Supplementary Information

Substrate-dependent Catalytic Activity of Single-atom Pt for CO Oxidation

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Table S1. Binding energy of Pt anchored on $SrBO_3$ (B = Ag, Co, Cu, Fe, Hf, Mg, Mn, Ni, Sc, Ti, Zr) with different types of surfaces.

	Binding Energy of Pt (eV)					
Facet	100		110		111	
Surface termination	SrO	BO_2	O_2	SrBO	B	SrO_3
Adsorption site	top^O	$hollow^{Sr}$	$hollow^O$	top^{Sr}	$hollow^{Sr}$	$hollow^{Sr}$
Ag	2.50	-3.77	0.71	0.96	3.29	0.87
Co	2.93	-1.34	-1.00	2.65	5.33	-2.38
Cu	2.17	-3.78	-3.31	1.59	5.11	-2.65
Fe	1.45	-0.30	0.94	2.94	5.37	2.92
Hf	2.79	4.43	-1.78	0.06	0.91	-2.51
Mg	1.82	-4.91	-4.91	2.01	4.58	-4.70
Mn	3.14	0.43	1.33	6.83	3.39	0.94
Ni	2.02	-3.42	-2.29	2.60	5.55	-1.79
Sc	1.65	-5.08	-4.37	2.58	4.20	-4.44
Ti	2.69	2.51	-1.11	1.42	1.30	-0.86
Zr	2.86	3.51	-3.55	0.49	1.48	-3.34

Table S2. Binding energy of Pt and Pt-O distance on Pt-$CaBO_3$ and Pt-$SrBO_3$ surfaces.

	Pt-O distance (Å)			Binding energy of Pt (eV)		
B-site elements	Pt-$CaBO_3$	Pt-$SrBO_3$	Pt-$BaBO_3$	Pt-$CaBO_3$	Pt-$SrBO_3$	Pt-$BaBO_3$
Ag	-	1.94	-	□-	-3.77	-
Al	-	1.93	1.94	□-	-2.92	-3.29
Au	-	1.97	1.97	□-	-1.62	-2.8
Co	1.95	1.95	1.92	-1.43	-1.34	-1.71
Cr	-	2	-	□-	1.09	-
Cu	1.91	1.92	1.92	-3.85	-3.78	-4.08
Fe	2	2	1.98	-0.85	-0.3	-1.18
Ge	2	2	1.99	0.99	0.78	-0.41
Hf	2.6	2.58	2.52	4.41	4.43	4.54
Mg	1.89	1.91	-	-4.68	-4.91	-
Mn	1.98	1.99	1.97	-0.79	0.43	-0.36
Mo	-	2.93	2.07	□-	4.37	4.31
Ni	-	1.91	1.92	□-	-3.42	-3.6
Os	2.69	2.64	2.03	3.83	4.01	2.85
Pd	-	1.94	-	□-	-2.77	-
Re	-	2.84	2.97	□-	3.62	4.32
Ru	2.48	2	2.01	3.91	1.35	1.17
Sc	-	1.9	1.93	-□	-5.08	-4.39
Si	-	2.51	2	-□	5.14	1.05
Sn	-	2.02	2.02	-□	0.15	0.38
Ta	-	3.03	3.03	-□	4.10	3.05
Ti	2.03	2.04	2.04	3.62	2.51	3.16
V	2.39	2.03	2.04	4.5	2.48	2.13
W	-	3	3.06	-	3.45	4.06
Zn	-	1.91	1.91	-□	-4.38	-4.4
Zr	2.34	2.34	2.37	4.29	3.51	4.26

Table S3. Distance between Pt and CO, C-O bond length in adsorbed CO (CO in gas phase: $d_{C\text{-}O}$ = 1.145 Å), adsorption energy of CO on Pt-$SrBO_3$, and charge transfer between Pt and C, in the first CO oxidation reaction step.

