Supporting information for

Molecular and Electronic structure of the Tetrabenzoporphyrin Metal Complexes, [TBPM (M = VO, TiO) and its Electochemical Study.

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Cartesian coordinates of VOTBP calculated at PBE0/def2-TZBP level of theory

H	7.542160000000	1.229241000000	-0.255130000000
H	-1.229262000000	7.542162000000	-0.255026000000
H	-7.542155000000	-1.229248000000	-0.255140000000
H	1.229236000000	7.542169000000	-0.255055000000
H	-7.542156000000	1.229248000000	-0.255108000000
H	-1.229246000000	-7.542164000000	-0.255050000000
H	7.542156000000	-1.229257000000	-0.255101000000
H	1.229251000000	-7.542163000000	-0.255022000000
N	0.000006000000	2.039486000000	0.011618000000
N	-2.039479000000	0.000001000000	0.011607000000
N	-0.000001000000	-2.039482000000	0.011617000000
N	2.039481000000	0.000002000000	0.011602000000
C	2.410165000000	2.410163000000	-0.033654000000
C	-2.410158000000	2.410164000000	-0.033611000000
C	-2.410163000000	-2.410163000000	-0.033654000000
C	2.410161000000	-2.410162000000	-0.033620000000
C	1.103758000000	2.841212000000	-0.029459000000
C	-2.841205000000	1.103756000000	-0.029454000000
C	-1.103754000000	-2.841206000000	-0.029458000000
C	2.841205000000	1.103754000000	-0.029481000000

C	-1.103749000000	2.841206000000	-0.029432000000
C	-2.841202000000	-1.103751000000	-0.029478000000
C	1.103753000000	-2.841208000000	-0.029437000000
C	2.841203000000	-1.103754000000	-0.029460000000
C	0.696633000000	4.226209000000	-0.093219000000
C	-4.226200000000	0.696633000000	-0.093242000000
C	-0.696631000000	-4.226205000000	-0.093217000000
C	4.226203000000	0.696628000000	-0.093261000000
C	-0.696628000000	4.226206000000	-0.093200000000
C	-4.226200000000	-0.696628000000	-0.093261000000
C	0.696629000000	-4.226205000000	-0.093205000000
C	4.226201000000	-0.696631000000	-0.093249000000
C	1.409594000000	5.420796000000	-0.153571000000
C	-5.420785000000	1.409600000000	-0.153594000000
C	-1.409597000000	-5.420790000000	-0.153569000000
C	5.420787000000	1.409593000000	-0.153628000000
C	-1.409601000000	5.420787000000	-0.153537000000
C	-5.420782000000	-1.409596000000	-0.153627000000
C	1.409599000000	-5.420789000000	-0.153540000000
C	5.420783000000	-1.409602000000	-0.153595000000
C	0.700604000000	6.599388000000	-0.210116000000
C	-6.599377000000	0.700615000000	-0.210171000000
C	-0.700613000000	-6.599384000000	-0.210111000000
C	6.599381000000	0.700607000000	-0.210183000000
C	-0.700623000000	6.599385000000	-0.210097000000
C	-6.599377000000	-0.700614000000	-0.210189000000
C	0.700616000000	-6.599383000000	-0.210097000000
C	6.599378000000	-0.700621000000	-0.210168000000
H	2.491514000000	5.432427000000	-0.154666000000
H	-5.432414000000	2.491520000000	-0.154659000000
H	-2.491517000000	-5.432416000000	-0.154656000000
H	5.432414000000	2.491513000000	-0.154719000000

H	-2.491521000000	5.432404000000	-0.154600000000
H	-5.432406000000	-2.491516000000	-0.154721000000
H	2.491518000000	-5.432414000000	-0.154606000000
H	5.432406000000	-2.491522000000	-0.154662000000
H	3.173962000000	3.173958000000	-0.068312000000
H	-3.173953000000	3.173960000000	-0.068254000000
H	-3.173959000000	-3.173957000000	-0.068318000000
H	3.173956000000	-3.173960000000	-0.068266000000
V	-0.000002000000	-0.000003000000	0.515318000000
O	0.000005000000	0.000000000000	2.071988000000

Cartesian coordinates of TiOTBP calculated at PBE0/def2-TZBP level of theory

H	4.472147000000	-6.210583000000	0.317349000000
H	6.210582000000	4.472145000000	0.317350000000
H	-4.472146000000	6.210583000000	0.317353000000
H	-6.210583000000	4.472145000000	0.317353000000
H	-4.472148000000	-6.210582000000	0.317349000000
H	6.210584000000	-4.472145000000	0.317347000000
H	4.472145000000	6.210583000000	0.317342000000
H	-6.210584000000	-4.472143000000	0.317344000000
N	1.458331000000	-1.458331000000	-0.031296000000
N	1.458330000000	1.458330000000	-0.031295000000
N	-1.458330000000	1.458330000000	-0.031296000000
N	-1.458330000000	-1.458331000000	-0.031296000000
C	0.000000000000	-3.415095000000	0.030399000000
C	3.415094000000	0.000000000000	0.030408000000
C	0.000000000000	3.415095000000	0.030397000000
C	-3.415094000000	0.000000000000	0.030413000000
C	-1.236088000000	-2.802673000000	0.022352000000
C	2.802673000000	-1.236089000000	0.022355000000
C	1.236088000000	2.802673000000	0.022353000000
C	-2.802672000000	-1.236088000000	0.022357000000
C	1.236088000000	-2.802674000000	0.022353000000

