Electronic Supplementary Material (ESI) for New Journal of Chemistry.

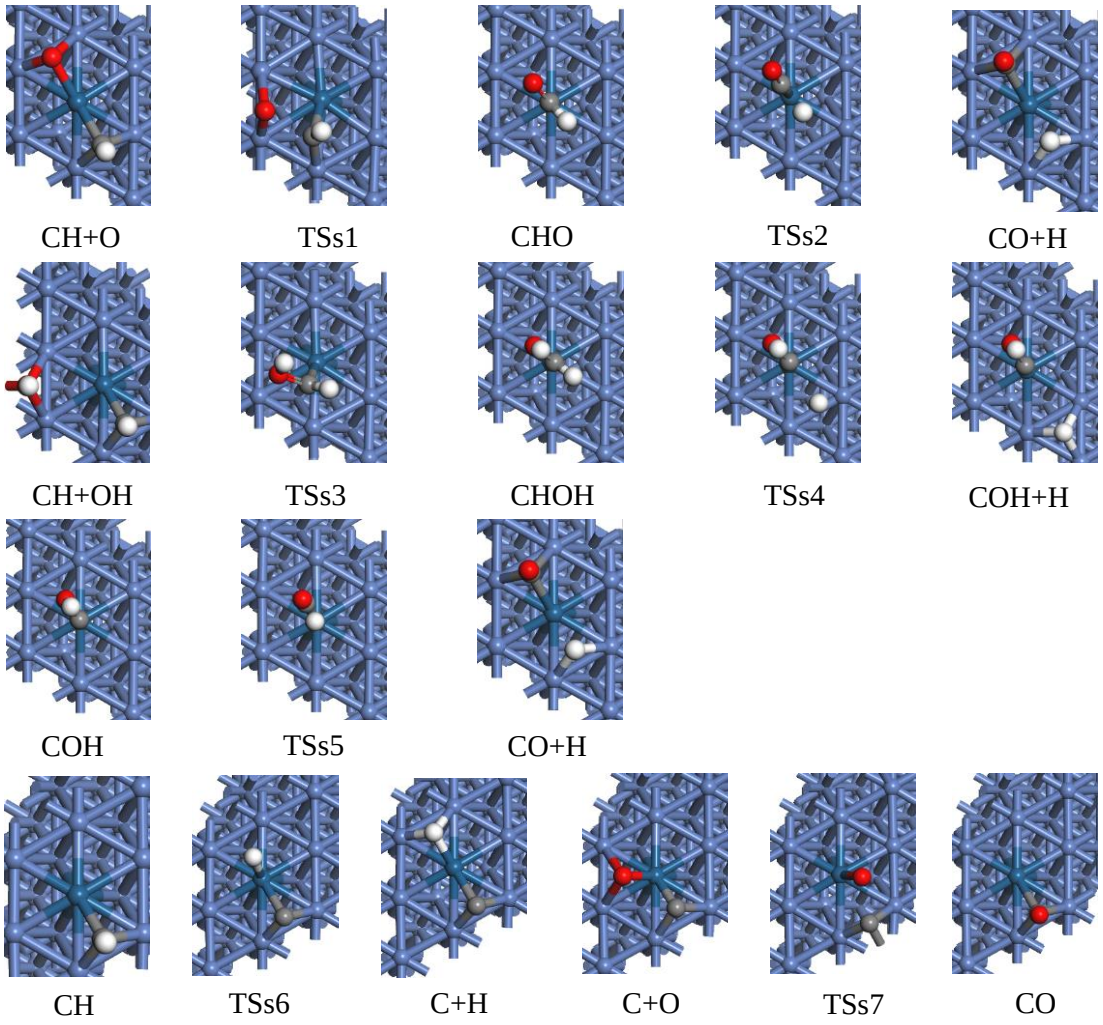

Figure s1 *The stable adsorption configurations and transition states in the three reactions of CO formation on the $Pt_1Ni(111)$ surface.*

