

## Supplementary Information

### **The rational design of high-performance graphene-based single-atom electrocatalysts for ORR using machine learning**

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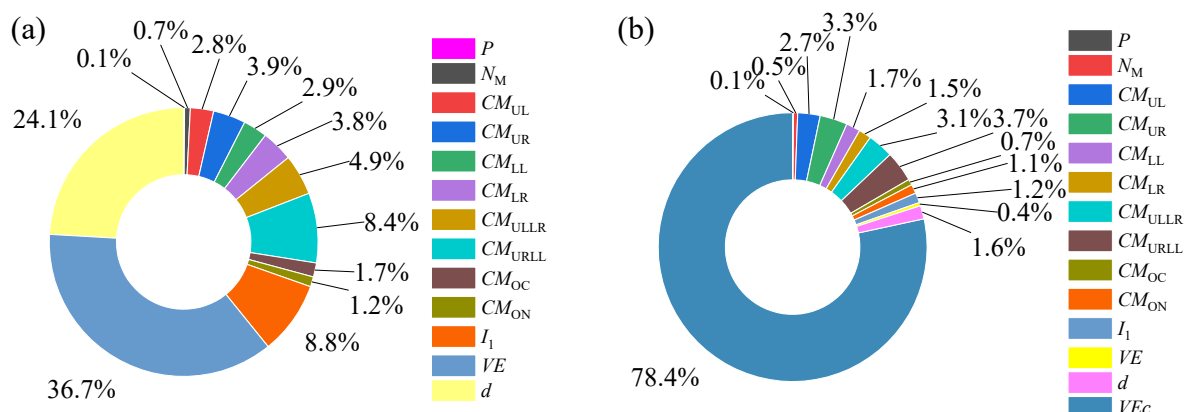
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## Supplementary Figures



**Figure S1.** The importance of each descriptor in descriptor group that consists of (a) central metal period ( $P$ ), the metal atomic number ( $N_M$ ), Coulomb matrix ( $CM_{UL}$ ,  $CM_{UR}$ ,  $CM_{LL}$ ,  $CM_{LR}$ ,  $CM_{ULLR}$ ,  $CM_{URLL}$ ,  $CM_{OC}$ ,  $CM_{ON}$ ),  $I_1$ , valence electron number ( $VE$ ),  $d$  electron number ( $E_d$ ); (b)  $P$ ,  $N_M$ ,  $CM$  ( $CM_{UL}$ ,  $CM_{UR}$ ,  $CM_{LL}$ ,  $CM_{LR}$ ,  $CM_{ULLR}$ ,  $CM_{URLL}$ ,  $CM_{OC}$ ,  $CM_{ON}$ ),  $I_1$ ,  $VE$ , valence electron correction ( $VEc$ ). Corresponding machine learning (ML) models chose the first two columns of K-dataset which in Table S1 as the dataset. The Random Forest algorithm was chosen as ML algorithm, corresponding hyperparameters was kept default.

## Supplementary Tables

**Table. S1** K-dataset (consist of ZA-MC<sub>4</sub>, ZA-MN<sub>1</sub>C<sub>3</sub>, ZA-MN<sub>2</sub>C<sub>2</sub>, ZA-MN<sub>2</sub>C<sub>2</sub>b, ZA-MN<sub>2</sub>C<sub>2</sub>c, ZA-MN<sub>3</sub>C<sub>1</sub>, ZA-MN<sub>4</sub>). The first two columns are the name of the catalysts and corresponding ORR overpotential ( $\eta_{ORR}$ ) and others columns are the descriptors.

Catalysts	$\eta_{ORR}$	$P$	$VEc$	$I_1 * \chi$	$DC$	$R_1$	$R_2$	$R_3$	$R_4$
ZA-ScC <sub>4</sub>	2.01	4	7.8	861.02	1.34	4	4	5	5
ZA-TiC <sub>4</sub>	2.34	4	8.8	1014.55	1.34	4	4	5	5
ZA-VC <sub>4</sub>	2.61	4	9.8	1060.97	1.34	4	4	5	5

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ZA-CrC <sub>4</sub>	2.16	4	10.8	1083.81	1.34	4	4	5	5
ZA-MnC <sub>4</sub>	2.15	4	11.8	1111.82	1.34	4	4	5	5
ZA-FeC <sub>4</sub>	1.27	4	12.8	1395.38	1.34	4	4	5	5
ZA-CoC <sub>4</sub>	1.05	4	13.8	1429.55	1.34	4	4	5	5
ZA-NiC <sub>4</sub>	0.35	4	14.8	1407.86	1.34	4	4	5	5
ZA-CuC <sub>4</sub>	1.13	4	15.8	1416.45	1.34	4	4	5	5
ZA-ZnC <sub>4</sub>	0.84	4	16.8	1495.56	1.34	4	4	5	5
ZA-YC <sub>4</sub>	1.99	5	7.8	731.88	1.34	4	4	5	5
ZA-ZrC <sub>4</sub>	2.25	5	8.8	851.33	1.34	4	4	5	5
ZA-NbC <sub>4</sub>	2.78	5	9.8	1043.36	1.34	4	4	5	5
ZA-MoC <sub>4</sub>	2.50	5	10.8	1478.09	1.34	4	4	5	5
ZA-TcC <sub>4</sub>	1.86	5	11.8	1475.04	1.34	4	4	5	5
ZA-RuC <sub>4</sub>	1.57	5	12.8	1562.44	1.34	4	4	5	5
ZA-RhC <sub>4</sub>	1.29	5	13.8	1640.92	1.34	4	4	5	5
ZA-PdC <sub>4</sub>	0.33	5	14.8	1769.68	1.34	4	4	5	5
ZA-AgC <sub>4</sub>	0.96	5	15.8	1410.83	1.34	4	4	5	5
ZA-CdC <sub>4</sub>	0.59	5	16.8	1466.58	1.34	4	4	5	5
ZA-LaC <sub>4</sub>	1.80	6	7.8	591.91	1.34	4	4	5	5
ZA-HfC <sub>4</sub>	2.66	6	8.8	856.05	1.34	4	4	5	5
ZA-TaC <sub>4</sub>	3.30	6	9.8	1092.60	1.34	4	4	5	5
ZA-WC <sub>4</sub>	2.90	6	10.8	1289.96	1.34	4	4	5	5
ZA-ReC <sub>4</sub>	1.29	6	11.8	1436.02	1.34	4	4	5	5
ZA-OsC <sub>4</sub>	1.22	6	12.8	1791.24	1.34	4	4	5	5
ZA-IrC <sub>4</sub>	1.69	6	13.8	1903.44	1.34	4	4	5	5
ZA-PtC <sub>4</sub>	0.54	6	14.8	1901.68	1.34	4	4	5	5
ZA-AuC <sub>4</sub>	1.11	6	15.8	2136.24	1.34	4	4	5	5
ZA-HgC <sub>4</sub>	0.90	6	16.8	1913.49	1.34	4	4	5	5
ZA-ScN <sub>1</sub> C <sub>3</sub>	1.86	4	8	861.02	0.81	4	5	5	6

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ZA-TiN <sub>1</sub> C <sub>3</sub>	2.82	4	9	1014.55	0.81	4	5	5	6
ZA-VN <sub>1</sub> C <sub>3</sub>	2.69	4	10	1060.97	0.81	4	5	5	6
ZA-CrN <sub>1</sub> C <sub>3</sub>	2.32	4	11	1083.81	0.81	4	5	5	6
ZA-MnN <sub>1</sub> C <sub>3</sub>	1.38	4	12	1111.82	0.81	4	5	5	6
ZA-FeN <sub>1</sub> C <sub>3</sub>	1.05	4	13	1395.38	0.81	4	5	5	6
ZA-CoN <sub>1</sub> C <sub>3</sub>	1.02	4	14	1429.55	0.81	4	5	5	6
ZA-NiN <sub>1</sub> C <sub>3</sub>	0.49	4	15	1407.86	0.81	4	5	5	6
ZA-CuN <sub>1</sub> C <sub>3</sub>	1.17	4	16	1416.45	0.81	4	5	5	6
ZA-ZnN <sub>1</sub> C <sub>3</sub>	0.46	4	17	1495.56	0.81	4	5	5	6
ZA-YN <sub>1</sub> C <sub>3</sub>	1.88	5	8	731.88	0.81	4	5	5	6
ZA-ZrN <sub>1</sub> C <sub>3</sub>	2.76	5	9	851.33	0.81	4	5	5	6
ZA-NbN <sub>1</sub> C <sub>3</sub>	2.82	5	10	1043.36	0.81	4	5	5	6
ZA-MoN <sub>1</sub> C <sub>3</sub>	2.57	5	11	1478.09	0.81	4	5	5	6
ZA-TcN <sub>1</sub> C <sub>3</sub>	1.58	5	12	1475.04	0.81	4	5	5	6
ZA-RuN <sub>1</sub> C <sub>3</sub>	2.11	5	13	1562.44	0.81	4	5	5	6
ZA-RhN <sub>1</sub> C <sub>3</sub>	0.81	5	14	1640.92	0.81	4	5	5	6
ZA-PdN <sub>1</sub> C <sub>3</sub>	0.35	5	15	1769.68	0.81	4	5	5	6
ZA-AgN <sub>1</sub> C <sub>3</sub>	1.14	5	16	1410.83	0.81	4	5	5	6
ZA-CdN <sub>1</sub> C <sub>3</sub>	1.05	5	17	1466.58	0.81	4	5	5	6
ZA-LaN <sub>1</sub> C <sub>3</sub>	1.62	6	8	591.91	0.81	4	5	5	6
ZA-HfN <sub>1</sub> C <sub>3</sub>	3.20	6	9	856.05	0.81	4	5	5	6
ZA-TaN <sub>1</sub> C <sub>3</sub>	3.39	6	10	1092.60	0.81	4	5	5	6
ZA-WN <sub>1</sub> C <sub>3</sub>	3.10	6	11	1289.96	0.81	4	5	5	6
ZA-ReN <sub>1</sub> C <sub>3</sub>	2.12	6	12	1436.02	0.81	4	5	5	6
ZA-OsN <sub>1</sub> C <sub>3</sub>	1.05	6	13	1791.24	0.81	4	5	5	6
ZA-IrN <sub>1</sub> C <sub>3</sub>	1.13	6	14	1903.44	0.81	4	5	5	6
ZA-PtN <sub>1</sub> C <sub>3</sub>	0.38	6	15	1901.68	0.81	4	5	5	6
ZA-AuN <sub>1</sub> C <sub>3</sub>	1.19	6	16	2136.24	0.81	4	5	5	6

