Supporting Information

Theoretical design of one-dimensional dual site metal-organic framework ribbon for CO_2RR

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Supplementary Figures

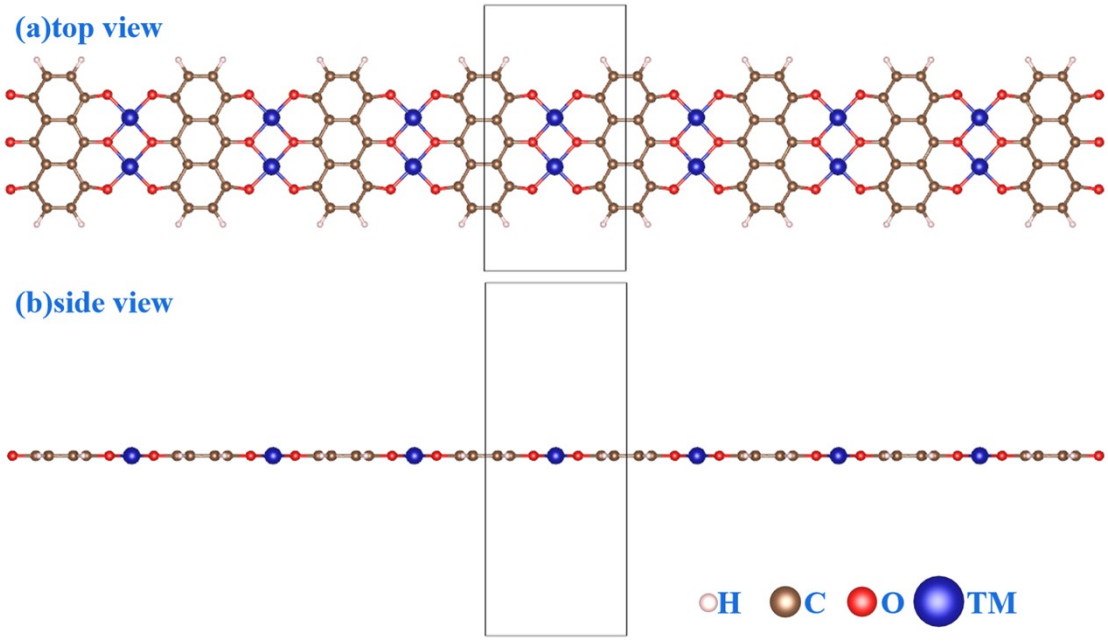
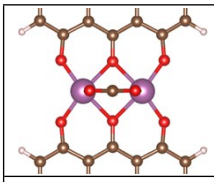
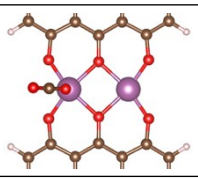
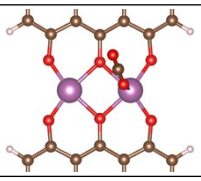
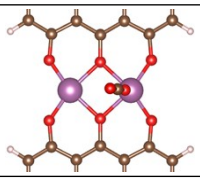
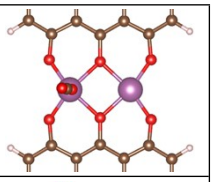
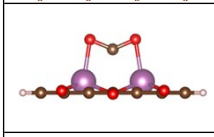
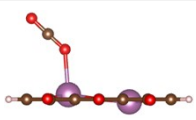
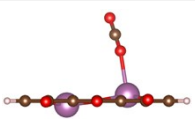
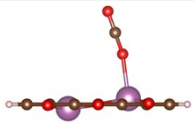
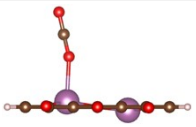


