Supporting Information

A computational study on CO$_2$ electrochemical reduction on the two dimensional metal -1,2,3,4,5,6,7,8,9,10,11,12-perthiolated coronene frameworks

Haoyan Zhang,[a,b] Lin Cheng,[a,*] Kai Li,[b] Ying Wang,[b] Wencheng Wang [c,*]

[a]College of Chemical Engineering, Inner Mongolia University of Technology, Inner Mongolia Key Laboratory of Theoretical and Computational Chemistry Simulation, Hohhot 010051, P. R. China
[b]State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China.
[c]Radiotherapy Laboratory, Jilin Cancer Hospital, Changchun 130012, P. R. China

*Corresponding authors. lcheng1983@aliyun.com; wencheng.w@163.com.

Table S1. The calculated metal-S bond distances, lattice parameters a, adsorption energies of CO_2, and the calculated U values.

	TM-S bond length（Å）	a(Å)	E_{ads}	U
Sc	2.43, 2.43, 2.43, 2.43	14.37	-0.09	0.08
Ti	2.40, 2.39, 2.40, 2.40	14.27	-0.10	3.97
V	2.34, 2.34, 2.34, 2.34	14.11	-0.49	4.60
Cr	2.37, 2.37, 2.37, 2.37	14.15	-0.14	4.70
Mn	2.37, 2.37, 2.37, 2.37	14.10	-0.14	5.52
Fe	2.23, 2.23, 2.23, 2.23	13.79	-0.15	4.29
Co	2.19, 2.19, 2.19, 2.19	13.69	-0.14	4.97
Ni	2.11, 2.12, 2.11, 2.11	13.54	-0.41	5.54
Cu	2.22, 2.22, 2.22, 2.22	13.69	-0.13	7.52
Zn	2.27, 2.28, 2.28, 2.28,	13.81	-0.15	5.67
Y	2.61, 2.61, 2.61, 2.61	14.82	-0.64	2.60
Zr	2.52, 2.48, 2.52, 2.49	14.45	-1.72	3.58
Nb	2.43, 2.33, 2.43, 2.33	14.27	-1.07	1.89
Mo	2.39, 2.37, 2.38, 2.38	14.22	-0.25	2.37
Ru	2.26, 2.26, 2.25, 2.26	13.91	-0.50	2.50
Rh	2.30, 2.18, 2.30, 2.18	13.77	-0.95	3.09
Pd	2.28, 2.28, 2.28, 2.28	13.85	-0.41	1.77
Ag	2.43, 2.43, 2.43, 2.43	14.60	-0.13	3.39
Sc-O	2.76, 2.76, 2.76, 2.76	14.37	-0.21	0.08
Ti-O	2.55, 2.54, 2.54, 2.54	14.27	-0.16	3.97
Zr-O	2.68, 2.69, 2.71, 2.70	14.45	-0.19	3.58
Nb-O	2.53, 2.51, 2.51, 2.49	14.27	-0.13	1.89
Mo-O	2.43, 2.43, 2.43, 2.44	14.22	-0.27	2.37

Table S2. Standard dissolution potentials (U_M^0, in V) of bulk metals and the calculated dissolution potentials (U_{dis}, in V) of TM for $TM + nH^+ \leftrightarrow TM^{n+} + n/2H_2$, at pH=0.

