Supplementary Information

Intercalation of First Row Transition Metals inside Covalent-Organic Frameworks (COF): a Strategy to Fine Tune the Electronic Properties of Porous Crystalline Materials

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Contents

1   Possible position of TM atoms intercalation in COF
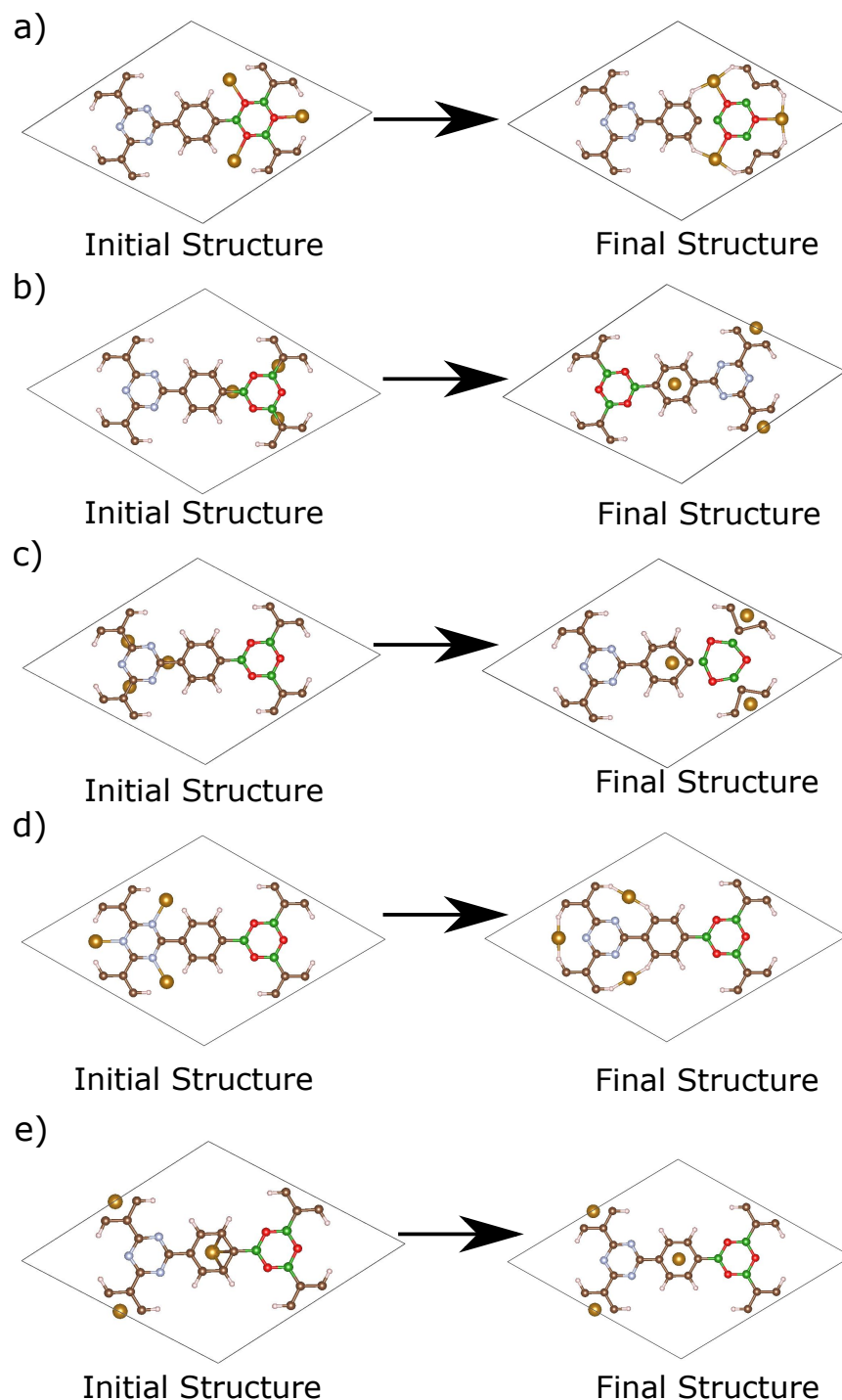
Figure S1: Various possible intercalation position of TM atoms in COF-TM-3, and the most stable configuration of the COF-TM-3: (a) the TM atoms initial positions are around the boroxine ring (high symmetry site: top); (b) the TM atoms position around the C=B bond bridging area between the boroxine and benzene rings; (c) the TM atoms position around C=C bond bridging area between the benzene and triazine rings;(d) the TM atoms position at adsorption site around the triazine ring (high symmetry site: top); and (e) the TM atoms position between benzene rings (benzene rings hollow site).

We investigated several possible intercalation and adsorption sites of TM atoms in COF-TM-3 materials (Figure S1) noted as:

(a) the TM atoms initial positions are around the boroxine ring (high symmetry site: top);

(b) the TM atoms position around the C=B bond bridging area between the boroxine and benzene rings;

(c) the TM atoms position around C=C bond bridging area between the benzene and triazine rings;

(d) the TM atoms position at adsorption site around the triazine ring (high symmetry site: top); and

(e) the TM atoms position between benzene rings (benzene rings hollow site).

Our present DFT-D computation found that the structures/conformers of the COF-TM-3 (a) to (d) are not stable conformers and they never converge to the minima. The TM atoms are trying to move to the inter-rings bridge sites of the COFs; see Figure S1b, c. We found that the inter-rings bridge sites i.e. at the centroid of the benzene rings of the TM-intercalated COFs, COF-TM-3 are the stable conformers. The total energy and configurations are shown for COF-TM-3 with Fe as example in Table S1 and Figure S1. The other TMs follows a similar trend.

Table S1: Various possible intercalation position of TM atoms in COF-TM-3 materials (see Figure S1). The total energy of the COFs are express in Hartree (a.u.). These energies corresponds to the Fe analog, however the other TMs follows a similar trend.

Configurations (See Fig. S1)	Energy of initial geometry (a.u.)	Energy of final geometry (a.u.)	Converge (YES/NO)
a	-5.069067467952E+03	-5.0624831931079E+03	NO
b	-5.070760915114E+03	-5.0624804225369E+03	NO
c	-5.061685373335E+03	-5.0624862210383E+03	NO
d	-5.069404676880E+03	-5.0624867651903E+03	NO
e	-5.062821123956E+03	-5.0712178203780E+03	YES

2   Figures of the COF-TM-x Materials

a)   b)   c)

COF-Ti-3   COF-Ti-4   COF-Ti-5

d)   e)   f)

COF-V-3   COF-V-4   COF-V-5

g)   h)   i)

COF-Cr-3   COF-Cr-4   COF-Cr-5

○ ≡ **H**   ● ≡ **B**   ● ≡ **C**   ● ≡ **N**   ● ≡ **O**   ● ≡ **Ti**   ● ≡ **V**   ● ≡ **Cr**

Figure S2: The structures obtained for the COF-TM-x (where x=3-5) with the perspective along the z-axis.

a) COF-Mn-3   b) COF-Mn-4   c) COF-Mn-5

d) COF-Fe-3   e) COF-Fe-4   f) COF-Fe-5

g) COF-Co-3   h) COF-Co-4   i) COF-Co-5

○ ≡ H   ● ≡ B   ● ≡ C   ● ≡ N   ● ≡ O   ● ≡ Mn   ● ≡ Fe   ● ≡ Co

Figure S3: The structures obtained for the COF-TM-x (where x=3-5) with the perspective along the z-axis.

