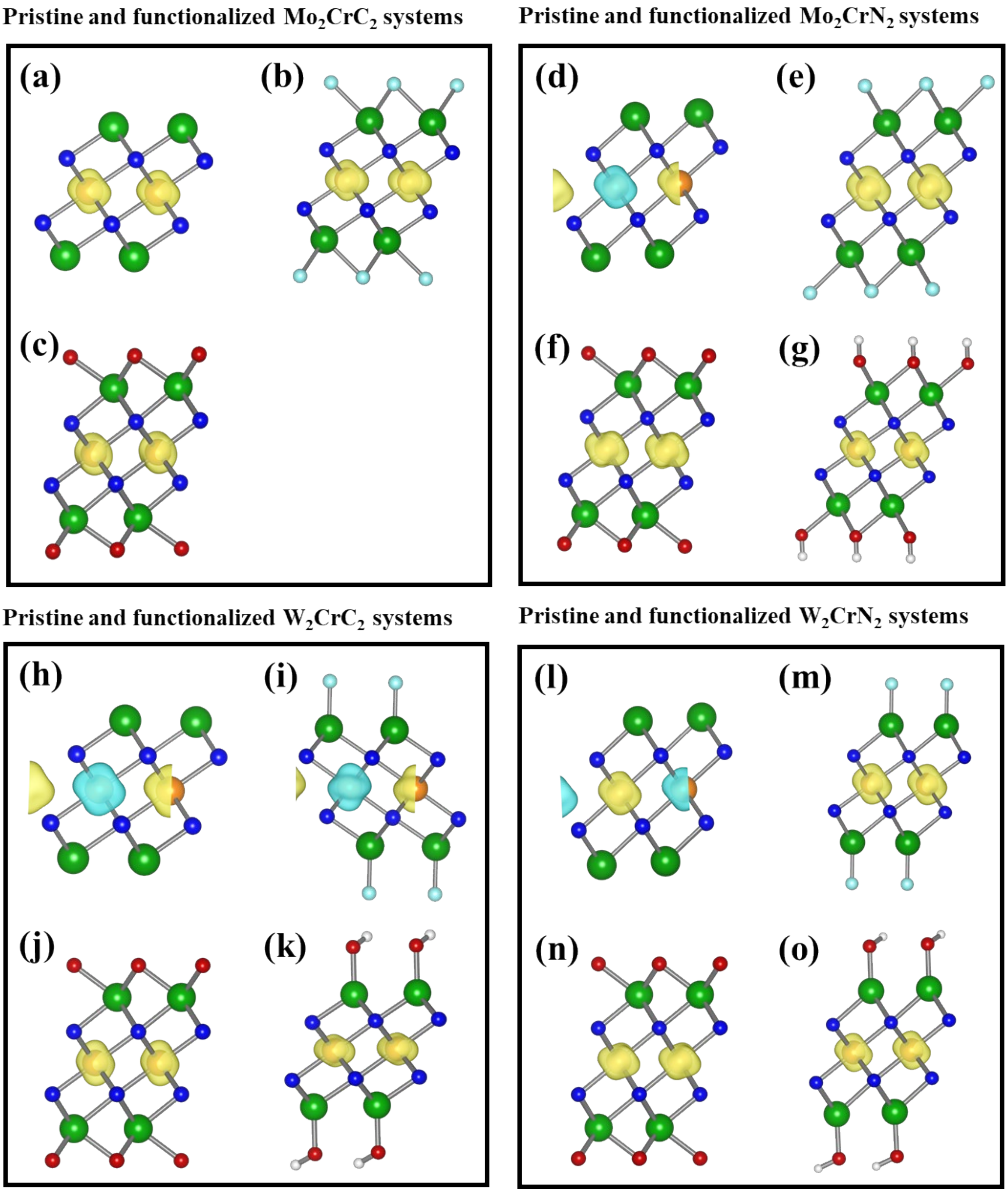

Fig. S9: Magnetic spin density distributions ($\Delta\rho = \rho\uparrow - \rho\downarrow$) side view for pristine M'_2CrX_2 and functionalized $M'_2CrX_2T_2$ (where M′= Mo/W, X = C/N, and T = –F/–OH/=O) MXenes. Top panel [(a)-(g)] for (a) Mo_2CrC_2, (b) $Mo_2CrC_2F_2$, (c) $Mo_2CrC_2O_2$, (d) Mo_2CrN_2, (e) $Mo_2CrN_2F_2$, (f) $Mo_2CrN_2O_2$, (g) $Mo_2CrN_2(OH)_2$ MXenes. Bottom panel [(h)-(o)] for (h) W_2CrC_2, (i) $W_2CrC_2F_2$, (j) $W_2CrC_2O_2$, (k) $W_2CrC_2(OH)_2$, (l) W_2CrN_2, (m) $W_2CrN_2F_2$, (n) $W_2CrN_2O_2$, and (o) $W_2CrN_2(OH)_2$ MXenes. The yellow and cyan isosurfaces indicate up and down spin densities, respectively.