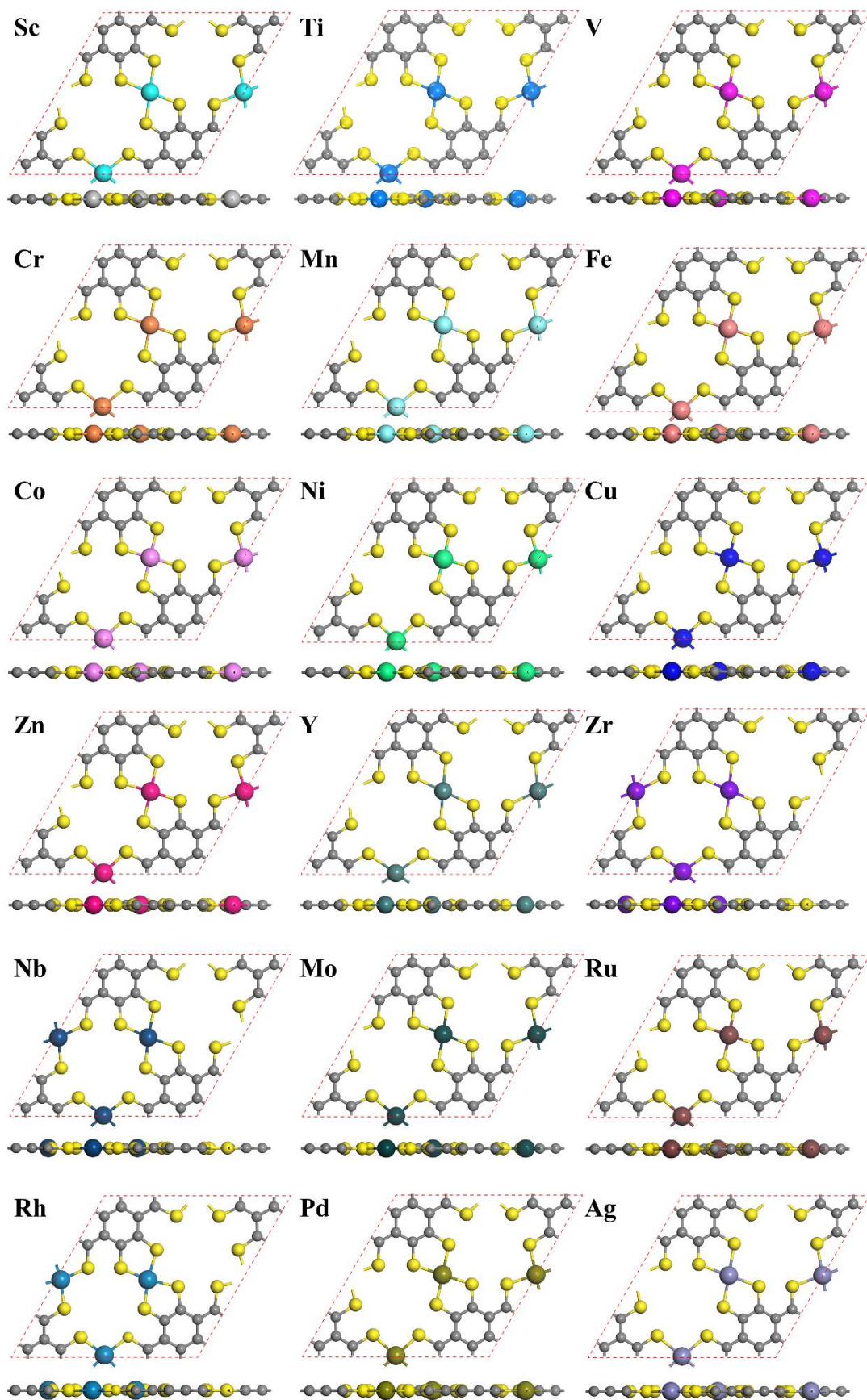|	E_M	Formation energy	U_M^0	n	U_{diss}
Sc	-6.34	-3.61	-2.08	3	-0.88
Ti	-5.16	-2.75	-1.63	2	-0.25
V	-5.66	-2.00	-1.18	2	-0.18
Cr	-6.04	-2.31	-0.91	2	0.25
Mn	-6.57	-1.71	-1.19	2	-0.33
Fe	-6.56	-0.87	-0.45	2	-0.01
Co	-3.81	-2.10	-0.28	2	0.77
Ni	-2.99	-1.64	-0.26	2	0.56
Cu	-2.38	-0.56	0.34	2	0.62
Zn	-0.34	-1.73	-0.76	2	0.11
Y	-5.77	-3.01	-2.37	3	-1.37
Zr	-6.90	-1.64	-1.45	4	-1.04
Nb	-9.00	-0.10	-1.10	3	-1.07
Mo	-8.08	-0.52	-0.20	3	-0.03
Ru	-7.69	-0.42	0.46	2	0.67
Rh	-5.24	-1.18	0.60	2	1.19
Pd	-3.38	-2.69	0.95	2	2.29
Ag	-2.53	0.07	0.80	1	0.73
Sc-O	-6.34	-8.35	-2.08	3	0.70
Ti-O	-5.16	-4.89	-1.63	2	0.81
Zr-O	-6.90	-9.09	-1.45	4	0.82
Nb-O	-9.00	-9.26	-1.10	3	1.99
Mo-O	-8.08	-8.10	-0.20	3	2.50