B-site elements	$d_{Pt\text{-}C}$ (Å)	$d_{C\text{-}O}$ (Å)	E_{ad} (eV)	Charge transfer (e)
Ag	1.792	1.166	-0.290	0.30
Al	1.824	1.167	-0.676	0.30
Au	1.806	1.165	-0.947	0.40
Co	1.828	1.170	-0.446	0.35
Cu	1.816	1.166	-0.381	0.23
Fe	1.867	1.168	-0.627	0.35
Mn	1.888	1.168	-1.210	0.38
Ni	1.833	1.163	-0.351	0.21
Pd	1.820	1.165	-0.137	0.32

Table S4. Distance between Pt and CO, C-O bond length in adsorbed CO, O-O bond length in adsorbed O_2 (O_2 in gas phase: d_{O-O} = 1.233 Å), and adsorption energy of CO on Pt-$SrBO_3$, in the second CO oxidation reaction step.

B-site elements	d_{Pt-C} (Å)	d_{C-O} (Å)	d_{O-O} (Å)	E_{ad} (eV)
Ag	1.818	1.166	1.388	-0.61
Al	1.822	1.162	1.472	-0.98
Au	1.832	1.168	1.398	-1.37
Co	1.832	1.167	1.398	-1.48
Cu	1.821	1.165	1.395	-0.68
Fe	1.827	1.167	1.388	-1.50
Mn	1.823	1.168	1.424	-1.70
Ni	1.830	1.163	1.390	-0.76
Pd	1.839	1.167	1.397	-0.82

Table S5. Adsorption energy of CO and O_2 (eV), energy barrier (eV) and tilted angle (°) in the first and second CO oxidation step on Pt-$SrBO_3$.

	First Oxidation Step			Second Oxidation Step			
B-site elements	E_a(CO)	Barrier	Tilted angle	E_a(O_2)	E_a(CO)	Barrier	Tilted angle
Ag	-0.29	-	3.8	-1.09	-0.61	0.71	17.9
Al	-0.68	0.19	15.7	-0.31	-0.98	1.38	20.7
Au	-0.95	0.06	10.4	-0.64	-1.37	1.09	20.0
Co	-0.45	0.13	6.2	-0.55	-1.48	1.74	20.5
Cu	-0.38	0.05	11.9	-0.72	-0.68	0.88	18.2
Fe	-0.63	0.21	12.6	-1.14	-1.50	1.81	22.4
Mn	-1.21	0.09	11.2	-1.03	-1.70	2.24	21.9
Ni	-0.35	-	6.8	-1.01	-0.76	0.64	11.8
Pd	-0.14	-	3.3	-1.01	-0.82	0.79	17.3