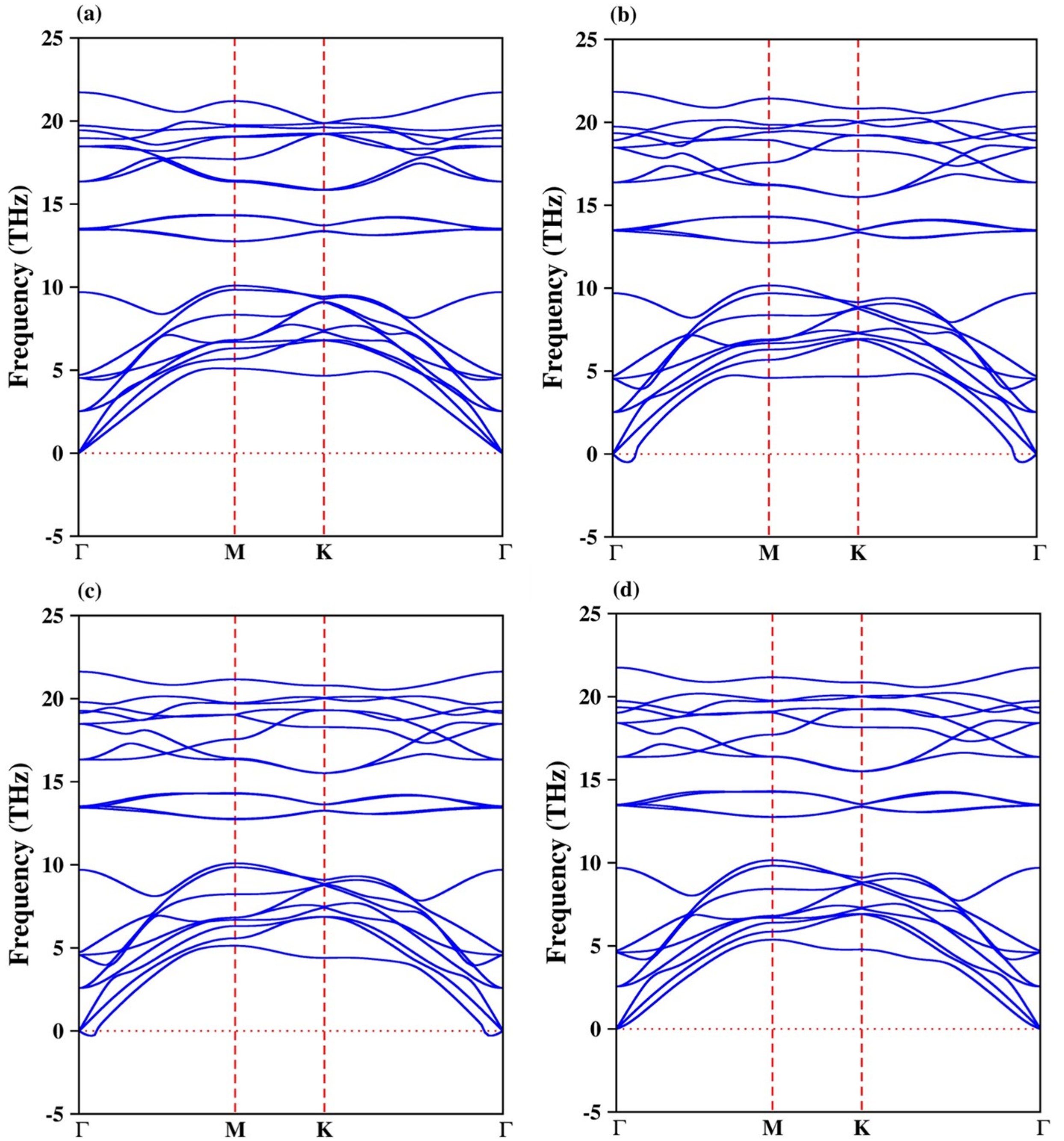

Fig. S10: The phonon dispersion calculated within PBE for $Mo_2CrC_2O_2$ (H_XH_X) MXenes (a) 2x2x1, (b) 3x3x1, (c) 4x4x1, and (d) 5x5x1 supercell. H_XH_X indicating, hollow site of C/N top for top and bottom surface of MXenes.

Table S1: Calculated relative energies (E_R in eV) for passivation of functional groups (T = –F/–OH/=O) at different sites of MXene surfaces (Model I-IV) without (w/o) and with vdW dispersion correction, magnetic moment at ferromagnetic state (MM in μ_B/unit cell), and magnetic energy difference $\Delta E = E_{AFM}$-E_{FM} (eV) for $Cr_2MoX_2T_2$ and $Cr_2WX_2T_2$ (X = C/N) systems with four modelled structures calculated with PBE.

Surface termina-ting group	**Models**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**
		$Cr_2MoC_2T_2$			**$Cr_2WC_2T_2$**		
-F	H_XH_X	0.00 (0.000)	4.69	1.195	0.02 (0.004)	4.72	1.188
	H_MH_X	0.74 (0.649)	4.72	0.435	0.00 (0.000)	4.71	1.209
	H_MH_M	0.03 (0.002)	4.69	1.169	0.09 (0.032)	4.71	1.119
	T_MT_M	0.97 (0.895)	2.92	0.061	1.10 (1.022)	3.11	0.067
-O	H_XH_X	0.54 (0.411)	0.00	—	0.69 (0.567)	0.00	—
	H_MH_X	0.39 (0.332)	1.74	0.264	0.86 (0.471)	0.01	0.062
	H_MH_M	0.00 (0.000)	4.24	0.041	0.00 (0.000)	4.27	0.834
	T_MT_M	1.36 (1.400)	0.00	—	1.54 (1.510)	0.03	0.083
-OH	H_XH_X	0.98 (1.008)	4.47	0.222	1.06 (1.062)	4.54	0.279
	H_MH_X	0.50 (0.507)	4.61	0.618	0.52 (0.533)	4.66	0.684
	H_MH_M	0.00 (0.000)	4.58	1.018	0.00 (0.000)	4.65	0.981
	T_MT_M	0.29 (0.453)	2.89	0.152	0.43 (0.578)	3.05	0.144

Surface termina-ting group	**Models**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**
		$Cr_2MoN_2T_2$			**$Cr_2WN_2T_2$**		
-F	H_XH_X	0.03 (0.006)	6.32	1.061	0.23 (0.238)	6.42	0.914
	H_MH_X	0.00 (0.000)	6.31	1.073	0.00 (0.000)	5.60	0.867
	H_MH_M	0.02 (0.025)	6.31	1.050	0.24 (0.233)	6.42	0.894
	T_MT_M	1.54 (1.540)	2.20	-0.002	1.70 (1.722)	2.44	0.108
-O	H_XH_X	0.64 (0.649)	0.00	—	0.91 (0.925)	0.00	—
	H_MH_X	0.58 (0.627)	3.04	0.339	0.73 (0.775)	2.50	0.409
	H_MH_M	0.00 (0.000)	5.39	1.044	0.00 (0.000)	5.65	1.177
	T_MT_M	2.90 (2.896)	0.00	—	3.33 (3.426)	0.00	—
-OH	H_XH_X	0.27 (0.213)	4.95	0.116	1.09 (0.267)	4.26	-0.393
	H_MH_X	0.18 (0.100)	6.16	0.513	0.68 (0.126)	5.11	0.478
	H_MH_M	0.00 (0.000)	6.17	0.867	0.00 (0.000)	5.91	-0.099
	T_MT_M	0.92 (0.895)	2.21	0.030	0.84 (0.887)	2.26	-0.271

Table S2: Calculated relative energies (E_R in eV) for passivation of functional groups (T = –F/–OH/=O) at different sites of MXene surfaces (Model I-IV) without (w/o) and with vdW dispersion correction, magnetic moment at ferromagnetic state (MM in μ_B/unit cell), and magnetic energy difference $\Delta E = E_{AFM}$-E_{FM} (eV) for $Mo_2CrX_2T_2$ and $Mo_2WX_2T_2$ (X = C/N)