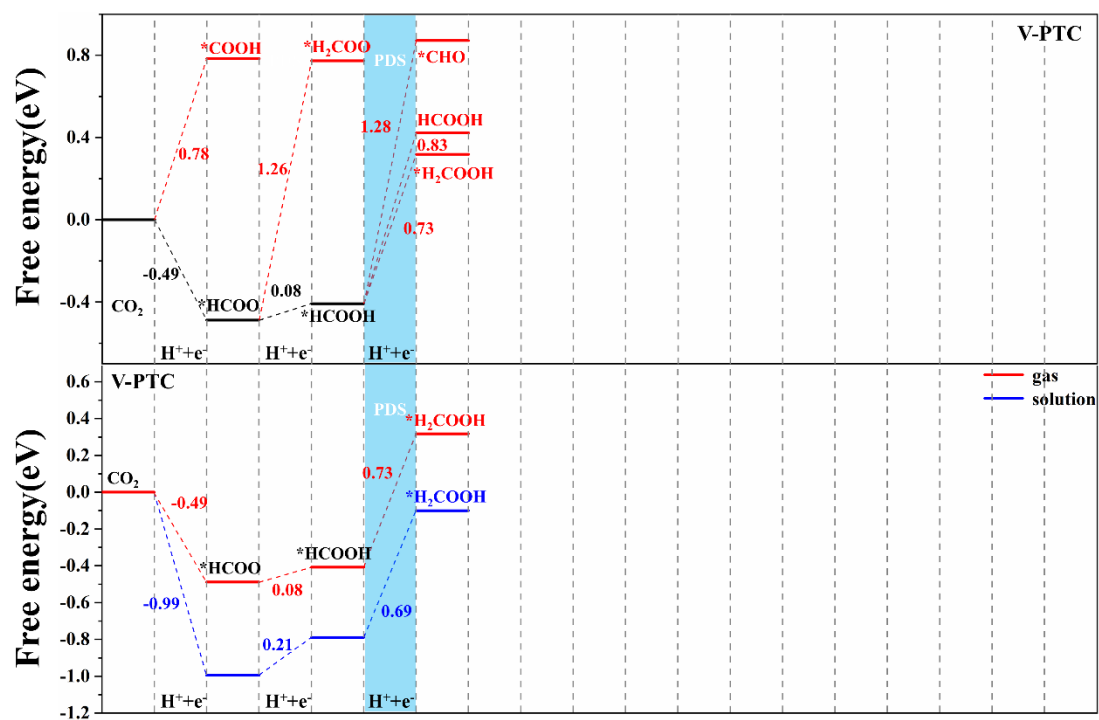**Figure S1.** The optimized structures of TM-PTC.

