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Supplementary Materials for

Designing less noble yet high-performing multimetallic catalysts for catalytic converters using a high-throughput approach

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Table S1. List of chemicals used in the present research

Chemical	Formula	Supplier	MW (g/mol)	Purity
Iridium (III) acetylacetonate	$Ir(C_5H_7O_2)_3$	Sigma Aldrich	489.54	97
Palladium (II) acetylacetonate	$Pd(C_5H_7O_2)_2$	Sigma Aldrich	304.64	99
Bis(acetylacetonato)platinum (II)	$Pt(C_5H_7O_2)_2$	Wako Chemical	393.3	98
Rhodium (III) acetylacetonate	$Rh(C_5H_7O_2)_3$	Sigma Aldrich	400.23	97
Silver acetylacetonate	$Ag(C_5H_7O_2)$	Sigma Aldrich	206.98	98
Cobalt (II) acetylacetonate	$Co(C_5H_7O_2)_2$	Sigma Aldrich	257.15	97
Nickel (II) acetylacetonate	$Ni(C_5H_7O_2)_2$	Sigma Aldrich	256.91	95
Iron (III) acetylacetonate	$Fe(C_5H_7O_2)_3$	Sigma Aldrich	353.17	97
Indium (III) acetylacetonate	$In(C_5H_7O_2)_3$	Sigma Aldrich	412.14	99.99
Chromium (III) acetylacetonate	$Cr(C_5H_7O_2)_3$	Sigma Aldrich	349.32	99.99
Manganese (II) acetylacetonate	$Mn(C_5H_7O_2)_2$	Sigma Aldrich	253.15	100
Ruthenium (III) acetylacetonate	$Ru(C_5H_7O_2)_3$	Sigma Aldrich	398.39	97
Copper (III) acetylacetonate	$Cu(C_5H_7O_2)_2$	Sigma Aldrich	261.76	99.9
Poly(vinylpyrrolidone) K30	$(C_6H_9NO)_n$	Wako Chemical	40,000	
1–methyl–2–pyrrolidone, anhydrous	C_5H_9NO	Sigma Aldrich	99.13	99.5
Triethylene glycol	$C_6H_{14}O_4$	Alfa Aesar	150.17	99
Lithium triethylborohydride	$Li(C_2H_5)_3BH$	Sigma Aldrich	105.95	
Methanol	CH_3OH	Kanto Chemical	32.04	99.8
Hexane	$CH_3(CH_2)_4CH_3$	Kanto Chemical	86.18	96.0
CeO_2–ZrO_2 (6:4 mole ratio based on oxides)*				

***Preparation of CeO_2-ZrO_2:** The CeO_2–ZrO_2 oxide (6:4 mole ratio based on oxides) was prepared by a coprecipitation method. $Ce(NO_3)_3 \cdot 6H_2O$ (Nacalai Tesque) and $ZrO(NO_3)_2 \cdot 2H_2O$ (Nacalai Tesque) were dissolved in deionized (DI) water. The pH of the solution was adjusted by adding aqueous ammonia solution until the pH reached 10. The solution was stirred for 12 h, and the precipitate was collected through centrifugation and washed with DI water until the supernatant was neutral. The resulting precipitate was dried at 110 °C and calcined in air at 973 K for 5 h.

Table S2. List of catalysts[a] and their T_{50}[b] for NO reduction, CO and C_3H_6 oxidation