Surface termina-ting group	**Models**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**	**E_R w/o vdW (E_R with vdW)**	**MM**
		$Mo_2CrC_2T_2$			**$Mo_2WC_2T_2$**	
-F	H_XH_X	0.07 (0.050)	1.85	0.086	0.00 (0.000)	0.00
	H_MH_X	0.00 (0.000)	1.78	0.178	0.14 (0.133)	0.00
	H_MH_M	0.19 (0.024)	0.00	–	0.09 (0.095)	0.00
	T_MT_M	0.43 (0.275)	0.95	-0.060	0.04 (0.076)	0.00
-O	H_XH_X	0.00 (0.000)	2.02	0.178	0.00 (0.000)	0.00
	H_MH_X	0.59 (0.627)	1.88	0.242	0.65 (0.669)	0.00
	H_MH_M	1.17 (1.242)	1.53	0.093	1.07 (1.087)	0.00
	T_MT_M	2.77 (2.908)	2.24	0.220	2.76 (2.697)	0.00
-OH	H_XH_X	0.00 (0.000)	0.00	–	0.19 (0.138)	0.00
	H_MH_X	0.18 (0.254)	1.52	0.174	0.26 (0.244)	0.00
	H_MH_M	0.39 (0.552)	1.29	0.257	0.35 (0.294)	0.00
	T_MT_M	0.08 (0.247)	0.88	0.041	0.00 (0.000)	0.00
Surface termina-ting group	**Models**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**	**E_R w/o vdW (E_R with vdW)**	**MM**
		$Mo_2CrN_2T_2$			**$Mo_2WN_2T_2$**	
-F	H_XH_X	0.63 (0.579)	1.66	0.512	0.00 (0.000)	0.00
	H_MH_X	0.00 (0.000)	2.92	0.502	0.70 (0.102)	0.00
	H_MH_M	0.01 (0.001)	2.92	0.439	0.70 (0.102)	0.00
	T_MT_M	0.39 (0.459)	2.25	0.585	0.96 (0.913)	0.00
-O	H_XH_X	0.00 (0.000)	3.54	0.144	0.00 (0.000)	0.00
	H_MH_X	0.43 (0.417)	2.64	-0.067	0.43 (0.459)	0.00
	H_MH_M	1.19 (1.131)	2.71	0.320	1.29 (1.109)	0.00
	T_MT_M	3.13 (3.168)	2.29	0.385	2.86 (2.975)	0.00
-OH	H_XH_X	0.93 (0.411)	0.00	–	0.37 (0.439)	0.00
	H_MH_X	0.24 (0.231)	2.62	0.535	0.11 (0.269)	0.00
	H_MH_M	0.00 (0.000)	2.83	0.599	0.02 (0.317)	0.00
	T_MT_M	0.14 (0.172)	2.40	0.548	0.00 (0.000)	0.00

systems with four modeled structures calculated with PBE.

Table S3: Calculated relative energies (E_R in eV) for passivation of functional groups (T = –F/–OH/=O) at different sites of MXene surfaces (Model I-IV) without (w/o) and with vdW dispersion correction, magnetic moment at ferromagnetic state (MM in μ_B/unit cell), and magnetic energy difference $\Delta E = E_{AFM}-E_{FM}$ (eV) for $W_2CrX_2T_2$ and $W_2MoX_2T_2$ (X = C/N) systems with four modeled structures calculated with PBE.

Surface termina-ting group	**Models**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**	**E_R w/o vdW (E_R with vdW)**	**MM**
		$W_2CrC_2T_2$			**$W_2MoC_2T_2$**	
-F	H_XH_X	0.25 (0.309)	1.77	0.148	0.44 (0.482)	0.00
	H_MH_X	0.35 (0.307)	0.01	0.042	0.41 (0.473)	0.00
	H_MH_M	0.38 (0.326)	0.01	0.013	0.42 (0.472)	0.00
	T_MT_M	0.00 (0.000)	1.19	-0.051	0.00 (0.000)	0.00
-O	H_XH_X	0.00 (0.000)	2.03	0.158	0.00 (0.000)	0.00
	H_MH_X	0.68 (0.707)	1.87	0.209	0.82 (0.813)	0.00
	H_MH_M	1.30 (1.361)	1.21	0.113	1.42 (1.379)	0.00
	T_MT_M	2.84 (2.984)	2.29	0.259	2.88 (2.801)	0.00
-OH	H_XH_X	0.39 (0.250)	2.28	0.169	0.57 (0.604)	0.00
	H_MH_X	0.97 (0.610)	0.00	—	0.51 (0.468)	0.00
	H_MH_M	1.19 (1.048)	1.35	0.162	0.29 (0.279)	0.00
	T_MT_M	0.00 (0.000)	1.32	0.096	0.00 (0.000)	0.00
Surface termina-ting group	**Models**	**E_R w/o vdW (E_R with vdW)**	**MM**	**ΔE**	**E_R w/o vdW (E_R with vdW)**	**MM**
		$W_2CrN_2T_2$			**$W_2MoN_2T_2$**	
-F	H_XH_X	0.73 (0.654)	3.12	-0.231	0.40 (0.466)	0.00
	H_MH_X	0.81 (0.691)	0.03	0.008	0.36 (0.337)	0.00
	H_MH_M	0.87 (0.783)	0.00	—	0.94 (0.319)	0.00
	T_MT_M	0.00 (0.000)	2.75	0.492	0.00 (0.000)	0.00
-O	H_XH_X	0.00 (0.000)	3.56	0.153	0.00 (0.000)	0.00
	H_MH_X	0.66 (0.641)	2.69	0.366	0.91 (0.830)	0.00
	H_MH_M	1.60 (1.548)	2.75	0.358	1.81 (1.720)	0.00
	T_MT_M	3.27 (3.298)	2.39	0.382	3.58 (3.456)	0.00
-OH	H_XH_X	1.31 (1.197)	0.01	-1.509	1.09 (1.082)	0.00
	H_MH_X	1.04 (0.931)	2.86	0.491	0.82 (0.783)	0.00
	H_MH_M	0.80 (0.755)	3.01	0.506	1.09 (0.557)	0.00

T_MT_M	0.00 (0.000)	2.72	0.598	0.00 (0.000)	0.00

Data S1: Representative input file (INCAR) for geometry optimization calculation with VASP software package by considering PBE functional. Each line giving individual statement for electronic optimization, and ionic relaxation.

```
#------------------System_Initial------------------
SYSTEM = MXene
ISTART = 0
ICHARG = 2
#------------------Convergence_Criteria----------
ENCUT = 400
LWAVE = .FALSE.
LREAL = .FALSE.
PREC = ACCURATE
ISMEAR = 0
SIGMA = 0.05
ISPIN = 2
NSW = 1000
ISIF = 3
IBRION = 2
NPAR = 4
```

Data S2: Representative input file (INCAR) for phonon calculation with VASP software package by considering PBE functional.

```
#------------------System_Initial-------------
SYSTEM = MXene
ISTART = 0
ICHARG = 2
#------------------Convergence_Criteria--------
EDIFF = 1E-6
ENCUT = 520
LWAVE = .FALSE.
LREAL = .FALSE.
LCHARG = .FALSE.
ADDGRID = .TRUE.
PREC = ACCURATE
ISMEAR = 1
SIGMA = 0.15
ISPIN = 2
MAGMOM = 50*1 50*1 25*4 50*1   ## NIONS vary with size of the supercell
NSW = 0
IBRION = -1
NPAR = 7
NELM = 200
ISYM = 0
NSIM = 8
```

Data S3: Relaxed geometries (CONTCAR) for 36 stable MXenes using VASP.

