Supporting Information

Confined Catalysis in the *g*-C_3N_4/Pt(111) Interface: Feasible Molecule Intercalation, Tunable Molecule-Metal Interaction and Enhanced Reaction Activity of CO Oxidation

*Shujiao Wang, Yingxin Feng, Ming'an Yu, Qiang Wan and Sen Lin**

State Key Laboratory of Photocatalysis on Energy and Environment, College of Chemistry, Fuzhou University, Fuzhou 350002, China

**Corresponding author.* Address: *Research Institute of Photocatalysis, Fuzhou University, Fuzhou 350002, China. Phone: +86-591-83969175. Email: slin@fzu.edu.cn*

Table S1 Calculated adsorption energies of CO, O_2, O, and CO_2 on Pt(111) surface with and without *g*-C_3N_4 cover.

Species	Adsorption sites	adsorption energy (eV)
CO	pore-fcc	-1.50
	pore-hcp	-1.40
	pore-top	-1.09
	fcc	-1.40
	hcp	-1.36
	top	-1.05
	Pt(111)-fcc	-1.84
	Pt(111)-hcp	-1.83
	Pt(111)-top	-1.66
O_2	pore-fcc	-0.82
	pore-hcp	-0.71
	fcc	-0.75
	hcp	-0.60
	Pt(111)-fcc	-0.93
	Pt(111)-hcp	-0.84
	surface	0.67
O	pore-fcc	-1.37
	pore-hcp	-1.03
	fcc	-1.41
	hcp	-0.94
	Pt(111)-fcc	-1.39
	Pt(111)-hcp	-1.03
CO_2	bent	0.45
	bent-pore	0.52
	linear	0.38
	linear-pore	0.15
	bent-Pt (111)	0.05
	linear-Pt(111)	-0.48

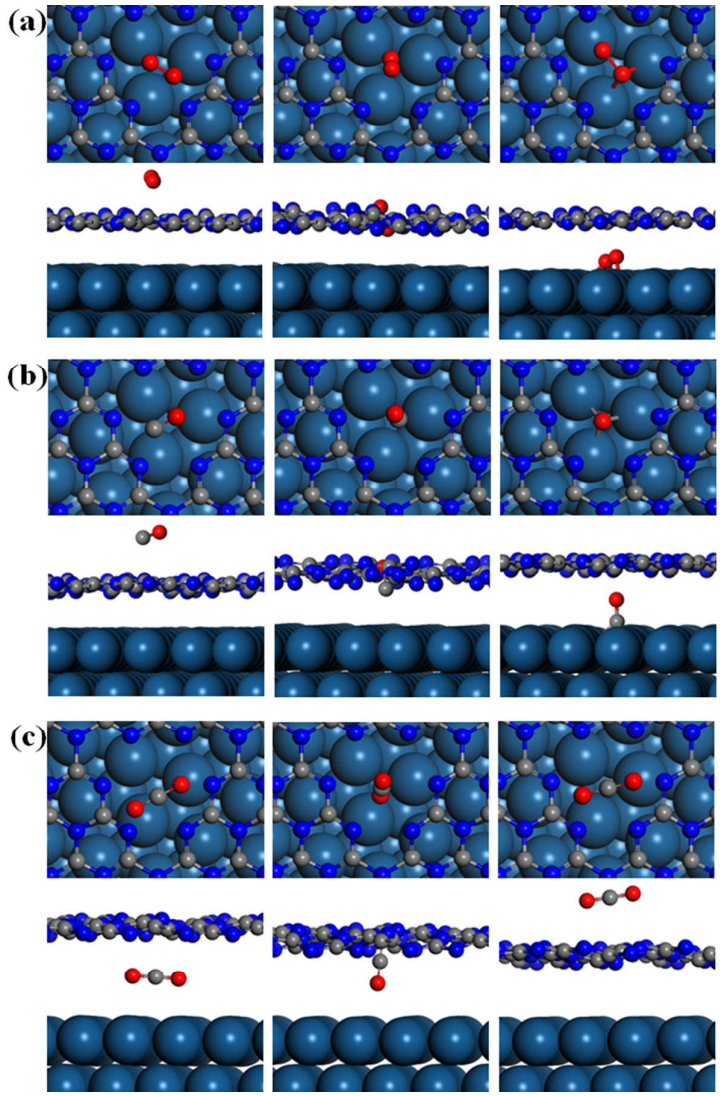

Fig. S1 Geometries of initial state (IS), transition state (TS) and final state (FS) of O_2 (a), CO (b) and CO_2 (c) intercalation at the *g*-C_3N_4/Pt(111) interface. Color scheme: C, grey; N, blue; O, red; Pt, indigo.