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ZA-HgN <sub>1</sub> C <sub>3</sub>	0.62	6	17	1913.49	0.81	4	5	5	6
ZA-ScN <sub>2</sub> C <sub>2</sub>	2.15	4	8.2	861.02	0.37	5	5	6	6
ZA-TiN <sub>2</sub> C <sub>2</sub>	2.97	4	9.2	1014.55	0.37	5	5	6	6
ZA-VN <sub>2</sub> C <sub>2</sub>	2.84	4	10.2	1060.97	0.37	5	5	6	6
ZA-CrN <sub>2</sub> C <sub>2</sub>	2.06	4	11.2	1083.81	0.37	5	5	6	6
ZA-MnN <sub>2</sub> C <sub>2</sub>	1.34	4	12.2	1111.82	0.37	5	5	6	6
ZA-FeN <sub>2</sub> C <sub>2</sub>	1.21	4	13.2	1395.38	0.37	5	5	6	6
ZA-CoN <sub>2</sub> C <sub>2</sub>	0.68	4	14.2	1429.55	0.37	5	5	6	6
ZA-NiN <sub>2</sub> C <sub>2</sub>	0.75	4	15.2	1407.86	0.37	5	5	6	6
ZA-CuN <sub>2</sub> C <sub>2</sub>	0.93	4	16.2	1416.45	0.37	5	5	6	6
ZA-ZnN <sub>2</sub> C <sub>2</sub>	0.83	4	17.2	1495.56	0.37	5	5	6	6
ZA-YN <sub>2</sub> C <sub>2</sub>	1.99	5	8.2	731.88	0.37	5	5	6	6
ZA-ZrN <sub>2</sub> C <sub>2</sub>	2.93	5	9.2	851.33	0.37	5	5	6	6
ZA-NbN <sub>2</sub> C <sub>2</sub>	3.35	5	10.2	1043.36	0.37	5	5	6	6
ZA-MoN <sub>2</sub> C <sub>2</sub>	1.73	5	11.2	1478.09	0.37	5	5	6	6
ZA-TcN <sub>2</sub> C <sub>2</sub>	1.02	5	12.2	1475.04	0.37	5	5	6	6
ZA-RuN <sub>2</sub> C <sub>2</sub>	1.00	5	13.2	1562.44	0.37	5	5	6	6
ZA-RhN <sub>2</sub> C <sub>2</sub>	0.92	5	14.2	1640.92	0.37	5	5	6	6
ZA-PdN <sub>2</sub> C <sub>2</sub>	0.83	5	15.2	1769.68	0.37	5	5	6	6
ZA-AgN <sub>2</sub> C <sub>2</sub>	1.05	5	16.2	1410.83	0.37	5	5	6	6
ZA-CdN <sub>2</sub> C <sub>2</sub>	0.46	5	17.2	1466.58	0.37	5	5	6	6
ZA-LaN <sub>2</sub> C <sub>2</sub>	1.54	6	8.2	591.91	0.37	5	5	6	6
ZA-HfN <sub>2</sub> C <sub>2</sub>	3.37	6	9.2	856.05	0.37	5	5	6	6
ZA-TaN <sub>2</sub> C <sub>2</sub>	1.34	6	10.2	1092.60	0.37	5	5	6	6
ZA-WN <sub>2</sub> C <sub>2</sub>	1.89	6	11.2	1289.96	0.37	5	5	6	6
ZA-ReN <sub>2</sub> C <sub>2</sub>	0.40	6	12.2	1436.02	0.37	5	5	6	6
ZA-OsN <sub>2</sub> C <sub>2</sub>	0.82	6	13.2	1791.24	0.37	5	5	6	6
ZA-IrN <sub>2</sub> C <sub>2</sub>	1.17	6	14.2	1903.44	0.37	5	5	6	6

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ZA-PtN <sub>2</sub> C <sub>2</sub>	0.76	6	15.2	1901.68	0.37	5	5	6	6
ZA-AuN <sub>2</sub> C <sub>2</sub>	1.17	6	16.2	2136.24	0.37	5	5	6	6
ZA-HgN <sub>2</sub> C <sub>2</sub>	1.52	6	17.2	1913.49	0.37	5	5	6	6
ZA-ScN <sub>2</sub> C <sub>2</sub> b	2.13	4	8.2	861.02	0.37	4	6	6	6
ZA-TiN <sub>2</sub> C <sub>2</sub> b	2.96	4	9.2	1014.55	0.37	4	6	6	6
ZA-VN <sub>2</sub> C <sub>2</sub> b	1.78	4	10.2	1060.97	0.37	4	6	6	6
ZA-CrN <sub>2</sub> C <sub>2</sub> b	1.14	4	11.2	1083.81	0.37	4	6	6	6
ZA-MnN <sub>2</sub> C <sub>2</sub> b	1.15	4	12.2	1111.82	0.37	4	6	6	6
ZA-FeN <sub>2</sub> C <sub>2</sub> b	0.96	4	13.2	1395.38	0.37	4	6	6	6
ZA-CoN <sub>2</sub> C <sub>2</sub> b	0.62	4	14.2	1429.55	0.37	4	6	6	6
ZA-NiN <sub>2</sub> C <sub>2</sub> b	0.78	4	15.2	1407.86	0.37	4	6	6	6
ZA-CuN <sub>2</sub> C <sub>2</sub> b	0.99	4	16.2	1416.45	0.37	4	6	6	6
ZA-ZnN <sub>2</sub> C <sub>2</sub> b	0.41	4	17.2	1495.56	0.37	4	6	6	6
ZA-YN <sub>2</sub> C <sub>2</sub> b	2.01	5	8.2	731.88	0.37	4	6	6	6
ZA-ZrN <sub>2</sub> C <sub>2</sub> b	2.96	5	9.2	851.33	0.37	4	6	6	6
ZA-NbN <sub>2</sub> C <sub>2</sub> b	3.30	5	10.2	1043.36	0.37	4	6	6	6
ZA-MoN <sub>2</sub> C <sub>2</sub> b	1.67	5	11.2	1478.09	0.37	4	6	6	6
ZA-TcN <sub>2</sub> C <sub>2</sub> b	1.18	5	12.2	1475.04	0.37	4	6	6	6
ZA-RuN <sub>2</sub> C <sub>2</sub> b	0.54	5	13.2	1562.44	0.37	4	6	6	6
ZA-RhN <sub>2</sub> C <sub>2</sub> b	0.90	5	14.2	1640.92	0.37	4	6	6	6
ZA-PdN <sub>2</sub> C <sub>2</sub> b	1.01	5	15.2	1769.68	0.37	4	6	6	6
ZA-AgN <sub>2</sub> C <sub>2</sub> b	1.13	5	16.2	1410.83	0.37	4	6	6	6
ZA-CdN <sub>2</sub> C <sub>2</sub> b	1.03	5	17.2	1466.58	0.37	4	6	6	6
ZA-LaN <sub>2</sub> C <sub>2</sub> b	1.58	6	8.2	591.91	0.37	4	6	6	6
ZA-HfN <sub>2</sub> C <sub>2</sub> b	3.41	6	9.2	856.05	0.37	4	6	6	6
ZA-TaN <sub>2</sub> C <sub>2</sub> b	1.48	6	10.2	1092.60	0.37	4	6	6	6
ZA-WN <sub>2</sub> C <sub>2</sub> b	1.69	6	11.2	1289.96	0.37	4	6	6	6
ZA-ReN <sub>2</sub> C <sub>2</sub> b	1.22	6	12.2	1436.02	0.37	4	6	6	6

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ZA-OsN <sub>2</sub> C <sub>2</sub> b	1.18	6	13.2	1791.24	0.37	4	6	6	6
ZA-IrN <sub>2</sub> C <sub>2</sub> b	0.92	6	14.2	1903.44	0.37	4	6	6	6
ZA-PtN <sub>2</sub> C <sub>2</sub> b	1.10	6	15.2	1901.68	0.37	4	6	6	6
ZA-AuN <sub>2</sub> C <sub>2</sub> b	1.18	6	16.2	2136.24	0.37	4	6	6	6
ZA-ScN <sub>2</sub> C <sub>2</sub> c	2.34	4	8.2	861.02	0.74	5	5	5	7
ZA-TiN <sub>2</sub> C <sub>2</sub> c	2.95	4	9.2	1014.55	0.74	5	5	5	7
ZA-VN <sub>2</sub> C <sub>2</sub> c	1.37	4	10.2	1060.97	0.74	5	5	5	7
ZA-CrN <sub>2</sub> C <sub>2</sub> c	0.94	4	11.2	1083.81	0.74	5	5	5	7
ZA-MnN <sub>2</sub> C <sub>2</sub> c	1.18	4	12.2	1111.82	0.74	5	5	5	7
ZA-FeN <sub>2</sub> C <sub>2</sub> c	0.64	4	13.2	1395.38	0.74	5	5	5	7
ZA-CoN <sub>2</sub> C <sub>2</sub> c	0.74	4	14.2	1429.55	0.74	5	5	5	7
ZA-NiN <sub>2</sub> C <sub>2</sub> c	0.74	4	15.2	1407.86	0.74	5	5	5	7
ZA-CuN <sub>2</sub> C <sub>2</sub> c	0.94	4	16.2	1416.45	0.74	5	5	5	7
ZA-ZnN <sub>2</sub> C <sub>2</sub> c	1.97	4	17.2	1495.56	0.74	5	5	5	7
ZA-YN <sub>2</sub> C <sub>2</sub> c	2.26	5	8.2	731.88	0.74	5	5	5	7
ZA-ZrN <sub>2</sub> C <sub>2</sub> c	2.99	5	9.2	851.33	0.74	5	5	5	7
ZA-NbN <sub>2</sub> C <sub>2</sub> c	1.31	5	10.2	1043.36	0.74	5	5	5	7
ZA-MoN <sub>2</sub> C <sub>2</sub> c	1.33	5	11.2	1478.09	0.74	5	5	5	7
ZA-TcN <sub>2</sub> C <sub>2</sub> c	1.16	5	12.2	1475.04	0.74	5	5	5	7
ZA-RuN <sub>2</sub> C <sub>2</sub> c	0.70	5	13.2	1562.44	0.74	5	5	5	7
ZA-RhN <sub>2</sub> C <sub>2</sub> c	0.80	5	14.2	1640.92	0.74	5	5	5	7
ZA-PdN <sub>2</sub> C <sub>2</sub> c	1.02	5	15.2	1769.68	0.74	5	5	5	7
ZA-AgN <sub>2</sub> C <sub>2</sub> c	1.03	5	16.2	1410.83	0.74	5	5	5	7
ZA-CdN <sub>2</sub> C <sub>2</sub> c	1.12	5	17.2	1466.58	0.74	5	5	5	7
ZA-LaN <sub>2</sub> C <sub>2</sub> c	1.82	6	8.2	591.91	0.74	5	5	5	7
ZA-HfN <sub>2</sub> C <sub>2</sub> c	3.46	6	9.2	856.05	0.74	5	5	5	7
ZA-TaN <sub>2</sub> C <sub>2</sub> c	3.76	6	10.2	1092.60	0.74	5	5	5	7
ZA-WN <sub>2</sub> C <sub>2</sub> c	1.20	6	11.2	1289.96	0.74	5	5	5	7