(1) $Cr_2MoC_2\_F_2$ (H_XH_X)

```
1.00000000000000
  3.0194730233058147   0.0108539064169124   0.2918603538733978
 -1.5037811454865952   2.6237183715436037  -0.2928616431855917
  2.9606693337342955  -1.9535371773001933  17.3838289465346811
C  Cr  Mo  F
2  2   1   2
Direct
0.1194396958149564  0.1693358689781292  0.2976186392154802
0.9413409858524147  0.3250139136849980  0.1401196160221075
0.7333849419436294  0.5655323876281098  0.3533093964489956
0.3300509017649078 -0.0716338848329798  0.0844047675543398
0.5320693059304588  0.7486674929430002  0.2189144305194618
0.3242334808838775 -0.0204445166479224  0.4258029291521790
0.7292306858097475  0.5120386822466600  0.0117201890874381
```

(2) $Cr_2MoC_2\_O_2$ (H_MH_M)

```
1.00000000000000
  2.9598016074086977   0.0001294751763667  -0.0159568213784646
 -1.4813202887517949   2.5618581313615745   0.0154869636016760
  0.0871480041214914  -0.1776521112038440  26.1958376399060739
C  Cr  Mo  O
2  2   1   2
Direct
0.1930761077387415  0.0784565747661857  0.2690541127926327
0.8567623340500105  0.4052649067069106  0.1687767496568261
0.8692821331062793  0.4106448266403501  0.3168901367484552
0.2002408560293898  0.0578956315122822  0.1209554475047660
0.5129029870734659  0.7510393465485256  0.2189423698071800
0.5338039391215369  0.7469605873168456  0.3516613478553254
0.5262116228805777  0.7290580625088988  0.0861097976348180
```

(3) $Cr_2MoC_2\_(OH)_2$ (H_MH_M)

```
1.00000000000000
```

```
   3.0567902819097985  -0.0016172912086575  -0.0161164416581772
  -1.5314333418193813   2.6441524652413482   0.0114311341463493
   0.1069298802025813  -0.2395672859522881  28.6487503518898130
 C   Cr   Mo   O    H
 2    2    1   2    2
Direct
 0.1959526194282371  0.0790692453178504  0.2654806724620090
 0.8573890335660891  0.4055593382194673  0.1742042859270105
 0.8638492741608379  0.4141155812363082  0.2977282044548590
 0.1894627170855080  0.0694406808867405  0.1415117227621897
 0.5268511204710323  0.7421216577247461  0.2199032586574130
 0.5348224638363938  0.7518976316365765  0.3406490843250859
 0.5200417688140400  0.7332939431644292  0.0984272259120632
 0.5486593863019362  0.7616486845111096  0.3745288084859072
 0.5020416483359261  0.7486832853027675  0.0646766850134616
```

(4) Cr_2MoN_2_F_2 (H_MH_X)

```
  1.00000000000000
   2.9742931160769444  -0.0041096748836750  -0.1443387239282156
  -1.4919052459824909   2.5858776823476926  -0.0018441216688113
  -0.9883680580331934  -1.0853584017909526  20.7008627066536093
 N   Cr   Mo   F
  2    2    1   2
Direct
 0.3602683433634011  0.1744728747538881  0.2870004018249818
 0.8763713506470792  0.4060482336549092  0.1484034080661537
 0.0780736807092199  0.5423749198971660  0.3360743545264526
 0.1591438036577398  0.0395506536260177  0.0989529044482292
 0.6109417309997665  0.7850498765723449  0.2174701648970881
-0.1921112791672815 -0.0823043105359659  0.3939543629172935
 0.4375123527900744  0.6709677080316390  0.0410643453198023
```

(5) Cr_2MoN_2_O_2 (H_MH_M)

```
  1.00000000000000
   2.9086887927084666   0.0023455572990920  -0.0341579871781104
  -1.4621686528419409   2.5169185336942284   0.0084300689702202
   0.1069966059623223  -0.0774774935235882  23.7125557719056808
 N   Cr   Mo   O
  2    2    1   2
Direct
 0.2490523726755754  0.2215262719465850  0.2481146917089875
 0.9051392402845710  0.5476130554191224  0.1336501167621903
```

```
0.9204870474252156  0.5580982713677733  0.3036792650796401
0.2344270585993006  0.2108998868575251  0.0781126722939640
0.5780417500977474  0.8846984173056966  0.1908996363346655
0.5909654181693168  0.8936199556614939  0.3415219828663195
0.5639971687482790  0.8752542574418064  0.0403316839542238
```

(6) $Cr_2MoN_2\_(OH)_2$ (H_MH_M)

```
  1.00000000000000
    2.9922972893810069    0.0001809684054022   -0.0163524874786575
   -1.4975843046677575    2.5921504762168048    0.0120798149851357
    0.0906232890790099   -0.2247250512891717   26.4919591092428703
  N    Cr   Mo   O    H
   2    2    1   2    2
Direct
  0.1962504986449595  0.0859103576723487  0.2729961278124594
  0.8558914041445427  0.4101548539699346  0.1664866224350111
  0.8661310072275565  0.4223305574799776  0.3116770791475098
  0.1860254260836008  0.0745794941287580  0.1276745713969569
  0.5267800283688978  0.7496890859976858  0.2197080434130121
  0.5353298930786878  0.7575948969274028  0.3562029915250972
  0.5171066578661121  0.7364573572591725  0.0830716158868955
  0.5278519882461401  0.7507822230603151  0.3929372802503049
  0.5277031283395033  0.7183312215044019  0.0463556161327517
```

(7) $Cr_2WC_2\_F_2$ (H_MH_X)

```
  1.00000000000000
    3.0421441137850387   -0.0046168858022502   -0.1630332238016560
   -1.5274809875490496    2.6346954280774040   -0.0057631910629097
   -0.9570525101531792   -0.9662650488680817   17.5163704941593110
  C    Cr   W    F
   2    2   1    2
Direct
  0.3572837246085680  0.1708956951915646  0.2930376568991265
  0.8818962444231149  0.4132139601562380  0.1421478665490490
  0.0742747488508077  0.5366764569979663  0.3474381381649529
  0.1655083672936730  0.0473353933392172  0.0876320569707024
  0.6197573828449566  0.7915929986644337  0.2176387265249684
 -0.1981738024872589 -0.0918891821717981  0.4179720535665383
  0.4296533174661380  0.6683346338223778  0.0170534433246644
```

(8) $Cr_2WC_2\_O_2$ (H_MH_M)

```
  1.00000000000000
    2.9788542630154247   -0.0002326615809175   -0.0153602832448907
   -1.4911749813620416    2.5792682720838944    0.0142804657010741
```

0.0931534059280480 -0.1886431929588830 26.1868029324750147
C Cr W O
2 2 1 2
Direct
0.1907433771905257 0.0806663929031478 0.2681863860117122
0.8547400661566502 0.4066608174203419 0.1697190122768444
0.8732459920048798 0.4069882205649991 0.3160596031679176
0.2033823417971101 0.0555032252824617 0.1216917240599102
0.5075447012717894 0.7556721859666022 0.2189605332890497
0.5344963283140287 0.7461883209408413 0.3505570599609403
0.5281271732650187 0.7276407729216047 0.0872156432336289

