

Electronic Supplementary Information

Electronic Structures of Two-Dimensional Covalent Organic Frameworks Based on Series of Period 4 Transition-metal Phthalocyanine and Ethynyl Moiety

Xin Chen and Xianran Xing*

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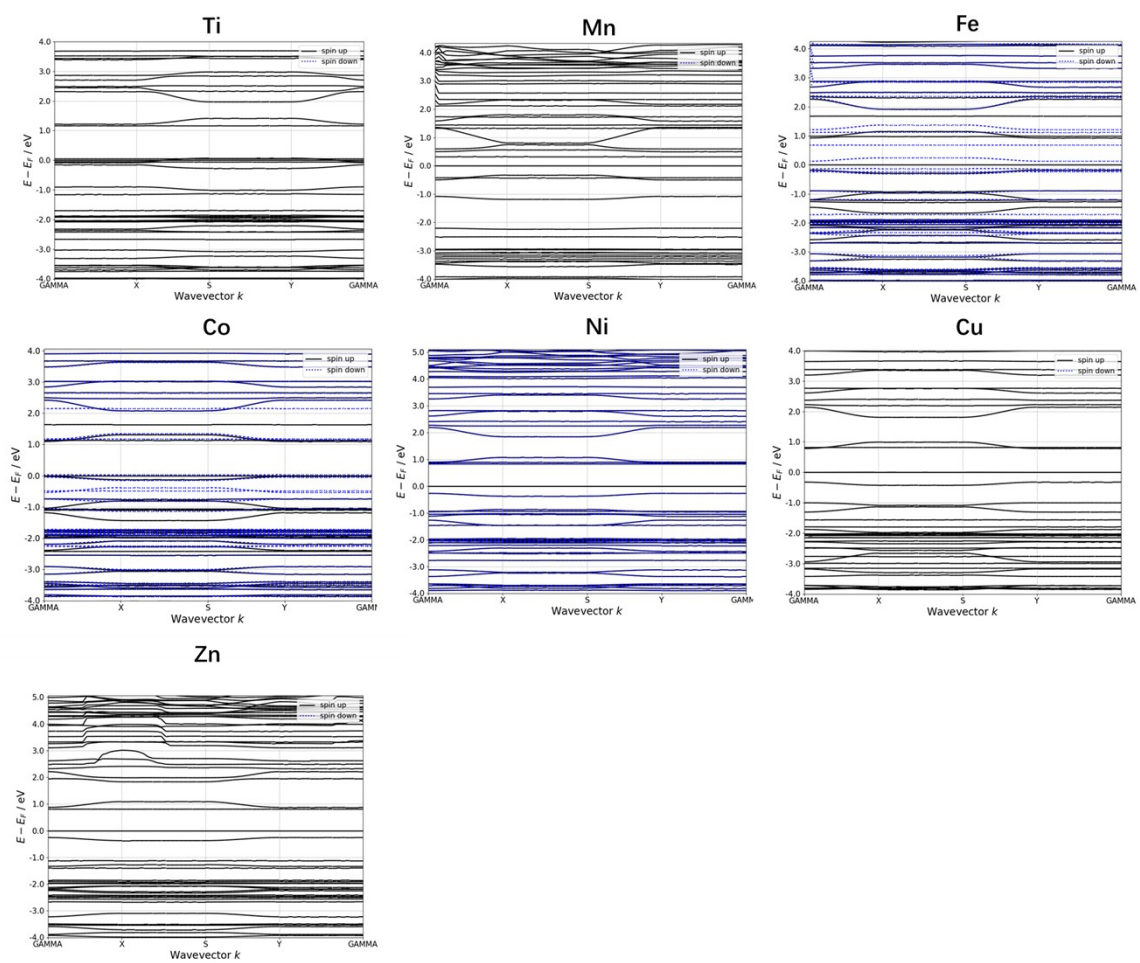


Figure S1. Electronic band structures of MPc COFs (M = Ti, Mn, Fe, Co, Ni, Cu and Zn).