C	2.802672000000	1.236088000000	0.022356000000
C	-1.236088000000	2.802673000000	0.022351000000
C	-2.802672000000	1.236088000000	0.022358000000
C	-2.505289000000	-3.491760000000	0.104124000000
C	3.491761000000	-2.505289000000	0.104122000000
C	2.505289000000	3.491760000000	0.104121000000
C	-3.491760000000	-2.505289000000	0.104120000000
C	2.505289000000	-3.491761000000	0.104125000000
C	3.491760000000	2.505288000000	0.104126000000
C	-2.505289000000	3.491760000000	0.104122000000
C	-3.491761000000	2.505289000000	0.104120000000
C	-2.845949000000	-4.839090000000	0.183375000000
C	4.839091000000	-2.845947000000	0.183379000000
C	2.845947000000	4.839090000000	0.183373000000
C	-4.839090000000	-2.845946000000	0.183377000000
C	2.845949000000	-4.839091000000	0.183377000000
C	4.839090000000	2.845947000000	0.183381000000
C	-2.845948000000	4.839090000000	0.183377000000
C	-4.839090000000	2.845947000000	0.183381000000
C	-4.180216000000	-5.170628000000	0.257970000000
C	5.170631000000	-4.180213000000	0.257972000000
C	4.180213000000	5.170630000000	0.257971000000
C	-5.170630000000	-4.180212000000	0.257970000000
C	4.180216000000	-5.170629000000	0.257971000000
C	5.170629000000	4.180214000000	0.257974000000
C	-4.180214000000	5.170629000000	0.257973000000
C	-5.170630000000	4.180214000000	0.257974000000
H	-2.089263000000	-5.612442000000	0.185053000000
H	5.612442000000	-2.089260000000	0.185052000000
H	2.089260000000	5.612441000000	0.185049000000
H	-5.612441000000	-2.089259000000	0.185049000000
H	2.089262000000	-5.612442000000	0.185053000000

H	5.612441000000	2.089260000000	0.185061000000
H	-2.089261000000	5.612441000000	0.185049000000
H	-5.612442000000	2.089260000000	0.185054000000
H	0.000000000000	-4.494959000000	0.078452000000
H	4.494958000000	0.000000000000	0.078462000000
H	0.000000000000	4.494959000000	0.078447000000
H	-4.494957000000	0.000000000000	0.078468000000
Ti	0.000000000000	-0.000001000000	-0.584507000000
O	0.000003000000	-0.000002000000	-2.183003000000

Frontier Molecular Orbitals diagram

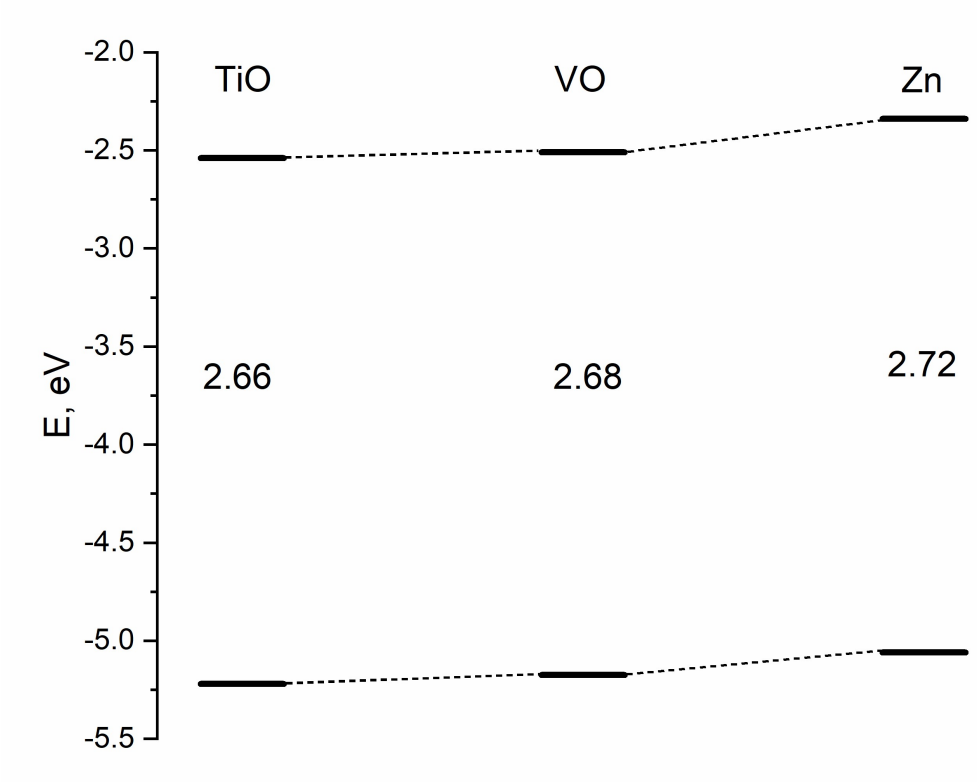

Figure S1. Frontier molecular orbitals diagram of MTBP(M= TiO, VO, Zn)