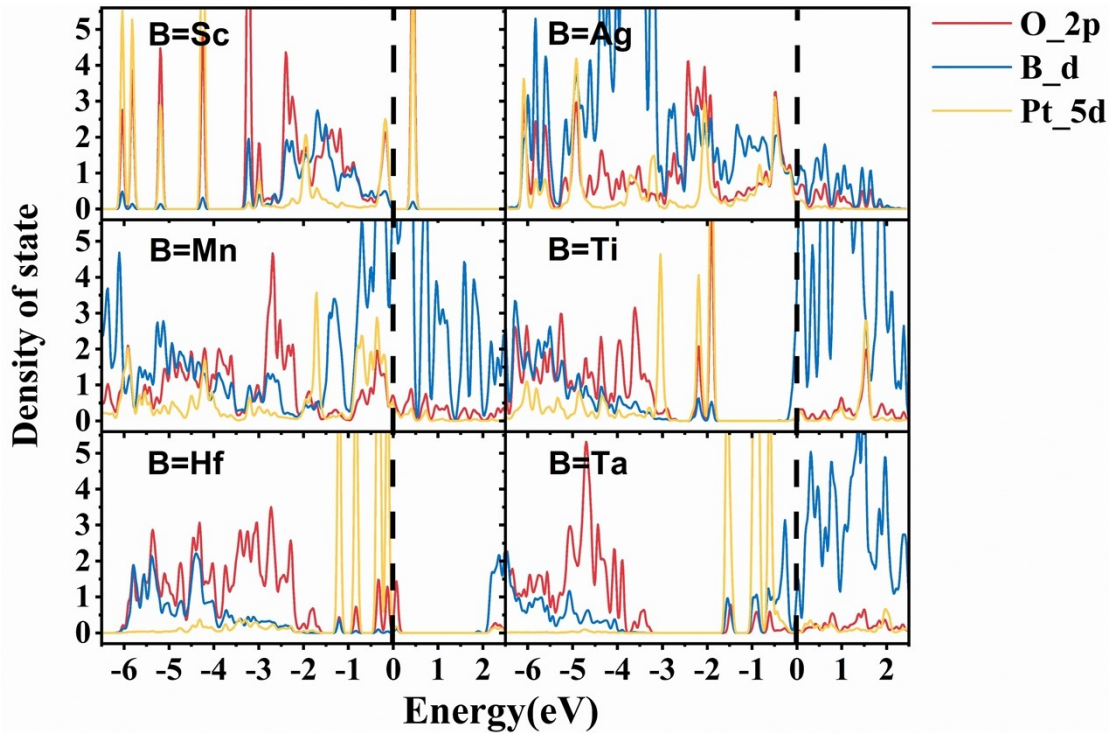

Fig. S1 Projected density of states for Pt-$SrBO_3$ (B = Sc, Ag, Mn, Ti, Hf, Ta). The red, blue and gold lines represent the partial density of states of O 2*p* orbital, B *d* orbital, and Pt 5*d* orbital, respectively.

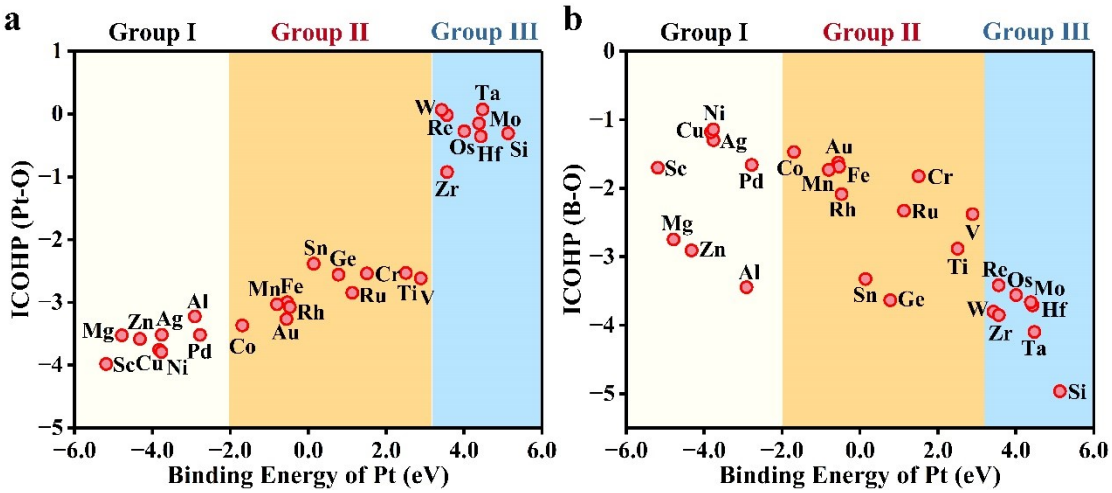

Fig. S2 (a) Relationship between Integrated COHP values (ICOHP) of Pt-O pair and binding energies of Pt. (b) Relationship between ICOHP values of B-O pair (the oxygen that connected to Pt) and binding energies of Pt.