(9) Cr_2WC_2_$(OH)_2$ (H_MH_M)
1.00000000000000
3.0581745762254977 -0.0018081793876647 -0.0166407017721858
-1.5322896280507610 2.6466603975277554 0.0117504436076580
0.1023165925024946 -0.2392492249549623 28.6852343801914493
C Cr W O H
2 2 1 2 2
Direct
0.1956346717197941 0.0792309610165515 0.2648174653437195
0.8576107010325223 0.4055012178678123 0.1744272118557983
0.8641369258458640 0.4142948004229189 0.2979983990592098
0.1893033544096145 0.0694100830263005 0.1413825845365747
0.5264855803447076 0.7424632044846903 0.2196064020766245
0.5351398519280099 0.7517153615080701 0.3408869363603369
0.5198951310037715 0.7336009020769333 0.0984858114231385
0.5483773278167322 0.7614447830676692 0.3747889985686110
0.5024864878989841 0.7481687345290500 0.0647161387759861

(10) Cr_2WN_2 F_2 (H_MH_X)
1.00000000000000
2.9244640698208686 0.0132248006028707 -0.2329388713731469
-1.4552478141816962 2.5365777555913551 0.2325954598582269
-1.7990278207399069 0.9198383821455168 22.6565945197397660
N Cr W F
2 2 1 2
Direct
0.3414581531758745 -0.0707542019607121 0.2818873253014664
0.8958363211123140 0.3662450420233130 0.1537013690971859
0.7178557719487050 0.5570951660225775 0.3302649723848399
0.1871251933247064 0.0715916764940173 0.1053546983659641
0.6144338665905141 0.6518033705353120 0.2159375196754988
0.0993491963592930 0.1794291039784031 0.3843807783615706

```
0.4741414804885934  0.7807497989070876  0.0513932788134757
```

(11) Cr_2WN_2_O_2 (H_MH_M)

```
  1.00000000000000
    2.9123786122883404    0.0001539044100996   -0.0268149798443073
   -1.4659618427849215    2.5184289392100938    0.0026903109510550
    0.1712535417009408   -0.0963439959125969   23.9285987267878539
  N    Cr   W    O
   2    2    1    2
Direct
  0.2498255483816884  0.2212114011791978  0.2466382536469763
  0.9056116523003369  0.5486829513741712  0.1351849132389906
  0.9218927648386019  0.5573504593431076  0.3041204387513190
  0.2327936238387277  0.2109773771267351  0.0776565212515293
  0.5772733542851263  0.8851810426888047  0.1909131697167369
  0.5909276229922481  0.8933343545455688  0.3410073590938854
  0.5637854893632765  0.8749725297424178  0.0407893933005534
```

(12) Cr_2WN_2_$(OH)_2$ (H_MH_M)

```
  1.00000000000000
    2.9899851138447882   -0.0010222027326404   -0.0161473974968597
   -1.4974750023592380    2.5898373897329128    0.0113956116649227
    0.1035107334998055   -0.2350091260358458   28.6972061037665149
  N    Cr   W    O    H
   2    2    1    2    2
Direct
  0.1975966384049578  0.0811424873594501  0.2673761994983666
  0.8546248325434476  0.4091533754910839  0.1714682551894309
  0.8677642650481256  0.4166110330994531  0.3046687066683931
  0.1851476287787165  0.0729962421145079  0.1347279537599458
  0.5280126944907110  0.7428805257982466  0.2194391005517270
  0.5370558366589538  0.7534438697165996  0.3453424125463576
  0.5151040116332877  0.7373771122268893  0.0943941493920601
  0.5401446591215375  0.7565324521272028  0.3792837430771271
  0.5136194653202635  0.7356929500665619  0.0604094273165909
```

(13) Mo_2CrC_2_F_2 (H_MH_X)

```
  1.00000000000000
    2.9679305371783502   -0.0255671378091718   -0.1131652737068239
   -1.5075916181173785    2.5566719482917835    0.1125814228908506
   -0.7506326346122515    0.3052182028564713   21.6781121766917195
  C    Mo   Cr   F
   2    2    1    2
Direct
```

```
0.1768808999038275  0.0940353828596949  0.2728540255880242
0.8009514822281816  0.4615453024990148  0.1622487100514595
0.8657566865825436  0.4095417025235997  0.3290649245453935
0.1041248714167482  0.1539378400005493  0.1062034547863806
0.4881762356222244  0.7784549081106288  0.2185956300098354
0.2324535517924203  0.0483072846294797  0.3976689678781675
0.6618562554540539  0.5903375353770318  0.0362842291407409
```

(14) $Mo_2CrC_2\_O_2$ (H_XH_X)

```
 1.00000000000000
   2.9127283337619838    0.0006052630092376   -0.0054000980748417
  -1.4574103145826991    2.5219285662496489    0.0031055651716204
   0.2197827052903442   -0.2607921515705078   24.6156797055470378
 C    Mo   Cr   O
 2     2    1   2
Direct
0.1955941961213418  0.0850198659126497  0.2681710225134262
0.8633486838776386  0.4081304774644515  0.1695131044215530
0.8629710788169808  0.4247554546419873  0.3220126134446884
0.1984157856971235  0.0701609411589931  0.1156585606266663
0.5270665580068811  0.7448229365053122  0.2188412045802054
0.1963166041144398  0.0968427868631898  0.3713550114320490
0.8660370913655938  0.3987774814534120  0.0663384509814063
```

(15) $Mo_2CrC_2\_(OH)_2$ (H_XH_X)

```
 1.00000000000000
   2.9551836975286139   -0.0040589408615725   -0.0042961925849719
  -1.4826940963525517    2.5551634571866488    0.0017434330582069
   0.2217269243411139   -0.2674243597296734   27.7449550361706905
 C    Mo   Cr   O    H
 2     2    1   2    2
Direct
0.1999756101796344  0.0871879325236573  0.2623437724944069
0.8645998823423067  0.4120706520677174  0.1766023109346419
0.8658217069604852  0.4252252622893538  0.3064548456091137
0.1968382799889475  0.0736192212254667  0.1324882693004092
0.5340585171908188  0.7500482856757209  0.2194416763965397
0.1981395203093730  0.0961721849090969  0.3574454977409783
0.8632464037577789  0.4030277791896380  0.0815675742174253
0.1981937490700429  0.0932679504205425  0.3928990024243019
0.8705962912006000  0.4111007186988008  0.0460469958821831
```

(16) $Mo_2CrN_2\_F_2$ (H_MH_X)

```
 1.00000000000000
```

```
2.8505191093052047    0.0035679621503344    0.1203447424322376
-1.4242678512748910    2.4724710645780119   -0.1246864851103163
1.3300217063632265   -0.9391822526181156   24.7697394706260141
N    Mo   Cr   F
2     2     1   2
Direct
0.1177535376426385  0.1628071986220019  0.2694585538591243
0.8392236004440640  0.4254618933143721  0.1682623577466447
0.7575448492048810  0.5309380220234309  0.3244300664482694
0.2048893992555536  0.0556742209504283  0.1132062971591684
0.4859917711492521  0.7928740712877246  0.2187695922067266
0.3843986110800499 -0.0901782094980814  0.3857563056983606
0.5688282102235618  0.6808927623001241  0.0520267798817092
```