a) COF-Ni-3   b) COF-Ni-4   c) COF-Ni-5

d) COF-Cu-3   e) COF-Cu-4   f) COF-Cu-5

g) COF-Zn-3   h) COF-Zn-4   i) COF-Zn-5

H **B** **C** **N** **O** **Ni** **Cu** **Zn**

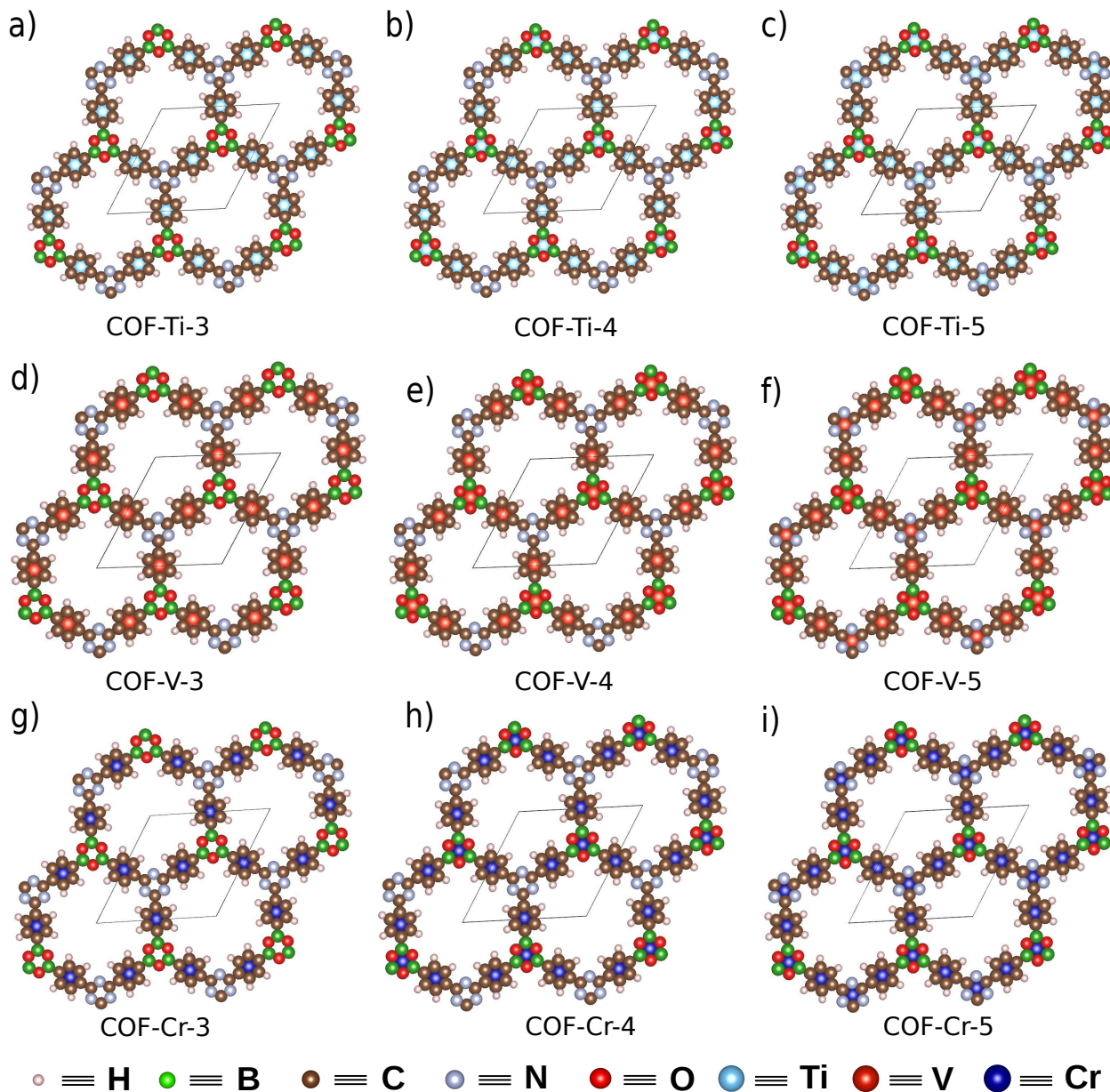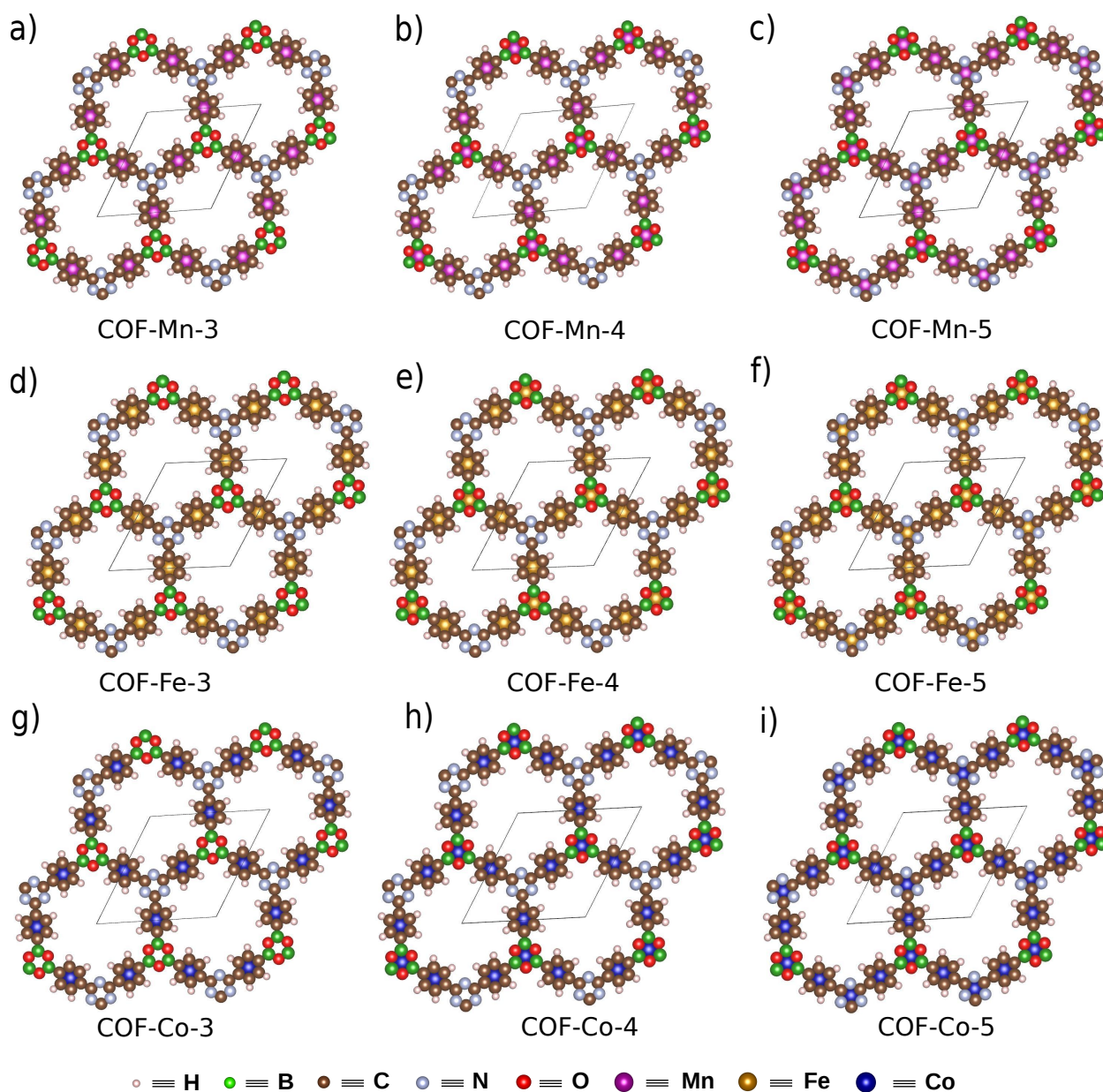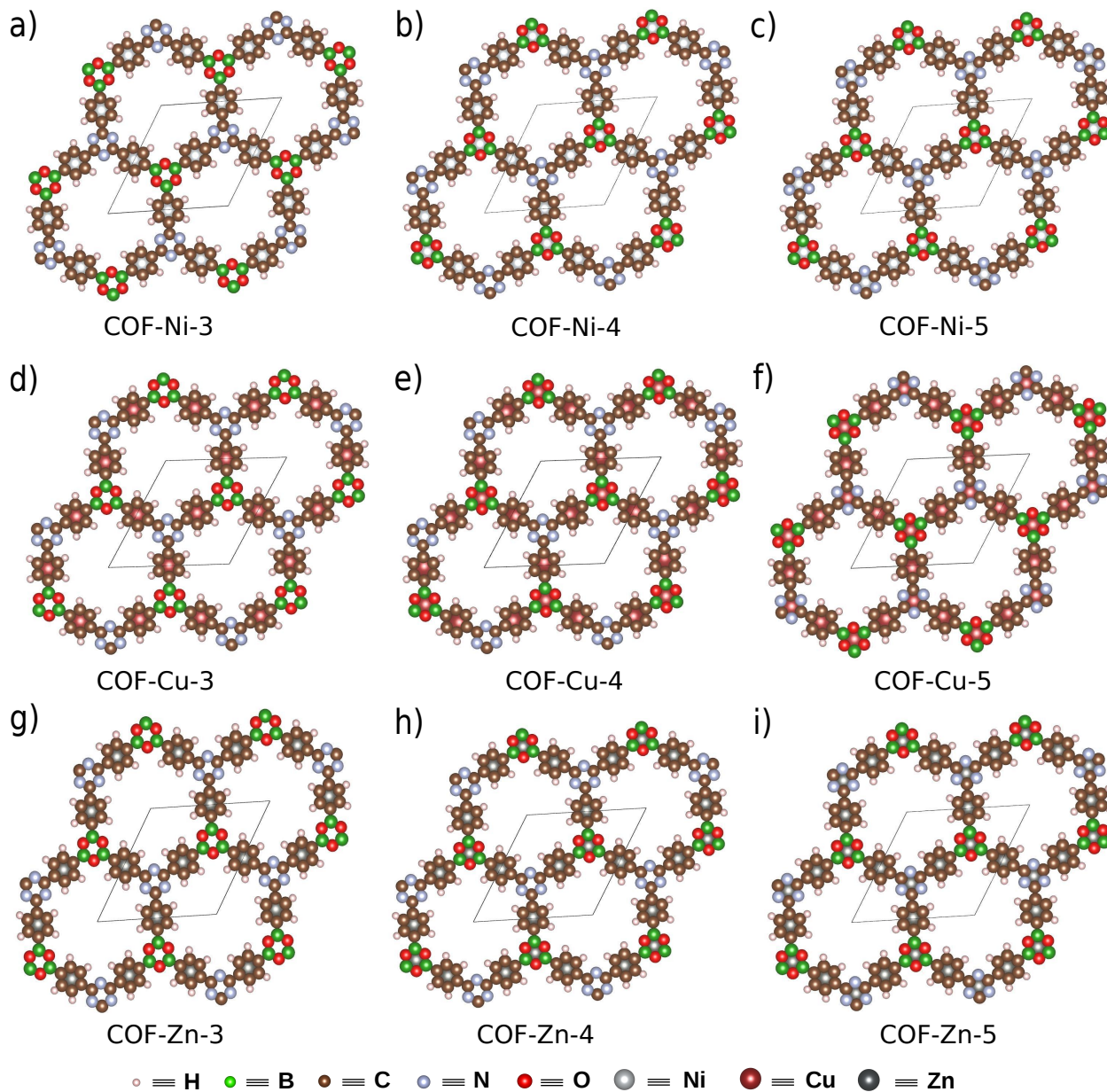Figure S4: The structures obtained for the COF-TM-x (where x=3-5) with the perspective along the z-axis.
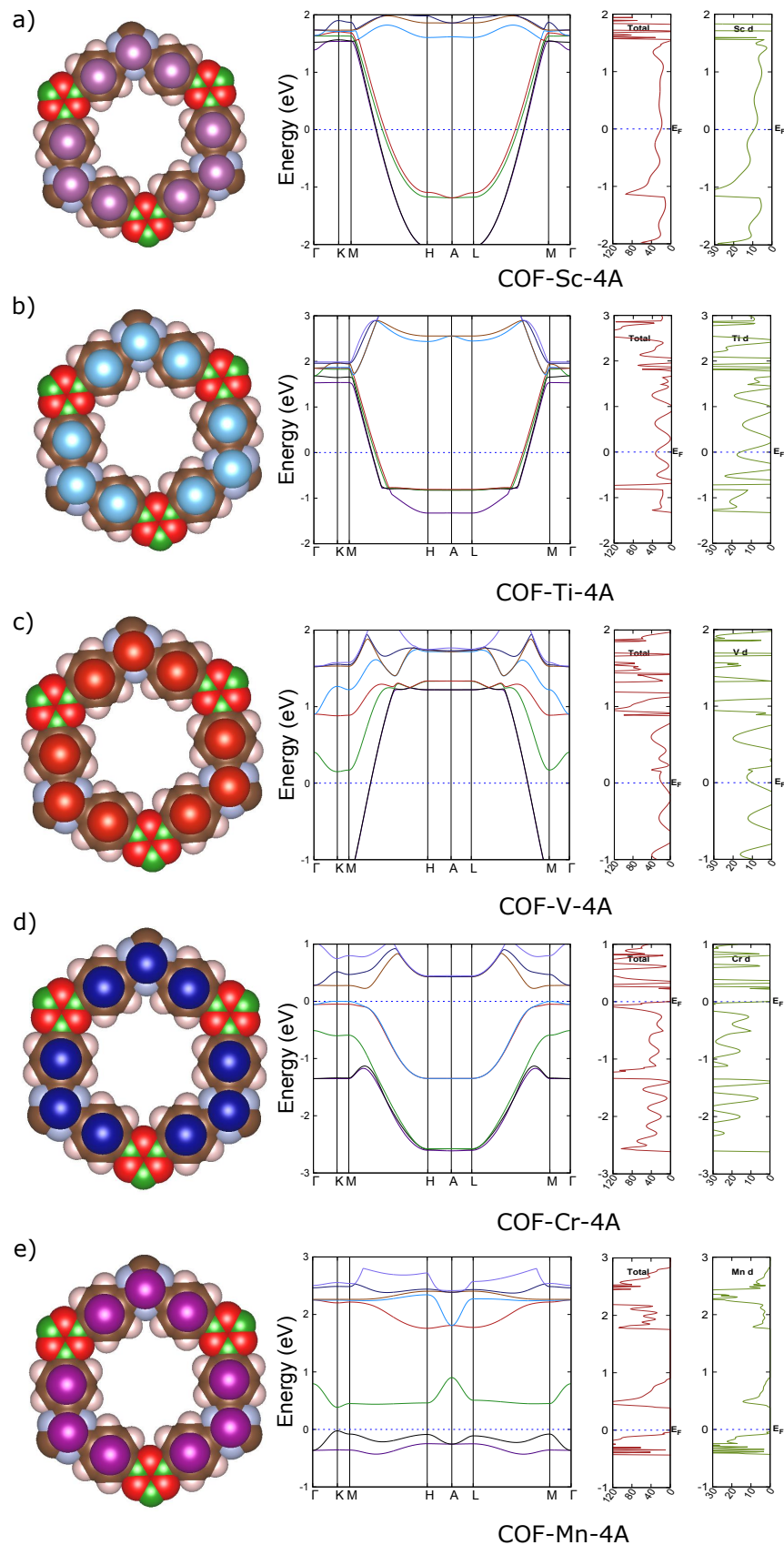
Figure S5: The equilibrium structures and electronic properties obtained for the COF-TM-4A with the perspective along the z-axis, (here TM is Sc - Mn).
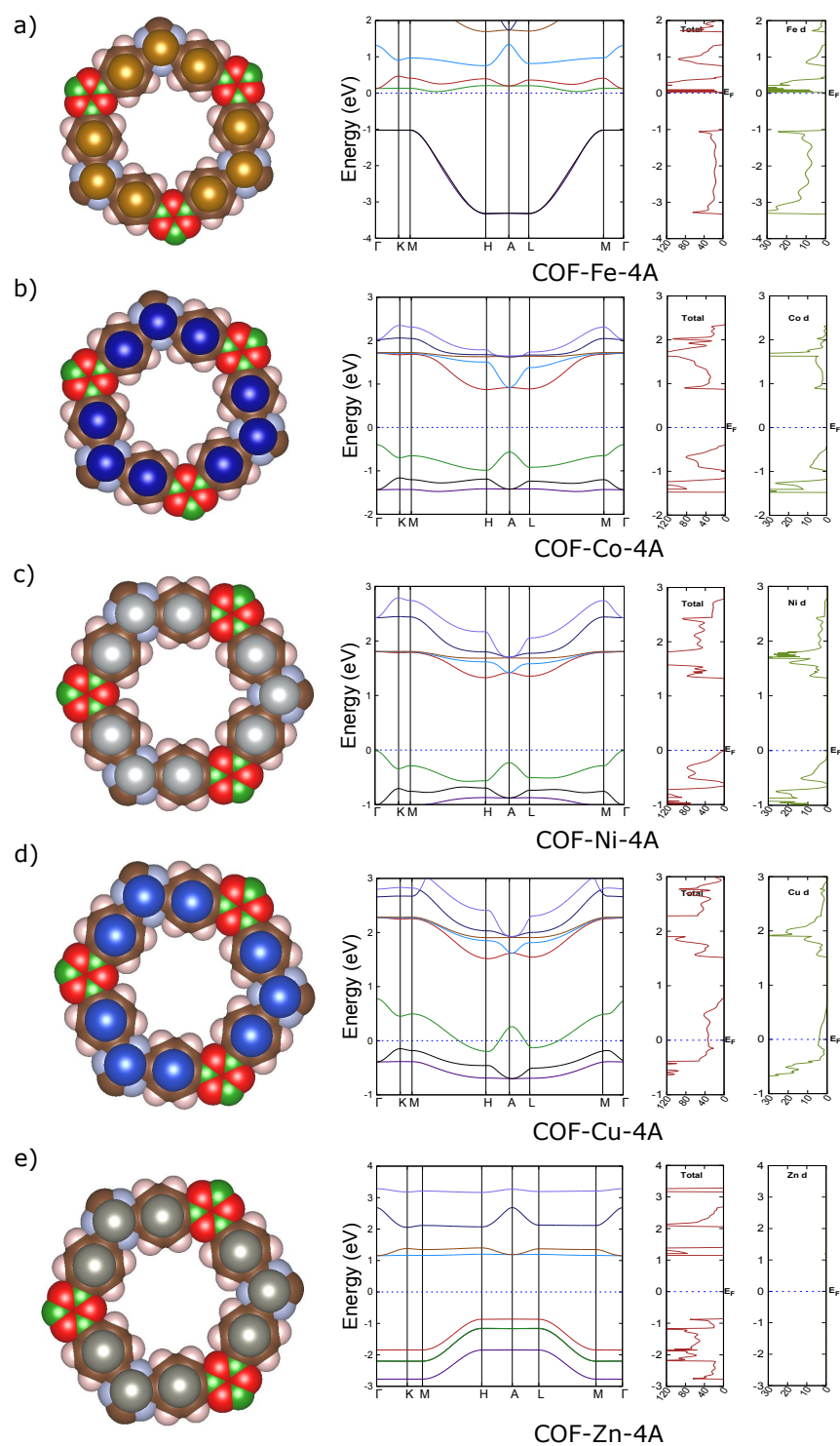
Figure S6: The equilibrium structures and electronic properties obtained for the COF-TM-4A with the perspective along the z-axis, (here TM is Fe - Zn).