Fig. S1. Atomic configuration of TM_2-MOF monolayer.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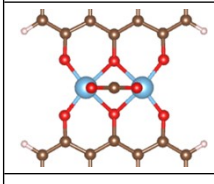	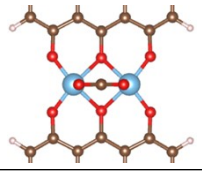	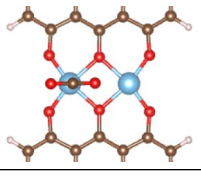	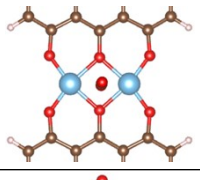	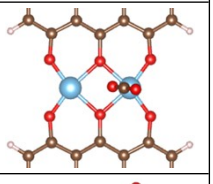
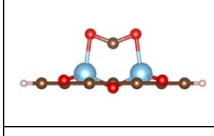	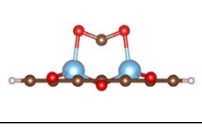	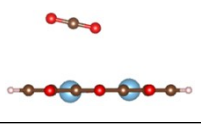	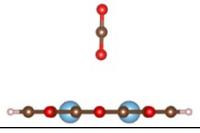	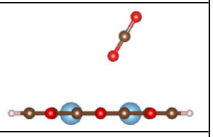
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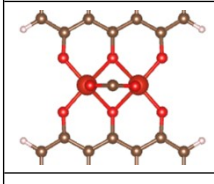	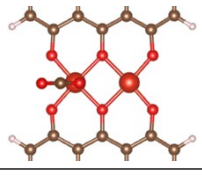	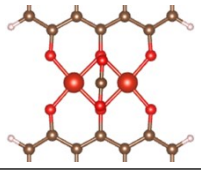	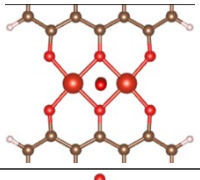	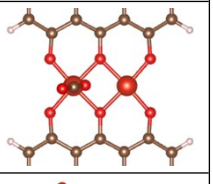
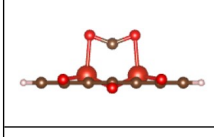	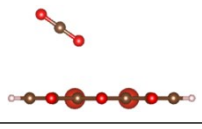	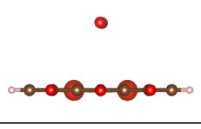	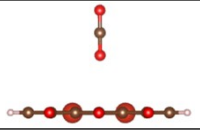	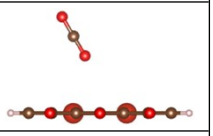