No.	Catalyst	T50_NO	T50_CO	T50_C_3H_6
1	Ru	500.0	354.9	382.1
2	Rh	308.6	281.4	303.5
3	Pd	295.0	283.7	285.0
4	Pt	338.8	345.5	321.7
5	Cr–Cr–Cr–Pd–Pd	329.4	287.5	293.2
6	Cr–Pt–Pt–Pt–Pt	500.0	393.0	413.0
7	Mn–Rh	500.0	274.0	300.0
8	Mn–Pt	358.2	325.0	335.0
9	Mn–Mn–Pt–Pt–Pt	500.0	356.4	368.0
10	Mn–Pd–Pd–Pd	308.6	275.3	276.3
11	Mn–Pt–Pt–Pt	500.0	336.5	344.9
12	Mn–Rh–Rh–Rh–Rh	322.6	255.0	286.0
13	Fe–Pt–Pt	500.0	351.4	368.8
14	Co–Pt–Pt	394.4	334.1	346.6
15	Co–Pt–Pt–Pt	358.9	327.9	328.2
16	Co–Rh–Rh–Rh–Rh	500.0	270.0	301.0
17	Ni–Pd	311.1	257.0	272.0
18	Cu–Rh	311.6	293.0	317.0
19	Cu–Pd	340.8	305.0	310.0
20	Cu–Pt	386.4	328.3	331.4
21	Cu–Pt–Pt	500.0	372.8	371.4
22	Cu–Pd–Pd–Pd–Pd	296.3	288.7	290.1
23	Ru–Ru–Ru–Ru–Pd	332.1	270.8	287.1
24	Ru–Ru–Ag	500.0	350.6	364.8
25	Ru–Rh	500.0	363.1	373.8
26	Ru–Pd	308.8	266.0	283.0
27	Ru–Pt	328.3	300.7	286.1
28	Rh–Pd	275.9	259.0	268.0
29	Rh–Pt	287.5	274.0	286.0
30	Rh–Pd–Pd–Pd–Pd	276.0	235.0	246.0
31	Rh–Pt–Pt–Pt–Pt	377.3	322.3	342.2
32	Pd–Pd–Pd–Pd–In	314.8	269.0	273.0
33	Pd–Pd–In	356.9	296.4	304.1
34	Pd–In	357.2	298.0	307.0
35	Pd–Pt	293.4	253.0	265.0
36	Pd–Pt–Pt	316.1	262.4	272.3
37	Pd–Pt–Pt–Pt–Pt	332.8	287.4	297.2
38	Ag–Pt–Pt	339.4	289.4	295.4
39	Ag–Pt–Pt–Pt	500.0	339.3	344.4
40	In–Pt	500.0	328.4	357.8

41	In–Pt–Pt	500.0	383.2	417.6
42	Cr–Cr–Pd–Pt	297.8	251.2	262.2
43	Cr–Cr–Rh–Rh–In	397.2	355.3	357.8
44	Cr–Cr–Rh–Pd–Pd	299.3	252.8	262.3
45	Cr–Cr–Pd–Pd–Ag	315.8	307.6	293.2
46	Cr–Pd–Pt–Pt	355.7	274.9	284.1
47	Cr–Co–Pd–Pd–Pd	369.3	323.5	329.9
48	Cr–Ni–Ni–Pt–Pt	500.0	323.3	371.0
49	Cr–Cu–Pt–Pt–Pt	500.0	339.0	360.0
50	Mn–Mn–Mn–Pd–Pt	385.9	349.5	358.7
51	Mn–Mn–Ru–Ru–Pt	500.0	382.2	395.6
52	Mn–Rh–Pd	305.4	266.0	278.0
53	Mn–Rh–Ag	372.0	280.0	308.0
54	Mn–Pd–Pt	313.1	261.0	275.0
55	Mn–Ni–Pt–Pt	500.0	321.0	337.3
56	Mn–Ni–Pt–Pt–Pt	398.9	339.9	353.0
57	Mn–Cu–Pd–Pd–Pd	318.4	288.0	291.0
58	Fe–Fe–Cu–Ag–Ag	500.0	299.0	353.0
59	Fe–Fe–Ru–Rh–Rh	500.0	294.0	313.0
60	Fe–Ru–Pd	311.0	265.0	282.0
61	Fe–Rh–Pd	299.0	258.0	283.0
62	Fe–Rh–Pt	296.7	261.0	284.0
63	Fe–Pd–Pt	303.6	291.0	294.0
64	Co–Ru–Pd	327.3	293.0	301.0
65	Co–Ru–Pt	339.0	287.0	328.0
66	Co–Rh–Pd	314.3	283.0	298.0
67	Co–Rh–Pt	308.1	272.0	292.0
68	Co–Pd–Pt	301.2	276.0	285.0
69	Co–Ag–Ag–Pt	500.0	347.0	379.0
70	Co–Pd–Pt–Pt–Pt	325.6	285.2	288.1
71	Co–Ag–Ag–Pt–Pt	500.0	322.3	407.7
72	Ni–Ni–Ni–Ru–Pt	312.9	290.7	297.1
73	Ni–Ni–Ag–Pt–Pt	335.5	330.7	318.2
74	Ni–Ru–Pd	323.6	278.0	291.0
75	Ni–Rh–Pd	298.2	257.0	285.0
76	Ni–Rh–Pt	296.9	244.0	272.0
77	Ni–Pd–Pt	311.7	258.0	273.0
78	Ni–Ir–Pt	397.1	304.0	348.0
79	Ni–Ru–Pd–Pd–Pd	284.1	265.7	274.8
80	Cu–Ru–Pd	298.5	259.5	262.6
81	Cu–Ru–Pt	500.0	391.8	405.1
82	Cu–Rh–Pd	307.3	266.0	291.0