Figure S2. Free energy change for V-PTC in the gas phase (top), and the comparison of the free energy change both in the gas phase and in solution (bottom).
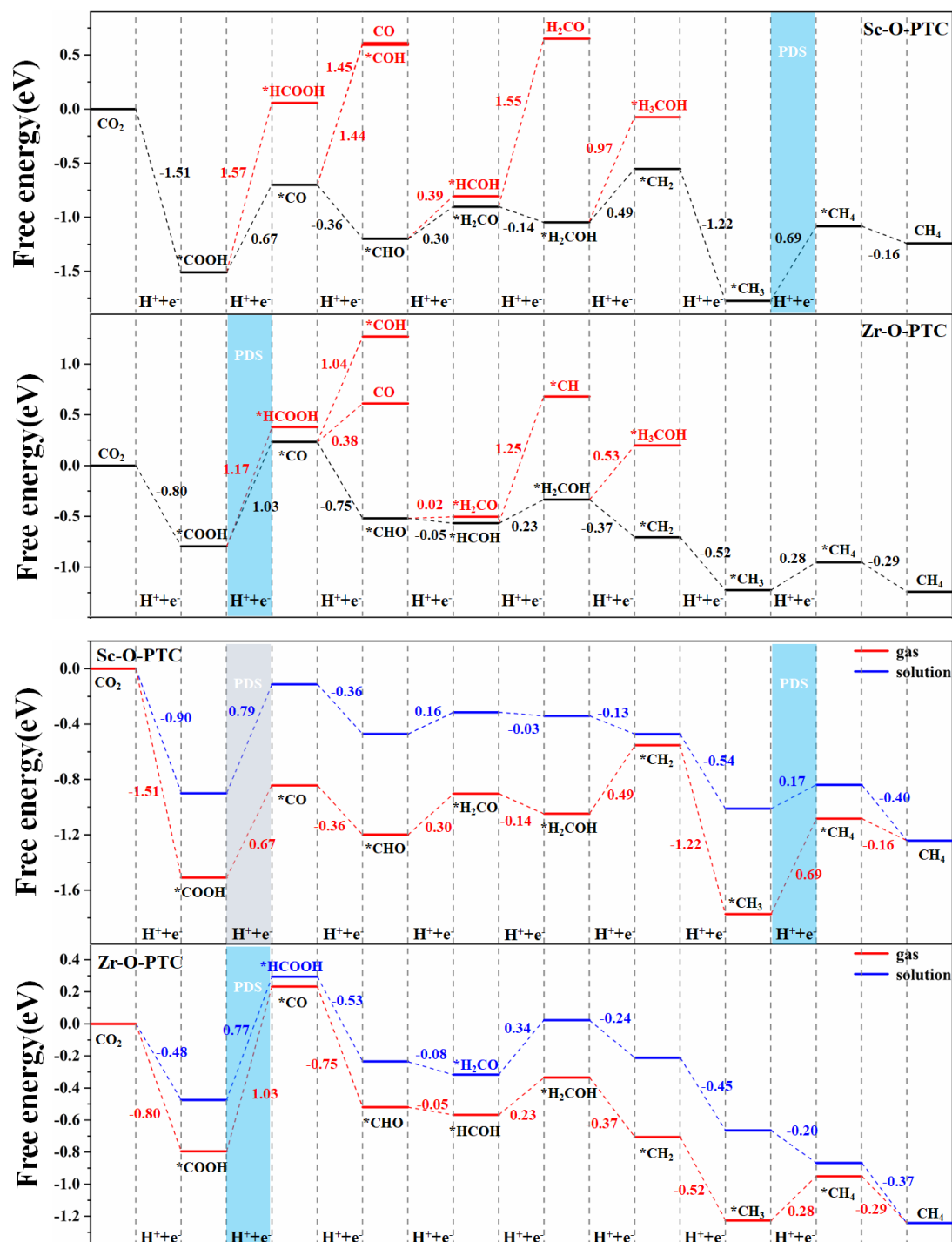
Figure S3. Free energy change in the gas phase (top two panels), and the comparison of the free energy change both in the gas phase and in solution (bottom two panels).