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

Electronic Supplementary Information (ESI)

Dissociative Adsorption of O_2 on Strained Pt(111)

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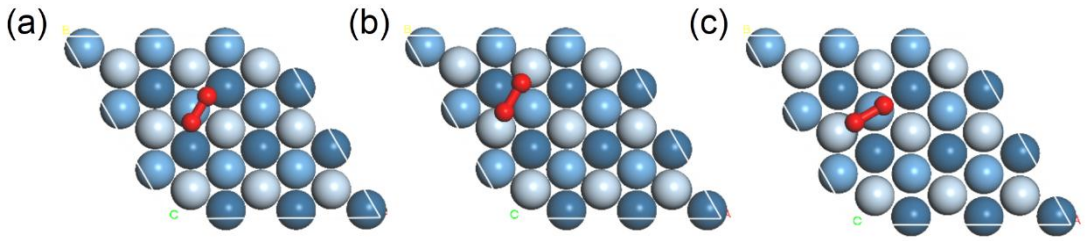

Fig S1 (a) The bhb configuration on Pt(111); (b) The tbt configuration on Pt(111) under 1%−3% strain; (c) The thb configuration on Pt(111) under 4% and 5% strain.

The bhb O_2 adsorption configuration on Pt(111) surface turned into tbt configuration under 1%−3% tensile strain (Fig S1b) *and* thb configuration under 4% and 5% tensile strain (Fig S1c) after geometry optimization.

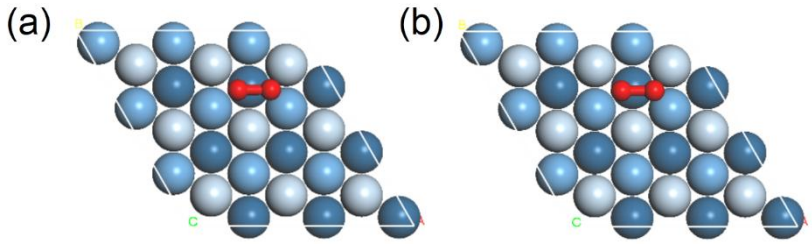

Fig S2 (a) The bfb configuration on Pt(111); (b) The tfb configuration on stretched Pt(111) (1%−5% tensile strain).

The bfb O_2 adsorption configuration on Pt(111) surface turned into tfb configuration (Fig S2b) under tensile strain after geometry optimization.

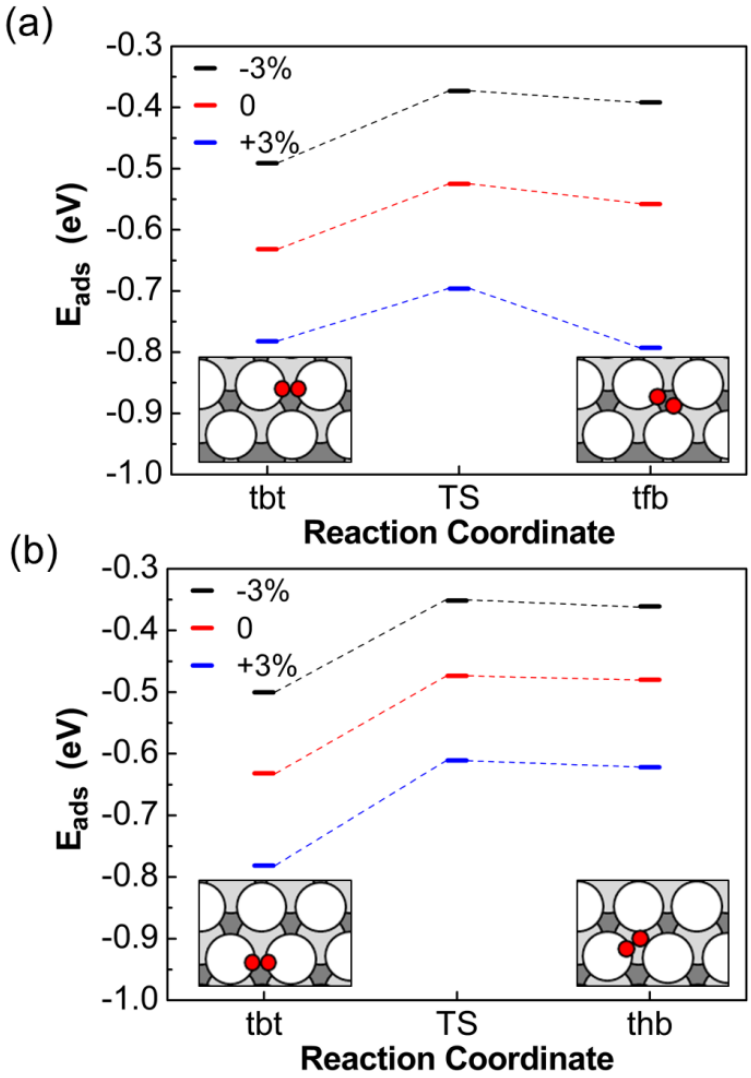

Fig. S3 Two O_2 diffusion pathways on the strained Pt(111) surface. (a) tbt→tfb and (b) tbt→thb.

