Supporting Information

Discovery of High-Efficient Dual-atom Catalysts for Propane Dehydrogenation Assisted by Machine Learning

Xianpeng Wang[a,b], Yanxia Ma[b], Youyong Li[a,b], Lu Wang[b*], Lifeng Chi[a,b*]

[a]*Macao Institute of Materials Science and Engineering, Macau University of Science and Technology, Taipa, Macau SAR 999078, China.*
[b]*Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Soochow University, Suzhou, Jiangsu 215123, China.*

Table S1. The 11 descriptors related to the DACs are summarized. The average bond lengths between M_1/M_2 atom and the surrounding O atoms ($d_{M1\text{-}O}$ and $d_{M2\text{-}O}$, Å), the distance of M_1 and M_2 atoms ($d_{M1\text{-}M2}$, Å), the electronegativity of M_1 and M_2 atoms (P_{M1} and P_{M2}), the electron affinity of M_1 and M_2 atoms (A_{M1} and A_{M2}, kJ/mol), the first ionization energy of M_1 and M_2 atoms (I_{M1} and I_{M2}, kJ/mol), and the number of *d*-electrons for M_1 and M_2 atoms ($N_{d\text{-}M1}$ and $N_{d\text{-}M2}$).

DACs	$d_{M1\text{-}O}$	$d_{M2\text{-}O}$	$d_{M1\text{-}M2}$	P_{M1}	P_{M2}	A_{M1}	A_{M2}	I_{M1}	I_{M2}	$N_{d\text{-}M1}$	$N_{d\text{-}M2}$
CuSc	1.85	2.11	2.88	1.90	1.36	118.40	18.10	745.50	633.10	10.00	0.00
CuTi	1.95	1.98	2.75	1.90	1.54	118.40	7.60	745.50	658.80	10.00	2.00
CuV	1.94	1.96	2.73	1.90	1.63	118.40	50.60	745.50	650.90	10.00	3.00
CuCr	1.85	2.04	2.87	1.90	1.66	118.40	64.30	745.50	652.90	10.00	5.00
CuMn	1.86	2.00	2.82	1.90	1.55	118.40	0.00	745.50	717.30	10.00	5.00
CuFe	1.85	2.07	2.89	1.90	1.83	118.40	15.70	745.50	762.50	10.00	6.00
CuCo	1.85	2.08	2.92	1.90	1.88	118.40	63.70	745.50	760.40	10.00	7.00
CuNi	1.85	2.04	2.85	1.90	1.91	118.40	112.00	745.50	737.10	10.00	8.00
CuZn	1.85	2.15	2.94	1.90	1.65	118.40	0.00	745.50	906.40	10.00	10.00
CuGa	1.85	2.04	2.89	1.90	1.81	118.40	28.90	745.50	578.80	10.00	10.00
CuGe	1.95	1.93	2.79	1.90	2.01	118.40	119.00	745.50	762.00	10.00	10.00
CuZr	1.95	2.10	2.78	1.90	1.33	118.40	41.10	745.50	640.10	10.00	2.00
CuNb	2.09	2.00	2.71	1.90	1.60	118.40	86.10	745.50	652.10	10.00	4.00
CuMo	1.96	2.04	2.72	1.90	2.16	118.40	71.90	745.50	684.30	10.00	5.00
CuRu	1.89	2.06	2.82	1.90	2.20	118.40	101.30	745.50	710.20	10.00	7.00
CuRh	1.85	2.10	2.88	1.90	2.28	118.40	109.70	745.50	719.70	10.00	8.00
CuPd	1.85	2.10	2.87	1.90	2.20	118.40	53.70	745.50	804.40	10.00	10.00
CuAg	1.85	2.21	2.90	1.90	1.93	118.40	125.60	745.50	731.00	10.00	10.00
CuIn	1.85	2.18	2.92	1.90	1.78	118.40	28.90	745.50	558.30	10.00	10.00
CuSn	1.94	2.07	2.86	1.90	1.96	118.40	107.30	745.50	708.60	10.00	10.00
CuHf	1.95	2.08	2.79	1.90	1.30	118.40	0.00	745.50	658.50	10.00	2.00
CuTa	2.10	2.00	2.70	1.90	1.50	118.40	31.00	745.50	761.00	10.00	3.00
CuW	2.01	2.01	2.72	1.90	2.36	118.40	78.60	745.50	770.00	10.00	4.00
CuRe	1.95	2.04	2.82	1.90	1.90	118.40	14.50	745.50	760.00	10.00	5.00
CuOs	1.94	2.03	2.81	1.90	2.20	118.40	106.10	745.50	840.00	10.00	6.00
CuIr	1.86	2.11	2.89	1.90	2.20	118.40	151.00	745.50	880.00	10.00	7.00
CuPt	1.85	2.09	2.87	1.90	2.28	118.40	205.30	745.50	870.00	10.00	9.00
CuAu	1.85	2.11	2.88	1.90	2.54	118.40	222.80	745.50	890.10	10.00	10.00
CuBi	1.85	2.28	2.93	1.90	2.02	118.40	91.20	745.50	703.00	10.00	10.00
PdAg	1.98	2.21	2.90	2.20	1.93	53.70	125.60	804.40	731.00	10.00	10.00
PdAu	1.99	2.10	2.89	2.20	2.54	53.70	222.80	804.40	890.10	10.00	10.00
PdBi	1.99	2.28	2.88	2.20	2.02	53.70	91.20	804.40	703.00	10.00	10.00
PdGa	1.99	2.03	2.90	2.20	1.81	53.70	28.90	804.40	578.80	10.00	10.00
PdGe	2.02	1.92	2.84	2.20	2.01	53.70	119.00	804.40	762.00	10.00	10.00
PdCo	1.99	2.09	2.87	2.20	1.88	53.70	63.70	804.40	760.40	10.00	7.00
PdCr	2.00	1.99	2.81	2.20	1.66	53.70	64.30	804.40	652.90	10.00	5.00