3   Discussion about the Less Stable TM-intercalated COFs

We studied the equilibrium structure and electronic properties of the other conformer of the COF-TM-4 configuration, i.e. COF-TM-4A (where TM = Sc - Zn) using the same level of theory, and they are shown in Figure S5 and S6. All of the COFs presented converged to honeycomb-like structures with the **bnn** topology. In the COF-TM-4A configuration, four TM atoms were intercalated per one unit cell, whereas three TM atoms were placed at the centroid of three benzene rings, and one TM atom was placed at the centroid of triazine ring. On the other hand for the COF-TM-4 configuration, the 4th TM atom was placed at the centroid of boroxine ring. We computed the total energy and relative energy of both the COF-TM-4A and COF-TM-4, and the values are reported in Table S2. These calculations showed that the COF-TM-4 is more stable than the COF-TM-4A (ΔE_R) by around 0.05 to 3.94 eV depending of the TMs. The electronic properties (the band structure and DOS) of the less stable one COF-TM-4A compound are shown in Figure S5 - S6. The present calculations found these COF-TM-4A has similar material properties to its most stable isomer COF-TM-4.

We computed the DOS of the minority carriers (i.e. the β electrons) of the COF-TM-4 materials, and they are shown in Figure S7 - S8. This calculation shows that the material properties are determined by majority α electrons, which are reported in the main manuscript.

Table S2: The total energy of the COF-TM-4 and COF-TM-4A materials, and their relative energy ΔE_R, with respect to COF-TM-4 are tabulated. Notice that in all cases, the COF-TM-4 configuration is the most stable. The unit of total energy is in Hartree (a.u.) and the relative energy is expressed in eV.

COFs/TMs (Figs. S5, S6)	Total Energy of COF-TM-4 (a.u.)	Total Energy of COF-TM-4A (a.u.)	ΔE_R w.r.t COF-TM-4 (eV)
Sc	-4.3147680531597E+03	-4.3146391718055E+03	-3.56
Ti	-4.6695620760279E+03	-4.6694190390317E+03	-3.94
V	-5.0477165763121E+03	-5.0475859492506E+03	-3.61
Cr	-5.4493984242043E+03	-5.449325659053E+03	-2.01
Mn	-5.8756309571364E+03	-5.8755419899986E+03	-2.46
Fe	-6.3263861642116E+03	-6.3263252615482E+03	-1.68
Co	-6.8027687585757E+03	-6.8026965760779E+03	-1.99
Ni	-7.3048867437303E+03	-7.3048491309491E+03	-1.04
Cu	-7.8333832665116E+03	-7.8333371110262E+03	-1.27
Zn	-8.3889674527633E+03	-8.3889657977528E+03	-0.05
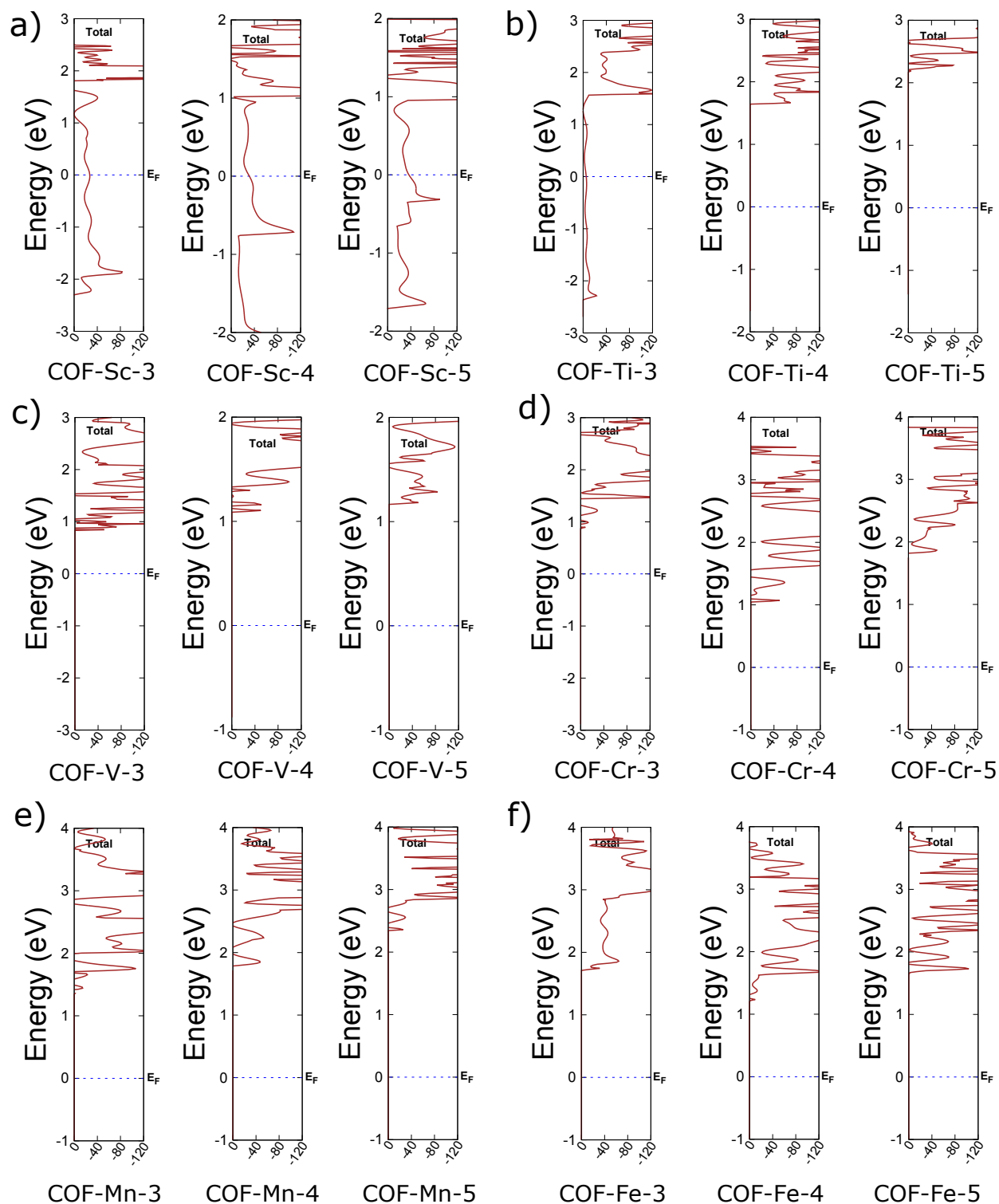
Figure S7: The total density of states of the beta electrons (minority carriers) of the COF-TM-xA (where x = 3-5 and TM is Sc - Fe).
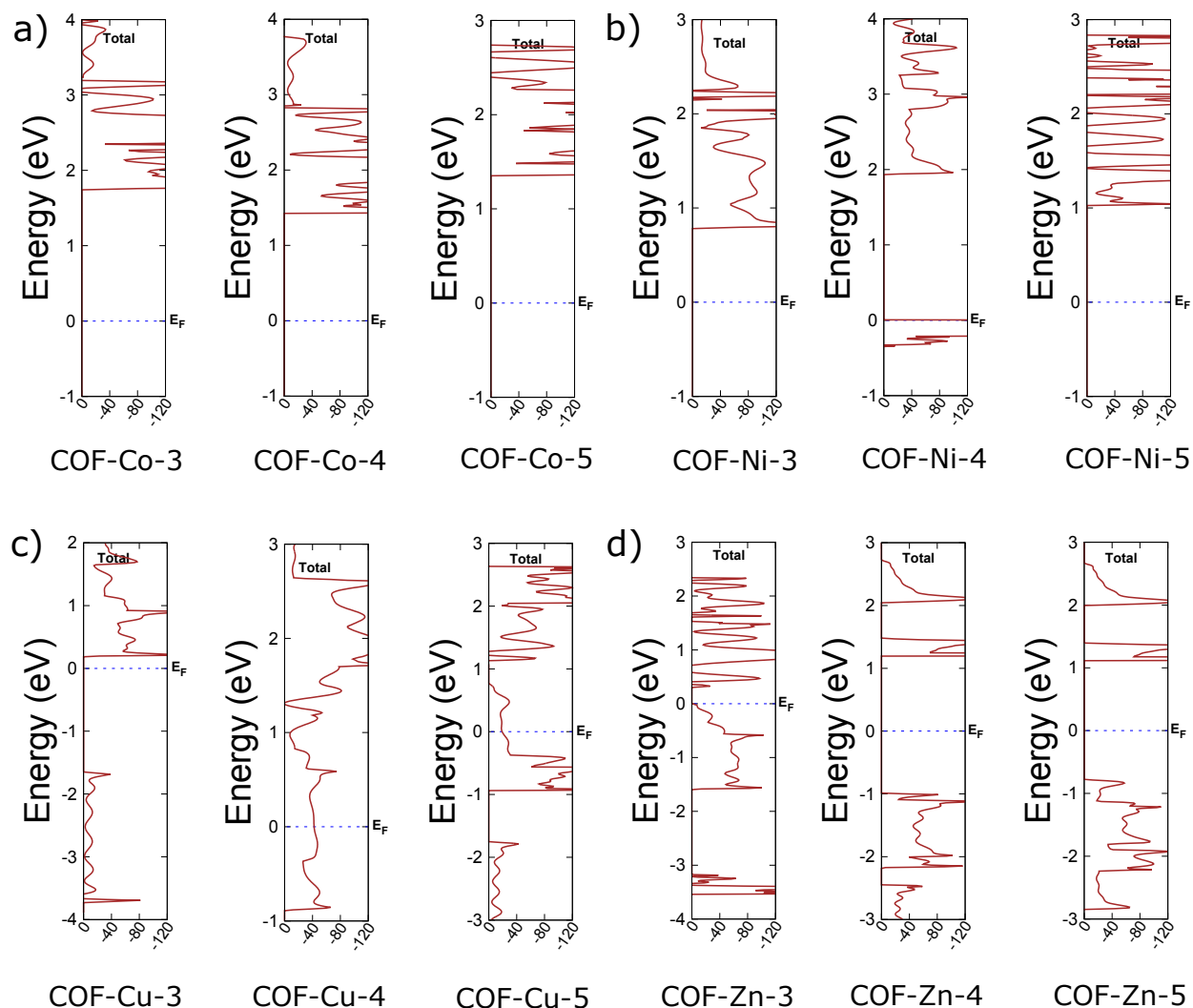
Figure S8: The total density of states of the beta electrons (minority carriers) of the COF-TM-xA (where x = 3-5 and TM is Co - Zn).

