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

New insights into O and OH adsorption on Pt-Co alloy surface: Effects of Pt/Co ratios and structures

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Supplementary Information

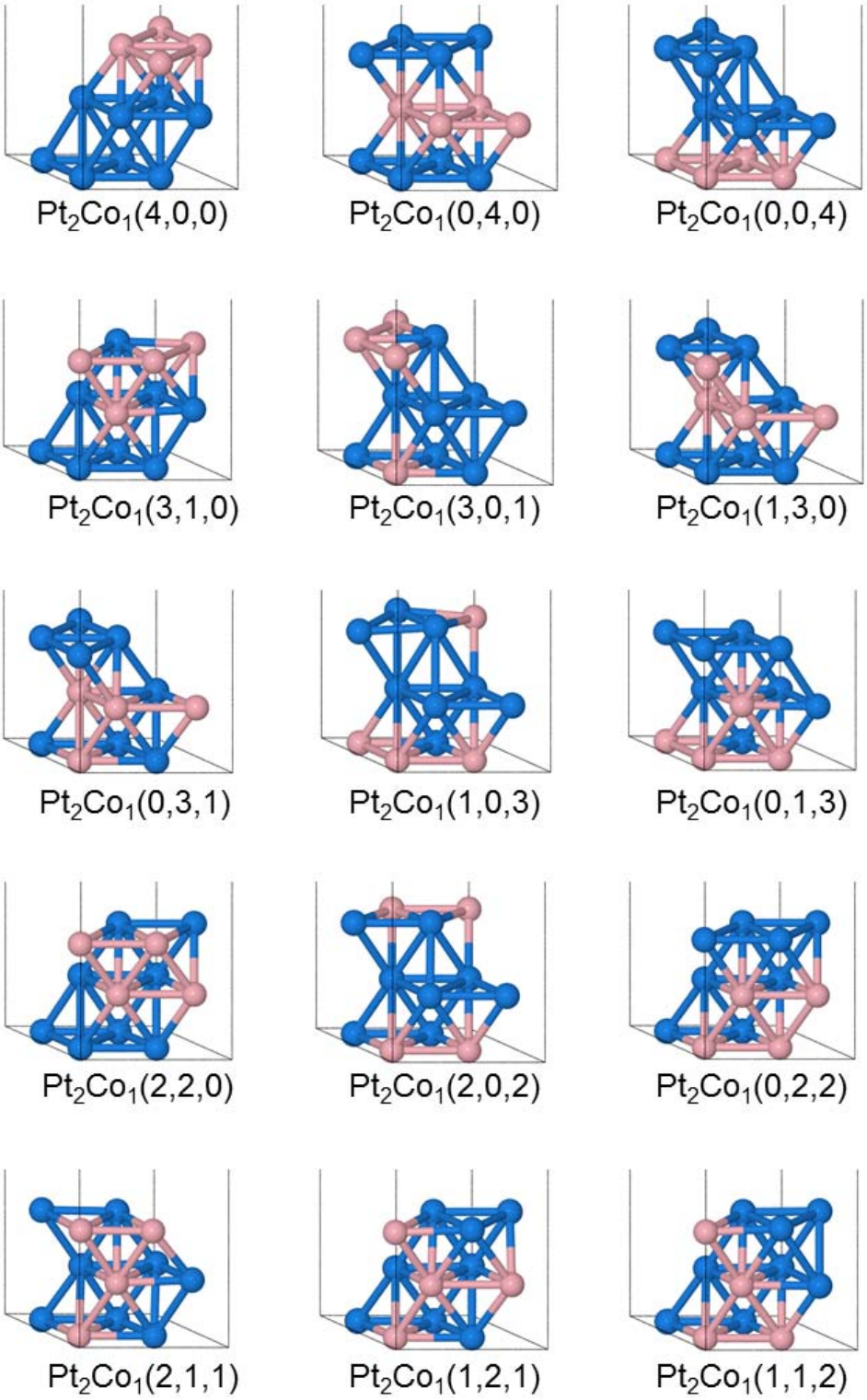

Fig. S1 The alloy configurations with Pt/Co atomic ratio of 2:1. The colors of Pt and Co atoms are blue and pink, respectively.