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ZA-ReN <sub>2</sub> C <sub>2c</sub>	1.35	6	12.2	1436.02	0.74	5	5	5	7
ZA-OsN <sub>2</sub> C <sub>2c</sub>	1.28	6	13.2	1791.24	0.74	5	5	5	7
ZA-IrN <sub>2</sub> C <sub>2c</sub>	1.28	6	14.2	1903.44	0.74	5	5	5	7
ZA-PtN <sub>2</sub> C <sub>2c</sub>	1.07	6	15.2	1901.68	0.74	5	5	5	7
ZA-AuN <sub>2</sub> C <sub>2c</sub>	1.12	6	16.2	2136.24	0.74	5	5	5	7
ZA-HgN <sub>2</sub> C <sub>2c</sub>	0.90	6	17.2	1913.49	0.74	5	5	5	7
ZA-ScN <sub>3</sub> C <sub>1</sub>	2.48	4	8.4	861.02	0.34	5	6	6	7
ZA-TiN <sub>3</sub> C <sub>1</sub>	3.36	4	9.4	1014.55	0.34	5	6	6	7
ZA-VN <sub>3</sub> C <sub>1</sub>	2.98	4	10.4	1060.97	0.34	5	6	6	7
ZA-CrN <sub>3</sub> C <sub>1</sub>	1.90	4	11.4	1083.81	0.34	5	6	6	7
ZA-MnN <sub>3</sub> C <sub>1</sub>	1.26	4	12.4	1111.82	0.34	5	6	6	7
ZA-FeN <sub>3</sub> C <sub>1</sub>	1.04	4	13.4	1395.38	0.34	5	6	6	7
ZA-CoN <sub>3</sub> C <sub>1</sub>	0.46	4	14.4	1429.55	0.34	5	6	6	7
ZA-NiN <sub>3</sub> C <sub>1</sub>	0.76	4	15.4	1407.86	0.34	5	6	6	7
ZA-CuN <sub>3</sub> C <sub>1</sub>	0.95	4	16.4	1416.45	0.34	5	6	6	7
ZA-ZnN <sub>3</sub> C <sub>1</sub>	0.54	4	17.4	1495.56	0.34	5	6	6	7
ZA-YN <sub>3</sub> C <sub>1</sub>	2.35	5	8.4	731.88	0.34	5	6	6	7
ZA-ZrN <sub>3</sub> C <sub>1</sub>	3.56	5	9.4	851.33	0.34	5	6	6	7
ZA-NbN <sub>3</sub> C <sub>1</sub>	1.82	5	10.4	1043.36	0.34	5	6	6	7
ZA-MoN <sub>3</sub> C <sub>1</sub>	1.50	5	11.4	1478.09	0.34	5	6	6	7
ZA-TcN <sub>3</sub> C <sub>1</sub>	1.03	5	12.4	1475.04	0.34	5	6	6	7
ZA-RuN <sub>3</sub> C <sub>1</sub>	0.40	5	13.4	1562.44	0.34	5	6	6	7
ZA-RhN <sub>3</sub> C <sub>1</sub>	0.42	5	14.4	1640.92	0.34	5	6	6	7
ZA-PdN <sub>3</sub> C <sub>1</sub>	1.09	5	15.4	1769.68	0.34	5	6	6	7
ZA-AgN <sub>3</sub> C <sub>1</sub>	1.05	5	16.4	1410.83	0.34	5	6	6	7
ZA-CdN <sub>3</sub> C <sub>1</sub>	1.13	5	17.4	1466.58	0.34	5	6	6	7
ZA-LaN <sub>3</sub> C <sub>1</sub>	1.91	6	8.4	591.91	0.34	5	6	6	7
ZA-HfN <sub>3</sub> C <sub>1</sub>	3.88	6	9.4	856.05	0.34	5	6	6	7



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ZA-TaN <sub>3</sub> C <sub>1</sub>	1.67	6	10.4	1092.60	0.34	5	6	6	7
ZA-WN <sub>3</sub> C <sub>1</sub>	1.43	6	11.4	1289.96	0.34	5	6	6	7
ZA-ReN <sub>3</sub> C <sub>1</sub>	1.48	6	12.4	1436.02	0.34	5	6	6	7
ZA-OsN <sub>3</sub> C <sub>1</sub>	0.92	6	13.4	1791.24	0.34	5	6	6	7
ZA-IrN <sub>3</sub> C <sub>1</sub>	0.54	6	14.4	1903.44	0.34	5	6	6	7
ZA-PtN <sub>3</sub> C <sub>1</sub>	1.10	6	15.4	1901.68	0.34	5	6	6	7
ZA-AuN <sub>3</sub> C <sub>1</sub>	1.13	6	16.4	2136.24	0.34	5	6	6	7
ZA-ScN <sub>4</sub>	3.21	4	8.6	861.02	0.31	6	6	7	7
ZA-TiN <sub>4</sub>	3.32	4	9.6	1014.55	0.31	6	6	7	7
ZA-VN <sub>4</sub>	0.83	4	10.6	1060.97	0.31	6	6	7	7
ZA-CrN <sub>4</sub>	1.40	4	11.6	1083.81	0.31	6	6	7	7
ZA-MnN <sub>4</sub>	0.86	4	12.6	1111.82	0.31	6	6	7	7
ZA-FeN <sub>4</sub>	0.67	4	13.6	1395.38	0.31	6	6	7	7
ZA-CoN <sub>4</sub>	0.39	4	14.6	1429.55	0.31	6	6	7	7
ZA-NiN <sub>4</sub>	1.02	4	15.6	1407.86	0.31	6	6	7	7
ZA-CuN <sub>4</sub>	0.95	4	16.6	1416.45	0.31	6	6	7	7
ZA-ZnN <sub>4</sub>	0.67	4	17.6	1495.56	0.31	6	6	7	7
ZA-YN <sub>4</sub>	3.08	5	8.6	731.88	0.31	6	6	7	7
ZA-ZrN <sub>4</sub>	3.80	5	9.6	851.33	0.31	6	6	7	7
ZA-NbN <sub>4</sub>	1.39	5	10.6	1043.36	0.31	6	6	7	7
ZA-MoN <sub>4</sub>	0.50	5	11.6	1478.09	0.31	6	6	7	7
ZA-TcN <sub>4</sub>	0.66	5	12.6	1475.04	0.31	6	6	7	7
ZA-RuN <sub>4</sub>	0.94	5	13.6	1562.44	0.31	6	6	7	7
ZA-RhN <sub>4</sub>	0.27	5	14.6	1640.92	0.31	6	6	7	7
ZA-PdN <sub>4</sub>	1.19	5	15.6	1769.68	0.31	6	6	7	7
ZA-AgN <sub>4</sub>	0.53	5	16.6	1410.83	0.31	6	6	7	7
ZA-CdN <sub>4</sub>	1.07	5	17.6	1466.58	0.31	6	6	7	7
ZA-LaN <sub>4</sub>	2.55	6	8.6	591.91	0.31	6	6	7	7

ZA-HfN <sub>4</sub>	4.02	6	9.6	856.05	0.31	6	6	7	7
ZA-TaN <sub>4</sub>	1.69	6	10.6	1092.60	0.31	6	6	7	7
ZA-WN <sub>4</sub>	1.28	6	11.6	1289.96	0.31	6	6	7	7
ZA-ReN <sub>4</sub>	0.58	6	12.6	1436.02	0.31	6	6	7	7
ZA-OsN <sub>4</sub>	0.88	6	13.6	1791.24	0.31	6	6	7	7
ZA-IrN <sub>4</sub>	0.28	6	14.6	1903.44	0.31	6	6	7	7
ZA-PtN <sub>4</sub>	1.21	6	15.6	1901.68	0.31	6	6	7	7
ZA-AuN <sub>4</sub>	0.93	6	16.6	2136.24	0.31	6	6	7	7

**Table. S2** Target-dataset (consist of ZZ-MC<sub>4</sub>, ZZ-MN<sub>1</sub>C<sub>3</sub>, ZZ-MN<sub>2</sub>C<sub>2</sub>, ZZ-MN<sub>2</sub>C<sub>2</sub>b, ZZ-MN<sub>3</sub>C<sub>1</sub>, ZZ-MN<sub>4</sub>). The first columns are the name of the catalysts and others columns are the descriptors.