4 Role of the different orbitals

We computed the total DOS of all the COFs studied here, and the contribution d-subshells electron density of states of the TM atoms in the intercalated COFs, COF-TM-x materials. We also calculated the contribution of the s- and p-subshells DOS of the TMs in COF-TM-x materials along with d-subshells DOS as shown in Figure S9 and S10. Our present computation shows that the contribution of the s- and p-subshells DOS of the TMs in the total DOS are negligible and the main contributing component in determining the properties of the TM-intercalated COFs are d-subshells DOS.
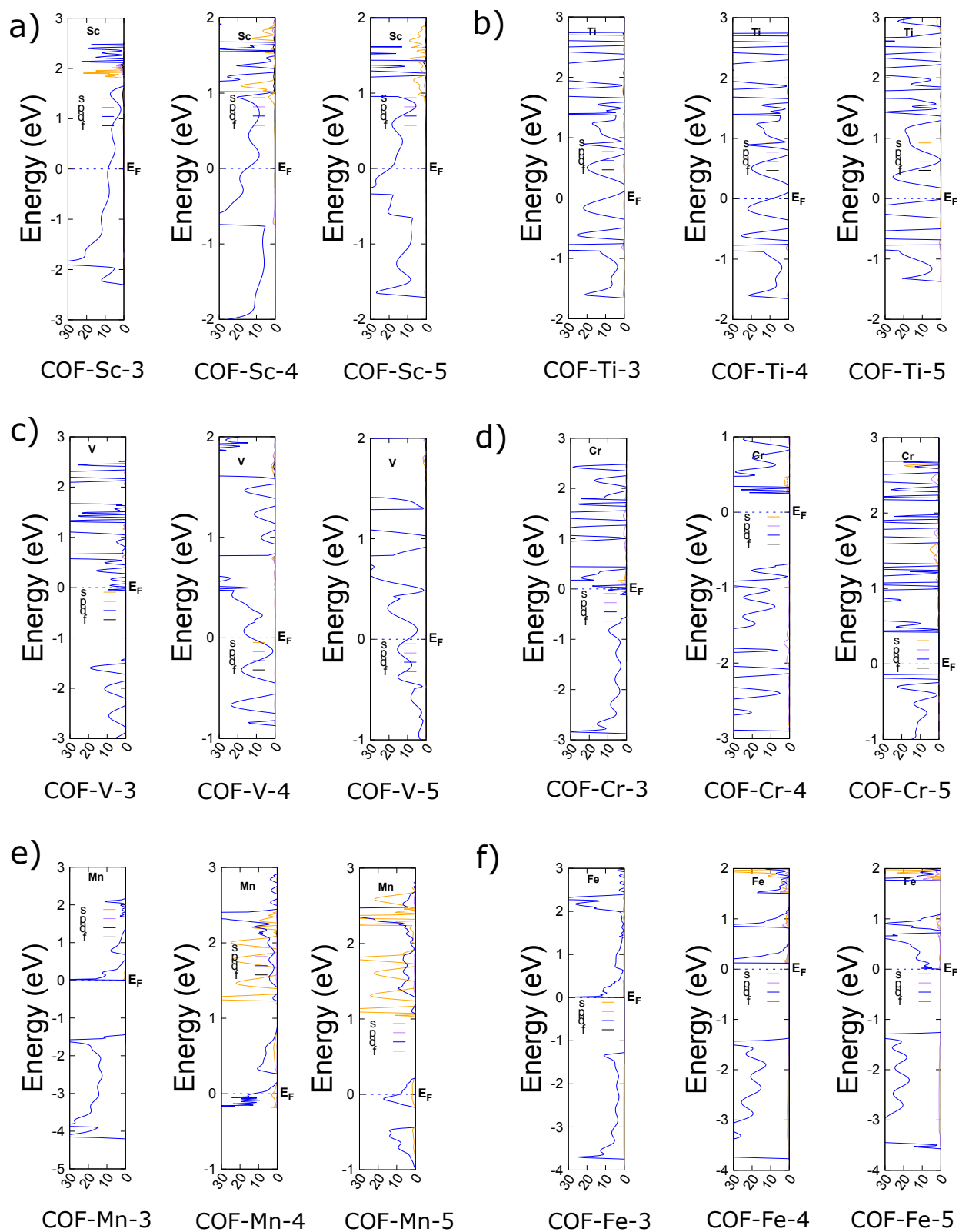
Figure S9: The subshells electron density of states of the TMs of the COF-TM-x materials (where x = 3-5 and TM is Sc - Fe) i.e. *s-*, *p-*, and *d*-subshells electron DOS of the TMs in the TM-intercalated COFs.
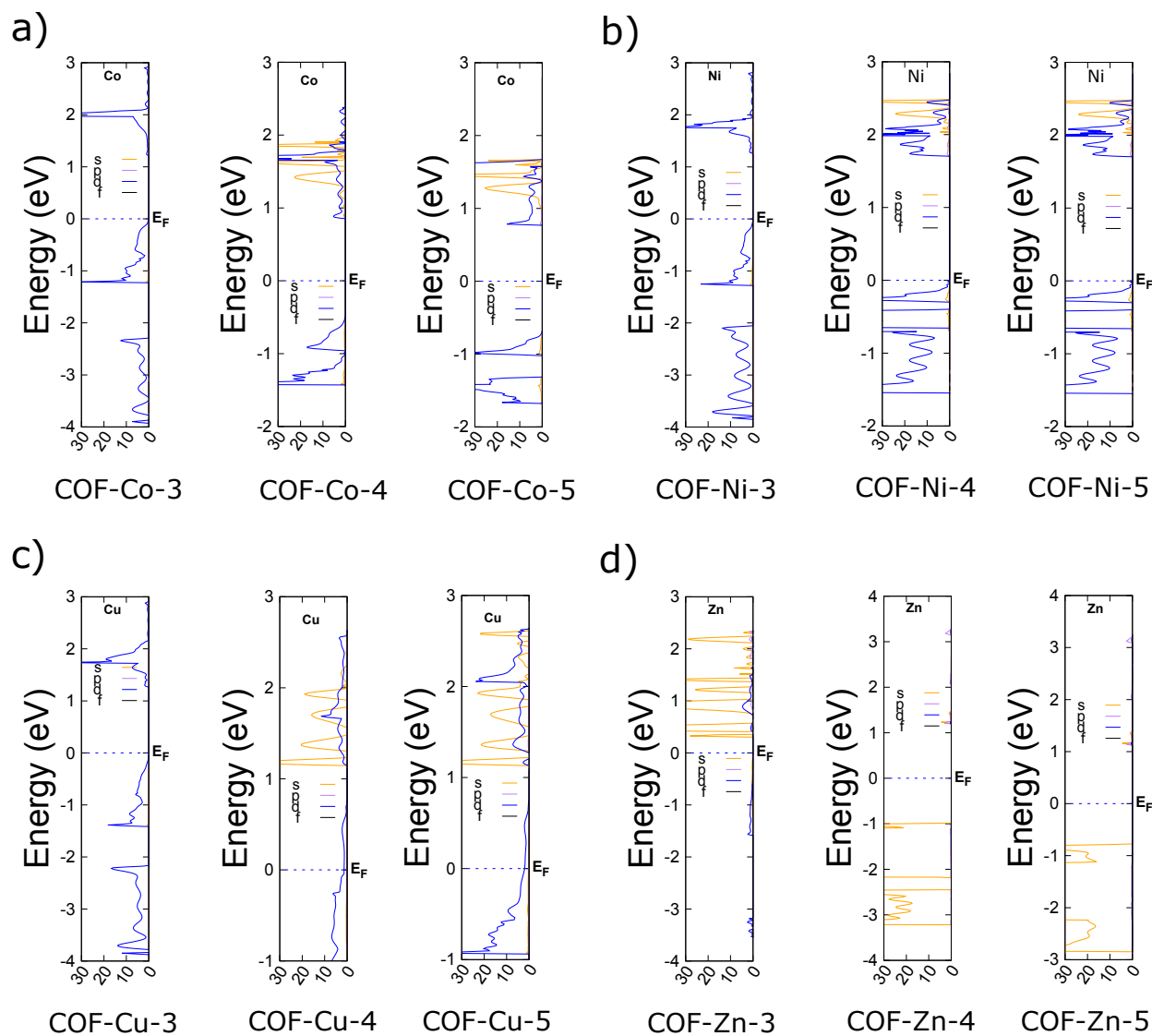
Figure S10: The subshells electron density of states of the TMs of the COF-TM-x materials (where x = 3-5 and TM is Co - Zn) i.e. *s*-, *p*-, and *d*-subshells electron DOS of the TMs in the TM-intercalated COFs.

