Supporting Information

"The decisive role of Au in the CO diffusion on Pt surfaces: a DFT study"

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CO Adsorption Energies on Pt(111) with and without Au

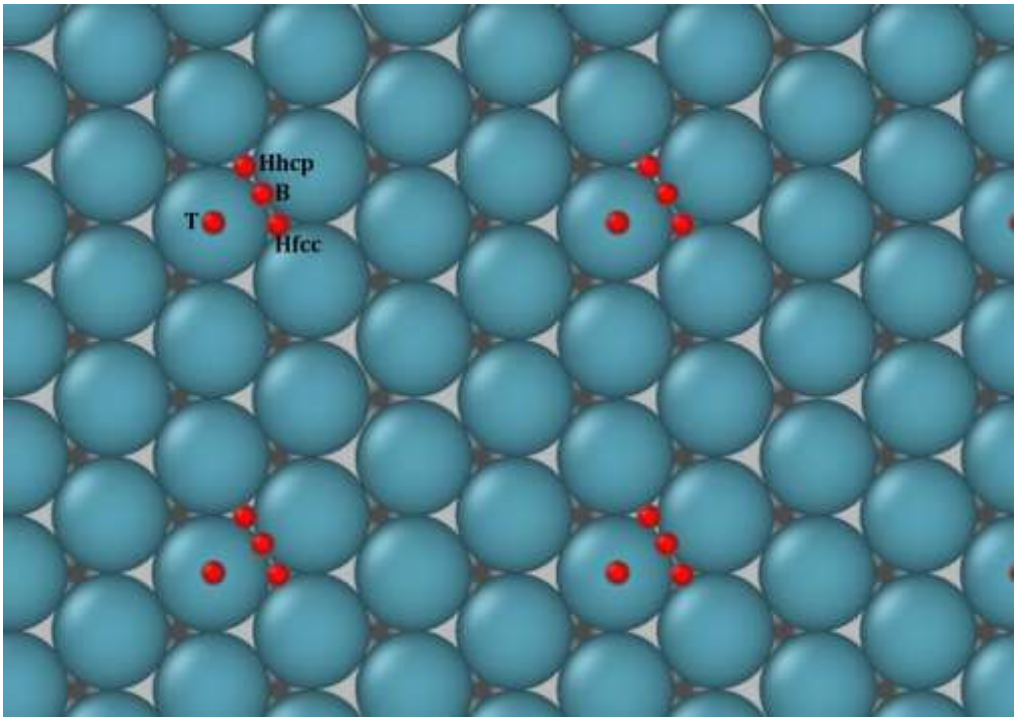

Figure S1: Top view of CO sites on Pt(111)

Site	E_{ad} (eV)
Bridge	-2.40
Hollow fcc	-2.49
Hollow hcp	-2.45
Top	-2.28

Table S1: Adsorbtion energies of CO on Pt(111)