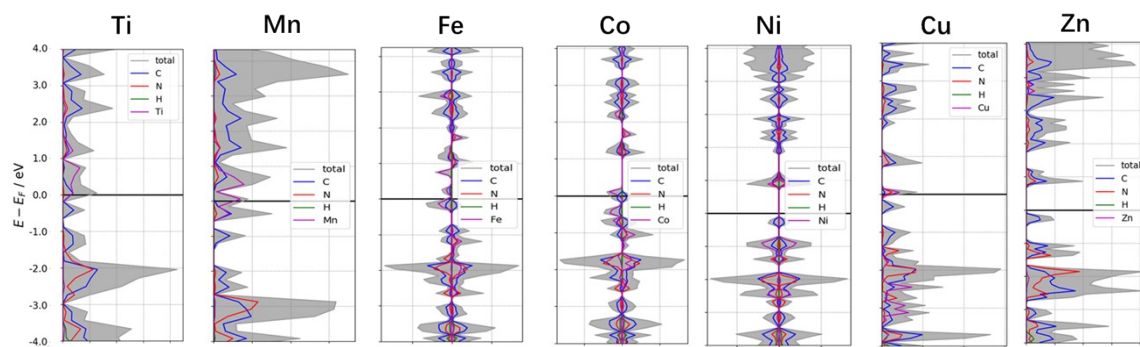


Figure S2. pDOS of MPc COFs (M = Ti, Mn, Fe, Co, Ni, Cu and Zn).

Table S1. Fraction coordinates for the optimized structures.

CrPC COF

1.0000000000000000		
17.3500003814352688	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
-3.5480074821132401	0.0000000000000000	16.9833493794633590

C	N	H	Cr
36	8	12	1

Direct

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MnPc COF

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0.0000000000000000 20.0000000000000000 0.0000000000000000

-3.5480074821132401 0.0000000000000000 16.9833493794633590

C N H Mn

36 8 12 1

Direct

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FePc COF

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0.0000000000000000 20.0000000000000000 0.0000000000000000
-3.5480074821132401 0.0000000000000000 16.9833493794633590
C N H Fe
36 8 12 1
  
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Direct

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CoPc COF

1.0000000000000000

17.3500003814352688	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
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C	N	H	Co
36	8	12	1

Direct

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NiPc COF

1.0000000000000000
17.3500003814352688 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
-3.5480074821132401 0.0000000000000000 16.9833493794633590
C N H Ni
36 8 12 1

Direct

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0.1373851961308513 0.0000000002390623 0.1754517394970733
0.1452847853445222 0.00000000013684074 0.9021500588934015
0.8860919973814868 -0.0000000001591992 0.6391906373529251
0.1298644387093809 0.0000000003976433 0.6137577168541795
0.1756071716805279 -0.0000000000767131 0.7615862026506940
0.3125068299194267 -0.0000000001363435 0.9243776577129467
0.4487408852923302 0.0000000001999740 0.1634914970322814
0.3281481501843863 0.0000000000811607 0.2157220931933272
0.1139080029425615 -0.0000000002068261 0.3608093627833227
0.8701355615578941 0.0000000003406179 0.3862422826658150
0.8243928275692703 0.000000000057326 0.2384137966468145
0.6874931700717751 -0.0000000001464334 0.0756223419758313
0.5512591154831121 0.0000000002148948 0.8365085031374392
0.6718518500723949 0.0000000001080135 0.7842779064756660
0.0000000034568506 0.0000000095678865 0.0000000020075112