<b>Catalysts</b>	<b><i>P</i></b>	<b><i>VEc</i></b>	<b><i>I</i><sub>1</sub><sup>*</sup><b><i>χ</i></b></b>	<b><i>DC</i></b>	<b><i>R</i><sub>1</sub></b>	<b><i>R</i><sub>2</sub></b>	<b><i>R</i><sub>3</sub></b>	<b><i>R</i><sub>4</sub></b>
ZZ-ScC <sub>4</sub>	4	7.8	861.02	0.80	5	5	5	5
ZZ-TiC <sub>4</sub>	4	8.8	1014.55	0.80	5	5	5	5
ZZ-VC <sub>4</sub>	4	9.8	1060.97	0.80	5	5	5	5
ZZ-CrC <sub>4</sub>	4	10.8	1083.81	0.80	5	5	5	5
ZZ-MnC <sub>4</sub>	4	11.8	1111.82	0.80	5	5	5	5
ZZ-FeC <sub>4</sub>	4	12.8	1395.38	0.80	5	5	5	5
ZZ-CoC <sub>4</sub>	4	13.8	1429.55	0.80	5	5	5	5
ZZ-NiC <sub>4</sub>	4	14.8	1407.86	0.80	5	5	5	5
ZZ-CuC <sub>4</sub>	4	15.8	1416.45	0.80	5	5	5	5
ZZ-ZnC <sub>4</sub>	4	16.8	1495.56	0.80	5	5	5	5
ZZ-YC <sub>4</sub>	5	7.8	731.88	0.80	5	5	5	5
ZZ-ZrC <sub>4</sub>	5	8.8	851.33	0.80	5	5	5	5
ZZ-NbC <sub>4</sub>	5	9.8	1043.36	0.80	5	5	5	5
ZZ-MoC <sub>4</sub>	5	10.8	1478.09	0.80	5	5	5	5

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ZZ-TcC <sub>4</sub>	5	11.8	1475.04	0.80	5	5	5	5
ZZ-RuC <sub>4</sub>	5	12.8	1562.44	0.80	5	5	5	5
ZZ-RhC <sub>4</sub>	5	13.8	1640.92	0.80	5	5	5	5
ZZ-PdC <sub>4</sub>	5	14.8	1769.68	0.80	5	5	5	5
ZZ-AgC <sub>4</sub>	5	15.8	1410.83	0.80	5	5	5	5
ZZ-CdC <sub>4</sub>	5	16.8	1466.58	0.80	5	5	5	5
ZZ-LaC <sub>4</sub>	6	7.8	591.91	0.80	5	5	5	5
ZZ-HfC <sub>4</sub>	6	8.8	856.05	0.80	5	5	5	5
ZZ-TaC <sub>4</sub>	6	9.8	1092.60	0.80	5	5	5	5
ZZ-WC <sub>4</sub>	6	10.8	1289.96	0.80	5	5	5	5
ZZ-ReC <sub>4</sub>	6	11.8	1436.02	0.80	5	5	5	5
ZZ-OsC <sub>4</sub>	6	12.8	1791.24	0.80	5	5	5	5
ZZ-IrC <sub>4</sub>	6	13.8	1903.44	0.80	5	5	5	5
ZZ-PtC <sub>4</sub>	6	14.8	1901.68	0.80	5	5	5	5
ZZ-AuC <sub>4</sub>	6	15.8	2136.24	0.80	5	5	5	5
ZZ-ScN <sub>1</sub> C <sub>3</sub>	4	8	861.02	0.55	5	5	6	6
ZZ-TiN <sub>1</sub> C <sub>3</sub>	4	9	1014.55	0.55	5	5	6	6
ZZ-VN <sub>1</sub> C <sub>3</sub>	4	10	1060.97	0.55	5	5	6	6
ZZ-CrN <sub>1</sub> C <sub>3</sub>	4	11	1083.81	0.55	5	5	6	6
ZZ-MnN <sub>1</sub> C <sub>3</sub>	4	12	1111.82	0.55	5	5	6	6
ZZ-FeN <sub>1</sub> C <sub>3</sub>	4	13	1395.38	0.55	5	5	6	6
ZZ-CoN <sub>1</sub> C <sub>3</sub>	4	14	1429.55	0.55	5	5	6	6
ZZ-NiN <sub>1</sub> C <sub>3</sub>	4	15	1407.86	0.55	5	5	6	6
ZZ-CuN <sub>1</sub> C <sub>3</sub>	4	16	1416.45	0.55	5	5	6	6
ZZ-ZnN <sub>1</sub> C <sub>3</sub>	4	17	1495.56	0.55	5	5	6	6
ZZ-YN <sub>1</sub> C <sub>3</sub>	5	8	731.88	0.55	5	5	6	6
ZZ-ZrN <sub>1</sub> C <sub>3</sub>	5	9	851.33	0.55	5	5	6	6
ZZ-NbN <sub>1</sub> C <sub>3</sub>	5	10	1043.36	0.55	5	5	6	6

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ZZ-MoN <sub>1</sub> C <sub>3</sub>	5	11	1478.09	0.55	5	5	6	6
ZZ-TcN <sub>1</sub> C <sub>3</sub>	5	12	1475.04	0.55	5	5	6	6
ZZ-RuN <sub>1</sub> C <sub>3</sub>	5	13	1562.44	0.55	5	5	6	6
ZZ-RhN <sub>1</sub> C <sub>3</sub>	5	14	1640.92	0.55	5	5	6	6
ZZ-PdN <sub>1</sub> C <sub>3</sub>	5	15	1769.68	0.55	5	5	6	6
ZZ-AgN <sub>1</sub> C <sub>3</sub>	5	16	1410.83	0.55	5	5	6	6
ZZ-CdN <sub>1</sub> C <sub>3</sub>	5	17	1466.58	0.55	5	5	6	6
ZZ-LaN <sub>1</sub> C <sub>3</sub>	6	8	591.91	0.55	5	5	6	6
ZZ-HfN <sub>1</sub> C <sub>3</sub>	6	9	856.05	0.55	5	5	6	6
ZZ-TaN <sub>1</sub> C <sub>3</sub>	6	10	1092.60	0.55	5	5	6	6
ZZ-WN <sub>1</sub> C <sub>3</sub>	6	11	1289.96	0.55	5	5	6	6
ZZ-ReN <sub>1</sub> C <sub>3</sub>	6	12	1436.02	0.55	5	5	6	6
ZZ-OsN <sub>1</sub> C <sub>3</sub>	6	13	1791.24	0.55	5	5	6	6
ZZ-IrN <sub>1</sub> C <sub>3</sub>	6	14	1903.44	0.55	5	5	6	6
ZZ-PtN <sub>1</sub> C <sub>3</sub>	6	15	1901.68	0.55	5	5	6	6
ZZ-AuN <sub>1</sub> C <sub>3</sub>	6	16	2136.24	0.55	5	5	6	6
ZZ-ScN <sub>2</sub> C <sub>2</sub>	4	8.2	861.02	0.34	6	6	6	6
ZZ-TiN <sub>2</sub> C <sub>2</sub>	4	9.2	1014.55	0.34	6	6	6	6
ZZ-VN <sub>2</sub> C <sub>2</sub>	4	10.2	1060.97	0.34	6	6	6	6
ZZ-CrN <sub>2</sub> C <sub>2</sub>	4	11.2	1083.81	0.34	6	6	6	6
ZZ-MnN <sub>2</sub> C <sub>2</sub>	4	12.2	1111.82	0.34	6	6	6	6
ZZ-FeN <sub>2</sub> C <sub>2</sub>	4	13.2	1395.38	0.34	6	6	6	6
ZZ-CoN <sub>2</sub> C <sub>2</sub>	4	14.2	1429.55	0.34	6	6	6	6
ZZ-NiN <sub>2</sub> C <sub>2</sub>	4	15.2	1407.86	0.34	6	6	6	6
ZZ-CuN <sub>2</sub> C <sub>2</sub>	4	16.2	1416.45	0.34	6	6	6	6
ZZ-ZnN <sub>2</sub> C <sub>2</sub>	4	17.2	1495.56	0.34	6	6	6	6
ZZ-YN <sub>2</sub> C <sub>2</sub>	5	8.2	731.88	0.34	6	6	6	6
ZZ-ZrN <sub>2</sub> C <sub>2</sub>	5	9.2	851.33	0.34	6	6	6	6

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ZZ-NbN <sub>2</sub> C <sub>2</sub>	5	10.2	1043.36	0.34	6	6	6	6
ZZ-MoN <sub>2</sub> C <sub>2</sub>	5	11.2	1478.09	0.34	6	6	6	6
ZZ-TcN <sub>2</sub> C <sub>2</sub>	5	12.2	1475.04	0.34	6	6	6	6
ZZ-RuN <sub>2</sub> C <sub>2</sub>	5	13.2	1562.44	0.34	6	6	6	6
ZZ-RhN <sub>2</sub> C <sub>2</sub>	5	14.2	1640.92	0.34	6	6	6	6
ZZ-PdN <sub>2</sub> C <sub>2</sub>	5	15.2	1769.68	0.34	6	6	6	6
ZZ-AgN <sub>2</sub> C <sub>2</sub>	5	16.2	1410.83	0.34	6	6	6	6
ZZ-CdN <sub>2</sub> C <sub>2</sub>	5	17.2	1466.58	0.34	6	6	6	6
ZZ-LaN <sub>2</sub> C <sub>2</sub>	6	8.2	591.91	0.34	6	6	6	6
ZZ-HfN <sub>2</sub> C <sub>2</sub>	6	9.2	856.05	0.34	6	6	6	6
ZZ-TaN <sub>2</sub> C <sub>2</sub>	6	10.2	1092.60	0.34	6	6	6	6
ZZ-WN <sub>2</sub> C <sub>2</sub>	6	11.2	1289.96	0.34	6	6	6	6
ZZ-ReN <sub>2</sub> C <sub>2</sub>	6	12.2	1436.02	0.34	6	6	6	6
ZZ-OsN <sub>2</sub> C <sub>2</sub>	6	13.2	1791.24	0.34	6	6	6	6
ZZ-IrN <sub>2</sub> C <sub>2</sub>	6	14.2	1903.44	0.34	6	6	6	6
ZZ-PtN <sub>2</sub> C <sub>2</sub>	6	15.2	1901.68	0.34	6	6	6	6
ZZ-AuN <sub>2</sub> C <sub>2</sub>	6	16.2	2136.24	0.34	6	6	6	6
ZZ-ScN <sub>2</sub> C <sub>2</sub> b	4	8.2	861.02	0.67	5	6	6	7
ZZ-TiN <sub>2</sub> C <sub>2</sub> b	4	9.2	1014.55	0.67	5	6	6	7
ZZ-VN <sub>2</sub> C <sub>2</sub> b	4	10.2	1060.97	0.67	5	6	6	7
ZZ-CrN <sub>2</sub> C <sub>2</sub> b	4	11.2	1083.81	0.67	5	6	6	7
ZZ-MnN <sub>2</sub> C <sub>2</sub> b	4	12.2	1111.82	0.67	5	6	6	7
ZZ-FeN <sub>2</sub> C <sub>2</sub> b	4	13.2	1395.38	0.67	5	6	6	7
ZZ-CoN <sub>2</sub> C <sub>2</sub> b	4	14.2	1429.55	0.67	5	6	6	7
ZZ-NiN <sub>2</sub> C <sub>2</sub> b	4	15.2	1407.86	0.67	5	6	6	7
ZZ-CuN <sub>2</sub> C <sub>2</sub> b	4	16.2	1416.45	0.67	5	6	6	7
ZZ-ZnN <sub>2</sub> C <sub>2</sub> b	4	17.2	1495.56	0.67	5	6	6	7
ZZ-YN <sub>2</sub> C <sub>2</sub> b	5	8.2	731.88	0.67	5	6	6	7

