Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Reversed selectivity of photocatalytic CO_2 reduction over metallic Pt and Pt (II) oxide cocatalysts

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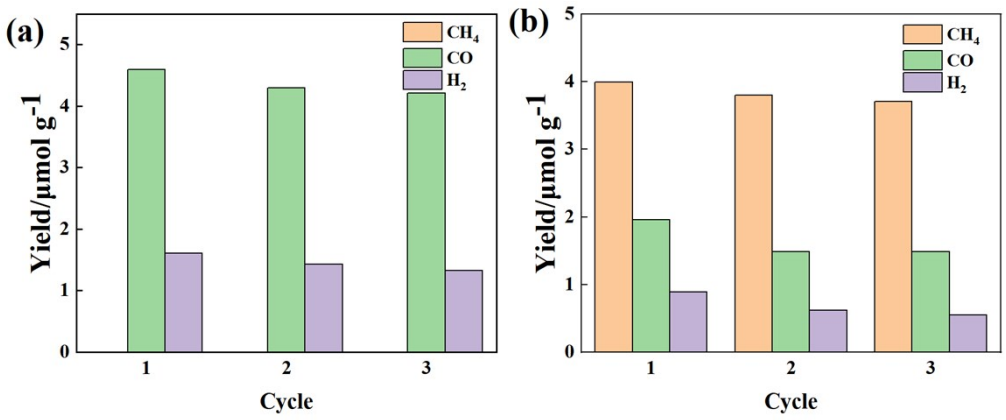

Fig. S1 Stability test on PtO/TiO_2 (a) and Pt/TiO_2 (b) photocatalytic CO_2 reduction.

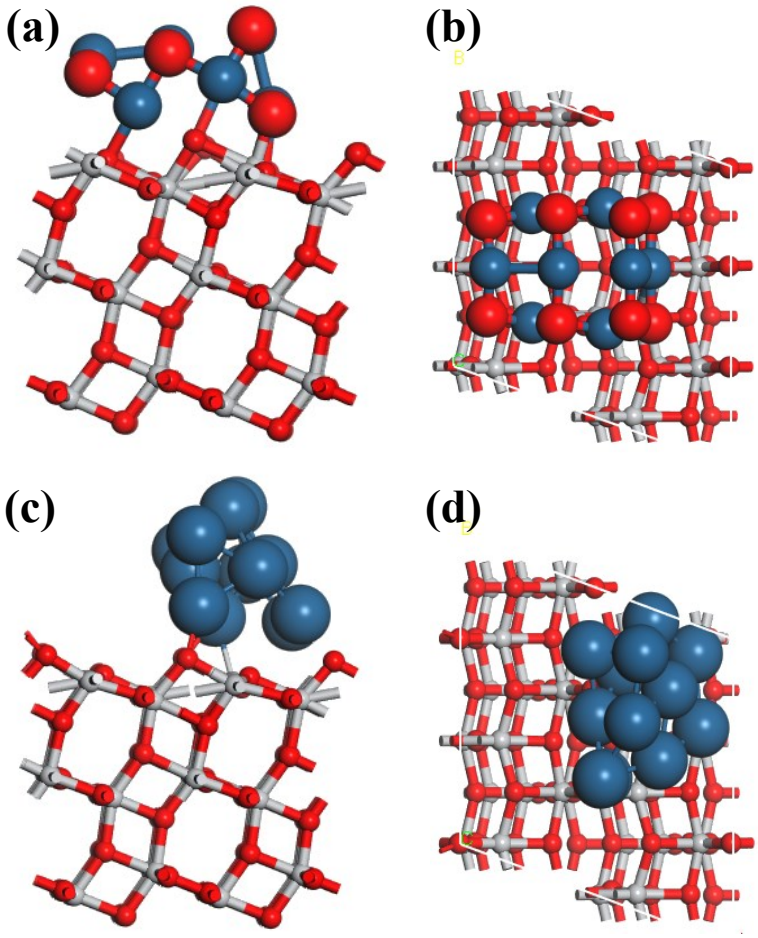

Fig. S2 The optimized geometry of $Pt_8O_8/TiO_2(101)$ on top view (a) and side view (b), and $Pt_{12}/TiO_2(101)$ on top view (c) and side view (d). Red, dark gray, blue and light gray balls represent O, C, Pt and Ti atoms, respectively.