PdFe	1.99	2.07	2.83	2.20	1.83	53.70	15.70	804.40	762.50	10.00	6.00
PdHf	2.02	2.09	2.72	2.20	1.30	53.70	0.00	804.40	658.50	10.00	2.00
PdIn	1.99	2.18	2.88	2.20	1.78	53.70	28.90	804.40	558.30	10.00	10.00
PdIr	2.01	2.05	2.79	2.20	2.20	53.70	151.00	804.40	880.00	10.00	7.00
PdMn	2.00	2.00	2.82	2.20	1.55	53.70	0.00	804.40	717.30	10.00	5.00
PdMo	2.01	2.07	2.64	2.20	2.16	53.70	71.90	804.40	684.30	10.00	5.00
PdNb	2.02	2.07	2.69	2.20	1.60	53.70	86.10	804.40	652.10	10.00	4.00
PdNi	1.99	2.01	2.86	2.20	1.91	53.70	112.00	804.40	737.10	10.00	8.00
PdOs	2.02	2.04	2.79	2.20	2.20	53.70	106.10	804.40	840.00	10.00	6.00
PdPt	1.99	2.08	2.89	2.20	2.28	53.70	205.30	804.40	870.00	10.00	9.00
PdRe	2.02	2.06	2.79	2.20	1.90	53.70	14.50	804.40	760.00	10.00	5.00
PdRh	1.99	2.07	2.88	2.20	2.28	53.70	109.70	804.40	719.70	10.00	8.00
PdRu	2.01	2.05	2.66	2.20	2.20	53.70	101.30	804.40	710.20	10.00	7.00
PdSc	1.99	2.12	2.83	2.20	1.36	53.70	18.10	804.40	633.10	10.00	0.00
PdSn	2.02	2.09	2.81	2.20	1.96	53.70	107.30	804.40	708.60	10.00	10.00
PdTa	2.19	2.01	2.58	2.20	1.50	53.70	31.00	804.40	761.00	10.00	3.00
PdTi	2.02	2.00	2.69	2.20	1.54	53.70	7.60	804.40	658.80	10.00	2.00
PdW	2.02	2.05	2.69	2.20	2.36	53.70	78.60	804.40	770.00	10.00	4.00
PdZn	1.98	2.16	2.97	2.20	1.65	53.70	0.00	804.40	906.40	10.00	10.00
PdZr	2.02	2.11	2.72	2.20	1.33	53.70	41.10	804.40	640.10	10.00	2.00
SnAg	2.00	2.28	2.92	1.96	1.93	107.30	125.60	708.60	731.00	10.00	10.00
SnAu	2.00	2.25	2.93	1.96	2.54	107.30	222.80	708.60	890.10	10.00	10.00
SnBi	2.12	2.28	2.98	1.96	2.02	107.30	91.20	708.60	703.00	10.00	10.00
SnCr	2.10	2.04	2.94	1.96	1.66	107.30	64.30	708.60	652.90	10.00	5.00
SnGa	2.09	2.03	2.99	1.96	1.81	107.30	28.90	708.60	578.80	10.00	10.00
SnGe	2.00	2.26	3.03	1.96	2.01	107.30	119.00	708.60	762.00	10.00	10.00
SnMn	2.11	1.99	2.92	1.96	1.55	107.30	0.00	708.60	717.30	10.00	5.00
SnPt	2.12	2.09	2.89	1.96	2.28	107.30	205.30	708.60	870.00	10.00	9.00
SnRh	2.12	2.09	2.86	1.96	2.28	107.30	109.70	708.60	719.70	10.00	8.00
SnCo	1.99	2.16	2.97	1.96	1.88	107.30	63.70	708.60	760.40	10.00	7.00
SnFe	2.00	2.17	2.95	1.96	1.83	107.30	15.70	708.60	762.50	10.00	6.00
SnHf	2.26	2.08	3.10	1.96	1.30	107.30	0.00	708.60	658.50	10.00	2.00
SnIn	2.11	2.18	3.02	1.96	1.78	107.30	28.90	708.60	558.30	10.00	10.00
SnIr	2.23	2.05	2.91	1.96	2.20	107.30	151.00	708.60	880.00	10.00	7.00
SnMo	2.27	2.04	3.00	1.96	2.16	107.30	71.90	708.60	684.30	10.00	5.00
SnNb	2.29	2.05	3.03	1.96	1.60	107.30	86.10	708.60	652.10	10.00	4.00
SnNi	1.99	2.14	2.96	1.96	1.91	107.30	112.00	708.60	737.10	10.00	8.00
SnOs	2.25	2.03	2.92	1.96	2.20	107.30	106.10	708.60	840.00	10.00	6.00
SnRe	2.24	2.05	2.99	1.96	1.90	107.30	14.50	708.60	760.00	10.00	5.00
SnRu	2.24	2.02	2.93	1.96	2.20	107.30	101.30	708.60	710.20	10.00	7.00
SnSc	2.11	2.11	3.01	1.96	1.36	107.30	18.10	708.60	633.10	10.00	0.00
SnTa	2.35	2.03	3.03	1.96	1.50	107.30	31.00	708.60	761.00	10.00	3.00
SnTi	2.26	1.99	3.07	1.96	1.54	107.30	7.60	708.60	658.80	10.00	2.00
SnW	2.29	2.03	2.99	1.96	2.36	107.30	78.60	708.60	770.00	10.00	4.00