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ZZ-ZrN <sub>2</sub> C <sub>2</sub> b	5	9.2	851.33	0.67	5	6	6	7
ZZ-NbN <sub>2</sub> C <sub>2</sub> b	5	10.2	1043.36	0.67	5	6	6	7
ZZ-MoN <sub>2</sub> C <sub>2</sub> b	5	11.2	1478.09	0.67	5	6	6	7
ZZ-TcN <sub>2</sub> C <sub>2</sub> b	5	12.2	1475.04	0.67	5	6	6	7
ZZ-RuN <sub>2</sub> C <sub>2</sub> b	5	13.2	1562.44	0.67	5	6	6	7
ZZ-RhN <sub>2</sub> C <sub>2</sub> b	5	14.2	1640.92	0.67	5	6	6	7
ZZ-PdN <sub>2</sub> C <sub>2</sub> b	5	15.2	1769.68	0.67	5	6	6	7
ZZ-AgN <sub>2</sub> C <sub>2</sub> b	5	16.2	1410.83	0.67	5	6	6	7
ZZ-CdN <sub>2</sub> C <sub>2</sub> b	5	17.2	1466.58	0.67	5	6	6	7
ZZ-LaN <sub>2</sub> C <sub>2</sub> b	6	8.2	591.91	0.67	5	6	6	7
ZZ-HfN <sub>2</sub> C <sub>2</sub> b	6	9.2	856.05	0.67	5	6	6	7
ZZ-TaN <sub>2</sub> C <sub>2</sub> b	6	10.2	1092.60	0.67	5	6	6	7
ZZ-WN <sub>2</sub> C <sub>2</sub> b	6	11.2	1289.96	0.67	5	6	6	7
ZZ-ReN <sub>2</sub> C <sub>2</sub> b	6	12.2	1436.02	0.67	5	6	6	7
ZZ-OsN <sub>2</sub> C <sub>2</sub> b	6	13.2	1791.24	0.67	5	6	6	7
ZZ-IrN <sub>2</sub> C <sub>2</sub> b	6	14.2	1903.44	0.67	5	6	6	7
ZZ-PtN <sub>2</sub> C <sub>2</sub> b	6	15.2	1901.68	0.67	5	6	6	7
ZZ-AuN <sub>2</sub> C <sub>2</sub> b	6	16.2	2136.24	0.67	5	6	6	7
ZZ-ScN <sub>3</sub> C <sub>1</sub>	4	8.4	861.02	0.77	6	6	7	7
ZZ-TiN <sub>3</sub> C <sub>1</sub>	4	9.4	1014.55	0.77	6	6	7	7
ZZ-VN <sub>3</sub> C <sub>1</sub>	4	10.4	1060.97	0.77	6	6	7	7
ZZ-CrN <sub>3</sub> C <sub>1</sub>	4	11.4	1083.81	0.77	6	6	7	7
ZZ-MnN <sub>3</sub> C <sub>1</sub>	4	12.4	1111.82	0.77	6	6	7	7
ZZ-FeN <sub>3</sub> C <sub>1</sub>	4	13.4	1395.38	0.77	6	6	7	7
ZZ-CoN <sub>3</sub> C <sub>1</sub>	4	14.4	1429.55	0.77	6	6	7	7
ZZ-NiN <sub>3</sub> C <sub>1</sub>	4	15.4	1407.86	0.77	6	6	7	7
ZZ-CuN <sub>3</sub> C <sub>1</sub>	4	16.4	1416.45	0.77	6	6	7	7
ZZ-ZnN <sub>3</sub> C <sub>1</sub>	4	17.4	1495.56	0.77	6	6	7	7

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ZZ-YN <sub>3</sub> C <sub>1</sub>	5	8.4	731.88	0.77	6	6	7	7
ZZ-ZrN <sub>3</sub> C <sub>1</sub>	5	9.4	851.33	0.77	6	6	7	7
ZZ-NbN <sub>3</sub> C <sub>1</sub>	5	10.4	1043.36	0.77	6	6	7	7
ZZ-MoN <sub>3</sub> C <sub>1</sub>	5	11.4	1478.09	0.77	6	6	7	7
ZZ-TcN <sub>3</sub> C <sub>1</sub>	5	12.4	1475.04	0.77	6	6	7	7
ZZ-RuN <sub>3</sub> C <sub>1</sub>	5	13.4	1562.44	0.77	6	6	7	7
ZZ-RhN <sub>3</sub> C <sub>1</sub>	5	14.4	1640.92	0.77	6	6	7	7
ZZ-PdN <sub>3</sub> C <sub>1</sub>	5	15.4	1769.68	0.77	6	6	7	7
ZZ-AgN <sub>3</sub> C <sub>1</sub>	5	16.4	1410.83	0.77	6	6	7	7
ZZ-CdN <sub>3</sub> C <sub>1</sub>	5	17.4	1466.58	0.77	6	6	7	7
ZZ-LaN <sub>3</sub> C <sub>1</sub>	6	8.4	591.91	0.77	6	6	7	7
ZZ-HfN <sub>3</sub> C <sub>1</sub>	6	9.4	856.05	0.77	6	6	7	7
ZZ-TaN <sub>3</sub> C <sub>1</sub>	6	10.4	1092.60	0.77	6	6	7	7
ZZ-WN <sub>3</sub> C <sub>1</sub>	6	11.4	1289.96	0.77	6	6	7	7
ZZ-ReN <sub>3</sub> C <sub>1</sub>	6	12.4	1436.02	0.77	6	6	7	7
ZZ-OsN <sub>3</sub> C <sub>1</sub>	6	13.4	1791.24	0.77	6	6	7	7
ZZ-IrN <sub>3</sub> C <sub>1</sub>	6	14.4	1903.44	0.77	6	6	7	7
ZZ-PtN <sub>3</sub> C <sub>1</sub>	6	15.4	1901.68	0.77	6	6	7	7
ZZ-AuN <sub>3</sub> C <sub>1</sub>	6	16.4	2136.24	0.77	6	6	7	7
ZZ-ScN <sub>4</sub>	4	8.6	861.02	1.14	7	7	7	7
ZZ-TiN <sub>4</sub>	4	9.6	1014.55	1.14	7	7	7	7
ZZ-VN <sub>4</sub>	4	10.6	1060.97	1.14	7	7	7	7
ZZ-CrN <sub>4</sub>	4	11.6	1083.81	1.14	7	7	7	7
ZZ-MnN <sub>4</sub>	4	12.6	1111.82	1.14	7	7	7	7
ZZ-FeN <sub>4</sub>	4	13.6	1395.38	1.14	7	7	7	7
ZZ-CoN <sub>4</sub>	4	14.6	1429.55	1.14	7	7	7	7
ZZ-NiN <sub>4</sub>	4	15.6	1407.86	1.14	7	7	7	7
ZZ-CuN <sub>4</sub>	4	16.6	1416.45	1.14	7	7	7	7

ZZ-ZnN <sub>4</sub>	4	17.6	1495.56	1.14	7	7	7	7
ZZ-YN <sub>4</sub>	5	8.6	731.88	1.14	7	7	7	7
ZZ-ZrN <sub>4</sub>	5	9.6	851.33	1.14	7	7	7	7
ZZ-NbN <sub>4</sub>	5	10.6	1043.36	1.14	7	7	7	7
ZZ-MoN <sub>4</sub>	5	11.6	1478.09	1.14	7	7	7	7
ZZ-TcN <sub>4</sub>	5	12.6	1475.04	1.14	7	7	7	7
ZZ-RuN <sub>4</sub>	5	13.6	1562.44	1.14	7	7	7	7
ZZ-RhN <sub>4</sub>	5	14.6	1640.92	1.14	7	7	7	7
ZZ-PdN <sub>4</sub>	5	15.6	1769.68	1.14	7	7	7	7
ZZ-AgN <sub>4</sub>	5	16.6	1410.83	1.14	7	7	7	7
ZZ-CdN <sub>4</sub>	5	17.6	1466.58	1.14	7	7	7	7
ZZ-LaN <sub>4</sub>	6	8.6	591.91	1.14	7	7	7	7
ZZ-HfN <sub>4</sub>	6	9.6	856.05	1.14	7	7	7	7
ZZ-TaN <sub>4</sub>	6	10.6	1092.60	1.14	7	7	7	7
ZZ-WN <sub>4</sub>	6	11.6	1289.96	1.14	7	7	7	7
ZZ-ReN <sub>4</sub>	6	12.6	1436.02	1.14	7	7	7	7
ZZ-OsN <sub>4</sub>	6	13.6	1791.24	1.14	7	7	7	7
ZZ-IrN <sub>4</sub>	6	14.6	1903.44	1.14	7	7	7	7
ZZ-PtN <sub>4</sub>	6	15.6	1901.68	1.14	7	7	7	7
ZZ-AuN <sub>4</sub>	6	16.6	2136.24	1.14	7	7	7	7

**Table. S3** the values of high-performance catalyst retention rate  $r_R$  and high-performance catalyst occupancy rate  $r_O$  for each of group in Table. 1.