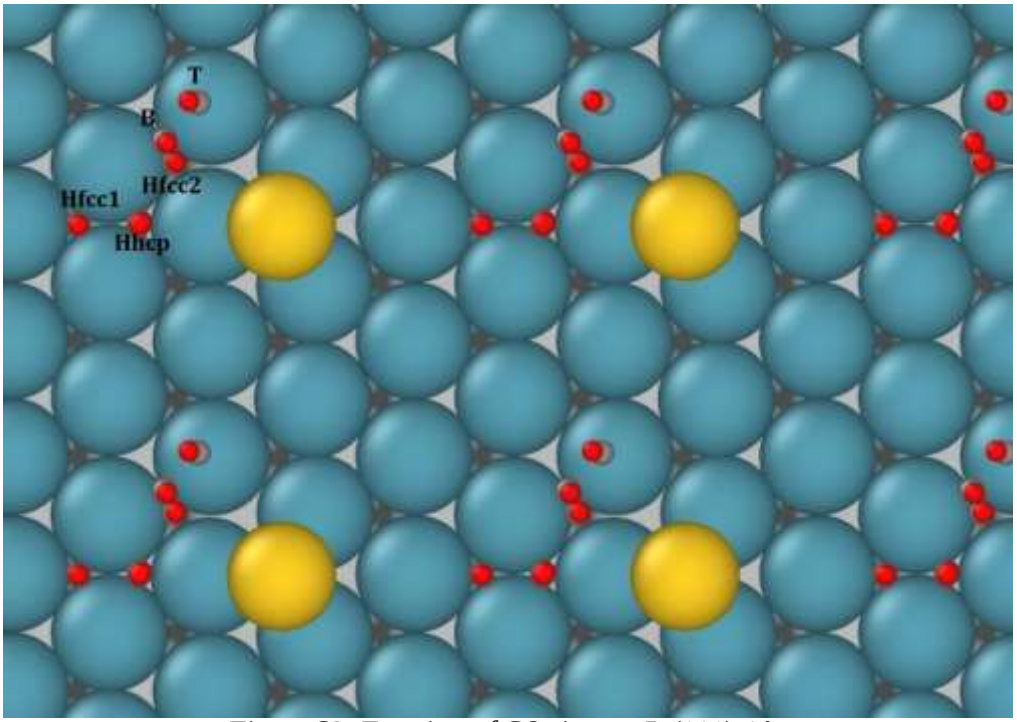

Figure S2: Top view of CO sites on Pt(111)-1Au

Site	E_{ad} (eV)
B	-2.37
Hfcc1	-2.49
Hfcc2	-2.37
Hhcp	-2.40
T	-2.06

Table S2: Adsorbtion energies of CO on Pt(111)-1Au

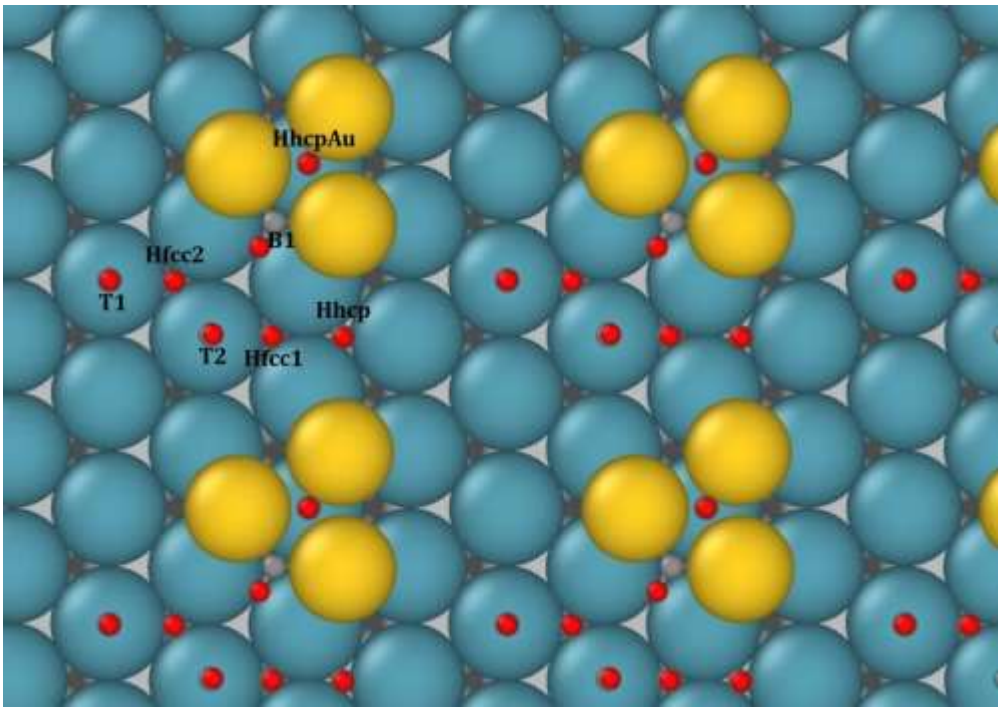

Figure S3: Top view of CO sites on Pt(111)-3Au

Site	E_{ad} (eV)
B1	-1.25
Hfcc1	-2.14
Hfcc2	-2.21
Hhcp Au	-1.15
Hhcp	-1.90
T1	-1.98
T2	-2.01

Table S3: Adsorbtion energies of CO on Pt(111)-3Au

NEB calculation over Pt(111)

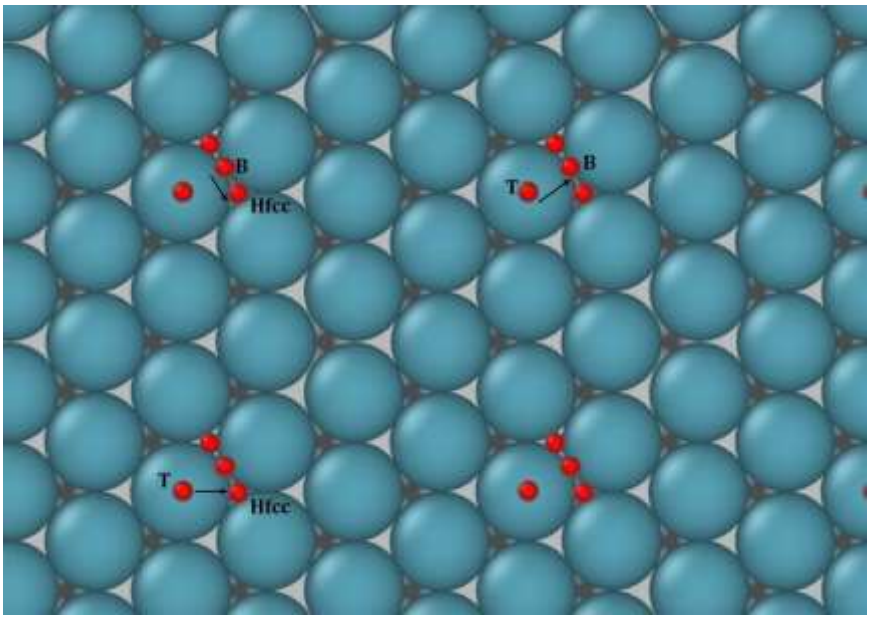

Figure S4: NEB path for CO over Pt(111)