SnZn	1.99	2.16	3.00	1.96	1.65	107.30	0.00	708.60	906.40	10.00	10.00
SnZr	2.26	2.10	3.10	1.96	1.33	107.30	41.10	708.60	640.10	10.00	2.00
PtAg	1.98	2.24	2.93	2.28	1.93	205.30	125.60	870.00	731.00	9.00	10.00
PtAu	2.00	2.12	2.92	2.28	2.54	205.30	222.80	870.00	890.10	9.00	10.00
PtBi	2.01	2.29	2.89	2.28	2.02	205.30	91.20	870.00	703.00	9.00	10.00
PtGa	2.01	2.02	2.92	2.28	1.81	205.30	28.90	870.00	578.80	9.00	10.00
PtGe	2.03	1.92	2.87	2.28	2.01	205.30	119.00	870.00	762.00	9.00	10.00
PtRh	2.00	2.06	2.86	2.28	2.28	205.30	109.70	870.00	719.70	9.00	8.00
PtCo	2.00	2.10	2.80	2.28	1.88	205.30	63.70	870.00	760.40	9.00	7.00
PtCr	2.01	2.03	2.87	2.28	1.66	205.30	64.30	870.00	652.90	9.00	5.00
PtFe	2.01	2.08	2.80	2.28	1.83	205.30	15.70	870.00	762.50	9.00	6.00
PtHf	2.03	2.11	2.67	2.28	1.30	205.30	0.00	870.00	658.50	9.00	2.00
PtIn	2.01	2.19	2.88	2.28	1.78	205.30	28.90	870.00	558.30	9.00	10.00
PtIr	2.01	2.07	2.76	2.28	2.20	205.30	151.00	870.00	880.00	9.00	7.00
PtMn	2.01	2.00	2.83	2.28	1.55	205.30	0.00	870.00	717.30	9.00	5.00
PtMo	2.02	2.09	2.59	2.28	2.16	205.30	71.90	870.00	684.30	9.00	5.00
PtNb	2.02	2.09	2.63	2.28	1.60	205.30	86.10	870.00	652.10	9.00	4.00
PtNi	1.99	2.11	2.84	2.28	1.91	205.30	112.00	870.00	737.10	9.00	8.00
PtOs	2.01	2.07	2.60	2.28	2.20	205.30	106.10	870.00	840.00	9.00	6.00
PtRe	2.03	2.07	2.74	2.28	1.90	205.30	14.50	870.00	760.00	9.00	5.00
PtRu	2.01	2.05	2.76	2.28	2.20	205.30	101.30	870.00	710.20	9.00	7.00
PtSc	2.01	2.12	2.81	2.28	1.36	205.30	18.10	870.00	633.10	9.00	0.00
PtTa	2.03	2.06	2.64	2.28	1.50	205.30	31.00	870.00	761.00	9.00	3.00
PtTi	2.02	2.03	2.60	2.28	1.54	205.30	7.60	870.00	658.80	9.00	2.00
PtW	2.02	2.07	2.63	2.28	2.36	205.30	78.60	870.00	770.00	9.00	4.00
PtZn	1.98	2.17	3.00	2.28	1.65	205.30	0.00	870.00	906.40	9.00	10.00
PtZr	2.02	2.13	2.67	2.28	1.33	205.30	41.10	870.00	640.10	9.00	2.00
VAg	1.84	2.35	2.92	1.63	1.93	50.60	125.60	650.90	731.00	3.00	10.00
VAu	1.86	2.35	2.80	1.63	2.54	50.60	222.80	650.90	890.10	3.00	10.00
VBi	1.93	2.28	2.98	1.63	2.02	50.60	91.20	650.90	703.00	3.00	10.00
VCo	1.88	2.14	2.81	1.63	1.88	50.60	63.70	650.90	760.40	3.00	7.00
VCr	1.90	2.06	2.91	1.63	1.66	50.60	64.30	650.90	652.90	3.00	5.00
VFe	1.89	2.14	2.79	1.63	1.83	50.60	15.70	650.90	762.50	3.00	6.00
VGa	1.93	2.04	2.94	1.63	1.81	50.60	28.90	650.90	578.80	3.00	10.00
VGe	1.88	2.29	3.14	1.63	2.01	50.60	119.00	650.90	762.00	3.00	10.00
VIn	1.92	2.19	2.98	1.63	1.78	50.60	28.90	650.90	558.30	3.00	10.00
VMn	1.88	2.15	2.91	1.63	1.55	50.60	0.00	650.90	717.30	3.00	5.00
VNi	1.88	2.14	2.84	1.63	1.91	50.60	112.00	650.90	737.10	3.00	8.00
VPd	1.88	2.16	2.75	1.63	2.20	50.60	53.70	650.90	804.40	3.00	10.00
VPt	1.90	2.11	2.65	1.63	2.28	50.60	205.30	650.90	870.00	3.00	9.00
VRh	1.90	2.13	2.63	1.63	2.28	50.60	109.70	650.90	719.70	3.00	8.00
VSn	1.88	2.37	3.17	1.63	1.96	50.60	107.30	650.90	708.60	3.00	10.00
VZn	1.87	2.17	2.96	1.63	1.65	50.60	0.00	650.90	906.40	3.00	10.00
VHf	1.97	2.10	2.75	1.63	1.30	50.60	0.00	650.90	658.50	3.00	2.00