<b>group</b>	<b>descriptors</b>	$r_O$	$r_R$
G1	$CM, I_1, N_M, VE, E_d, P$	0.222	0.360
G2	$CM, I_1, N_M, VE, E_d, P, VEc, DC$	0.385	0.529
G3	$P, VEc, DC$	0.413	0.648



G4	$P, VEc, I_1^*\chi$	0.382	0.652
G5	$CM, P, VEc, DC, I_1^*\chi$	0.401	0.577
G6	$P, VEc, DC, I_1^*\chi$	<b>0.421</b>	<b>0.671</b>
G7	$P, VEc, DC, I_1^*\chi, n_N$	0.411	0.656
G8	$P, VEc, DC, I_1^*\chi, n_N, \eta_{ORR}^*n_N$	0.409	0.848
G9	$P, VEc, DC, I_1^*\chi, \varphi$	0.396	0.633
G10	$P, DC, I_1^*\chi, \varphi$	0.233	0.431

\* The maximum of  $r_O$  and  $r_R$  are marked with bold font (G8 with the descriptor  $\eta_{ORR}^*n_N$  and is ignored in evaluating).

**Table. S4** ORR overpotential  $\eta_{model}$  of catalysts of ZZ-MN<sub>x</sub>C<sub>y</sub> system predicted by the ML model, which using descriptors  $VEc, DC, I_1^*\chi$  and  $P$  as catalysts feature.

Catalysts	$\eta_{model}$	Catalysts	$\eta_{model}$	Catalysts	$\eta_{model}$
ZZ-ScC <sub>4</sub>	2.007	ZZ-ScN <sub>2</sub> C <sub>2</sub>	2.120	ZZ-ScN <sub>3</sub> C <sub>1</sub>	2.394
ZZ-TiC <sub>4</sub>	2.867	ZZ-TiN <sub>2</sub> C <sub>2</sub>	2.984	ZZ-TiN <sub>3</sub> C <sub>1</sub>	3.244
ZZ-VC <sub>4</sub>	3.004	ZZ-VN <sub>2</sub> C <sub>2</sub>	2.620	ZZ-VN <sub>3</sub> C <sub>1</sub>	2.266
ZZ-CrC <sub>4</sub>	1.809	ZZ-CrN <sub>2</sub> C <sub>2</sub>	1.857	ZZ-CrN <sub>3</sub> C <sub>1</sub>	1.502
ZZ-MnC <sub>4</sub>	1.627	ZZ-MnN <sub>2</sub> C <sub>2</sub>	1.194	ZZ-MnN <sub>3</sub> C <sub>1</sub>	1.218
ZZ-FeC <sub>4</sub>	0.964	ZZ-FeN <sub>2</sub> C <sub>2</sub>	0.915	ZZ-FeN <sub>3</sub> C <sub>1</sub>	0.946
ZZ-CoC <sub>4</sub>	0.755	ZZ-CoN <sub>2</sub> C <sub>2</sub>	0.717	ZZ-CoN <sub>3</sub> C <sub>1</sub>	0.517
ZZ-NiC <sub>4</sub>	0.491	ZZ-NiN <sub>2</sub> C <sub>2</sub>	0.772	ZZ-NiN <sub>3</sub> C <sub>1</sub>	0.812
ZZ-CuC <sub>4</sub>	1.052	ZZ-CuN <sub>2</sub> C <sub>2</sub>	0.945	ZZ-CuN <sub>3</sub> C <sub>1</sub>	0.963
ZZ-ZnC <sub>4</sub>	0.646	ZZ-ZnN <sub>2</sub> C <sub>2</sub>	0.760	ZZ-ZnN <sub>3</sub> C <sub>1</sub>	0.588
ZZ-YC <sub>4</sub>	1.966	ZZ-YN <sub>2</sub> C <sub>2</sub>	2.011	ZZ-YN <sub>3</sub> C <sub>1</sub>	2.312
ZZ-ZrC <sub>4</sub>	2.835	ZZ-ZrN <sub>2</sub> C <sub>2</sub>	3.021	ZZ-ZrN <sub>3</sub> C <sub>1</sub>	3.432
ZZ-NbC <sub>4</sub>	3.212	ZZ-NbN <sub>2</sub> C <sub>2</sub>	3.100	ZZ-NbN <sub>3</sub> C <sub>1</sub>	2.450
ZZ-MoC <sub>4</sub>	1.891	ZZ-MoN <sub>2</sub> C <sub>2</sub>	1.774	ZZ-MoN <sub>3</sub> C <sub>1</sub>	1.614

ZZ-TcC <sub>4</sub>	1.609	ZZ-TcN <sub>2</sub> C <sub>2</sub>	1.020	ZZ-TcN <sub>3</sub> C <sub>1</sub>	1.110
ZZ-RuC <sub>4</sub>	0.983	ZZ-RuN <sub>2</sub> C <sub>2</sub>	0.890	ZZ-RuN <sub>3</sub> C <sub>1</sub>	0.645
ZZ-RhC <sub>4</sub>	0.809	ZZ-RhN <sub>2</sub> C <sub>2</sub>	0.909	ZZ-RhN <sub>3</sub> C <sub>1</sub>	0.577
ZZ-PdC <sub>4</sub>	0.470	ZZ-PdN <sub>2</sub> C <sub>2</sub>	0.851	ZZ-PdN <sub>3</sub> C <sub>1</sub>	1.055
ZZ-AgC <sub>4</sub>	1.096	ZZ-AgN <sub>2</sub> C <sub>2</sub>	1.019	ZZ-AgN <sub>3</sub> C <sub>1</sub>	1.066
ZZ-CdC <sub>4</sub>	0.837	ZZ-CdN <sub>2</sub> C <sub>2</sub>	0.761	ZZ-CdN <sub>3</sub> C <sub>1</sub>	0.866
ZZ-LaC <sub>4</sub>	1.692	ZZ-LaN <sub>2</sub> C <sub>2</sub>	1.585	ZZ-LaN <sub>3</sub> C <sub>1</sub>	1.936
ZZ-HfC <sub>4</sub>	2.914	ZZ-HfN <sub>2</sub> C <sub>2</sub>	3.342	ZZ-HfN <sub>3</sub> C <sub>1</sub>	3.679
ZZ-TaC <sub>4</sub>	3.219	ZZ-TaN <sub>2</sub> C <sub>2</sub>	1.809	ZZ-TaN <sub>3</sub> C <sub>1</sub>	1.769
ZZ-WC <sub>4</sub>	1.661	ZZ-WN <sub>2</sub> C <sub>2</sub>	1.806	ZZ-WN <sub>3</sub> C <sub>1</sub>	1.537
ZZ-ReC <sub>4</sub>	1.702	ZZ-ReN <sub>2</sub> C <sub>2</sub>	0.636	ZZ-ReN <sub>3</sub> C <sub>1</sub>	1.049
ZZ-OsC <sub>4</sub>	1.024	ZZ-OsN <sub>2</sub> C <sub>2</sub>	0.910	ZZ-OsN <sub>3</sub> C <sub>1</sub>	0.988
ZZ-IrC <sub>4</sub>	1.004	ZZ-IrN <sub>2</sub> C <sub>2</sub>	1.081	ZZ-IrN <sub>3</sub> C <sub>1</sub>	0.685
ZZ-PtC <sub>4</sub>	0.498	ZZ-PtN <sub>2</sub> C <sub>2</sub>	0.857	ZZ-PtN <sub>3</sub> C <sub>1</sub>	1.096
ZZ-AuC <sub>4</sub>	1.154	ZZ-AuN <sub>2</sub> C <sub>2</sub>	1.162	ZZ-AuN <sub>3</sub> C <sub>1</sub>	1.134
ZZ-ScN <sub>1</sub> C <sub>3</sub>	1.977	ZZ-ScN <sub>2</sub> C <sub>2</sub> b	2.120	ZZ-ScN <sub>4</sub>	2.839
ZZ-TiN <sub>1</sub> C <sub>3</sub>	2.896	ZZ-TiN <sub>2</sub> C <sub>2</sub> b	2.984	ZZ-TiN <sub>4</sub>	2.997
ZZ-VN <sub>1</sub> C <sub>3</sub>	2.962	ZZ-VN <sub>2</sub> C <sub>2</sub> b	2.620	ZZ-VN <sub>4</sub>	1.371
ZZ-CrN <sub>1</sub> C <sub>3</sub>	2.063	ZZ-CrN <sub>2</sub> C <sub>2</sub> b	1.857	ZZ-CrN <sub>4</sub>	1.412
ZZ-MnN <sub>1</sub> C <sub>3</sub>	1.763	ZZ-MnN <sub>2</sub> C <sub>2</sub> b	1.194	ZZ-MnN <sub>4</sub>	0.972
ZZ-FeN <sub>1</sub> C <sub>3</sub>	1.059	ZZ-FeN <sub>2</sub> C <sub>2</sub> b	0.915	ZZ-FeN <sub>4</sub>	0.734
ZZ-CoN <sub>1</sub> C <sub>3</sub>	0.776	ZZ-CoN <sub>2</sub> C <sub>2</sub> b	0.717	ZZ-CoN <sub>4</sub>	0.445
ZZ-NiN <sub>1</sub> C <sub>3</sub>	0.537	ZZ-NiN <sub>2</sub> C <sub>2</sub> b	0.772	ZZ-NiN <sub>4</sub>	0.957
ZZ-CuN <sub>1</sub> C <sub>3</sub>	1.015	ZZ-CuN <sub>2</sub> C <sub>2</sub> b	0.945	ZZ-CuN <sub>4</sub>	0.940
ZZ-ZnN <sub>1</sub> C <sub>3</sub>	0.726	ZZ-ZnN <sub>2</sub> C <sub>2</sub> b	0.760	ZZ-ZnN <sub>4</sub>	1.367
ZZ-YN <sub>1</sub> C <sub>3</sub>	1.922	ZZ-YN <sub>2</sub> C <sub>2</sub> b	2.011	ZZ-YN <sub>4</sub>	2.765
ZZ-ZrN <sub>1</sub> C <sub>3</sub>	2.905	ZZ-ZrN <sub>2</sub> C <sub>2</sub> b	3.021	ZZ-ZrN <sub>4</sub>	3.340
ZZ-NbN <sub>1</sub> C <sub>3</sub>	3.155	ZZ-NbN <sub>2</sub> C <sub>2</sub> b	3.100	ZZ-NbN <sub>4</sub>	1.473