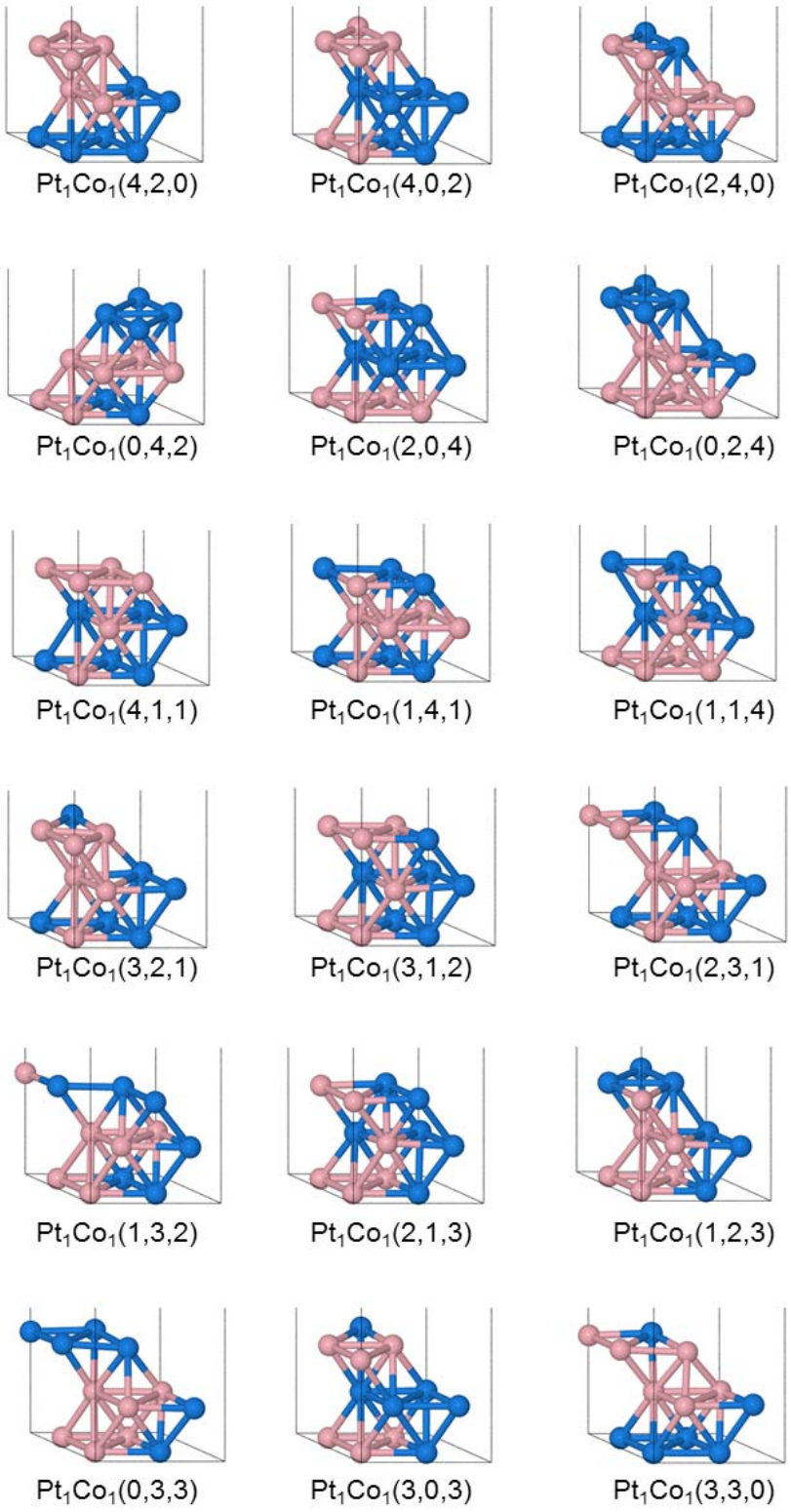

Fig. S2 The alloy configurations with Pt/Co atomic ratio of 1:1. The colors of Pt and Co atoms are blue and pink, respectively.