83	Cu–Rh–Pt	305.8	264.0	287.0
84	Cu–Pd–Pt	327.5	287.0	297.0
85	Cu–In–Pt–Pt	395.9	327.0	365.6
86	Cu–Pd–Pd–Pd–Ag	282.1	255.8	250.7
87	Ru–Rh–Pd	304.6	272.0	293.0
88	Ru–Rh–Pt	309.8	264.0	289.0
89	Ru–Pd–Pt	321.3	268.0	289.0
90	Ru–Pd–In–In	500.0	341.5	355.6
91	Ru–Pd–Pd–Pd–Pt	287.0	256.6	253.5
92	Ru–Ag–In–In–In	500.0	396.0	402.0
93	Rh–Pd–Pt	273.4	264.0	268.0
94	Rh–Ag–In	500.0	360.0	359.0
95	Rh–Ag–Pt	500.0	277.3	322.5
96	Rh–Pd–Pt–Pt–Pt	333.1	265.9	282.0
97	Rh–Ag–In–In–In	500.0	381.0	393.0
98	Pd–Pd–Ag–Pt–Pt	338.5	303.5	315.2
99	Pd–In–Pt	500.0	266.0	315.9
100	Pd–Ag–Ag–Ag–Pt	338.9	276.0	290.3
101	Pd–In–Pt–Pt–Pt	377.8	340.0	345.9
102	Cr–Mn–Mn–Ru–Pd	339.5	283.7	294.0
103	Cr–Mn–Ag–Ag–In	500.0	350.0	363.0
104	Cr–Ru–Pd–Ag–Ag	284.6	260.1	253.4
105	Cr–Pd–Ag–Ag–Pt	500.0	350.0	363.0
106	Cr–Pd–In–In–Pt	329.3	286.7	292.2
107	Mn–Mn–Ni–Ru–Pd	311.6	295.2	283.5
108	Mn–Co–Pd–Pt	319.6	288.7	288.9
109	Mn–Cu–Ru–Rh	500.0	284.0	317.0
110	Mn–Fe–Ru–Pt–Pt	500.0	297.9	358.7
111	Mn–Cu–Ru–Ru–Pd	317.1	283.9	284.5
112	Mn–Cu–Rh–Pt–Pt	348.7	306.0	314.0
113	Mn–Rh–Ag–In–In	500.0	335.0	351.0
114	Fe–Co–Rh–Pd	323.3	288.0	305.0
115	Fe–Cu–Rh–Pd	330.3	261.0	298.0
116	Fe–Rh–Pd–Pt	316.8	278.0	296.0
117	Fe–Co–Pd–Pd–In	384.1	341.9	343.0
118	Fe–Cu–Rh–Ag–Ag	354.8	269.0	309.0
119	Co–Cu–Rh–Pd	314.0	284.0	297.0
120	Co–Ru–Ag–Pt–Pt	500.0	379.8	406.5
121	Ni–Pd–Ag–Pt–Pt	270.7	240.2	241.8
122	Ni–Pd–In–Pt–Pt	500.0	358.4	371.1
123	Cu–Rh–Pd–Pt	318.4	291.0	317.0
124	Ru–Rh–Pd–In	291.9	255.6	259.3
125	Ru–Pd–In–Pt	361.6	290.5	308.9