5 Vibrational Analysis of the Pristine and COF-Fe-3

Table S3: Frequencies and nodes of vibration of the pristine COF and COF-Fe-3.

Nodes	COF-pristine Frequencies	Raman	COF-Fe-3 Frequencies	Raman
1	0.0000	A	0.0000	A
2	0.0000	A	0.0000	A
3	0.0000	I	0.0000	I
5	53.0270	A	30.0563	A
6	68.0895	I	66.0512	I
7	70.2789	I	91.3247	I
9	134.4108	A	103.9850	A
10	145.7328	I	111.6951	A
12	147.5666	A	132.8971	I
13	157.7700	I	138.1795	A
15	208.2918	A	146.7856	A
17	225.6108	A	164.7425	A
18	245.3316	I	183.4669	I
20	269.9500	A	226.4919	A
22	294.5406	A	227.8719	I
23	330.3431	I	228.8113	A
24	351.4716	A	271.3749	I
26	424.9787	A	299.8980	A
27	456.0535	I	303.6884	I
29	456.2964	A	307.4341	A
31	484.1818	A	331.3277	A
33	510.3174	A	368.9833	I
34	530.1794	I	382.6535	A
35	562.4860	I	417.1592	A
36	632.7975	I	431.1689	A
38	639.6387	A	473.7861	A
40	646.2557	A	473.9172	I
41	663.8382	I	474.0555	A
43	667.8886	A	483.1162	I
44	702.0151	I	540.7916	I
46	725.0360	A	573.9709	A
47	758.8260	I	598.8206	I
48	763.2503	A	626.4383	A
50	786.9339	A	627.8402	I
52	798.9929	A	647.8368	I
53	809.4229	A	661.0449	A
54	872.5563	I	670.3523	A
56	877.7697	A	718.4170	I
58	918.5354	A	732.8542	A
59	924.5207	I	762.3750	A
61	925.2738	A	764.2704	A
62	932.6617	I	805.7117	A
63	994.4447	A	844.4458	I
65	1024.5866	A	851.4999	A
66	1026.0425	I	880.0937	A
67	1027.7854	A	883.9609	I

Continued on next page

Table S3 – *Continued from previous page*

Nodes	COF-pristine Frequencies	Raman	COF-Fe-3 Frequencies	Raman
68	1044.8815	I	906.2513	I
70	1045.5197	A	907.9315	A
72	1063.6005	A	951.5577	I
73	1100.1634	A	953.0741	A
75	1118.8749	A	966.0528	A
76	1159.9144	I	973.3075	A
78	1165.1586	A	975.0762	I
79	1167.2571	A	993.3314	A
80	1187.1464	I	999.4365	A
82	1195.2105	A	1021.3651	A
84	1234.2862	A	1055.1000	A
85	1246.0253	I	1069.8964	A
86	1263.2837	A	1099.0435	I
88	1323.3611	A	1105.2691	A
90	1358.5617	A	1132.4704	A
91	1370.7829	I	1132.6660	A
93	1373.6798	A	1176.2283	A
95	1383.4070	A	1191.3340	I
96	1386.5706	I	1264.3357	A
97	1431.0342	A	1270.5327	I
99	1438.3886	A	1284.2668	I
100	1475.2348	I	1295.4016	A
101	1483.5502	A	1300.9974	A
103	1483.7117	A	1315.7999	I
105	1570.5195	A	1331.3021	A
107	1587.3630	A	1353.4503	A
108	1620.7821	I	1402.2918	A
109	1634.9499	A	1410.9533	A
111	1643.1347	A	1421.8302	I
113	1693.5645	A	1423.6632	A
114	1699.2162	A	1433.2116	I
116	3151.1038	A	1466.6770	A
117	3167.2126	I	1479.9307	A
119	3172.4750	A	1511.3801	A
120	3177.0513	A	1541.1002	A
122	3195.1177	A	1565.8221	A
123	3208.3486	I	1626.9350	A
125	3219.3855	A	3133.9786	A
126	3349.4621	A	3172.6629	A
127	NA	NA	3185.4328	I
128	NA	NA	3196.2384	I
129	NA	NA	3197.4543	A
130	NA	NA	3199.9310	A
132	NA	NA	3204.8224	A
134	NA	NA	3226.4304	A

6 Optimized Structures (.cif format)

The optimized structures of the pristine and first row TM atoms (Sc-Zn) intercalated COF materials are provided below in .cif format.

6.1 COF: Pristine COF

Total Energy E_{COF} = -1271.9764747 a.u.

```
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loop_
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  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
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  x,x-y,-z
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C007   C     0.04784   -0.39468   -0.00000    0.00000   Uiso    1.00
H013   H     0.40727    0.10371   -0.00000    0.00000   Uiso    1.00
H019   H    -0.40041   -0.30980    0.00000    0.00000   Uiso    1.00
C025   C    -0.38476    0.38476   -0.00000    0.00000   Uiso    1.00
C028   C    -0.44247    0.44247    0.00000    0.00000   Uiso    1.00
B031   B     0.38811   -0.38811   -0.00000    0.00000   Uiso    1.00
N034   N    -0.27996    0.27996   -0.00000    0.00000   Uiso    1.00
C037   C     0.44818   -0.44818   -0.00000    0.00000   Uiso    1.00
O040   O     0.27968   -0.27968    0.00000    0.00000   Uiso    1.00
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6.2   COF-Sc-3: Sc-intercalated COF

Total Energy $E_{COF-Sc-3}$ = **-3554.0883204 a.u.**

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  x,y,-z
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C007    C     0.04891   -0.39105    0.00000    0.01267   Uiso    1.00
H013    H     0.40708    0.10577   -0.00000    0.01267   Uiso    1.00
H019    H    -0.39921   -0.30744    0.00000    0.01267   Uiso    1.00
C025    C    -0.38427    0.38427   -0.00000    0.01267   Uiso    1.00
C028    C    -0.44040    0.44040   -0.00000    0.01267   Uiso    1.00
B031    B     0.38761   -0.38761   -0.00000    0.01267   Uiso    1.00
N034    N    -0.28005    0.28005   -0.00000    0.01267   Uiso    1.00
C037    C     0.44616   -0.44616   -0.00000    0.01267   Uiso    1.00
O040    O     0.27989   -0.27989    0.00000    0.01267   Uiso    1.00
SC043   Sc   -0.49807    0.49807   -0.50000    0.01267   Uiso    1.00
```

6.3   COF-Sc-4: Sc-intercalated COF

Total Energy $E_{COF-Sc-4}$ = **-4314.6391718 a.u.**

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  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
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_atom_site_occupancy
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H019   H    -0.39833   -0.31216    0.00000    0.01267   Uiso   1.00
C025   C    -0.38363    0.38363    0.00000    0.01267   Uiso   1.00
C028   C    -0.43911    0.43911    0.00000    0.01267   Uiso   1.00
B031   B     0.39148   -0.39148   -0.00000    0.01267   Uiso   1.00
N034   N    -0.28070    0.28070    0.00000    0.01267   Uiso   1.00
C037   C     0.44859   -0.44859   -0.00000    0.01267   Uiso   1.00
O040   O     0.28031   -0.28031   -0.00000    0.01267   Uiso   1.00
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SC046  Sc    0.33333   -0.33333    0.50000    0.01267   Uiso   1.00
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6.4 COF-Sc-5: Sc-intercalated COF

Total Energy $E_{COF-Sc-5}$ = **-5075.3170461 a.u.**

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 -x+y,-x,z
 x,y,-z
 -y,x-y,-z
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 -y,-x,z
 -x+y,y,z
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_atom_site_fract_z
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_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38733  -0.44914   0.00000   0.01267  Uiso   1.00
C007   C     0.04728  -0.39441   0.00000   0.01267  Uiso   1.00
H013   H     0.40966   0.10402  -0.00000   0.01267  Uiso   1.00
H019   H    -0.40063  -0.31259   0.00000   0.01267  Uiso   1.00
C025   C    -0.38617   0.38617  -0.00000   0.01267  Uiso   1.00
C028   C    -0.44091   0.44091  -0.00000   0.01267  Uiso   1.00
B031   B     0.39083  -0.39083   0.00000   0.01267  Uiso   1.00
N034   N    -0.27932   0.27932  -0.00000   0.01267  Uiso   1.00
C037   C     0.44746  -0.44746   0.00000   0.01267  Uiso   1.00
O040   O     0.28075  -0.28075   0.00000   0.01267  Uiso   1.00
SC043  Sc   -0.49824   0.49824  -0.50000   0.01267  Uiso   1.00
SC046  Sc    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
SC047  Sc   -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.5   COF-Ti-3: Ti-intercalated COF

Total Energy $E_{COF-Ti-3}$ = **-3820.1885996 a.u.**

```
data_COF-Ti-3
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
```

```
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                14.8635
_cell_length_b                14.8635
_cell_length_c                3.3867
_cell_angle_alpha             90.0000
_cell_angle_beta              90.0000
_cell_angle_gamma             120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38451  -0.44615   0.00000   0.01267  Uiso   1.00
C007   C     0.04939  -0.39077   0.00000   0.01267  Uiso   1.00
H013   H     0.40650   0.10550  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39917  -0.30706   0.00000   0.01267  Uiso   1.00
C025   C    -0.38423   0.38423  -0.00000   0.01267  Uiso   1.00
C028   C    -0.44046   0.44046  -0.00000   0.01267  Uiso   1.00
B031   B     0.38756  -0.38756   0.00000   0.01267  Uiso   1.00
N034   N    -0.28012   0.28012  -0.00000   0.01267  Uiso   1.00
C037   C     0.44615  -0.44615   0.00000   0.01267  Uiso   1.00
O040   O     0.27993  -0.27993   0.00000   0.01267  Uiso   1.00
TI043  Ti   -0.49728   0.49728  -0.50000   0.01267  Uiso   1.00
```

6.6   COF-Ti-4: Ti-intercalated COF

Total Energy $E_{COF-Ti-4}$ = **-4669.4190390 a.u.**

```
data_COF-Ti-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
```

```
 x,x-y,z
 -y,-x,-z
 -x+y,y,-z
 x,x-y,-z
_cell_length_a                  15.0729
_cell_length_b                  15.0729
_cell_length_c                  3.4082
_cell_angle_alpha               90.0000
_cell_angle_beta                90.0000
_cell_angle_gamma               120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38401  -0.44917   0.00000   0.01267  Uiso   1.00
C007   C     0.04453  -0.39487   0.00000   0.01267  Uiso   1.00
H013   H     0.40968   0.10803  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39839  -0.31226   0.00000   0.01267  Uiso   1.00
C025   C    -0.38351   0.38351   0.00000   0.01267  Uiso   1.00
C028   C    -0.43895   0.43895   0.00000   0.01267  Uiso   1.00
B031   B     0.39174  -0.39174  -0.00000   0.01267  Uiso   1.00
N034   N    -0.28084   0.28084   0.00000   0.01267  Uiso   1.00
C037   C     0.44892  -0.44892  -0.00000   0.01267  Uiso   1.00
O040   O     0.28033  -0.28033  -0.00000   0.01267  Uiso   1.00
TI043  Ti   -0.49391   0.49391  -0.50000   0.01267  Uiso   1.00
TI046  Ti    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
```

6.7   COF-Ti-5: Ti-intercalated COF

Total Energy $E_{COF-Ti-5}$ = -5518.7896859 a.u.

```
data_COF-Ti-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -y,x-y,z
 -x+y,-x,z
 x,y,-z
 -y,x-y,-z
 -x+y,-x,-z
 -y,-x,z
 -x+y,y,z
 x,x-y,z
 -y,-x,-z
 -x+y,y,-z
 x,x-y,-z
```

```
_cell_length_a                    15.2172
_cell_length_b                    15.2172
_cell_length_c                    3.4267
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38700  -0.44881   0.00000   0.01267  Uiso   1.00
C007   C     0.04716  -0.39433   0.00000   0.01267  Uiso   1.00
H013   H     0.40952   0.10415  -0.00000   0.01267  Uiso   1.00
H019   H    -0.40050  -0.31252   0.00000   0.01267  Uiso   1.00
C025   C    -0.38636   0.38636   0.00000   0.01267  Uiso   1.00
C028   C    -0.44102   0.44102   0.00000   0.01267  Uiso   1.00
B031   B     0.39111  -0.39111  -0.00000   0.01267  Uiso   1.00
N034   N    -0.27932   0.27932   0.00000   0.01267  Uiso   1.00
C037   C     0.44774  -0.44774  -0.00000   0.01267  Uiso   1.00
O040   O     0.28084  -0.28084  -0.00000   0.01267  Uiso   1.00
TI043  Ti   -0.49683   0.49683  -0.50000   0.01267  Uiso   1.00
TI046  Ti    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
TI047  Ti   -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.8   COF-V-3: V-intercalated COF

Total Energy $E_{COF-V-3}$ = -4103.8136388 a.u.

