

Supporting Information

Indirect Design of OCM Catalysts through Machine Learning of Catalyst Surface Oxygen Species

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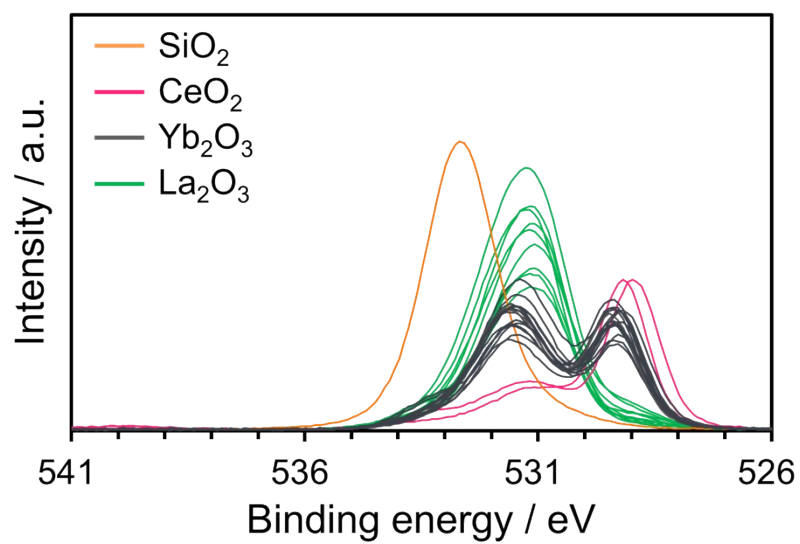


Fig. S1 O1s XPS spectra of the predicted 28 catalysts.

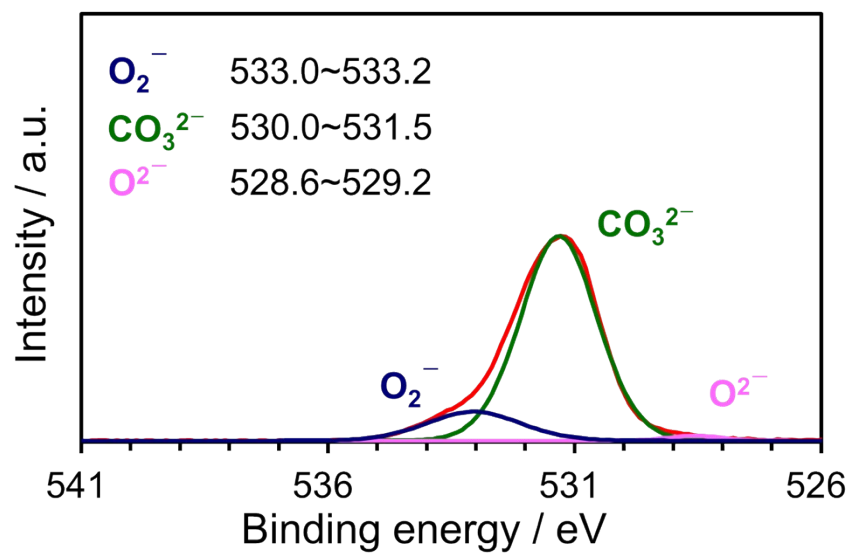


Fig. S2 Peak deconvolution of the O1s XPS spectrum of Ba-In-Rb/La₂O₃.

Table. S1 Binding energies of the three deconvoluted O1s XPS peaks of the 51 catalysts reported in the previous study (*Catal. Sci. Technol.*, 2021, **11**, 524).

Catalyst	Peak Binding energy		
	O ₂ ⁻	CO ₃ ²⁻	O ²⁻
In / CeO ₂	533.58	531.77	529.24
In / Pr ₆ O ₁₁	533.63	531.41	528.46
In / Nd ₂ O ₃	533.64	531.62	529.11
In / Sm ₂ O ₃	533.59	531.66	529.20
In / Eu ₂ O ₃	533.00	531.42	529.07
In / Gd ₂ O ₃	533.65	531.86	529.15
In / Dy ₂ O ₃	533.00	531.42	529.07
In / Yb ₂ O ₃	533.65	531.86	529.15
Li / La ₂ O ₃	532.80	531.44	528.83
Na / La ₂ O ₃	533.40	531.20	528.52
Mg / La ₂ O ₃	532.68	531.53	529.51
K / La ₂ O ₃	532.65	531.54	529.02
Ca / La ₂ O ₃	533.70	531.61	528.96
V / La ₂ O ₃	533.74	531.71	529.25
Cr / La ₂ O ₃	533.51	531.48	528.63
Mn / La ₂ O ₃	533.69	531.60	528.95
Fe / La ₂ O ₃	533.55	531.61	528.87
Co / La ₂ O ₃	533.61	531.63	528.96
Ni / La ₂ O ₃	533.49	531.62	528.87
Cu / La ₂ O ₃	533.99	531.59	528.91
Zn / La ₂ O ₃	533.41	531.64	529.01
Rb / La ₂ O ₃	533.47	531.41	528.74
Sr / La ₂ O ₃	533.34	531.63	528.98
Mo / La ₂ O ₃	533.35	531.35	528.66
Pd / La ₂ O ₃	533.53	531.63	529.01
Ag / La ₂ O ₃	532.70	531.48	528.96
Sn / La ₂ O ₃	532.49	531.36	529.10
Cs / La ₂ O ₃	532.69	531.21	528.74
Ba / La ₂ O ₃	533.47	531.81	529.67
W / La ₂ O ₃	533.50	531.56	528.86
Re / La ₂ O ₃	532.34	531.34	528.84
Pt / La ₂ O ₃	533.59	531.68	529.01
In / La ₂ O ₃	533.00	531.46	528.88