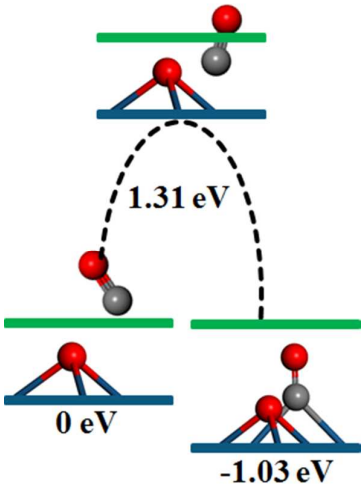

Fig. S2 Diagrams of initial state (IS), transition state (TS) and final state (FS) CO intercalation at the *g*-C_3N_4/Pt(111) interface in the presence of adsorbed atomic oxygen. The green and blue bars are used to represent *g*-C_3N_4 and Pt(111), respectively. Color scheme: C, grey; O, red.

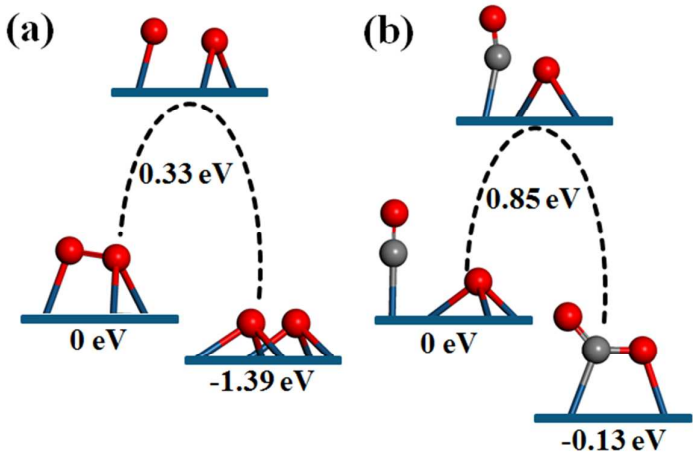

Fig. S3 Diagrams of IS, TS and FS for O_2 dissociation (a) and CO oxidation (b) on the Pt (111). The blue bars are used to represent Pt(111). Color scheme: C, grey; O, red.

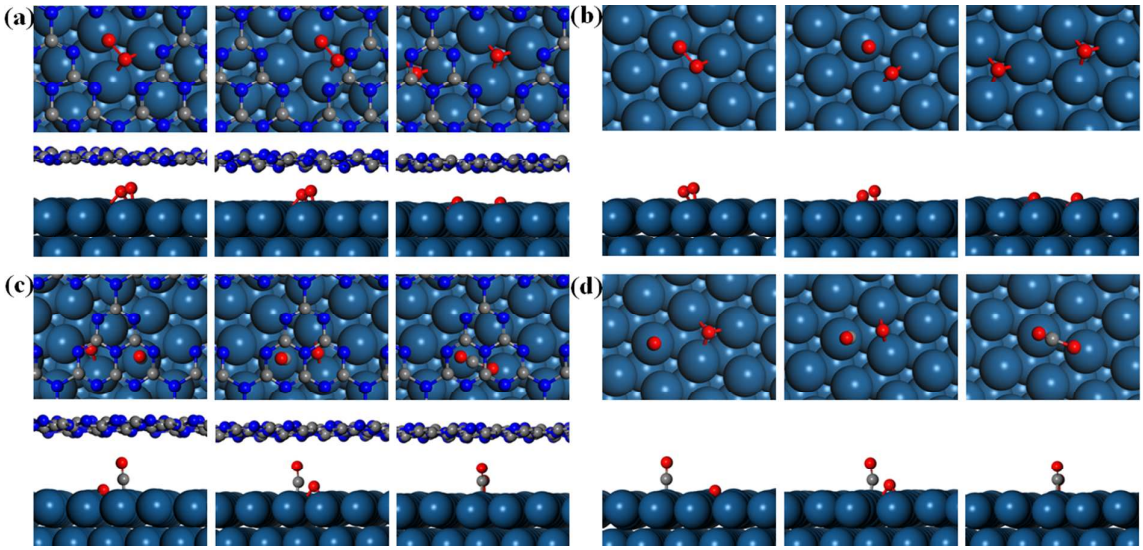

Fig. S4 Geometries of IS, TS and FS for O_2 dissociation and CO oxidation at the *g*-C_3N_4/Pt (111) interface (a and c) and on the pure Pt(111) surface (b and d). Color scheme: C, grey; N, blue; O, red; Pt, indigo.

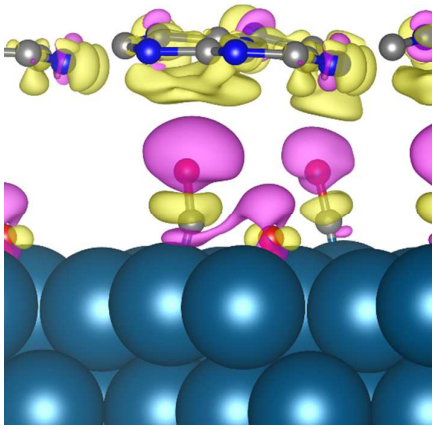

Fig. S5 Calculated differential charge density of TS for CO oxidation at the *g*-C_3N_4/Pt(111) interface in the presence of an adsorbed CO molecule. Yellow and purple represent charge depletion and accumulation, respectively. Color scheme: C, grey; N, blue; O, red; Pt, indigo.