```
data_COF-V-3
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.8627
_cell_length_b                    14.8627
_cell_length_c                    3.3567
```

```
_cell_angle_alpha              90.0000
_cell_angle_beta               90.0000
_cell_angle_gamma             120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38518  -0.44672   0.00000   0.01267  Uiso   1.00
C007   C     0.04922  -0.39127   0.00000   0.01267  Uiso   1.00
H013   H     0.40726   0.10554  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39947  -0.30764   0.00000   0.01267  Uiso   1.00
C025   C    -0.38423   0.38423   0.00000   0.01267  Uiso   1.00
C028   C    -0.44050   0.44050  -0.00000   0.01267  Uiso   1.00
B031   B     0.38754  -0.38754   0.00000   0.01267  Uiso   1.00
N034   N    -0.28003   0.28003  -0.00000   0.01267  Uiso   1.00
C037   C     0.44617  -0.44617   0.00000   0.01267  Uiso   1.00
O040   O     0.27993  -0.27993   0.00000   0.01267  Uiso   1.00
V043   V    -0.49774   0.49774  -0.50000   0.01267  Uiso   1.00
```

6.9   COF-V-4: V-intercalated COF

Total Energy $E_{COF-V-4}$ = -5047.5859492 a.u.

```
data_COF-V-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                 15.0534
_cell_length_b                 15.0534
_cell_length_c                  3.3879
_cell_angle_alpha              90.0000
_cell_angle_beta               90.0000
_cell_angle_gamma             120.0000
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001    C    -0.38470   -0.44948   -0.00000    0.01267   Uiso    1.00
C007    C     0.04491   -0.39512    0.00000    0.01267   Uiso    1.00
H013    H     0.41006    0.10777    0.00000    0.01267   Uiso    1.00
H019    H    -0.39909   -0.31250   -0.00000    0.01267   Uiso    1.00
C025    C    -0.38357    0.38357   -0.00000    0.01267   Uiso    1.00
C028    C    -0.43912    0.43912   -0.00000    0.01267   Uiso    1.00
B031    B     0.39113   -0.39113    0.00000    0.01267   Uiso    1.00
N034    N    -0.28071    0.28071   -0.00000    0.01267   Uiso    1.00
C037    C     0.44881   -0.44881    0.00000    0.01267   Uiso    1.00
O040    O     0.27977   -0.27977    0.00000    0.01267   Uiso    1.00
V043    V    -0.49450    0.49450   -0.50000    0.01267   Uiso    1.00
V046    V     0.33333   -0.33333   -0.50000    0.01267   Uiso    1.00
```

6.10   COF-V-5: V-intercalated COF

Total Energy $E_{COF-Fe-0}$ = **-5991.48736748 a.u.**

```
data_COF-V-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    15.1897
_cell_length_b                    15.1897
_cell_length_c                    3.3931
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001    C    -0.38732   -0.44883    0.00000    0.01267   Uiso    1.00
C007    C     0.04740   -0.39457    0.00000    0.01267   Uiso    1.00
H013    H     0.40946    0.10385   -0.00000    0.01267   Uiso    1.00
H019    H    -0.40115   -0.31271    0.00000    0.01267   Uiso    1.00
C025    C    -0.38636    0.38636    0.00000    0.01267   Uiso    1.00
C028    C    -0.44119    0.44119   -0.00000    0.01267   Uiso    1.00
B031    B     0.39060   -0.39060    0.00000    0.01267   Uiso    1.00
N034    N    -0.27927    0.27927    0.00000    0.01267   Uiso    1.00
C037    C     0.44777   -0.44777    0.00000    0.01267   Uiso    1.00
O040    O     0.28026   -0.28026    0.00000    0.01267   Uiso    1.00
V043    V    -0.49682    0.49682   -0.50000    0.01267   Uiso    1.00
V046    V     0.33333   -0.33333   -0.50000    0.01267   Uiso    1.00
V047    V    -0.33333    0.33333   -0.50000    0.01267   Uiso    1.00
```

6.11 COF-Cr-3: Cr-intercalated COF

Total Energy $E_{COF-Cr-3}$ **= -4405.0711792 a.u.**

```
data_COF-Cr-3
_symmetry_space_group_name_H-M      'P-6M2'
_symmetry_Int_Tables_number         187
_symmetry_cell_setting              hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                      14.9296
_cell_length_b                      14.9296
_cell_length_c                      3.3661
_cell_angle_alpha                   90.0000
_cell_angle_beta                    90.0000
_cell_angle_gamma                   120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
```

```
C001   C    -0.38694   -0.44876    0.00000    0.01267   Uiso   1.00
C007   C     0.04937   -0.39337    0.00000    0.01267   Uiso   1.00
H013   H     0.40752    0.10370   -0.00000    0.01267   Uiso   1.00
H019   H    -0.39999   -0.31011    0.00000    0.01267   Uiso   1.00
C025   C    -0.38402    0.38402   -0.00000    0.01267   Uiso   1.00
C028   C    -0.43964    0.43964   -0.00000    0.01267   Uiso   1.00
B031   B     0.38732   -0.38732    0.00000    0.01267   Uiso   1.00
N034   N    -0.28021    0.28021   -0.00000    0.01267   Uiso   1.00
C037   C     0.44538   -0.44538    0.00000    0.01267   Uiso   1.00
O040   O     0.28007   -0.28007   -0.00000    0.01267   Uiso   1.00
CR043  Cr   -0.49727    0.49727   -0.50000    0.01267   Uiso   1.00
```

6.12   COF-Cr-4: Cr-intercalated COF

Total Energy $E_{COF-Cr-4}$ **= -5449.2665368 a.u.**

```
data_COF-Cr-4
_symmetry_space_group_name_H-M     'P-6M2'
_symmetry_Int_Tables_number        187
_symmetry_cell_setting             hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                     15.0824
_cell_length_b                     15.0824
_cell_length_c                     3.4061
_cell_angle_alpha                  90.0000
_cell_angle_beta                   90.0000
_cell_angle_gamma                  120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38660   -0.45093    0.00000    0.01267   Uiso   1.00
C007   C     0.04653   -0.39635   -0.00000    0.01267   Uiso   1.00
H013   H     0.40964    0.10530   -0.00000    0.01267   Uiso   1.00
H019   H    -0.40018   -0.31390    0.00000    0.01267   Uiso   1.00
C025   C    -0.38349    0.38349    0.00000    0.01267   Uiso   1.00
```

```
C028   C    -0.43865    0.43865    0.00000    0.01267   Uiso    1.00
B031   B     0.38993   -0.38993   -0.00000    0.01267   Uiso    1.00
N034   N    -0.28075    0.28075    0.00000    0.01267   Uiso    1.00
C037   C     0.44731   -0.44731   -0.00000    0.01267   Uiso    1.00
O040   O     0.27902   -0.27902   -0.00000    0.01267   Uiso    1.00
CR043  Cr   -0.49391    0.49391    0.50000    0.01267   Uiso    1.00
CR046  Cr    0.33333   -0.33333    0.50000    0.01267   Uiso    1.00
```

6.13   COF-Cr-5: Cr-intercalated COF

Total Energy $E_{COF-Cr-5}$ **= -6493.6513435 a.u.**

```
data_COF-Cr-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    15.1665
_cell_length_b                    15.1665
_cell_length_c                    3.4451
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38876   -0.45096    0.00000    0.01267   Uiso    1.00
C007   C     0.04807   -0.39570    0.00000    0.01267   Uiso    1.00
H013   H     0.41013    0.10323   -0.00000    0.01267   Uiso    1.00
H019   H    -0.40117   -0.31375    0.00000    0.01267   Uiso    1.00
C025   C    -0.38545    0.38545   -0.00000    0.01267   Uiso    1.00
C028   C    -0.44010    0.44010    0.00000    0.01267   Uiso    1.00
B031   B     0.38953   -0.38953   -0.00000    0.01267   Uiso    1.00
N034   N    -0.27844    0.27844   -0.00000    0.01267   Uiso    1.00
C037   C     0.44658   -0.44658    0.00000    0.01267   Uiso    1.00
```

```
O040    O     0.27942  -0.27942   0.00000   0.01267  Uiso   1.00
CR043  Cr    -0.49789   0.49789  -0.50000   0.01267  Uiso   1.00
CR046  Cr     0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
CR047  Cr    -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.14   COF-Mn-3: Mn-intercalated COF

Total Energy $E_{COF-Mn-3}$ = **-4724.7346886 a.u.**

```
data_COF-Mn-3
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.8580
_cell_length_b                    14.8580
_cell_length_c                    3.5541
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38564  -0.44702   0.00000   0.01267  Uiso   1.00
C007   C     0.04852  -0.39206   0.00000   0.01267  Uiso   1.00
H013   H     0.40729   0.10523  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39936  -0.30831   0.00000   0.01267  Uiso   1.00
C025   C    -0.38434   0.38434   0.00000   0.01267  Uiso   1.00
C028   C    -0.44042   0.44042   0.00000   0.01267  Uiso   1.00
B031   B     0.38762  -0.38762  -0.00000   0.01267  Uiso   1.00
N034   N    -0.27991   0.27991   0.00000   0.01267  Uiso   1.00
C037   C     0.44617  -0.44617  -0.00000   0.01267  Uiso   1.00
O040   O     0.27982  -0.27982   0.00000   0.01267  Uiso   1.00
MN043  Mn   -0.49889   0.49889   0.50000   0.01267  Uiso   1.00
```

6.15   COF-Mn-4: Mn-intercalated COF

Total Energy $E_{COF-Mn-4}$ = **-5875.5419899 a.u.**

```
data_COF-Mn-3
_symmetry_space_group_name_H-M     'P-6M2'
_symmetry_Int_Tables_number        187
_symmetry_cell_setting             hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                     14.9922
_cell_length_b                     14.9922
_cell_length_c                     3.6025
_cell_angle_alpha                  90.0000
_cell_angle_beta                   90.0000
_cell_angle_gamma                  120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001    C    -0.38533   -0.44856    0.00000    0.01267   Uiso    1.00
C007    C     0.04556   -0.39479    0.00000    0.01267   Uiso    1.00
H013    H     0.40898    0.10648   -0.00000    0.01267   Uiso    1.00
H019    H    -0.39885   -0.31171    0.00000    0.01267   Uiso    1.00
C025    C    -0.38388    0.38388    0.00000    0.01267   Uiso    1.00
C028    C    -0.43932    0.43932    0.00000    0.01267   Uiso    1.00
B031    B     0.39076   -0.39076   -0.00000    0.01267   Uiso    1.00
N034    N    -0.28030    0.28030    0.00000    0.01267   Uiso    1.00
C037    C     0.44789   -0.44789   -0.00000    0.01267   Uiso    1.00
O040    O     0.27950   -0.27950   -0.00000    0.01267   Uiso    1.00
MN043   Mn   -0.49252    0.49252   -0.50000    0.01267   Uiso    1.00
MN046   Mn    0.33333   -0.33333   -0.50000    0.01267   Uiso    1.00
```