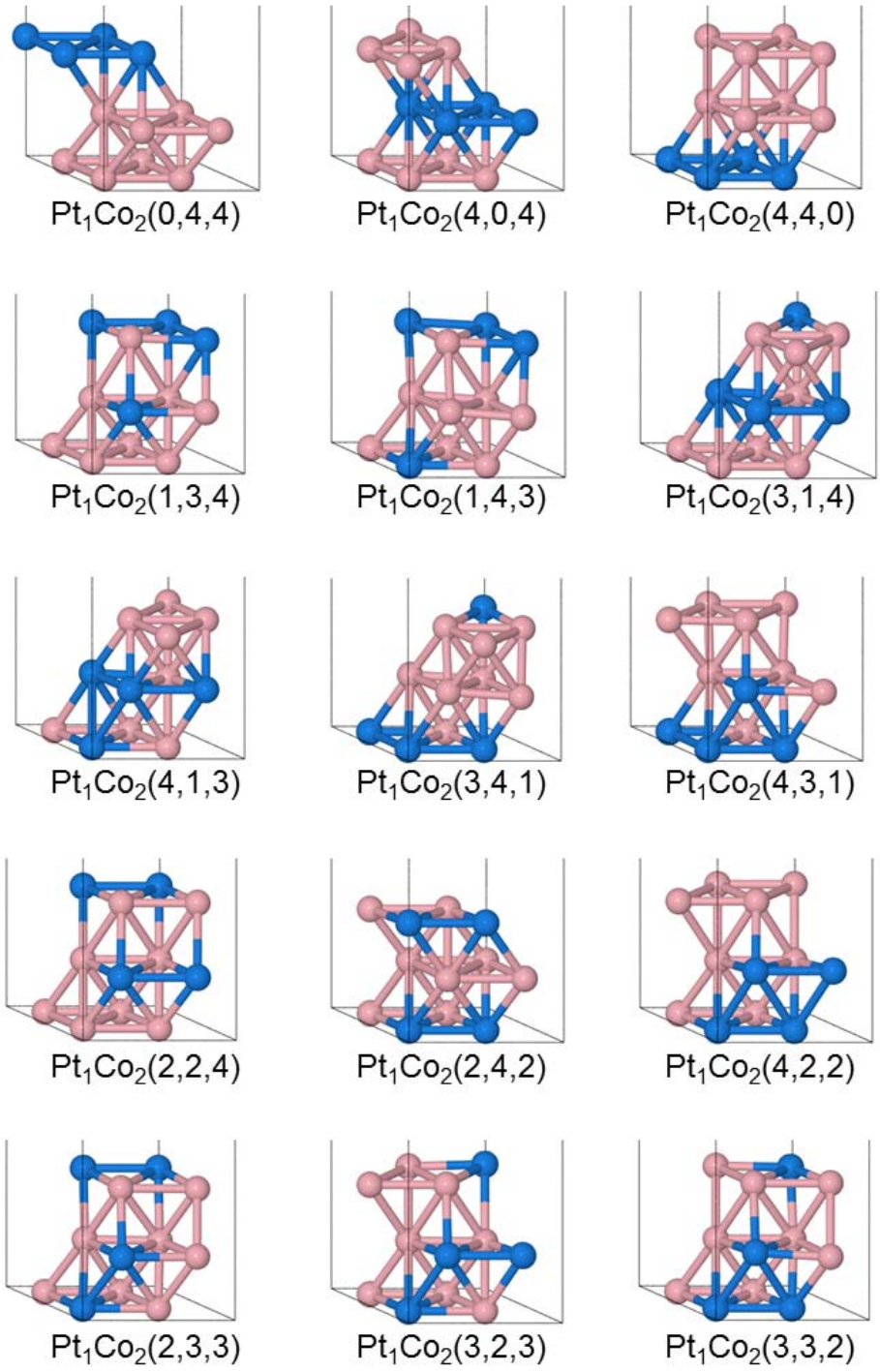

Fig. S3 The alloy configurations with Pt/Co atomic ratio of 1:2. The colors of Pt and Co atoms are blue and pink, respectively.