ZZ-MoN <sub>1</sub> C <sub>3</sub>	2.090	ZZ-MoN <sub>2</sub> C <sub>2</sub> b	1.774	ZZ-MoN <sub>4</sub>	1.539
ZZ-TcN <sub>1</sub> C <sub>3</sub>	1.708	ZZ-TcN <sub>2</sub> C <sub>2</sub> b	1.020	ZZ-TcN <sub>4</sub>	0.995
ZZ-RuN <sub>1</sub> C <sub>3</sub>	1.311	ZZ-RuN <sub>2</sub> C <sub>2</sub> b	0.890	ZZ-RuN <sub>4</sub>	0.873
ZZ-RhN <sub>1</sub> C <sub>3</sub>	0.909	ZZ-RhN <sub>2</sub> C <sub>2</sub> b	0.909	ZZ-RhN <sub>4</sub>	0.436
ZZ-PdN <sub>1</sub> C <sub>3</sub>	0.512	ZZ-PdN <sub>2</sub> C <sub>2</sub> b	0.851	ZZ-PdN <sub>4</sub>	1.107
ZZ-AgN <sub>1</sub> C <sub>3</sub>	1.043	ZZ-AgN <sub>2</sub> C <sub>2</sub> b	1.019	ZZ-AgN <sub>4</sub>	0.797
ZZ-CdN <sub>1</sub> C <sub>3</sub>	0.736	ZZ-CdN <sub>2</sub> C <sub>2</sub> b	0.761	ZZ-CdN <sub>4</sub>	1.195
ZZ-LaN <sub>1</sub> C <sub>3</sub>	1.599	ZZ-LaN <sub>2</sub> C <sub>2</sub> b	1.585	ZZ-LaN <sub>4</sub>	2.649
ZZ-HfN <sub>1</sub> C <sub>3</sub>	3.119	ZZ-HfN <sub>2</sub> C <sub>2</sub> b	3.342	ZZ-HfN <sub>4</sub>	3.677
ZZ-TaN <sub>1</sub> C <sub>3</sub>	2.938	ZZ-TaN <sub>2</sub> C <sub>2</sub> b	1.809	ZZ-TaN <sub>4</sub>	2.001
ZZ-WN <sub>1</sub> C <sub>3</sub>	1.874	ZZ-WN <sub>2</sub> C <sub>2</sub> b	1.806	ZZ-WN <sub>4</sub>	1.603
ZZ-ReN <sub>1</sub> C <sub>3</sub>	1.747	ZZ-ReN <sub>2</sub> C <sub>2</sub> b	0.636	ZZ-ReN <sub>4</sub>	0.889
ZZ-OsN <sub>1</sub> C <sub>3</sub>	1.003	ZZ-OsN <sub>2</sub> C <sub>2</sub> b	0.910	ZZ-OsN <sub>4</sub>	1.029
ZZ-IrN <sub>1</sub> C <sub>3</sub>	1.065	ZZ-IrN <sub>2</sub> C <sub>2</sub> b	1.081	ZZ-IrN <sub>4</sub>	0.460
ZZ-PtN <sub>1</sub> C <sub>3</sub>	0.553	ZZ-PtN <sub>2</sub> C <sub>2</sub> b	0.857	ZZ-PtN <sub>4</sub>	1.122
ZZ-AuN <sub>1</sub> C <sub>3</sub>	1.164	ZZ-AuN <sub>2</sub> C <sub>2</sub> b	1.162	ZZ-AuN <sub>4</sub>	0.928

**Table. S5** ORR overpotential  $\eta_{\text{model}}$  of catalysts of ZZ-MN<sub>x</sub>C<sub>y</sub> system predicted by the ML model, which using descriptors  $VEc$ ,  $DC$ ,  $I_1^*\chi$ ,  $P$ ,  $R_1$ ,  $R_2$ ,  $R_3$  and  $R_4$  as catalysts feature.

Catalysts	$\eta_{\text{model}}$	Catalysts	$\eta_{\text{model}}$	Catalysts	$\eta_{\text{model}}$
ZZ-ScC <sub>4</sub>	2.041	ZZ-ScN <sub>2</sub> C <sub>2</sub>	2.142	ZZ-ScN <sub>3</sub> C <sub>1</sub>	2.529
ZZ-TiC <sub>4</sub>	2.706	ZZ-TiN <sub>2</sub> C <sub>2</sub>	3.104	ZZ-TiN <sub>3</sub> C <sub>1</sub>	3.378
ZZ-VC <sub>4</sub>	2.957	ZZ-VN <sub>2</sub> C <sub>2</sub>	2.497	ZZ-VN <sub>3</sub> C <sub>1</sub>	2.280
ZZ-CrC <sub>4</sub>	2.196	ZZ-CrN <sub>2</sub> C <sub>2</sub>	1.588	ZZ-CrN <sub>3</sub> C <sub>1</sub>	1.478
ZZ-MnC <sub>4</sub>	1.804	ZZ-MnN <sub>2</sub> C <sub>2</sub>	1.078	ZZ-MnN <sub>3</sub> C <sub>1</sub>	1.031
ZZ-FeC <sub>4</sub>	1.077	ZZ-FeN <sub>2</sub> C <sub>2</sub>	0.869	ZZ-FeN <sub>3</sub> C <sub>1</sub>	0.840

ZZ-CoC <sub>4</sub>	0.860	ZZ-CoN <sub>2</sub> C <sub>2</sub>	0.661	ZZ-CoN <sub>3</sub> C <sub>1</sub>	0.487
ZZ-NiC <sub>4</sub>	0.501	ZZ-NiN <sub>2</sub> C <sub>2</sub>	0.777	ZZ-NiN <sub>3</sub> C <sub>1</sub>	0.784
ZZ-CuC <sub>4</sub>	1.045	ZZ-CuN <sub>2</sub> C <sub>2</sub>	0.940	ZZ-CuN <sub>3</sub> C <sub>1</sub>	0.917
ZZ-ZnC <sub>4</sub>	0.765	ZZ-ZnN <sub>2</sub> C <sub>2</sub>	0.718	ZZ-ZnN <sub>3</sub> C <sub>1</sub>	0.752
ZZ-YC <sub>4</sub>	1.995	ZZ-YN <sub>2</sub> C <sub>2</sub>	2.053	ZZ-YN <sub>3</sub> C <sub>1</sub>	2.482
ZZ-ZrC <sub>4</sub>	2.672	ZZ-ZrN <sub>2</sub> C <sub>2</sub>	3.167	ZZ-ZrN <sub>3</sub> C <sub>1</sub>	3.570
ZZ-NbC <sub>4</sub>	3.040	ZZ-NbN <sub>2</sub> C <sub>2</sub>	3.016	ZZ-NbN <sub>3</sub> C <sub>1</sub>	2.254
ZZ-MoC <sub>4</sub>	2.215	ZZ-MoN <sub>2</sub> C <sub>2</sub>	1.646	ZZ-MoN <sub>3</sub> C <sub>1</sub>	1.489
ZZ-TcC <sub>4</sub>	1.760	ZZ-TcN <sub>2</sub> C <sub>2</sub>	0.952	ZZ-TcN <sub>3</sub> C <sub>1</sub>	0.916
ZZ-RuC <sub>4</sub>	1.279	ZZ-RuN <sub>2</sub> C <sub>2</sub>	0.771	ZZ-RuN <sub>3</sub> C <sub>1</sub>	0.680
ZZ-RhC <sub>4</sub>	0.928	ZZ-RhN <sub>2</sub> C <sub>2</sub>	0.848	ZZ-RhN <sub>3</sub> C <sub>1</sub>	0.566
ZZ-PdC <sub>4</sub>	0.502	ZZ-PdN <sub>2</sub> C <sub>2</sub>	0.897	ZZ-PdN <sub>3</sub> C <sub>1</sub>	1.074
ZZ-AgC <sub>4</sub>	1.057	ZZ-AgN <sub>2</sub> C <sub>2</sub>	0.996	ZZ-AgN <sub>3</sub> C <sub>1</sub>	0.926
ZZ-CdC <sub>4</sub>	0.796	ZZ-CdN <sub>2</sub> C <sub>2</sub>	0.734	ZZ-CdN <sub>3</sub> C <sub>1</sub>	0.900
ZZ-LaC <sub>4</sub>	1.713	ZZ-LaN <sub>2</sub> C <sub>2</sub>	1.643	ZZ-LaN <sub>3</sub> C <sub>1</sub>	2.063
ZZ-HfC <sub>4</sub>	2.823	ZZ-HfN <sub>2</sub> C <sub>2</sub>	3.425	ZZ-HfN <sub>3</sub> C <sub>1</sub>	3.765
ZZ-TaC <sub>4</sub>	3.059	ZZ-TaN <sub>2</sub> C <sub>2</sub>	1.936	ZZ-TaN <sub>3</sub> C <sub>1</sub>	2.015
ZZ-WC <sub>4</sub>	2.103	ZZ-WN <sub>2</sub> C <sub>2</sub>	1.697	ZZ-WN <sub>3</sub> C <sub>1</sub>	1.444
ZZ-ReC <sub>4</sub>	1.860	ZZ-ReN <sub>2</sub> C <sub>2</sub>	0.672	ZZ-ReN <sub>3</sub> C <sub>1</sub>	0.874
ZZ-OsC <sub>4</sub>	1.194	ZZ-OsN <sub>2</sub> C <sub>2</sub>	0.929	ZZ-OsN <sub>3</sub> C <sub>1</sub>	0.909
ZZ-IrC <sub>4</sub>	1.140	ZZ-IrN <sub>2</sub> C <sub>2</sub>	0.968	ZZ-IrN <sub>3</sub> C <sub>1</sub>	0.571
ZZ-PtC <sub>4</sub>	0.586	ZZ-PtN <sub>2</sub> C <sub>2</sub>	0.896	ZZ-PtN <sub>3</sub> C <sub>1</sub>	1.053
ZZ-AuC <sub>4</sub>	1.205	ZZ-AuN <sub>2</sub> C <sub>2</sub>	1.149	ZZ-AuN <sub>3</sub> C <sub>1</sub>	1.060
ZZ-ScN <sub>1</sub> C <sub>3</sub>	2.031	ZZ-ScN <sub>2</sub> C <sub>2</sub> b	2.238	ZZ-ScN <sub>4</sub>	2.986
ZZ-TiN <sub>1</sub> C <sub>3</sub>	2.900	ZZ-TiN <sub>2</sub> C <sub>2</sub> b	3.102	ZZ-TiN <sub>4</sub>	3.291
ZZ-VN <sub>1</sub> C <sub>3</sub>	2.923	ZZ-VN <sub>2</sub> C <sub>2</sub> b	2.577	ZZ-VN <sub>4</sub>	1.202
ZZ-CrN <sub>1</sub> C <sub>3</sub>	2.273	ZZ-CrN <sub>2</sub> C <sub>2</sub> b	1.606	ZZ-CrN <sub>4</sub>	1.184
ZZ-MnN <sub>1</sub> C <sub>3</sub>	1.696	ZZ-MnN <sub>2</sub> C <sub>2</sub> b	1.196	ZZ-MnN <sub>4</sub>	0.889

