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Oxygen reduction reaction on Pt(111) and Pt(100) surfaces substituted by the subsurface Cu: a theoretical perspective

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Table S1 The adsorption energies (eV) of ORR intermediates on Pt/Cu(111) and Pt/Cu(100) surfaces.

	Pt/Cu(111)				Pt/Cu(100)		
	bri	fcc	hcp	top	bri	ff	top
O_2*	-0.14	—	—	—	-0.81	—	—
OOH*	-0.60	—	—	—	-1.01	—	—
H_2O_2*	-0.20	—	—	—	-0.27	—	—
OH*	-1.87	—	—	-1.87	-2.68		-2.25
O*	—	-3.94	-3.77	-2.76	-4.36	-4.20	-3.35
H*	—	-2.58	-2.58	-2.25	-2.70	—	-2.40
H_2O*	—	—	—	-0.12	—	—	-0.17

Table S2 The energy barrier (ΔE_a, eV) and reaction energy (ΔH, eV) of each elementary reaction on Pt(100) with different potentials.

	PAW-PBE		USPP-PBE		Ref. 36 (USPP-PW91)	
	ΔE_a	ΔH	ΔE_a	ΔH	ΔE_a	ΔH
Protonation						
$O_2+H \rightarrow OOH$	-	-	0.53	0.28	0.48	0.26
$OOH+H \rightarrow H_2O_2$	-	-	0.37	0.19	-	-
$O+H \rightarrow OH$	0.42	-0.29	0.36	-0.41	0.36	-0.43
$OH+H \rightarrow H_2O$	0.76	0.16	0.73	-0.01	0.80	0.06
O_2 dissociation						
$O_2 \rightarrow O+O$	0.13	-1.28	0.13	-1.13	0.15	-1.01
$OOH \rightarrow OH+O$	-	-	0.00	-2.13	0.00	-1.95
$H_2O_2 \rightarrow OH+OH$	-	-	0.08	-2.69	0.11	-2.56