Initial Site	Final Site	E_{act} (eV) ->	E_{act} (eV) <-
B	Hfcc	0.00	0.05
T	B	0.10	0.18
T	Hfcc	0.12	0.24

Table S4: Activation energies for CO over Pt(111)

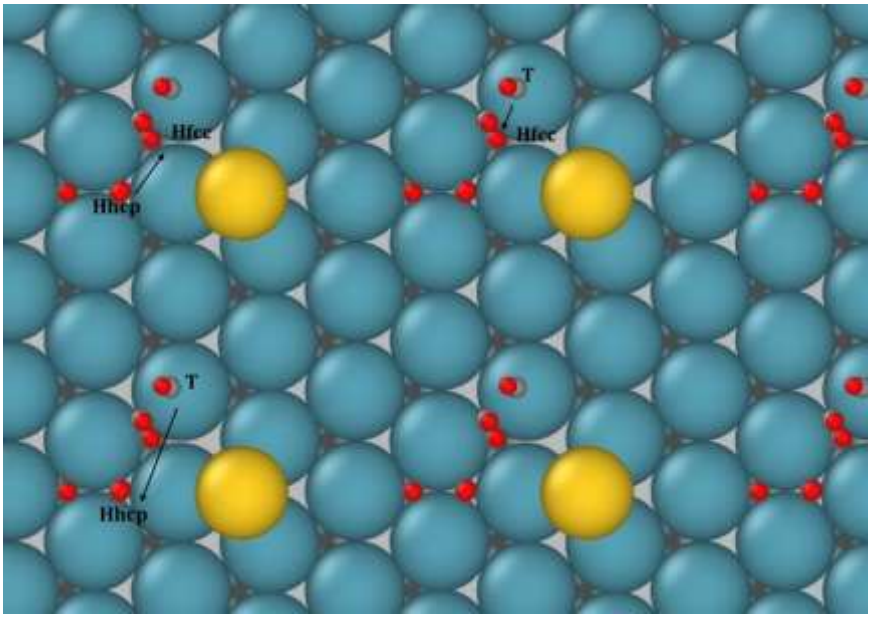

Figure S5: NEB path for CO over Pt(111)-1Au

Initial Site	Final Site	E_{act} (eV) ->	E_{act} (eV) <-
Hhcp	Hfcc	0.06	0.06
T	Hfcc	0.16	0.21
T	Hhcp	0.07	0.11

Table S5: Activation energies for CO over Pt(111)-1Au

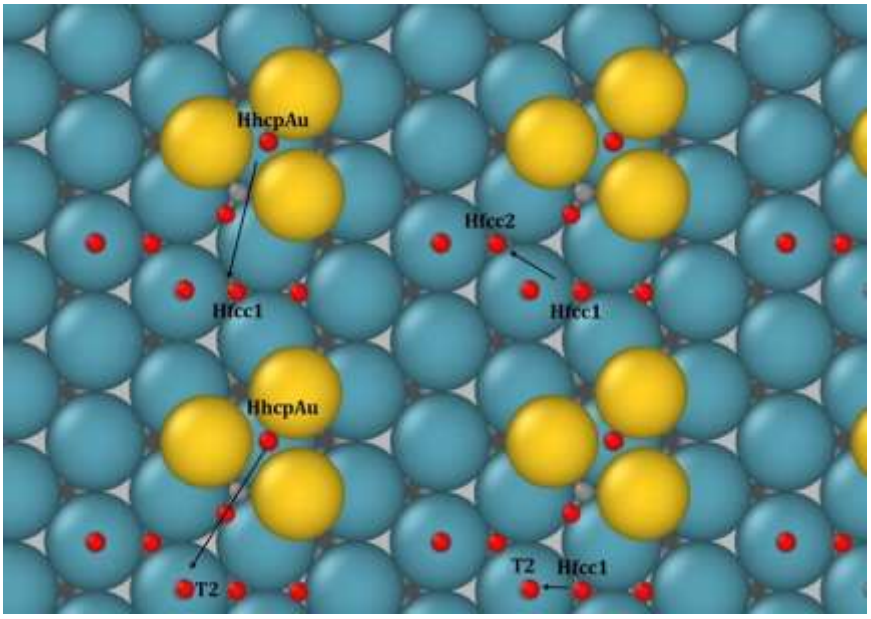

Figure S6: NEB path for CO over Pt(111)-3Au

Initial Site	Final Site	E_{act} (eV) ->	E_{act} (eV) <-
Hhcp Au	Hfcc1	0.00	0.91
Hhcp Au	T2	0.03	0.94
Hfcc1	Hfcc2	0.13	0.22
Hfcc1	T2	0.21	0.21

Table S6: Activation energies for CO over Pt(111)-3Au