6.16   COF-Mn-5: Mn-intercalated COF

Total Energy $E_{COF-Mn-5}$ = **-7026.4449277 a.u.**

```
data_COF-Mn-5
```

```
_symmetry_space_group_name_H-M     'P-6M2'
_symmetry_Int_Tables_number        187
_symmetry_cell_setting             hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                     15.0849
_cell_length_b                     15.0849
_cell_length_c                     3.6666
_cell_angle_alpha                  90.0000
_cell_angle_beta                   90.0000
_cell_angle_gamma                  120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001    C     -0.38728   -0.44819    0.00000    0.01267  Uiso    1.00
C007    C      0.04681   -0.39455    0.00000    0.01267  Uiso    1.00
H013    H      0.40822    0.10333   -0.00000    0.01267  Uiso    1.00
H019    H     -0.39984   -0.31197    0.00000    0.01267  Uiso    1.00
C025    C     -0.38639    0.38639    0.00000    0.01267  Uiso    1.00
C028    C     -0.44036    0.44036    0.00000    0.01267  Uiso    1.00
B031    B      0.39043   -0.39043   -0.00000    0.01267  Uiso    1.00
N034    N     -0.27862    0.27862    0.00000    0.01267  Uiso    1.00
C037    C      0.44684   -0.44684   -0.00000    0.01267  Uiso    1.00
O040    O      0.27986   -0.27986   -0.00000    0.01267  Uiso    1.00
MN043   Mn    -0.49780    0.49780    0.50000    0.01267  Uiso    1.00
MN046   Mn     0.33333   -0.33333    0.50000    0.01267  Uiso    1.00
MN047   Mn    -0.33333    0.33333    0.50000    0.01267  Uiso    1.00
```

6.17   COF-Fe-3: Fe-intercalated COF

Total Energy $E_{COF-Fe-0}$ = -5062.8211239 a.u.

```
data_COF-Fe-3
_symmetry_space_group_name_H-M     'P-6M2'
_symmetry_Int_Tables_number        187
_symmetry_cell_setting             hexagonal
```

```
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                 14.8311
_cell_length_b                 14.8311
_cell_length_c                 3.4436
_cell_angle_alpha              90.0000
_cell_angle_beta               90.0000
_cell_angle_gamma              120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38597   -0.44685    0.00000    0.00000   Uiso    1.00
C007   C     0.04847   -0.39240    0.00000    0.00000   Uiso    1.00
H013   H     0.40659    0.10439   -0.00000    0.00000   Uiso    1.00
H019   H    -0.39936   -0.30842    0.00000    0.00000   Uiso    1.00
C025   C    -0.38441    0.38441   -0.00000    0.00000   Uiso    1.00
C028   C    -0.44073    0.44073   -0.00000    0.00000   Uiso    1.00
B031   B     0.38771   -0.38771    0.00000    0.00000   Uiso    1.00
N034   N    -0.28000    0.28000   -0.00000    0.00000   Uiso    1.00
C037   C     0.44649   -0.44649    0.00000    0.00000   Uiso    1.00
O040   O     0.27983   -0.27983    0.00000    0.00000   Uiso    1.00
FE043  Fe   -0.49763    0.49763   -0.50000    0.00000   Uiso    1.00
```

6.18   COF-Fe-4: Fe-intercalated COF

Total Energy $E_{COF-Fe-0}$ = -6326.3861850 a.u.

```
data_COF-Fe-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
```

```
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a              14.9482
_cell_length_b              14.9482
_cell_length_c              3.4482
_cell_angle_alpha           90.0000
_cell_angle_beta            90.0000
_cell_angle_gamma           120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38561   -0.44844    0.00000   0.01267   Uiso   1.00
C007   C     0.04584   -0.39468    0.00000   0.01267   Uiso   1.00
H013   H     0.40834    0.10584   -0.00000   0.01267   Uiso   1.00
H019   H    -0.39919   -0.31132    0.00000   0.01267   Uiso   1.00
C025   C    -0.38400    0.38400   -0.00000   0.01267   Uiso   1.00
C028   C    -0.43988    0.43988    0.00000   0.01267   Uiso   1.00
B031   B     0.39010   -0.39010    0.00000   0.01267   Uiso   1.00
N034   N    -0.28041    0.28041   -0.00000   0.01267   Uiso   1.00
C037   C     0.44820   -0.44820    0.00000   0.01267   Uiso   1.00
O040   O     0.27953   -0.27953   -0.00000   0.01267   Uiso   1.00
FE043  Fe   -0.49468    0.49468   -0.50000   0.01267   Uiso   1.00
FE046  Fe    0.33333   -0.33333   -0.50000   0.01267   Uiso   1.00
```

6.19   COF-Fe-5: Fe-intercalated COF

Total Energy $E_{COF-Fe-0}$ = **-7589.8886945 a.u.**

```
data_COF-Fe-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
```

```
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                      15.0303
_cell_length_b                      15.0303
_cell_length_c                      3.4398
_cell_angle_alpha                   90.0000
_cell_angle_beta                    90.0000
_cell_angle_gamma                   120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38724  -0.44830   0.00000   0.01267  Uiso   1.00
C007   C     0.04713  -0.39421   0.00000   0.01267  Uiso   1.00
H013   H     0.40853   0.10397  -0.00000   0.01267  Uiso   1.00
H019   H    -0.40016  -0.31134   0.00000   0.01267  Uiso   1.00
C025   C    -0.38578   0.38578  -0.00000   0.01267  Uiso   1.00
C028   C    -0.44123   0.44123  -0.00000   0.01267  Uiso   1.00
B031   B     0.38976  -0.38976   0.00000   0.01267  Uiso   1.00
N034   N    -0.27898   0.27898  -0.00000   0.01267  Uiso   1.00
C037   C     0.44767  -0.44767   0.00000   0.01267  Uiso   1.00
O040   O     0.27980  -0.27980   0.00000   0.01267  Uiso   1.00
FE043  Fe   -0.49787   0.49787  -0.50000   0.01267  Uiso   1.00
FE046  Fe    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
FE047  Fe   -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.20   COF-Co-3: Co-intercalated COF

Total Energy $E_{COF-Co-3}$ = -5420.0991868 a.u.

```
data_COF-Co-3
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
```

```
  -x+y,y,-z
   x,x-y,-z
_cell_length_a                  14.8593
_cell_length_b                  14.8593
_cell_length_c                  3.4114
_cell_angle_alpha               90.0000
_cell_angle_beta                90.0000
_cell_angle_gamma               120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38641  -0.44691   0.00000   0.01267  Uiso   1.00
C007   C     0.04775  -0.39299   0.00000   0.01267  Uiso   1.00
H013   H     0.40682   0.10403  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39913  -0.30919   0.00000   0.01267  Uiso   1.00
C025   C    -0.38446   0.38446   0.00000   0.01267  Uiso   1.00
C028   C    -0.44009   0.44009   0.00000   0.01267  Uiso   1.00
B031   B     0.38766  -0.38766  -0.00000   0.01267  Uiso   1.00
N034   N    -0.27983   0.27983   0.00000   0.01267  Uiso   1.00
C037   C     0.44603  -0.44603  -0.00000   0.01267  Uiso   1.00
O040   O     0.27974  -0.27974   0.00000   0.01267  Uiso   1.00
CO043  Co   -0.49763   0.49763   0.50000   0.01267  Uiso   1.00
```

6.21   COF-Co-4: Co-intercalated COF

Total Energy $E_{COF-Co-4}$ = **-6802.6965761 a.u.**

```
data_COF-Co-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                  14.9497
_cell_length_b                  14.9497
_cell_length_c                  3.4706
```

```
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38630  -0.44843   0.00000   0.01267  Uiso   1.00
C007   C     0.04526  -0.39485   0.00000   0.01267  Uiso   1.00
H013   H     0.40849   0.10533  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39824  -0.31153   0.00000   0.01267  Uiso   1.00
C025   C    -0.38413   0.38413   0.00000   0.01267  Uiso   1.00
C028   C    -0.43946   0.43946   0.00000   0.01267  Uiso   1.00
B031   B     0.39031  -0.39031  -0.00000   0.01267  Uiso   1.00
N034   N    -0.28017   0.28017   0.00000   0.01267  Uiso   1.00
C037   C     0.44723  -0.44723  -0.00000   0.01267  Uiso   1.00
O040   O     0.27896  -0.27896  -0.00000   0.01267  Uiso   1.00
CO043  Co   -0.49547   0.49547   0.50000   0.01267  Uiso   1.00
CO046  Co    0.33333  -0.33333   0.50000   0.01267  Uiso   1.00
```

6.22   COF-Co-5: Co-intercalated COF

Total Energy $E_{COF-Co-5}$ = -8185.3674296 a.u.

```
data_COF-Co-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    15.0153
_cell_length_b                    15.0153
_cell_length_c                    3.5105
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38767  -0.44761   0.00000   0.01267  Uiso   1.00
C007   C     0.04683  -0.39463   0.00000   0.01267  Uiso   1.00
H013   H     0.40733   0.10245  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39989  -0.31165   0.00000   0.01267  Uiso   1.00
C025   C    -0.38655   0.38655  -0.00000   0.01267  Uiso   1.00
C028   C    -0.44041   0.44041  -0.00000   0.01267  Uiso   1.00
B031   B     0.38982  -0.38982   0.00000   0.01267  Uiso   1.00
N034   N    -0.27860   0.27860  -0.00000   0.01267  Uiso   1.00
C037   C     0.44664  -0.44664   0.00000   0.01267  Uiso   1.00
O040   O     0.27920  -0.27920   0.00000   0.01267  Uiso   1.00
CO043  Co   -0.49770   0.49770   0.50000   0.01267  Uiso   1.00
CO046  Co    0.33333  -0.33333   0.50000   0.01267  Uiso   1.00
CO047  Co   -0.33333   0.33333   0.50000   0.01267  Uiso   1.00
```

6.23   COF-Ni-3: Ni-intercalated COF

Total Energy $E_{COF-Ni-3}$ = **-5796.6548376 a.u.**

```
data_COF-Ni-3
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.9930
_cell_length_b                    14.9930
_cell_length_c                    3.5875
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C   -0.38856  -0.44885   0.00000   0.01267  Uiso   1.00
C007   C    0.04732  -0.39542   0.00000   0.01267  Uiso   1.00
H013   H    0.40763   0.10207  -0.00000   0.01267  Uiso   1.00
H019   H   -0.40012  -0.31225   0.00000   0.01267  Uiso   1.00
C025   C   -0.38540   0.38540  -0.00000   0.01267  Uiso   1.00
C028   C   -0.43988   0.43988  -0.00000   0.01267  Uiso   1.00
B031   B    0.38849  -0.38849   0.00000   0.01267  Uiso   1.00
N034   N   -0.27858   0.27858  -0.00000   0.01267  Uiso   1.00
C037   C    0.44595  -0.44595  -0.00000   0.01267  Uiso   1.00
O040   O    0.27875  -0.27875   0.00000   0.01267  Uiso   1.00
NI043  Ni  -0.49829   0.49829  -0.50000   0.01267  Uiso   1.00
NI046  Ni   0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
NI047  Ni  -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.24   COF-Ni-4: Ni-intercalated COF