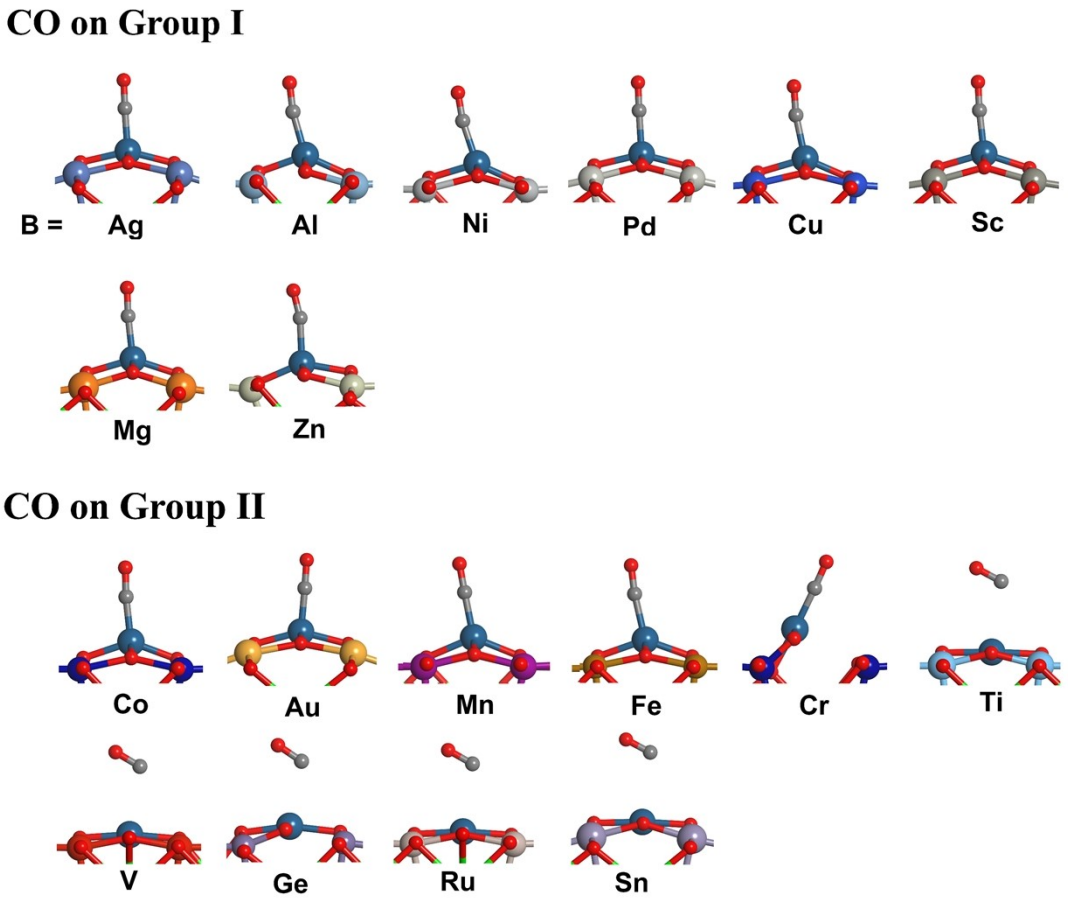

Fig. S3 Optimized configurations of CO adsorbed on Pt site of Pt-$SrBO_3$ surface in the first oxidation step.

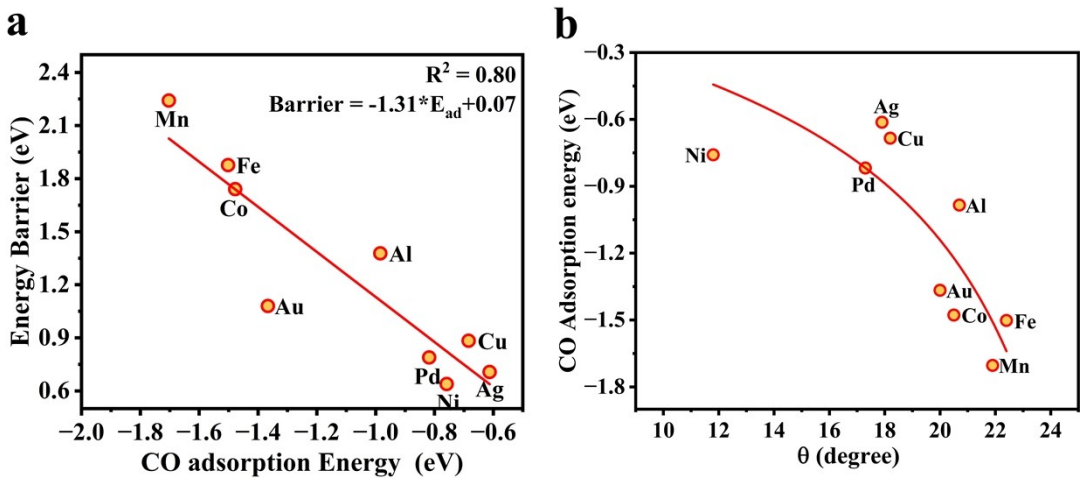

Fig. S4 (a) Relationship between CO adsorption energy and energy barrier in second oxidation step. (b) Relationship between the θ (tilted angle between adsorbed CO and z axis) and adsorption energy of CO in the second oxidation step.