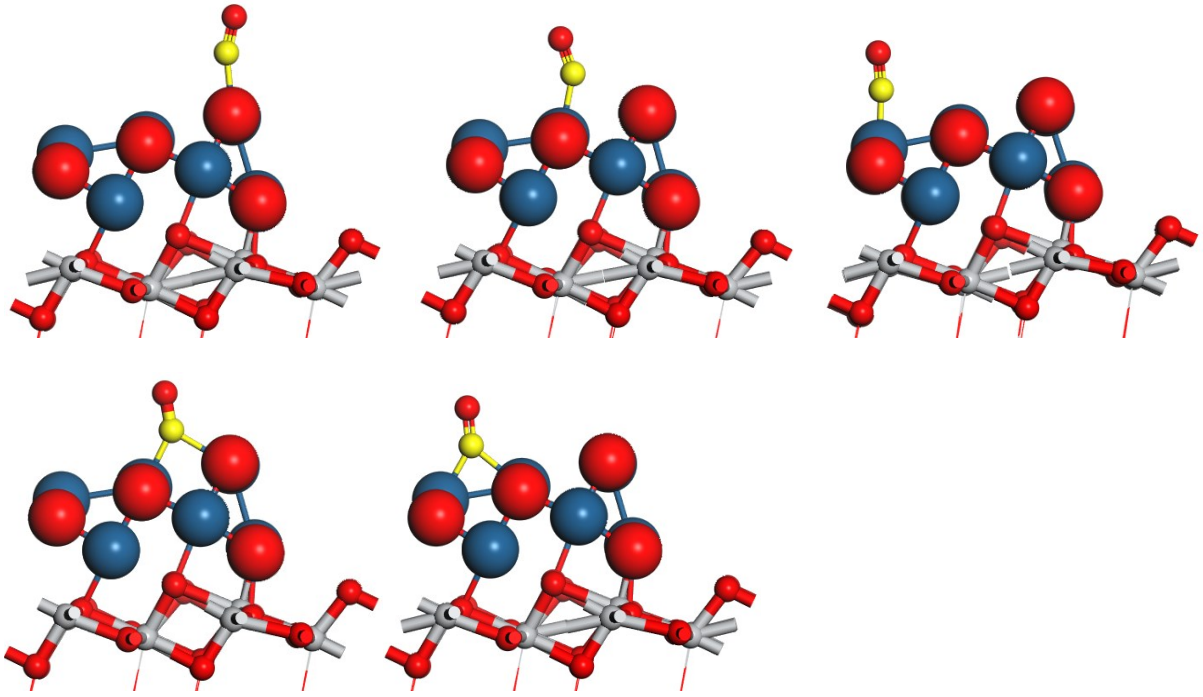

Fig. S3 The CO adsorption sites of $Pt_8O_8/TiO_2(101)$.

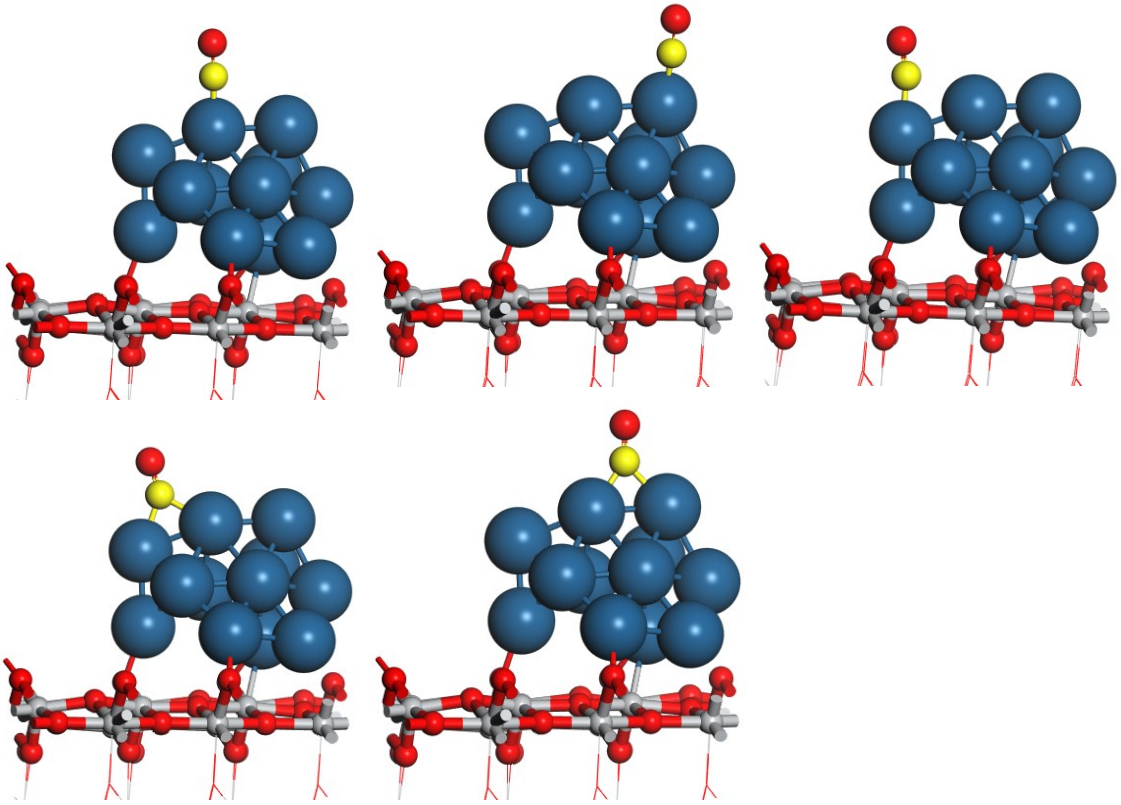

Fig. S4 The CO adsorption sites of $Pt_{12}/TiO_2(101)$.

Table S1 adsorption energies and Mulliken charge CO of $Pt_8O_8/TiO_2(101)$ and $Pt_{12}/TiO_2(101)$ surfaces.

Surface	Site		E_{ads}/eV	Mulliken Charge		
				C	O	Total
PtO/TiO_2	Top	1	-0.79	0.31	-0.31	0
		2	**-0.70**	**0.23**	**-0.31**	**-0.08**
		3	-0.86	0.27	-0.32	-0.05
	Bridge	1	-0.81	0.12	-0.30	-0.18
		2	**-1.25**	**0.11**	**-0.32**	**-0.21**
Pt/TiO_2	Top	1	-2.65	0.21	-0.35	-0.14
		2	-2.48	0.21	-0.35	-0.14
		3	**-2.06**	**0.14**	**-0.33**	**-0.19**
	Bridge	1	-2.16	0.04	-0.34	-0.30
		2	**-2.63**	**0.02**	**-0.36**	**-0.34**
Free CO				0.42	-0.42	0