126	Ru–Rh–In–Pt–Pt	500.0	317.2	344.2
127	Rh–Ag–In–Ir	500.0	347.0	365.0
128	Cr–Mn–Pd–In–Pt	500.0	371.6	373.0
129	Cr–Ru–Rh–Pd–Pt	311.4	264.0	287.0
130	Mn–Ni–Cu–Ru–Pd	339.5	322.6	314.0
131	Mn–Ru–Rh–Pd–Pt	315.1	287.0	311.0
132	Mn–Pd–In–Ir–Pt	398.8	312.0	335.0
133	Fe–Co–Ni–Pd–Pt	332.8	313.0	317.0
134	Fe–Co–Rh–Pd–Pt	339.5	281.0	325.0
135	Fe–Ni–Rh–Pd–Pt	313.2	313.0	311.0
136	Co–Ni–Rh–Pd–Pt	326.2	275.0	315.0
137	Co–Rh–Pd–Ag–Pt	334.6	286.0	328.0
138	Ni–Rh–Pd–In–Pt	298.9	294.0	296.0
139	Ru–Rh–Pd–Ag–Pt	334.3	297.0	345.0
140	Rh–Pd–Ag–Ir–Pt	320.9	283.0	318.0

[a]Catalyst compositions are denoted by their elemental symbols, and it should be noted that they assume an equal molar ratio among components. Repeated symbols indicate a proportional increase in the molar ratio of that element. For example, the designation M1–M2 represents a 50:50 molar ratio, M1–M2–M3–M4–M5 is 20% for each element, and M1–M1–M2–M3 has a 50% molar ratio for M1 with 25% each for M2 and M3.

[b]The T_{50} values, representing the temperatures corresponding to 50% conversion, were derived by interpolating the acquired conversions at discrete temperature points. When a catalyst did not reach 50% conversion up to 400 °C, the T_{50} value was assigned as 500 °C.

Table S3. Abundance values[a] of all the used elements and its log to the base 10

Element	**Abundance (ppm)**	**log(A)**
Cr	102	2.0
Mn	950	3.0
Fe	56300	4.8
Co	25	1.4
Ni	84	1.9
Cu	60	1.8
Ru	0.001	–3.0
Rh	0.001	–3.0
Pd	0.015	–1.8
Ag	0.075	–1.1
In	0.25	–0.6
Ir	0.001	–3.0
Pt	0.005	–2.3

[a]Haynes WM, Lide DR, Bruno TJ, editors. Geophysics, Astronomy, and Acoustics. In: CRC Handbook of Chemistry and Physics. 97th edn CRC Press; 2016.

Table S4. Performance comparison of classification models evaluated on the same training–testing split (Class 0 vs Class 3).

Model	**F1-score**
XGBoost	0.9474
Logistic regression	0.9000
Support vector machine (RBF kernel)	0.9000
Random forest	0.8889
k-nearest neighbours (k = 7)	0.6316

Note: Feature scaling was applied where required (SVM, logistic regression, k-NN), while XGBoost model was used without scaling.