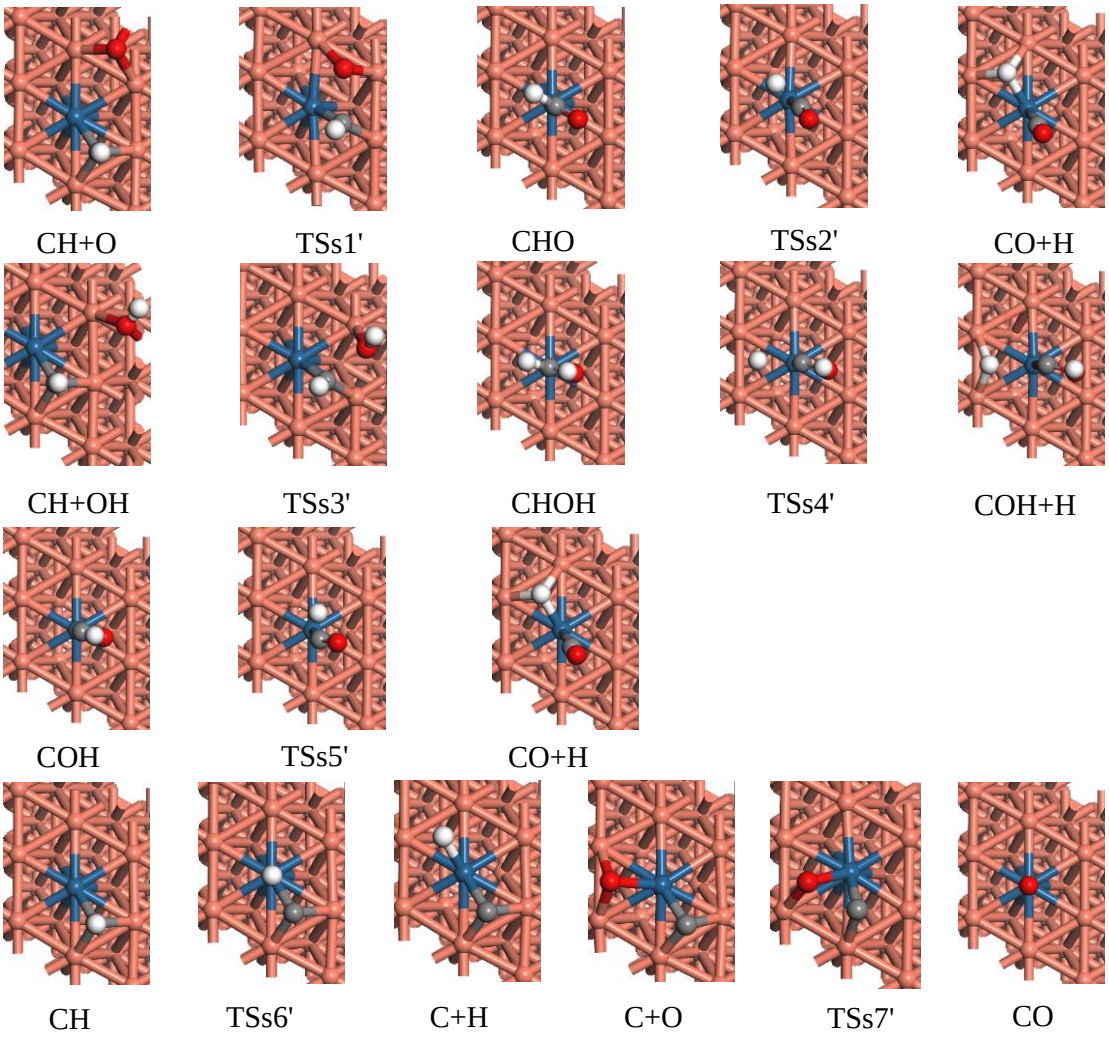

Figure s2 *The stable adsorption configurations and transition states in the three reactions of CO formation on the $Pt_1Cu(111)$ surface.*

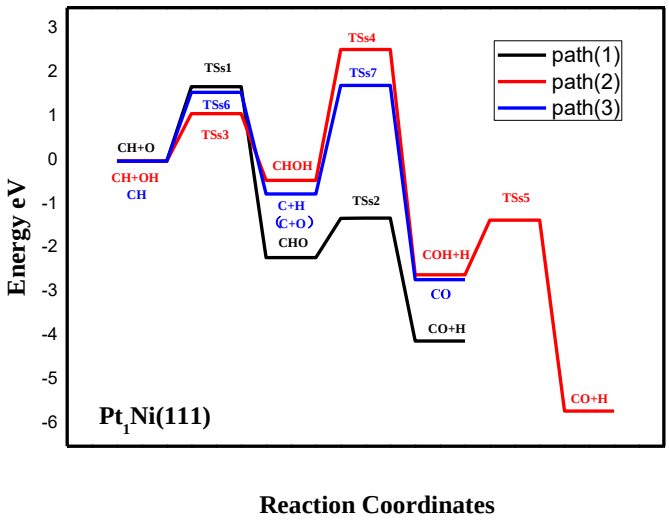

Figure s3 Three reaction energy change curve of *CO formation* on $Pt_1Ni(111)$ surface.

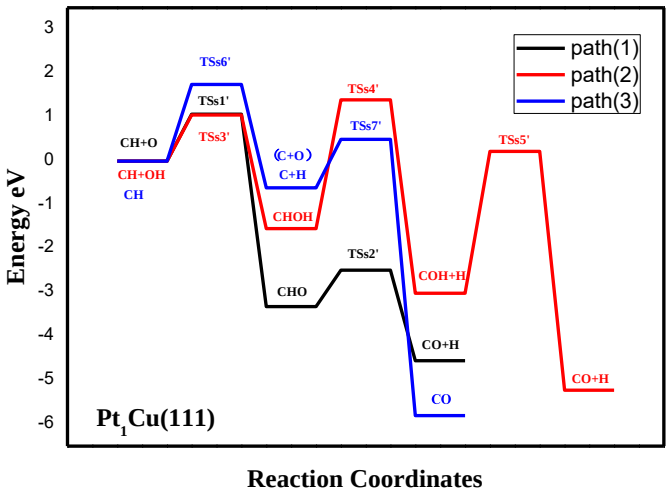

Figure s4 Three reaction energy change curve of *CO formation* on $Pt_1Cu(111)$ surface.

Table s1 *Energies of three reactions of CO formation on the $Pt_1Ni(111)$ and $Pt_1Cu(111)$, and surfaces (eV).*

	$Pt_1Ni(111)$		$Pt_1Cu(111)$	
	Ea(eV)	Ef(eV)	Ea(eV)	Ef(eV)
CH+O→CHO	1.71	-2.21	1.07	-3.32
CHO→CO+H	0.90	-1.90	0.83	-1.24
CH+OH→CHOH	1.08	-0.44	1.05	-1.54
CHOH→COH+H	2.98	-2.15	2.94	-1.48
COH→CO+H	0.81	-3.55	1.70	-3.75
CH→C+H	1.57	-0.75	1.75	-0.61
C+O→CO	2.47	-1.96	1.10	-5.20