ZZ-FeN <sub>1</sub> C <sub>3</sub>	1.015	ZZ-FeN <sub>2</sub> C <sub>2</sub> b	0.878	ZZ-FeN <sub>4</sub>	0.715
ZZ-CoN <sub>1</sub> C <sub>3</sub>	0.766	ZZ-CoN <sub>2</sub> C <sub>2</sub> b	0.664	ZZ-CoN <sub>4</sub>	0.459
ZZ-NiN <sub>1</sub> C <sub>3</sub>	0.539	ZZ-NiN <sub>2</sub> C <sub>2</sub> b	0.777	ZZ-NiN <sub>4</sub>	0.901
ZZ-CuN <sub>1</sub> C <sub>3</sub>	1.002	ZZ-CuN <sub>2</sub> C <sub>2</sub> b	0.945	ZZ-CuN <sub>4</sub>	0.956
ZZ-ZnN <sub>1</sub> C <sub>3</sub>	0.748	ZZ-ZnN <sub>2</sub> C <sub>2</sub> b	0.784	ZZ-ZnN <sub>4</sub>	1.144
ZZ-YN <sub>1</sub> C <sub>3</sub>	1.973	ZZ-YN <sub>2</sub> C <sub>2</sub> b	2.160	ZZ-YN <sub>4</sub>	2.937
ZZ-ZrN <sub>1</sub> C <sub>3</sub>	2.914	ZZ-ZrN <sub>2</sub> C <sub>2</sub> b	3.201	ZZ-ZrN <sub>4</sub>	3.548
ZZ-NbN <sub>1</sub> C <sub>3</sub>	3.096	ZZ-NbN <sub>2</sub> C <sub>2</sub> b	2.770	ZZ-NbN <sub>4</sub>	1.469
ZZ-MoN <sub>1</sub> C <sub>3</sub>	2.209	ZZ-MoN <sub>2</sub> C <sub>2</sub> b	1.603	ZZ-MoN <sub>4</sub>	1.368
ZZ-TcN <sub>1</sub> C <sub>3</sub>	1.656	ZZ-TcN <sub>2</sub> C <sub>2</sub> b	1.034	ZZ-TcN <sub>4</sub>	0.782
ZZ-RuN <sub>1</sub> C <sub>3</sub>	1.277	ZZ-RuN <sub>2</sub> C <sub>2</sub> b	0.679	ZZ-RuN <sub>4</sub>	0.844
ZZ-RhN <sub>1</sub> C <sub>3</sub>	0.905	ZZ-RhN <sub>2</sub> C <sub>2</sub> b	0.773	ZZ-RhN <sub>4</sub>	0.503
ZZ-PdN <sub>1</sub> C <sub>3</sub>	0.518	ZZ-PdN <sub>2</sub> C <sub>2</sub> b	0.898	ZZ-PdN <sub>4</sub>	1.132
ZZ-AgN <sub>1</sub> C <sub>3</sub>	1.036	ZZ-AgN <sub>2</sub> C <sub>2</sub> b	0.999	ZZ-AgN <sub>4</sub>	0.781
ZZ-CdN <sub>1</sub> C <sub>3</sub>	0.724	ZZ-CdN <sub>2</sub> C <sub>2</sub> b	0.825	ZZ-CdN <sub>4</sub>	1.100
ZZ-LaN <sub>1</sub> C <sub>3</sub>	1.624	ZZ-LaN <sub>2</sub> C <sub>2</sub> b	1.724	ZZ-LaN <sub>4</sub>	2.767
ZZ-HfN <sub>1</sub> C <sub>3</sub>	3.122	ZZ-HfN <sub>2</sub> C <sub>2</sub> b	3.485	ZZ-HfN <sub>4</sub>	3.818
ZZ-TaN <sub>1</sub> C <sub>3</sub>	2.912	ZZ-TaN <sub>2</sub> C <sub>2</sub> b	2.184	ZZ-TaN <sub>4</sub>	1.698
ZZ-WN <sub>1</sub> C <sub>3</sub>	2.104	ZZ-WN <sub>2</sub> C <sub>2</sub> b	1.611	ZZ-WN <sub>4</sub>	1.429
ZZ-ReN <sub>1</sub> C <sub>3</sub>	1.731	ZZ-ReN <sub>2</sub> C <sub>2</sub> b	0.751	ZZ-ReN <sub>4</sub>	0.725
ZZ-OsN <sub>1</sub> C <sub>3</sub>	1.017	ZZ-OsN <sub>2</sub> C <sub>2</sub> b	0.927	ZZ-OsN <sub>4</sub>	0.961
ZZ-IrN <sub>1</sub> C <sub>3</sub>	1.061	ZZ-IrN <sub>2</sub> C <sub>2</sub> b	0.945	ZZ-IrN <sub>4</sub>	0.446
ZZ-PtN <sub>1</sub> C <sub>3</sub>	0.562	ZZ-PtN <sub>2</sub> C <sub>2</sub> b	0.898	ZZ-PtN <sub>4</sub>	1.107
ZZ-AuN <sub>1</sub> C <sub>3</sub>	1.185	ZZ-AuN <sub>2</sub> C <sub>2</sub> b	1.147	ZZ-AuN <sub>4</sub>	0.915

**Table. S6** catalysts with  $\eta_{\text{model}} \leq 0.8$  V in Table S5.

<b>Catalysts</b>	<b><math>\eta_{\text{model}}</math></b>	<b>Catalysts</b>	<b><math>\eta_{\text{model}}</math></b>	<b>Catalysts</b>	<b><math>\eta_{\text{model}}</math></b>
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ZZ-CoN <sub>4</sub>	0.459	ZZ-ZnN <sub>2</sub> C <sub>2</sub>	0.718	ZZ-CoN <sub>1</sub> C <sub>3</sub>	0.766
ZZ-CoN <sub>3</sub> C <sub>1</sub>	0.487	ZZ-CdN <sub>1</sub> C <sub>3</sub>	0.724	ZZ-NiN <sub>2</sub> C <sub>2</sub> b	0.777
ZZ-NiC <sub>4</sub>	0.500	ZZ-ReN <sub>4</sub>	0.725	ZZ-NiN <sub>2</sub> C <sub>2</sub>	0.777
ZZ-NiN <sub>1</sub> C <sub>3</sub>	0.539	ZZ-CdN <sub>2</sub> C <sub>2</sub>	0.734	ZZ-ZnN <sub>2</sub> C <sub>2</sub> b	0.784
ZZ-CoN <sub>2</sub> C <sub>2</sub>	0.661	ZZ-ZnN <sub>1</sub> C <sub>3</sub>	0.748	ZZ-NiN <sub>3</sub> C <sub>1</sub>	0.784
ZZ-CoN <sub>2</sub> C <sub>2</sub> b	0.664	ZZ-ReN <sub>2</sub> C <sub>2</sub> b	0.751	ZZ-CdC <sub>4</sub>	0.796
ZZ-ReN <sub>2</sub> C <sub>2</sub>	0.672	ZZ-ZnN <sub>3</sub> C <sub>1</sub>	0.752	-	-
ZZ-FeN <sub>4</sub>	0.715	ZZ-ZnC <sub>4</sub>	0.765	-	-

**Table. S7**  $\Delta G$  of each reaction step,  $\eta_{\text{DFT}}$  and  $\eta_{\text{model}}$  of catalysts of ZZ-MN<sub>x</sub>C<sub>y</sub> system with  $\eta_{\text{model}} \leq 0.7\text{V}$ .

Catalysts	$\Delta G_1$	$\Delta G_2$	$\Delta G_3$	$\Delta G_4$	$\eta_{\text{DFT}}$	$\eta_{\text{model}}$
ZZ-NiC <sub>4</sub>	-1.251	0.265	0.281	0.704	0.704	0.462
ZZ-CdN <sub>1</sub> C <sub>3</sub>	-1.211	-0.720	1.216	0.716	1.216	0.724
ZZ-NiN <sub>1</sub> C <sub>3</sub>	-1.246	0.104	0.579	0.563	0.579	0.526
ZZ-CoN <sub>2</sub> C <sub>2</sub>	-0.490	0.785	-0.077	-0.218	0.785	0.661
ZZ-CoN <sub>3</sub> C <sub>1</sub>	-0.544	0.498	0.167	-0.121	0.498	0.487
ZZ-CoN <sub>4</sub>	-0.666	0.457	0.141	0.067	0.457	0.436
ZZ-FeN <sub>4</sub>	-0.434	0.940	-0.241	-0.265	0.940	0.715