(17) Mo_2CrN_2_O_2 (H_XH_X)

```
1.00000000000000
2.8810515440279749    0.0061213431664169    0.0087722504226989
-1.4457528674633608    2.4911168643091153   -0.0093905761697199
0.4144506110124115    0.0108253223820867   21.0001722157750770
N    Mo   Cr   O
2     2     1   2
Direct
0.2199509959956426  0.2731224377988160  0.2962564693536437
0.9021110607586926  0.6078140569590108  0.1735883351763276
0.8761672253809127  0.6076656200371598  0.3600683341082240
0.2457987411070736  0.2734447470884330  0.1097924820550407
0.5654493104372098  0.9375001828632701  0.2349809876654563
0.9219781624509297  0.6055646607198868  0.0526974396411672
0.2002045528695476  0.2753184505334292  0.4171759690001369
```

(18) Mo_2CrN_2_$(OH)_2$ (H_MH_M)

```
1.00000000000000
2.8914682416682660   -0.0041143335920487   -0.0254974326206795
-1.4508058476189867    2.5015445678114405    0.0211007965675573
-0.0284098746516607   -0.1524438719111458   26.7033710265827864
N    Mo   Cr   O    H
2     2     1   2     2
Direct
0.1985090811120470  0.0785283797804402  0.2652337527692896
0.8534240869850711  0.4108815093678852  0.1740775785149554
0.8745559328798266  0.4100196747697429  0.3164614125990372
0.1783510298409903  0.0801770888484501  0.1229433318088360
0.5248998298251039  0.7460791154495798  0.2197130227427747
0.5435055248088907  0.7479555446103932  0.3705163145749629
```

```
0.5109535267782875  0.7412196846166287  0.0688617156148214
0.5215315530786840  0.7735101961846415  0.4069004343441465
0.5333394666910989  0.7174588543722333  0.0324023850311751
```

(19) Mo_2WC_2_F_2 (H_XH_X)

```
  1.00000000000000
    3.0483628251964485  -0.0377511985246832   0.1303960080720092
   -1.5587856491976539   2.6190171945339187  -0.1304225336367184
    1.4898796552192564  -0.9718583022550447  23.6422508098756019
  C   Mo   W   F
   2    2   1   2
Direct
  0.1676955553441953  0.1142376587097624  0.2749255459124728
  0.8913990167737432  0.3800331764610550  0.1627504046376424
  0.8189485341164480  0.4679755449792394  0.3233140238614063
  0.2423155222305222  0.0267524479296431  0.1143474926520801
  0.5296431340725737  0.7460827942518815  0.2187774861699717
  0.2446549172184048  0.0474386356583695  0.3889972092851163
  0.8150933182441061  0.4459896860100451  0.0487778054813119
```

(20) Mo_2WC_2_O_2 (H_XH_X)

```
  1.00000000000000
    2.9113559213125115   0.0000751708663267  -0.0021975001001110
   -1.4571688105607685   2.5200692177614070  -0.0004633291760816
    0.2579294019352728  -0.2883831023801108  26.9070051631350218
  C   Mo   W   O
   2    2   1   2
Direct
  0.1958270690470237  0.0850968562685080  0.2710012814858642
  0.8632031482794627  0.4081302304470389  0.1666746064196657
  0.8626567499341374  0.4242840137213129  0.3211792268306690
  0.1975397755458326  0.0698387164592681  0.1165023173852777
  0.5294509833756676  0.7464037035453785  0.2188584900871673
  0.1957102360435760  0.0966023739734741  0.3663904865763299
  0.8653620357742923  0.3981540495850153  0.0712835592150279
```

(21) Mo_2WC_2_$(OH)_2$ (T_MT_M)

```
  1.00000000000000
    3.0366699624141682  -0.0039663584098953   0.0658522532957345
   -1.5218501201181358   2.6377503328346994   0.0322312165165011
    0.8538566694311811   0.4693526247388432  26.7039445524386423
  C   Mo   W   O   H
   2    2   1   2   2
Direct
```

```
  0.1651310490373846  0.0215693171922354  0.2655883439482930
  0.8991480663375084  0.3953609941648671  0.1681654460015915
  0.8065871924168406  0.3440059648631335  0.3093765019740154
  0.2635515957246758  0.0847025371857656  0.1245401264559939
  0.5331309123305724  0.7101876773259772  0.2168088473575677
  0.7635315233298413  0.2996659460869763  0.3823579054445906
  0.3151670465565177  0.1129469208275228  0.0517916597162364
  0.9767672725710596  0.6240539096165835  0.3980666808135160
  0.0054852326955981  0.0515466397369384  0.0362344122881983
```

(22) $Mo_2WN_2\_F_2$ (H_XH_X)

```
   1.00000000000000
     2.8138659315810952    0.0185266846240602   -0.0112841531624515
    -1.4008804698978625    2.4088779339300883    0.2987010393422840
     0.0604467227970783    3.1354726463010483   22.6238693271372568
   N    Mo   W    F
     2     2   1     2
Direct
  0.2797964067241776  0.2530757048762545  0.2996771998791266
  0.8197102428415393  0.3187630280729052  0.1446972816270467
  0.8728778026239687  0.4459564238281864  0.3589486313627938
  0.2291086956956050  0.1397550788963078  0.0795860041960063
  0.3985685439554411  0.4860997542596048  0.2105451057402947
  0.4572707022552003  0.6118852247012992  0.4275217888868472
  0.6524176039040598 -0.0270252706345627  0.0109139563078860
```

(23) $Mo_2WN_2\_O_2$ (H_XH_X)

```
   1.00000000000000
     2.8374493803295677   -0.0049084244782584    0.0029619870437912
    -1.4184915215224816    2.4600485209586371   -0.0019265175348771
     0.1916599580663285   -0.2513239619473481   23.7984173138130259
   N    Mo   W    O
     2     2   1     2
Direct
  0.2113621340125803  0.0966649630145744  0.2824533629420866
  0.8743995938772915  0.4178219234746732  0.1551086052701595
  0.8654292291160102  0.4280428202967140  0.3412640228873901
  0.2001282837563388  0.0702894251178346  0.0964227392723875
  0.4921185429591801  0.7166768949445388  0.2188990223806637
  0.1969291546794097  0.1005550197725681  0.3928629591500282
  0.8693730665991903  0.3984690503790977  0.0448792920972747
```

(24) $Mo_2WN_2\_(OH)_2$ (T_MT_M)

```
   1.00000000000000
     2.8402522642995747   -0.0047118586327211    0.0597650298177147
    -1.4257273253277332    2.4661367707613429    0.0187262373284937
     0.8589128051506812    0.3451442428243934   28.3510379937947086
   N    Mo   W    O    H
     2     2    1    2    2
Direct
  0.1450182849802906 -0.0058385843952194  0.2691349930460498
  0.8994739204899577  0.3790682260404413  0.1648399518285232
  0.7773188507826727  0.3386782588028157  0.3193413791300900
  0.2770419510874855  0.0936721445860371  0.1144269523384698
  0.5318818455475574  0.7445067055175977  0.2169367571323223
  0.7280277775012053  0.3233231743371460  0.3872080084443488
  0.3345367551444169  0.1306105687753732  0.0467144528429272
  0.0523380714638072  0.6175429067019961  0.4012300610570316
 -0.0171375659973950  0.0224765066338122  0.0330973681802401
```