CuPc COF

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1.0000000000000000
  17.3500003814352688   0.0000000000000000   0.0000000000000000
    0.0000000000000000  20.0000000000000000   0.0000000000000000
   -3.5480074821132401   0.0000000000000000   16.9833493794633590
C     N     H     Cu
  36     8    12     1
  
```

Direct

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0.1655689551024091  0.0000000188457205  0.1095917536564722
0.2505723982934412  0.0000000028090551  0.1023689500161734
0.2508033877687586 -0.0000000042762514  0.0207413940170496
0.1679768269268742  0.0000000071577830  0.9806024365002970
0.7491966105469784 -0.0000000146597137  0.9792586185748409
0.7494276184913728 -0.0000000037941167  0.8976310545123297
0.8320231671725824 -0.0000000058381562  0.0193975785836050
0.8344310288326764  0.0000000007038980  0.8904082410771980
0.0717860624309739 -0.0000000005774936  0.8633255755807627
0.0571903297474173  0.0000000036797748  0.7790059287625192
0.9751728351992834 -0.0000000002040964  0.7492814424610519
0.9395472709807442  0.0000000078354715  0.8219728811784380
0.0604527187958062  0.0000000204146861  0.1780271080009909
0.0248271688580613  0.0000000119849462  0.2507185565837386
0.9428096809088232  0.0000000165783728  0.2209940769074198
0.9282139010928754  0.0000000041333614  0.1366744364318276
0.9494224667425984 -0.0000000141273077  0.6664066377477336
0.0070261047825406 -0.0000000199260977  0.6180624853064243
0.0888594119775072 -0.0000000041424984  0.6528198296818012
0.1142899525000175  0.0000000067693781  0.7331789401119119
0.3196428207421306 -0.0000000042601213  0.9895927159217734
0.3950287129631016 -0.0000000097169577  0.0406142243001735
0.3941356653183792 -0.0000000128598058  0.1230847031287205
0.3249792284675940 -0.0000000035283546  0.1535539032372663
0.0505775464064906 -0.0000000008068257  0.3335933759629556
0.9929739056540858 -0.0000000109546558  0.3819375418324114
  
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0.9111406151144553	0.0000000011944592	0.3471801913859544
0.8857100690749958	0.0000000145312002	0.2668210666264538
0.6803571798439478	-0.0000000069185501	0.0104072864958669
0.6049712524423458	-0.0000000109821165	0.9593857434598747
0.6058643213066868	-0.0000000176713039	0.8769152756851157
0.6750207966564381	-0.0000000133412668	0.8464460709680306
0.0054413947622812	-0.0000000250707399	0.4659752817073230
0.9945586324100724	-0.0000000296382007	0.5340247405463704
0.4686266317981809	-0.0000000056140226	0.0118761097873928
0.5313733240767170	-0.0000000037591056	0.9881238678956371
0.1199028079728236	0.0000000150518086	0.0341810324157629
0.8800972076132255	-0.0000000090165269	0.9658189989775176
0.0015080787034572	0.0000000004121344	0.8878566085387449
0.9984918970388162	0.0000000022320491	0.1121433533531526
0.8626572339997781	0.0000000193728866	0.8237562785400686
0.8542710717524318	-0.0000000001632935	0.0967800746806816
0.1373427952208822	0.0000000330188778	0.1762437309196712
0.1457289308816649	0.0000000082991213	0.9032199350031553
0.8869106555455878	-0.0000000228007927	0.6389276723329826
0.1306740596534117	-0.0000000005637132	0.6137400422177046
0.1764532269468750	0.0000000177746864	0.7615547649858437
0.3143960818259752	0.0000000132698915	0.9257945313776529
0.4505836557389807	0.0000000059138132	0.1647436515980132
0.3303274078668245	-0.0000000015316559	0.2173630159933835
0.1130893605677067	-0.0000000056567023	0.3610723399997942
0.8693259614043777	-0.0000000049176024	0.3862599931400957
0.8235467745447046	0.0000000242474965	0.2384452575393260
0.6856039193601053	0.0000000029553837	0.0742054774026899