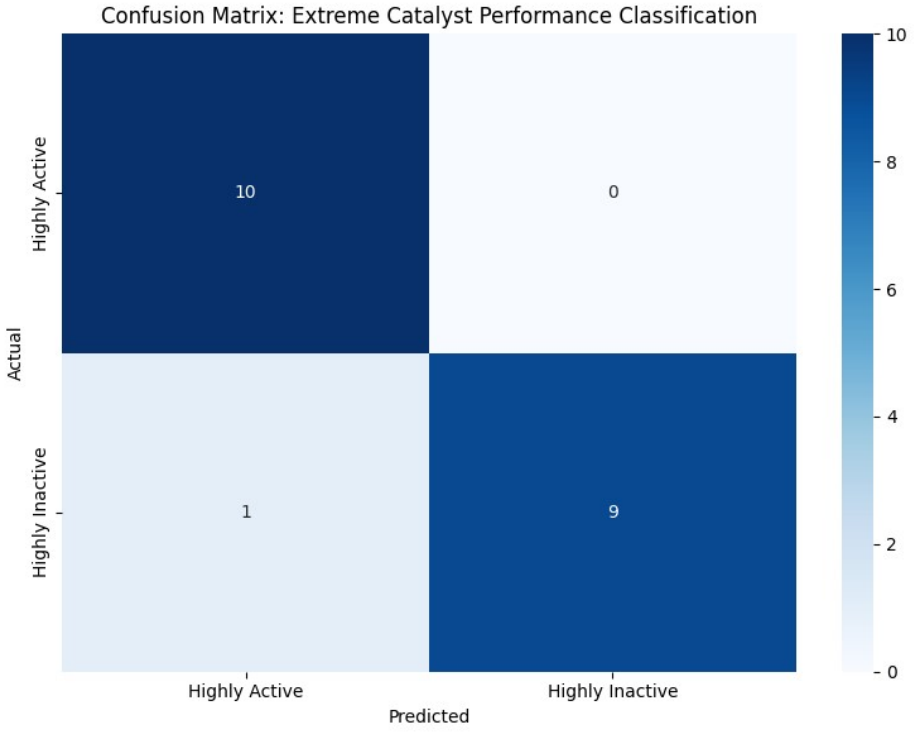

Fig. S1 Confusion matrix showing the accuracy of the classification model on the two extreme performance classes, i.e., class 0 (270.7–313.2 °C) and class 3 (398.9–500 °C).

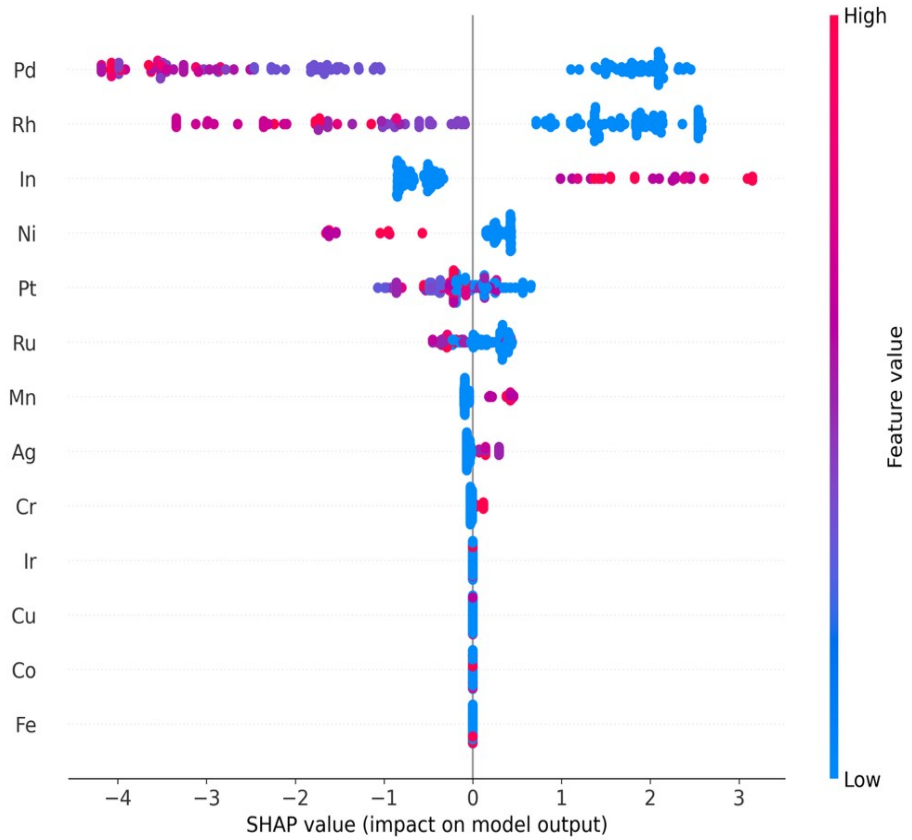

Fig. S2 SHAP beeswarm plot obtained using all 140 catalyst samples (Jenks Classes 0–3), evaluated with the XGBoost model trained on extreme performers (Class 0 vs Class 3). The feature importance ranking and qualitative trends closely match those observed in Fig. 7 in the main MS, demonstrating the robustness of the SHAP-based interpretation.