(25) W_2CrC_2_F_2 (T_MT_M)

```
   1.00000000000000
     3.0054912609749329   -0.0011020595323671   -0.0069634004256382
    -1.5053116513772637    2.6013176425358218    0.0092142820670801
     0.1991177016379197   -0.2103688724279944   27.4347679613102358
   C    W    Cr   F
     2    2     1    2
Direct
  0.1918810481454369  0.0755281827541978  0.2601366674635803
  0.8592884047168344  0.4050446802654692  0.1752659225469046
  0.8586811020651010  0.4098185205551184  0.3021945837805285
  0.1923958267500837  0.0698036549792635  0.1332359499182647
  0.5254389696257695  0.7404503451555161  0.2176914004189222
  0.8584825061037308  0.4105955293139576  0.3706256677414904
  0.1925520815930402  0.0645290189764719  0.0647597561303128
```

(26) W_2CrC_2_O_2 (H_XH_X)

```
   1.00000000000000
     2.9032949271834885    0.0013045509995570   -0.0051968028629703
    -1.4520833092542278    2.5140990311113511    0.0029112944169149
     0.2206896071075969   -0.2607968218407347   24.6598911680438775
   C    W    Cr   O
     2    2     1    2
Direct
  0.1956552324743639  0.0850502116369395  0.2683811219806857
  0.8633602850967428  0.4081533199035965  0.1693000125826529
  0.8628652913002229  0.4248167446156170  0.3221296992681755
```

```
0.1984579172167334  0.0700557343351441  0.1155508696298184
0.5272253973931684  0.7449479940601433  0.2188426631193577
0.1962881260104215  0.0967753498016267  0.3718990422301060
0.8658977485083462  0.3987105896469282  0.0657865591891983
```

(27) W_2CrC_2_$(OH)_2$ (T_MT_M)

```
   1.00000000000000
     3.0287747237419795   -0.0093413919622641    0.0660082725467998
    -1.5224557116794908    2.6239519044734947    0.0343434496549689
     0.8448172893380212    0.4094572151178283   26.2000765424494304
   C    W    Cr   O    H
     2    2     1    2     2
Direct
  0.1699946977295806  0.0286530615622716  0.2618476857599365
  0.8946208887760211  0.3994730364144432  0.1724097468963179
  0.8125748526230180  0.3465377914418429  0.3051624137168906
  0.2548089932645371  0.0838486976695598  0.1288611848468700
  0.5342929539255563  0.7170528845433554  0.2170125967831526
  0.7638791279768854  0.2901100641715222  0.3793617285190880
  0.3112677830522507  0.0937141097568927  0.0547358555852345
  0.9696654505174517  0.6164920365355494  0.3956866037826592
  0.0173951431346978  0.0681582249045622  0.0378521081098536
```

(28) W_2CrN_2_F_2 (T_MT_M)

```
   1.00000000000000
     2.8768307190813003    0.0136449029936176   -0.0036141411801608
    -1.4316424885494055    2.4956742951495583    0.0034760394578724
     0.0635902176920363   -0.1063353601031048   23.5678738990266758
   N    W    Cr   F
     2    2     1    2
Direct
  0.1908757300714017  0.0784732908315195  0.2701757611026765
  0.8601721092818463  0.4037192527087941  0.1652281936419339
  0.8556622208998833  0.4145651535184298  0.3291581424057428
  0.1953519102351815  0.0645468695298956  0.1062562369769129
  0.5256891297527525  0.7418116094232103  0.2177005852386253
  0.8574148624491108  0.4117498661119674  0.4080976307449765
  0.1935539313098273  0.0609038538761742  0.0273035058891337
```

(29) W_2CrN_2_O_2 (H_XH_X)

```
   1.00000000000000
     2.8740774553179138    0.0054464761912134    0.0001336915036973
    -1.4428201964595124    2.4848669509598795   -0.0011732492516855
```

0.3508809266806742 0.0435527679844099 21.3113486827809275
N W Cr O
2 2 1 2
Direct
0.2172155689305878 0.2754048886566766 0.2977853049787679
0.9063520317684073 0.6045492913706675 0.1720859976210102
0.8755887949353480 0.6081742905176145 0.3601870509370969
0.2473340967596118 0.2721967047514331 0.1096884837322263
0.5622902515128335 0.9396867271689205 0.2349384789222967
0.9214015061497717 0.6061757570036901 0.0524880059190346
0.2014777989434489 0.2742424965310030 0.4173866948895639

(30) W_2CrN_2_$(OH)_2$ (T_MT_M)
1.00000000000000
2.8930436313489496 0.0017363466442043 0.0506325148255084
-1.4456852202937285 2.4957735088377380 0.0486439888440670
0.7047810319059368 0.6622968949014131 26.8799001734008698
N W Cr O H
2 2 1 2 2
Direct
0.1566420790132269 0.0049111850290903 0.2627195913039720
0.8960051162219251 0.3966424284233239 0.1712296744560682
0.7991715234644019 0.3302382616564851 0.3145398907484545
0.2752290241502535 0.1045422499371888 0.1194249813986834
0.5289967274520928 0.7114645834558372 0.2170360646931243
0.7597807768719920 0.2935301651790825 0.3862455056762524
0.3389815416148147 0.1558308006112816 0.0477482871516448
0.9837609713279591 0.6399608427110878 0.4009397418415092
-0.0100678691166677 0.0069193899966226 0.0330461867302944

(31) W_2MoC_2_F_2 (T_MT_M)
1.00000000000000
3.0321763418085901 -0.0013204640642119 -0.0074650219053059
-1.5188465288956980 2.6239298650463097 0.0090844027680048
0.1920508380721701 -0.2132207404475435 27.1278871087198645
C W Mo F
2 2 1 2
Direct
0.1918277405639556 0.0760374975992351 0.2668764447391355
0.8596567111472325 0.4034162128804728 0.1685491403249794
0.8580429120187437 0.4121912181685952 0.3091028807548662
0.1936231021671794 0.0675265933868121 0.1262804294004217
0.5248355305494677 0.7382663352525072 0.2177096721197991
0.8567279358351541 0.4154780356782672 0.3783194194872182

```
  0.1940060067182638  0.0628540390341050  0.0570719611735837
```

(32) W_2MoC_2_O_2 (H_XH_X)

```
   1.00000000000000
     2.9106671143556846    0.0035470115773323   -0.0052377359090470
    -1.4538319609917871    2.5214186737743569    0.0030680093748030
     0.2236707617992934   -0.2603420011871568   26.2128955145483822
   C    W    Mo   O
     2    2      1    2
Direct
  0.1948048419295817  0.0853288101653538  0.2729820641496680
  0.8629767464137228  0.4070698600932457  0.1648211564674124
  0.8627439347024685  0.4248679912896843  0.3236397436626993
  0.1987799495342889  0.0701780971946423  0.1139202368523103
  0.5259248467815617  0.7439611067797560  0.2187491142672472
  0.1976756508842409  0.0975179426434936  0.3705102723084058
  0.8668440277541276  0.3995861358338191  0.0672673802922588
```