0.5494163086406575	0.0000000031893691	0.8352563095457253
0.6696725953632199	-0.0000000095551582	0.7826369403383528
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ZnPc COF

1.0000000000000000

17.3500003814352688	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
-3.5480074821132401	0.0000000000000000	16.9833493794633590

C	N	H	Zn
36	8	12	1

Direct

0.1668505661305616	0.0000000464745868	0.1107753217107520
0.2520590618395300	0.0000000814388724	0.1039300939676080
0.2524778728595631	0.0000001487136193	0.0221844900024372
0.1698686357364270	0.0000001136845335	0.9815446650907257
0.7475221284484165	0.9999998509580481	0.9778155095808635
0.7479409389691641	0.9999999186388797	0.8960699066371820
0.8301313649529157	0.9999998866521821	0.0184553348905567
0.8331494332648824	-0.0000000458278477	0.8892246795705347
0.0730341171748200	0.0000000586929953	0.8630337472268048
0.0584917727466893	-0.0000000042093297	0.7787424165494655
0.9762781453668337	-0.0000000721764922	0.7490192327130029
0.9400775062183586	-0.0000000625950767	0.8212202851427296
0.0599224933339158	0.0000000618756021	0.1787797139903870
0.0237218529540621	0.0000000731471759	0.2509807674597206
0.9415082283923581	0.0000000060299852	0.2212575843135460
0.9269658823784108	0.9999999413937095	0.1369662515397252
0.9505707556934778	0.9999999101692713	0.6663511102794831
0.0079736090053404	0.9999999225738687	0.6179707823712337
0.0898783059098340	-0.0000000577547023	0.6523723873481015
0.1154133139365446	-0.0000000088332555	0.7327155001942045
0.3212250015487668	0.0000001501647760	0.9913612398197654
0.3964110568831578	0.0000000828146486	0.0424474439870012
0.3957122845299219	0.0000000062869146	0.1248773954156970
0.3263946199469677	0.0000000396509243	0.1551129118491061
0.0494292445889810	0.0000000904650794	0.3336488900213989
0.9920263913762376	0.0000000771104352	0.3820292174095786

0.9101216940030191	0.0000000591410018	0.3476276121017800
0.8845866853218839	0.0000000109603703	0.2672845003190578
0.6787749979652504	-0.0000001508933811	0.0086387599776153
0.6035889442099568	-0.0000000838366004	0.9575525556962962
0.6042877151557049	-0.0000000072474763	0.8751226045900370
0.6736053804961873	-0.0000000400818943	0.8448870874023461
0.0051403970582299	0.0000000133140388	0.4659106308724017
0.9948596036003479	-0.0000000160281930	0.5340893674544149
0.4692064569217747	0.0000000182503702	0.0128273476957778
0.5307935424967406	-0.0000000195429671	0.9871726521340057
0.1220890942488009	0.0000000097232387	0.0351916443218611
0.8779109057612142	-0.0000000086621913	0.9648083575226195
0.0022282968220164	-0.0000000018946174	0.8867927026774665
0.9977717017752676	-0.0000000000355543	0.1132072956291560
0.8628895569842365	0.9999999192012473	0.8231093508976622
0.8530980305380418	-0.0000001685700452	0.0960725696902024
0.1371104414326958	0.0000000804059074	0.1768906512481991
0.1469019704604566	0.0000001686388350	0.9039274312808852
0.8880145839793357	-0.0000000566034779	0.6393073900673695
0.1314016284032769	-0.0000001187996041	0.6129884023174578
0.1775788326215535	0.9999999875598079	0.7610287105123565
0.3159301779658690	0.0000001838980338	0.9276008818375363
0.4521819142014937	0.9999999592182178	0.1665583057221016
0.3313708357995061	0.0000000388684657	0.2188688333470197
0.1119854163944711	0.0000000564382782	0.3606926098567694
0.8685983716808507	0.0000001199890010	0.3870115975987348
0.8224211672215880	0.0000000140439306	0.2389712893084534
0.6840698220992392	0.9999998143675642	0.0723991180198916
0.5478180858035508	0.0000000412433514	0.8334416939129976
0.6686291643246788	-0.0000000382824526	0.7811311662875503
0.0000000000665936	-0.0000000003225879	0.0000000006183639