VIr	1.91	2.11	2.57	1.63	2.20	50.60	151.00	650.90	880.00	3.00	7.00
VMo	1.93	2.14	2.48	1.63	2.16	50.60	71.90	650.90	684.30	3.00	5.00
VNb	1.95	2.12	2.71	1.63	1.60	50.60	86.10	650.90	652.10	3.00	4.00
VOs	1.94	2.11	2.48	1.63	2.20	50.60	106.10	650.90	840.00	3.00	6.00
VRe	1.93	2.11	2.43	1.63	1.90	50.60	14.50	650.90	760.00	3.00	5.00
VRu	1.92	2.12	2.56	1.63	2.20	50.60	101.30	650.90	710.20	3.00	7.00
VSc	1.90	2.12	2.89	1.63	1.36	50.60	18.10	650.90	633.10	3.00	0.00
VTa	1.98	2.08	2.58	1.63	1.50	50.60	31.00	650.90	761.00	3.00	3.00
VTi	1.94	2.07	2.68	1.63	1.54	50.60	7.60	650.90	658.80	3.00	2.00
VW	1.96	2.08	2.78	1.63	2.36	50.60	78.60	650.90	770.00	3.00	4.00
VZr	1.97	2.13	2.75	1.63	1.33	50.60	41.10	650.90	640.10	3.00	2.00

Table S2. Machine learning hyperparameters.

Algorithm	Hyperparameter
ABR	learning_rate = 0.85, n_estimators = 67, random_state = 55
RFR	n_estimators = 6, random_state = 72
XGBR	n_estimators = 5, learning_rate = 0.75, max_depth = 3, random_state = 1
GBR	n_estimators = 135, max_depth = 4, learning_rate = 0.04, subsample = 0.45, min_samples_split = 3, loss = 'huber', random_state = 894