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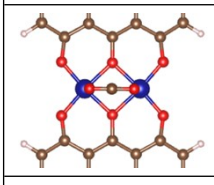	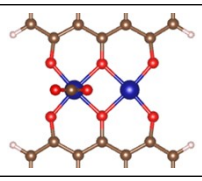	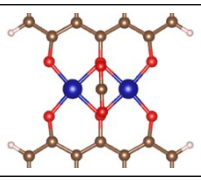	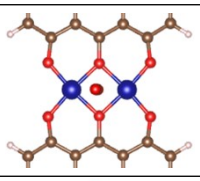	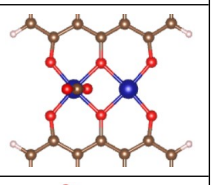
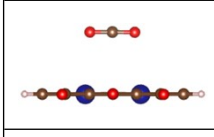	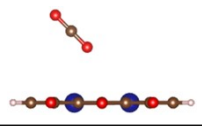	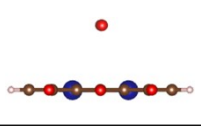	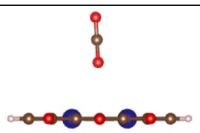	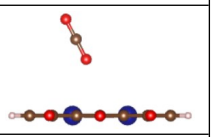
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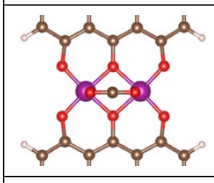	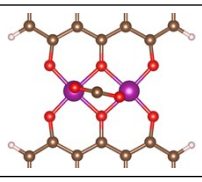	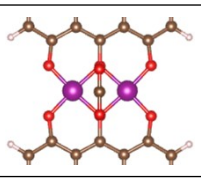	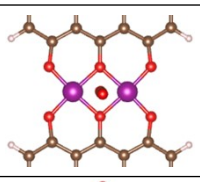	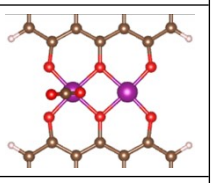
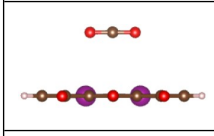	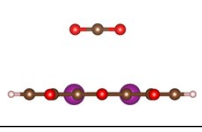	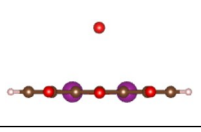	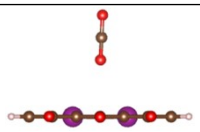	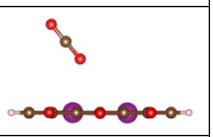
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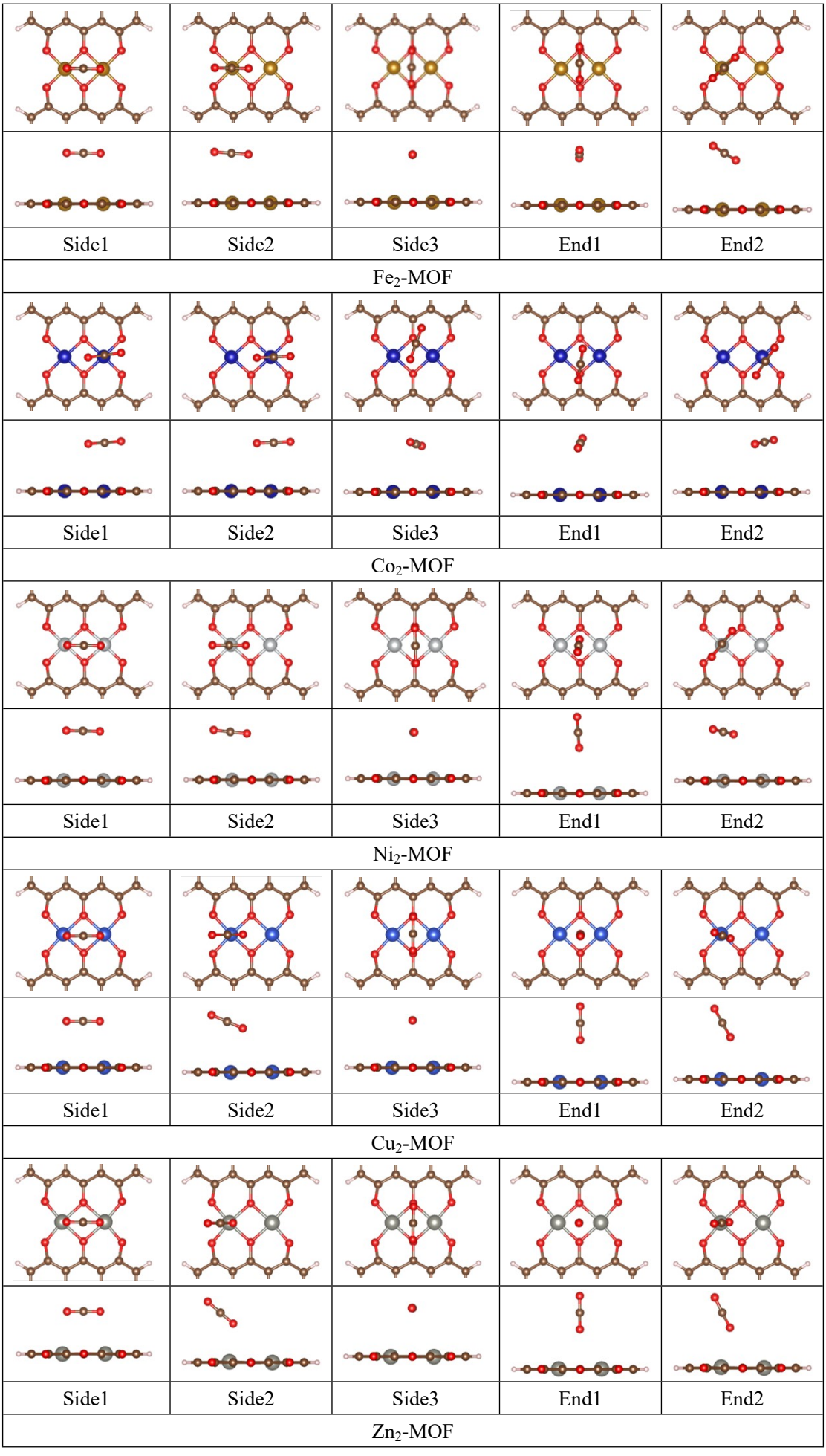