(33) W_2MoC_2_$(OH)_2$ (T_MT_M)

```
   1.00000000000000
     3.0368419232295016   -0.0016366585992540    0.0637794675461221
    -1.5201701657288083    2.6342516145413999    0.0287331675348510
     0.8555320189514132    0.4236245526393939   26.9974652212564443
   C    W    Mo   O    H
     2    2      1    2    2
Direct
  0.1658469811459577  0.0261469150185323  0.2664289875659157
  0.9008250836515194  0.3996642907844943  0.1674243054952627
  0.8079573202005745  0.3454962531072234  0.3088679389235288
  0.2629292553753591  0.0848151860616960  0.1251194842384918
  0.5302297402203459  0.7157075813959933  0.2168789763851259
  0.7644133124659858  0.2944340605113052  0.3808220440691357
  0.3116893713077730  0.0974720116720401  0.0532037672266610
  0.9728954413044887  0.6179459885607083  0.3966656828385152
  0.0117133853279945  0.0623576198880072  0.0375187372573663
```

(34) W_2MoN_2_F_2 (T_MT_M)

```
   1.00000000000000
     2.8217497464229324    0.0142483017272326   -0.0092187952362492
    -1.4000392376723909    2.4498166502193142    0.0097625882655583
     0.1183295967183361   -0.1766940523251262   27.7380489865041717
   N    W    Mo   F
     2    2      1   2
Direct
```

```
0.1893462557060205  0.0791841177713603  0.2717198363470100
0.8614510419539364  0.3985488880790104  0.1637082178708225
0.8556758614925780  0.4164426113874687  0.3230563794077173
0.1953964369651301  0.0625616544946413  0.1123603471581431
0.5251783852789805  0.7437780747448193  0.2177280321159348
0.8570123295691819  0.4146694107919420  0.3901196791650272
0.1946596280341703  0.0605851747307522  0.0452174559353482
```

(35) $W_2MoN_2\_O_2$ (H_XH_X)

```
1.00000000000000
  2.8402603388353604    0.0077590036319767    0.0001325592452846
 -1.4237827360374689    2.4519866368678822   -0.0005718393969076
  0.3515734603853733    0.0480182119371003   23.0821546896869059
N    W    Mo   O
2    2    1    2
Direct
0.2216945241899864  0.2694354159444912  0.3021675753074894
0.9142107990066085  0.5998460585091704  0.1674970701944603
0.8779661573245653  0.6067202293461512  0.3607311440395498
0.2497511545075697  0.2701415382585596  0.1091629721310945
0.5398935982411713  0.9554836813210079  0.2351710186196954
0.9229049161215356  0.6052913652916705  0.0557193871539968
0.2052388996085646  0.2735118673289546  0.4141108495537171
```

(36) $W_2MoN_2\_(OH)_2$ (T_MT_M)

```
1.00000000000000
  2.8382617448602687    0.0045528880553579    0.0527252800085940
 -1.4160196262203837    2.4615771943308484    0.0323371208508517
  0.7732733629289572    0.5036713053905263   27.8952668158493324
N    W    Mo   O    H
2    2    1    2    2
Direct
0.1443069256670854 -0.0057138960007589  0.2705863695687175
0.8976002103388145  0.3825232143631855  0.1631710911472679
0.7830617044568494  0.3341793830524739  0.3215991375200041
0.2772568481886536  0.0958296049886817  0.1123240183409769
0.5368915642059365  0.7332345887479734  0.2169371419700873
0.7345898129600897  0.3100002216043540  0.3903682680744129
0.3398038907139539  0.1380400770261609  0.0435948437280966
0.0257060163216051  0.6316182769216746  0.4048604891374287
-0.0107170818529896  0.0243284362962548  0.0294885645130110
```

Data S4: Optimized structures used for lattice dynamical calculations for $Mo_2CrC_2O_2$ (H_XH_X), $Mo_2CrN_2O_2$ (H_XH_X), $W_2CrC_2O_2$(H_XH_X), and $W_2CrN_2O_2$ (H_XH_X) MXenes.

(1) $Mo_2CrC_2\_O_2$ (H_XH_X)

```
  1.0
    2.9100057363937517    0.0000000000000000    0.0000000000000000
   -1.4550028681968759    2.5201388928754316    0.0000000000000000
    0.0000000000000000    0.0000000000000000   24.6149922244057038
  C    Mo   Cr   O
  2    2    1    2
Direct
  0.6666666666666666  0.3333333333333333  0.0492260347595916
  0.3333333333333334  0.6666666666666667  0.9507739652404084
  0.3333333333333333  0.6666666666666666  0.1031540611578237
  0.6666666666666667  0.3333333333333334  0.8968459388421763
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.6666666666666666  0.3333333333333333  0.1525899848742398
  0.3333333333333334  0.6666666666666667  0.8474100151257602
```

(2) $Mo_2CrN_2\_O_2$ (H_XH_X)

```
  1.0
    2.8987147890419500    0.0000000000000000    0.0000000000000000
   -1.4493573945209750    2.5103606456359784    0.0000000000000000
    0.0000000000000000    0.0000000000000000   21.5421185775140707
  N    Mo   Cr   O
  2    2    1    2
Direct
  0.6666666666666666  0.3333333333333333  0.9407965787992864
  0.3333333333333334  0.6666666666666667  0.0592034212007136
  0.3333333333333333  0.6666666666666666  0.8783377362290138
  0.6666666666666667  0.3333333333333334  0.1216622637709862
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.3333333333333333  0.6666666666666666  0.1774206269209344
  0.6666666666666667  0.3333333333333334  0.8225793730790656
```

(3) $W_2CrC_2\_O_2$ (H_XH_X)

```
  1.0
    2.9121152874061176    0.0000000000000000    0.0000000000000000
```

-1.4560576437030588   2.5219658176427195   0.0000000000000000
0.0000000000000000   0.0000000000000000   24.7152055762789367
C   W   Cr   O
2   2   1   2
Direct
0.3333333333333333 0.6666666666666666 0.5494769142340772
0.6666666666666667 0.3333333333333334 0.4505230857659228
0.6666666666666666 0.3333333333333333 0.6030573015598790
0.3333333333333334 0.6666666666666667 0.3969426984401210
0.0000000000000000 0.0000000000000000 0.5000000000000000
0.3333333333333333 0.6666666666666666 0.6526770068696877
0.6666666666666667 0.3333333333333334 0.3473229931303123

(4) W_2CrN_2_O_2 (H_XH_X)

1.0
2.8937985520210612   0.0000000000000000   0.0000000000000000
-1.4468992760105306   2.5061030594848632   0.0000000000000000
0.0000000000000000   0.0000000000000000   21.9175791711258334
N   W   Cr   O
2   2   1   2
Direct
0.6666666666666666 0.3333333333333333 0.9386368212240868
0.3333333333333334 0.6666666666666667 0.0613631787759132
0.3333333333333333 0.6666666666666666 0.8781992870587700
0.6666666666666667 0.3333333333333334 0.1218007129412300
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.3333333333333333 0.6666666666666666 0.1771968929054353
0.6666666666666667 0.3333333333333334 0.8228031070945647