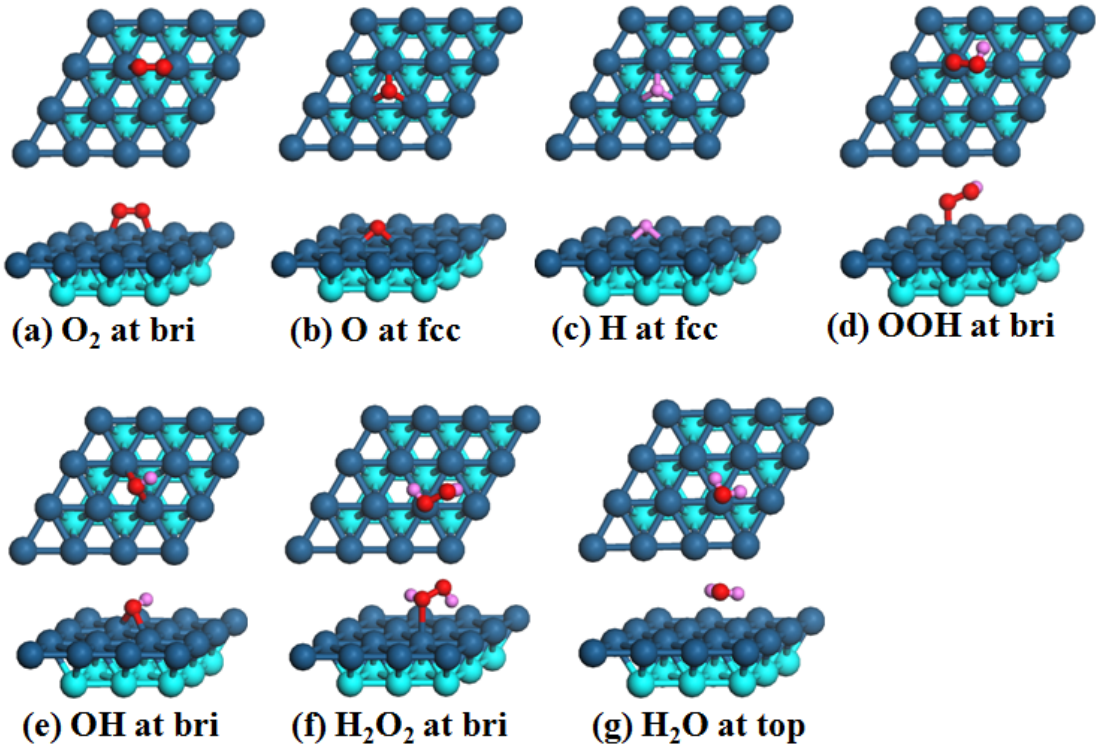

Fig. S1 The most stable adsorption on Pt/Cu(111). Red and pink balls denote the O and H, respectively.

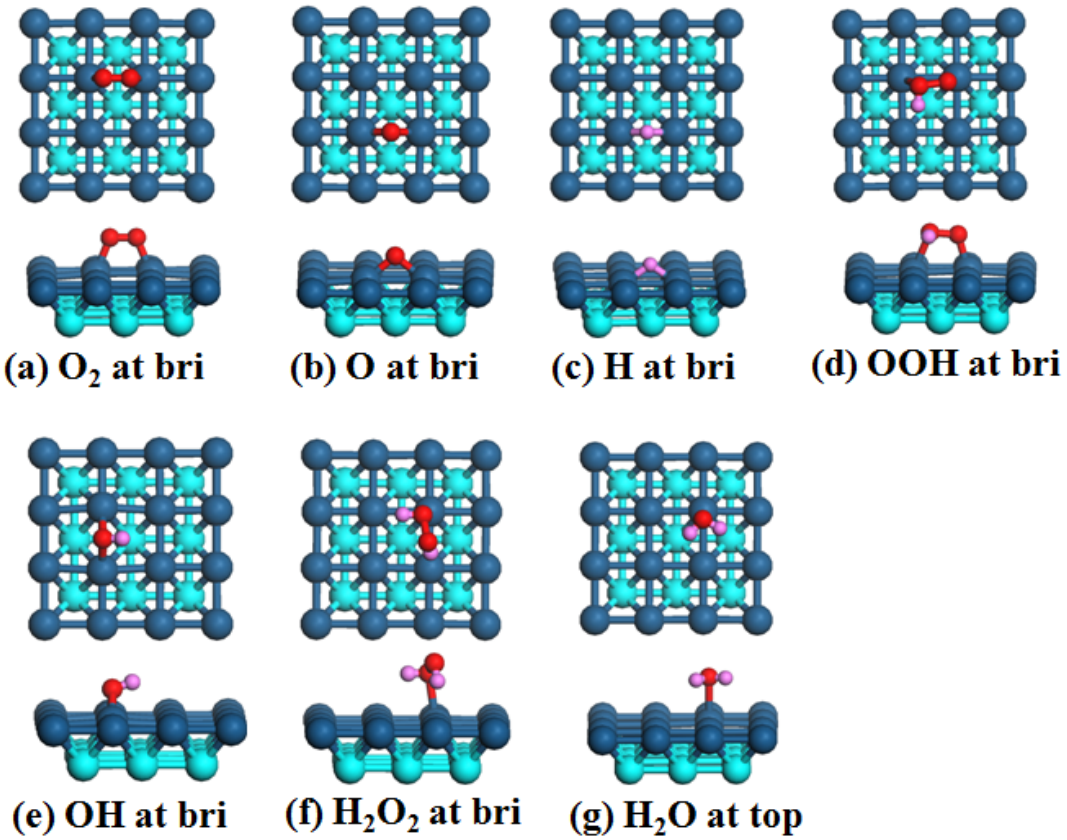

Fig. S2 The most stable adsorption for Pt/Cu(100). Red and pink balls denote the O and H, respectively.