Fig. S2. Optimized configuration of CO_2 molecule adsorbed on pristine TM_2-MOF.

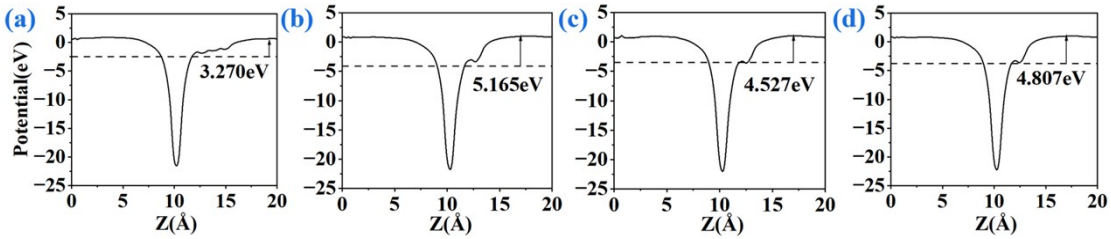

Fig. S3. Work function of (a) CO_2-end on Sc_2-MOF, (b) CO_2-side on Sc_2-MOF, (c) CO_2-side on Ti_2-MOF, (d) CO_2-side on V_2-MOF.

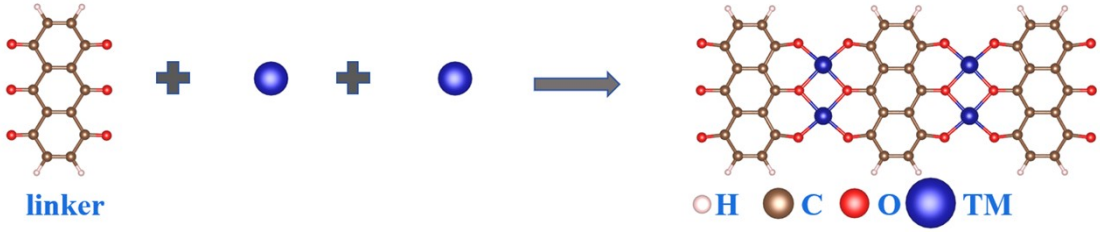

Fig. S4. Synthesis process of TM_2-MOF monolayer, Linker + 2TM → TM_2-MOF.