In(0.5 wt%) / La ₂ O ₃	533.00	531.41	528.78
In(0.1 wt%) / La ₂ O ₃	533.00	531.39	528.81
none / La ₂ O ₃	533.58	531.58	528.79
none / Pr ₆ O ₁₁	533.49	531.39	528.56
none / Nd ₂ O ₃	533.00	531.33	528.71
none / Sm ₂ O ₃	533.00	531.40	528.89
none / Eu ₂ O ₃	533.20	531.43	529.09
none / Gd ₂ O ₃	533.42	531.61	529.12
none / Dy ₂ O ₃	533.85	531.76	529.20
none / Yb ₂ O ₃	533.00	531.76	529.54
none / MgO	532.49	530.66	528.80
none / Al ₂ O ₃	532.53	530.66	528.85
none / ZnO	533.05	531.65	530.00
none / ZrO ₂	531.77	529.85	527.82
none / Nb ₂ O ₅	531.51	530.06	528.73
none / TiO ₂	532.32	530.46	529.79
none / FeO	533.27	531.45	529.98
none / SnO	532.78	530.95	529.89

Table S2 Binding energies of the three deconvoluted O1s XPS peaks of the 28 catalysts prepared in this study.

Catalyst	Peak binding energy (eV)		
	O ₂ ⁻	CO ₃ ²⁻	O ²⁻
Cs-In-Rb / La ₂ O ₃	532.99	531.43	528.93
Ba-Rb-Yb / La ₂ O ₃	532.87	531.27	528.68
Bi-Rb-Yb / La ₂ O ₃	532.57	531.20	528.77
Ba-In-Rb / La ₂ O ₃	532.80	531.34	528.53
In-Rb-Yb / La ₂ O ₃	533.18	531.33	528.51
In-Rb-Sm / La ₂ O ₃	532.66	531.27	528.67
Bi-In-Rb / La ₂ O ₃	532.78	531.28	528.65
Ba-In-Yb / La ₂ O ₃	533.23	531.27	528.62
Bi-In-Yb / La ₂ O ₃	532.48	531.15	528.94
Ce-In-Rb / La ₂ O ₃	532.71	531.26	528.78
Ba-Cs-Hf / CeO ₂	533.53	531.35	529.38
Ba-Cs-Sm / CeO ₂	533.57	531.47	529.24
Ba-Cs-Hf / Yb ₂ O ₃	532.86	531.58	529.53
Ba-Cs-Sm / Yb ₂ O ₃	533.02	531.58	529.51
Hf-In-Sm / Yb ₂ O ₃	532.99	531.71	529.58
Hf-In-Nd / Yb ₂ O ₃	532.99	531.66	529.55
Bi-In-Sm / Yb ₂ O ₃	532.86	531.60	529.48
Bi-Hf-Sm / Yb ₂ O ₃	532.98	531.68	529.61
Eu-Hf-Nd / Yb ₂ O ₃	532.87	531.73	529.53
Eu-Hf-Sm / Yb ₂ O ₃	532.87	531.75	529.56
Ba-Hf / Yb ₂ O ₃	532.98	531.63	529.58
Cs-Hf / Yb ₂ O ₃	532.81	531.73	529.60
Sm-Hf / Yb ₂ O ₃	532.96	531.72	529.58
Ce-Hf / Yb ₂ O ₃	532.77	531.63	529.38
Cu-Hf / Yb ₂ O ₃	533.00	531.59	529.50
Zn-Hf / Yb ₂ O ₃	532.75	531.70	529.52
Zn-W / Yb ₂ O ₃	532.84	531.56	529.43
Ba-Ce-Cs / SiO ₂	534.83	532.77	530.67