Total Energy $E_{COF-Ni-4}$ = -7304.8867437 a.u.

```
data_COF-Ni-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.9930
_cell_length_b                    14.9930
_cell_length_c                    3.5875
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
```

```
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38856   -0.44885    0.00000    0.01267   Uiso    1.00
C007   C     0.04732   -0.39542    0.00000    0.01267   Uiso    1.00
H013   H     0.40763    0.10207   -0.00000    0.01267   Uiso    1.00
H019   H    -0.40012   -0.31225    0.00000    0.01267   Uiso    1.00
C025   C    -0.38540    0.38540   -0.00000    0.01267   Uiso    1.00
C028   C    -0.43988    0.43988   -0.00000    0.01267   Uiso    1.00
B031   B     0.38849   -0.38849    0.00000    0.01267   Uiso    1.00
N034   N    -0.27858    0.27858   -0.00000    0.01267   Uiso    1.00
C037   C     0.44595   -0.44595   -0.00000    0.01267   Uiso    1.00
O040   O     0.27875   -0.27875    0.00000    0.01267   Uiso    1.00
NI043  Ni   -0.49829    0.49829   -0.50000    0.01267   Uiso    1.00
NI046  Ni    0.33333   -0.33333   -0.50000    0.01267   Uiso    1.00
NI047  Ni   -0.33333    0.33333   -0.50000    0.01267   Uiso    1.00
```

6.25 COF-Ni-5: Ni-intercalated COF

Total Energy $E_{COF-Ni-5}$ = **-8813.03418713 a.u.**

```
data_COF-Ni-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.9930
_cell_length_b                    14.9930
_cell_length_c                    3.5875
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38856   -0.44885    0.00000    0.01267   Uiso    1.00
```

```
C007   C     0.04732  -0.39542   0.00000   0.01267   Uiso   1.00
H013   H     0.40763   0.10207  -0.00000   0.01267   Uiso   1.00
H019   H    -0.40012  -0.31225   0.00000   0.01267   Uiso   1.00
C025   C    -0.38540   0.38540  -0.00000   0.01267   Uiso   1.00
C028   C    -0.43988   0.43988  -0.00000   0.01267   Uiso   1.00
B031   B     0.38849  -0.38849   0.00000   0.01267   Uiso   1.00
N034   N    -0.27858   0.27858  -0.00000   0.01267   Uiso   1.00
C037   C     0.44595  -0.44595  -0.00000   0.01267   Uiso   1.00
O040   O     0.27875  -0.27875   0.00000   0.01267   Uiso   1.00
NI043  Ni   -0.49829   0.49829  -0.50000   0.01267   Uiso   1.00
NI046  Ni    0.33333  -0.33333  -0.50000   0.01267   Uiso   1.00
NI047  Ni   -0.33333   0.33333  -0.50000   0.01267   Uiso   1.00
```

6.26   COF-Cu-3: Cu-intercalated COF

Total Energy $E_{COF-Cu-3}$ **= -6193.0306926 a.u.**

```
data_COF-Cu-3
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.8268
_cell_length_b                    14.8268
_cell_length_c                    3.4614
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38660  -0.44687   0.00000   0.01267   Uiso   1.00
C007   C     0.04768  -0.39326   0.00000   0.01267   Uiso   1.00
H013   H     0.40659   0.10381  -0.00000   0.01267   Uiso   1.00
H019   H    -0.39922  -0.30924   0.00000   0.01267   Uiso   1.00
```

```
C025   C    -0.38462   0.38462  -0.00000   0.01267  Uiso   1.00
C028   C    -0.44026   0.44026   0.00000   0.01267  Uiso   1.00
B031   B     0.38783  -0.38783  -0.00000   0.01267  Uiso   1.00
N034   N    -0.27973   0.27973   0.00000   0.01267  Uiso   1.00
C037   C     0.44617  -0.44617  -0.00000   0.01267  Uiso   1.00
O040   O     0.27964  -0.27964   0.00000   0.01267  Uiso   1.00
CU043  Cu   -0.49735   0.49735  -0.50000   0.01267  Uiso   1.00
```

6.27   COF-Cu-4: Cu-intercalated COF

Total Energy $E_{COF-Cu-4}$ = **-7833.3371110 a.u.**

```
data_COF-Cu-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.9292
_cell_length_b                    14.9292
_cell_length_c                    3.4926
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38692  -0.44741   0.00000   0.01267  Uiso   1.00
C007   C     0.04647  -0.39514   0.00000   0.01267  Uiso   1.00
H013   H     0.40701   0.10334  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39927  -0.31160   0.00000   0.01267  Uiso   1.00
C025   C    -0.38410   0.38410  -0.00000   0.01267  Uiso   1.00
C028   C    -0.43943   0.43943  -0.00000   0.01267  Uiso   1.00
B031   B     0.39050  -0.39050  -0.00000   0.01267  Uiso   1.00
N034   N    -0.27995   0.27995  -0.00000   0.01267  Uiso   1.00
C037   C     0.44677  -0.44677  -0.00000   0.01267  Uiso   1.00
```

```
O040   O     0.27921  -0.27921  -0.00000   0.01267  Uiso   1.00
CU043  Cu   -0.48342   0.48342  -0.50000   0.01267  Uiso   1.00
CU046  Cu    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
```

6.28   COF-Cu-5: Cu-intercalated COF

Total Energy $E_{COF-Cu-5}$ = -9473.7028001 a.u.

```
data_COF-Cu-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.9510
_cell_length_b                    14.9510
_cell_length_c                    3.5388
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38751  -0.44674   0.00000   0.01267  Uiso   1.00
C007   C     0.04715  -0.39472   0.00000   0.01267  Uiso   1.00
H013   H     0.40623   0.10184  -0.00000   0.01267  Uiso   1.00
H019   H    -0.39980  -0.31129   0.00000   0.01267  Uiso   1.00
C025   C    -0.38614   0.38614   0.00000   0.01267  Uiso   1.00
C028   C    -0.44003   0.44003   0.00000   0.01267  Uiso   1.00
B031   B     0.39038  -0.39038   0.00000   0.01267  Uiso   1.00
N034   N    -0.27833   0.27833   0.00000   0.01267  Uiso   1.00
C037   C     0.44644  -0.44644  -0.00000   0.01267  Uiso   1.00
O040   O     0.27944  -0.27944  -0.00000   0.01267  Uiso   1.00
CU043  Cu   -0.48796   0.48796  -0.50000   0.01267  Uiso   1.00
CU046  Cu    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
CU047  Cu   -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.29   COF-Zn-3: Zn-intercalated COF

Total Energy $E_{COF-Zn-3}$ = -6609.4788758 a.u.

```
data_COF-Zn-3
_symmetry_space_group_name_H-M     'P-6M2'
_symmetry_Int_Tables_number        187
_symmetry_cell_setting             hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                     14.7283
_cell_length_b                     14.7283
_cell_length_c                     5.9055
_cell_angle_alpha                  90.0000
_cell_angle_beta                   90.0000
_cell_angle_gamma                  120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38812   -0.44845    0.00000    0.01267   Uiso   1.00
C007   C     0.04776   -0.39477    0.00000    0.01267   Uiso   1.00
H013   H     0.40721    0.10376   -0.00000    0.01267   Uiso   1.00
H019   H    -0.40030   -0.30987    0.00000    0.01267   Uiso   1.00
C025   C    -0.38478    0.38478   -0.00000    0.01267   Uiso   1.00
C028   C    -0.44229    0.44229   -0.00000    0.01267   Uiso   1.00
B031   B     0.38809   -0.38809    0.00000    0.01267   Uiso   1.00
N034   N    -0.27991    0.27991   -0.00000    0.01267   Uiso   1.00
C037   C     0.44818   -0.44818    0.00000    0.01267   Uiso   1.00
O040   O     0.27959   -0.27959    0.00000    0.01267   Uiso   1.00
ZN043  Zn   -0.49370    0.49370   -0.50000    0.01267   Uiso   1.00
ZN046  Zn    0.33333   -0.33333   -0.50000    0.01267   Uiso   1.00
ZN047  Zn   -0.33333    0.33333   -0.50000    0.01267   Uiso   1.00
```

6.30   COF-Zn-4: Zn-intercalated COF

Total Energy $E_{COF-Zn-4}$ = -8388.9674528 a.u.

```
data_COF-Zn-4
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
_symmetry_cell_setting            hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                    14.7283
_cell_length_b                    14.7283
_cell_length_c                    5.9055
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C    -0.38812  -0.44845   0.00000   0.01267  Uiso   1.00
C007   C     0.04776  -0.39477   0.00000   0.01267  Uiso   1.00
H013   H     0.40721   0.10376  -0.00000   0.01267  Uiso   1.00
H019   H    -0.40030  -0.30987   0.00000   0.01267  Uiso   1.00
C025   C    -0.38478   0.38478  -0.00000   0.01267  Uiso   1.00
C028   C    -0.44229   0.44229  -0.00000   0.01267  Uiso   1.00
B031   B     0.38809  -0.38809   0.00000   0.01267  Uiso   1.00
N034   N    -0.27991   0.27991  -0.00000   0.01267  Uiso   1.00
C037   C     0.44818  -0.44818   0.00000   0.01267  Uiso   1.00
O040   O     0.27959  -0.27959   0.00000   0.01267  Uiso   1.00
ZN043  Zn   -0.49370   0.49370  -0.50000   0.01267  Uiso   1.00
ZN046  Zn    0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
ZN047  Zn   -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```

6.31   COF-Zn-5: Zn-intercalated COF

Total Energy $E_{COF-Zn-5}$ = -10168.2415578 a.u.

```
data_COF-Zn-5
_symmetry_space_group_name_H-M    'P-6M2'
_symmetry_Int_Tables_number       187
```

```
_symmetry_cell_setting          hexagonal
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -y,x-y,z
  -x+y,-x,z
  x,y,-z
  -y,x-y,-z
  -x+y,-x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
  -y,-x,-z
  -x+y,y,-z
  x,x-y,-z
_cell_length_a                  14.7283
_cell_length_b                  14.7283
_cell_length_c                  5.9055
_cell_angle_alpha               90.0000
_cell_angle_beta                90.0000
_cell_angle_gamma               120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C001   C   -0.38812  -0.44845   0.00000   0.01267  Uiso   1.00
C007   C    0.04776  -0.39477   0.00000   0.01267  Uiso   1.00
H013   H    0.40721   0.10376  -0.00000   0.01267  Uiso   1.00
H019   H   -0.40030  -0.30987   0.00000   0.01267  Uiso   1.00
C025   C   -0.38478   0.38478  -0.00000   0.01267  Uiso   1.00
C028   C   -0.44229   0.44229  -0.00000   0.01267  Uiso   1.00
B031   B    0.38809  -0.38809   0.00000   0.01267  Uiso   1.00
N034   N   -0.27991   0.27991  -0.00000   0.01267  Uiso   1.00
C037   C    0.44818  -0.44818   0.00000   0.01267  Uiso   1.00
O040   O    0.27959  -0.27959   0.00000   0.01267  Uiso   1.00
ZN043  Zn  -0.49370   0.49370  -0.50000   0.01267  Uiso   1.00
ZN046  Zn   0.33333  -0.33333  -0.50000   0.01267  Uiso   1.00
ZN047  Zn  -0.33333   0.33333  -0.50000   0.01267  Uiso   1.00
```