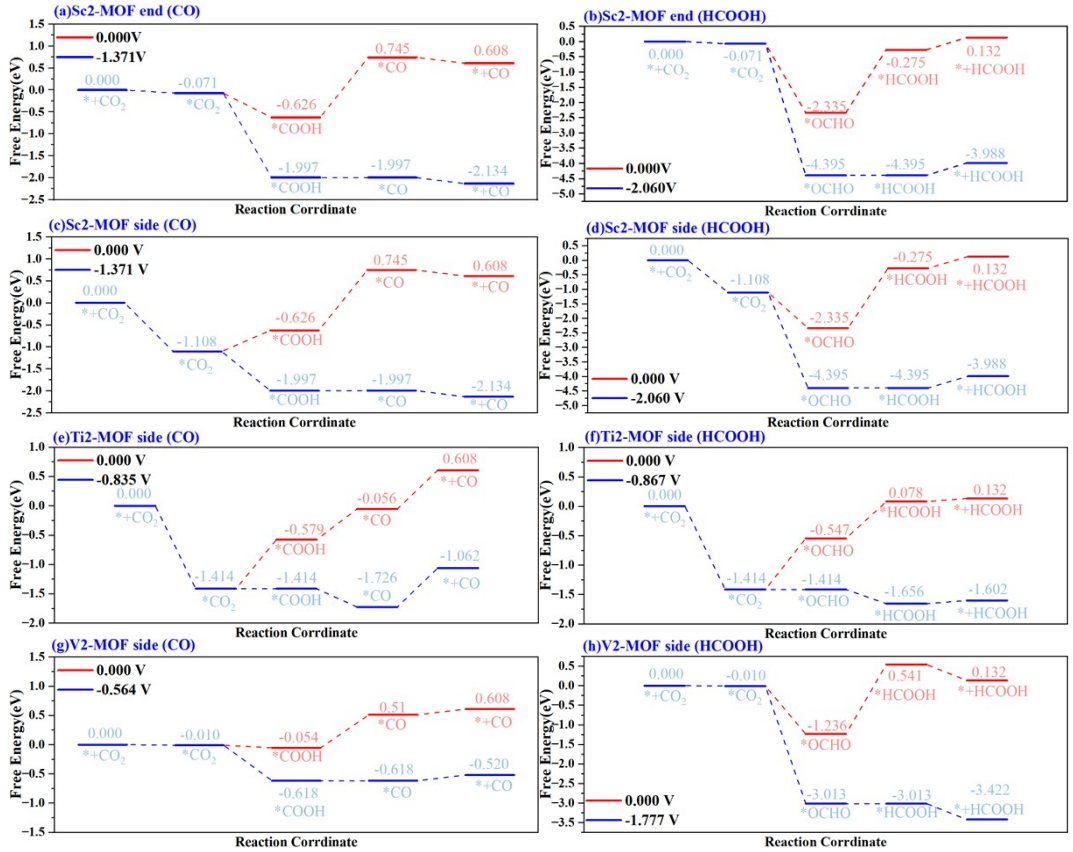

Fig. S5. Free energy diagrams at zero and applied potentials for (a) Sc2-MOF end CO, (b) Sc_2-MOF end HCOOH, (c) Sc2-MOF side CO, (d) Sc_2-MOF side HCOOH, (e) Ti2-MOF side CO, (f) Ti_2-MOF side HCOOH, (g) V2-MOF side CO, (h) V_2-MOF side HCOOH structures.

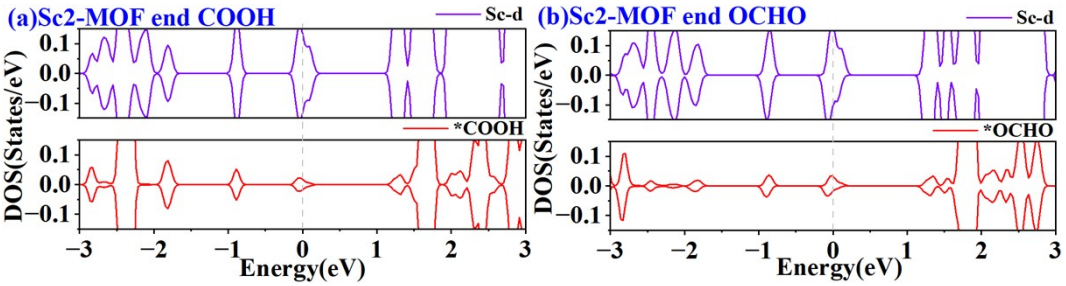

Fig. S6. PDOS of TM and LDOS of COOH or OCHO in (a) Sc_2-MOF end COOH, (b) Sc_2-MOF end OCHO structures.

Supplementary Tables

Table S1 Specific applied U value (U_{eff}) of 3d metals for DFT calculations [1].

3d	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
U_{eff}	2.11	2.58	2.73	2.79	3.06	3.29	3.42	3.40	3.87	4.12

Table S2 Contributions to the adsorbate free energy from zero-point energy correction (*ZPE*), enthalpic temperature correction, and entropy contribution (at 300 K), respectively.

Species	ΔZPE (eV)	$\int C_p dT$ (eV)	$T\Delta S$ (eV)
CO	0.14	0.09	0.57
CO_2	0.31	0.10	0.57
HCOOH	0.90	0.16	0.59
H_2	0.27	0.09	0.42
*H	0.27	0.005	0.006
*COOH	0.659	0.079	0.154
*OCHO	0.665	0.065	0.118
*HCOOH	0.943	0.102	0.218
*CO	0.253	0.046	0.085

References

[1] I V Solovyev, P H Dederichs, V I Anisimov, Physical Review B 1994 50, 16861.