Table S1 Activation barriers (E_a) and reaction energies (ΔE) of O_2 diffusion.

strain (%)	E_a (eV)		ΔE (eV)	
	tbt→tfb	tbt→thb	tbt→tfb	tbt→thb
−3	0.12	0.15	0.10	0.14
0	0.11	0.16	0.07	0.15
+3	0.09	0.17	−0.01	0.16

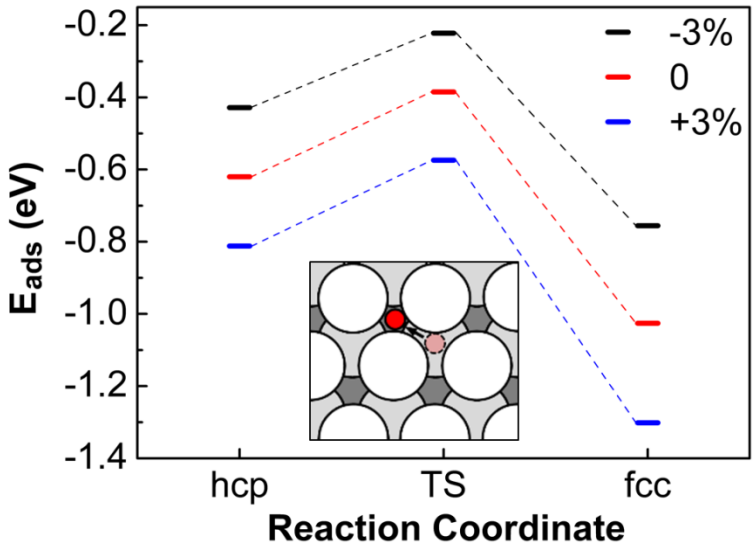

Fig. S4 O diffusion on a clean Pt(111) surface.

Table S2 Energies for key states in O diffusion on a clean Pt(111) surface.

strain (%)	$E_{ads,IS}$ (eV)	$E_{ads,TS}$ (eV)	$E_{ads,FS}$ (eV)	E_a (eV)
−3	−0.43	−0.22	−0.76	0.21
0	−0.62	−0.38	−1.03	0.24
+3	−0.81	−0.57	−1.30	0.24

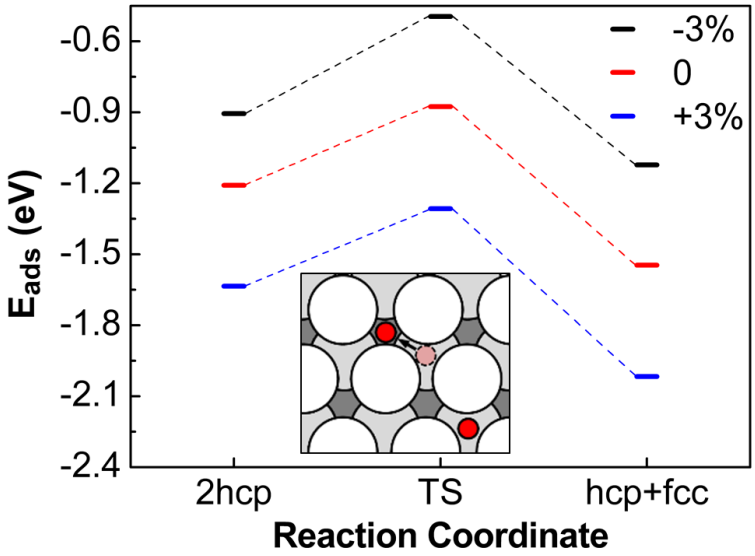

Fig. S5 O diffusion with a nearby O* adatom.

Table S3 Energies for key states in O diffusion on a Pt(111) surface with a first nearest neighboring h site O* adatom.

strain (%)	$E_{ads,IS}$ (eV)	$E_{ads,TS}$ (eV)	$E_{ads,FS}$ (eV)	E_a (eV)
−3	−0.90	−0.50	−1.12	0.41
0	−1.21	−0.88	−1.55	0.33
+3	−1.63	−1.31	−2.02	0.33