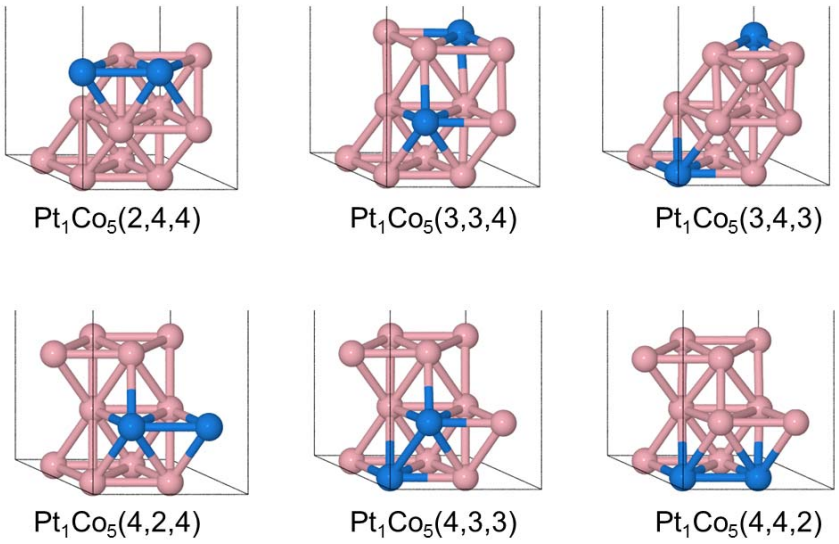

Fig. S4 The alloy configurations with Pt/Co atomic ratio of 1:5. The colors of Pt and Co atoms are blue and pink, respectively.

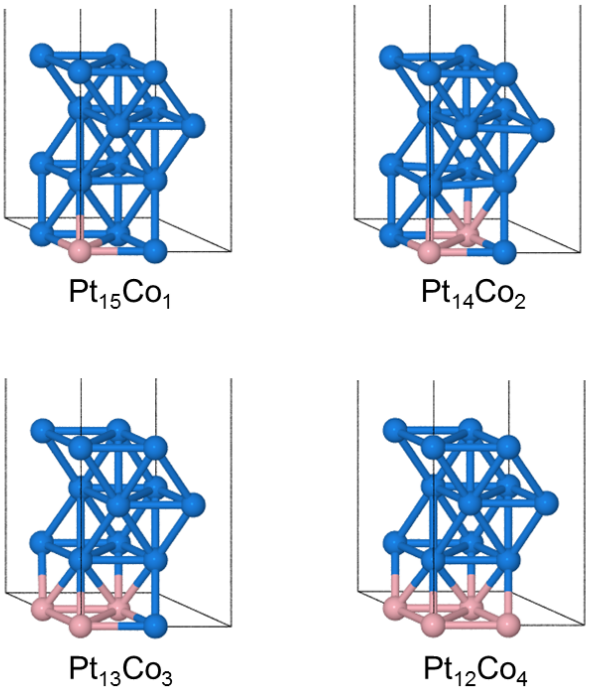

Fig. S5 The alloy configurations with different Pt/Co atomic ratio in the fourth atomic layer. The colors of Pt and Co atoms are blue and pink, respectively.

Table S1. The number of charge transfer of Co atoms in different alloy compositions. Here, '+' represents the loss of electrons. ΔQt represents the total value of charge transfers for all Co atoms in the corresponding structure, and ΔQa represents the average value for per Co atom. All values shown in the table are the results of averaging all structures of the same composition.

Pt/Co ratio	ΔQt	ΔQa
5:1	+1.09	+0.55
2:1	+1.73	+0.43
1:1	+2.10	+0.35
1:2	+1.66	+0.21
1:5	+1.22	+0.12

Table S2. Adsorption energy (E_{ads}, in eV) of O and OH on Pt_5Co_1 alloy surfaces with coverage of 1/4 and 1/16 ML

Configuration	Coverage (in ML)	E_{ads}(O)	E_{ads}(OH)
Pt_5Co_1(0,2,0)	1/4	-3.86	-2.41
	1/16	-3.84	-2.38
Pt_5Co_1(0,1,1)	1/4	-4.23	-2.27
	1/16	-4.21	-2.25
Pt_5Co_1(0,0,2)	1/4	-4.60	-2.45
	1/16	-4.58	-2.44
Pt_5Co_1(1,1,0)	1/4	-4.59	-3.06
	1/16	-4.56	-3.05
Pt_5Co_1(1,0,1)	1/4	-4.75	-2.63
	1/16	-4.71	-2.62
Pt_5Co_1(2,0,0)	1/4	-5.65	-2.83
	1/16	-5.62	-2.81

Table S3. Adsorption energy (E_{ads}, in eV) of O and OH on selected Pt-Co alloy surfaces. The corresponding configurations are displayed in Fig. S5.

Configuration	E_{ads}(O)	E_{ads}(OH)
$Pt_{15}Co_1$	-4.65	-2.46
$Pt_{14}Co_2$	-4.63	-2.46
$Pt_{13}Co_3$	-4.65	-2.48
$Pt_{12}Co_4$	-4.68	-2.47