Supporting Information

Building Up "Genome" of Bi-atom Catalysts toward the Efficient HER/OER/ORR

Lihong Zhang[1], Xiangyu Guo[2,3]*, Shengli Zhang[4]*, Shiping Huang[1]*

[1] State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, Beijing, 100029, China

[2] Shenzhen JL Computational Science and Applied Research Institute, Shenzhen 518110 China

[3] Beijing Computational Science Research Center (CSRC), Beijing 100193 China

[4] MIIT Key Laboratory of Advanced Display Materials and Devices, Ministry of Industry and Information Technology, Institute of Optoelectronics & Nanomaterials, Nanjing University of Science and Technology, Nanjing, 210094, China

Corresponding E-mails:

E-mail: xiangyuguochem@gmail.com

E-mail: zhangslvip@njust.edu.cn

E-mail: huangsp@mail.buct.edu.cn

DFT-D3 method

Since GGA correlation functionals do not account for long-range correlations, the DFT-D method proposed by Grimme[1] is widely used to solve the dispersion problem of DFT. Compared with the DFT-D1 and DFT-D2, the DFT-D3 takes the the number of neighbors in the atomic environment into account, and further enhancing the accuracy of the results. Patel et al [2] applied the DFT-D3 to all hybrid and GGA functional calculations, and found that the PBE-D3 can better describe the vdW interactions. Moreover, some literatures[3,4] have performed comparisons between DFT-D3 correction and experiments, and validate the reliability of DFT-D3.

Gibbs free energy computations

With regard to HER, the overall reaction scheme can be described as follows[5]:

$$H^+ + e^- + * \rightarrow H*$$

(S1)

$$H* + H^+ + e^- \rightarrow H_2(g) + *$$

(S2)

where * denotes the active site, and (g) denotes the gas phases. Under standard conditions (pH = 0, U = 0 V vs standard hydrogen electrode (SHE)), the Gibbs free energy change for hydrogen adsorption (ΔG_{H*}) can be calculated by:

$$\Delta G_{H*} = \Delta E_{H*} + \Delta E_{ZPE} - T\Delta S_H \quad \text{(S3)}$$

where ΔE_{H*} stands for the hydrogen adsorption energy. ΔE_{ZPE} and ΔS_H are the zero-point energy and entropy differences between gas phase and adsorbed state for hydrogen, respectively. *T* represents a temperature of 298.15 K herein.

The OER proceeds via four elementary reaction steps as follows[6]:

$$H_2O(l) + * \overset{\Delta G_1}{\rightarrow} OH* + e^- + H^+ \quad \text{(S4)}$$

$$OH* \overset{\Delta G_2}{\rightarrow} O* + e^- + H^+ \quad \text{(S5)}$$

$$H_2O(l) + O* \xrightarrow{\Delta G_3} OOH* + e^- + H^+ \quad \text{(S6)}$$

$$OOH* \xrightarrow{\Delta G_4} O_2(g) + e^- + H^+ \quad \text{(S7)}$$

where (l) represents the liquid phases. Moreover, OH*, O*, and OOH* stand for the oxygenated intermediates.

The ORR can be treated as the inverse of ORR, and proceeds according following four elementary reaction steps[7]:

$$* + O_2(g) + e^- + H^+ \xrightarrow{\Delta G_a} OOH \quad \text{(S8)}$$

$$OOH* + e^- + H^+ \xrightarrow{\Delta G_b} H_2O(l) + O \quad \text{(S9)}$$

$$O* + e^- + H^+ \xrightarrow{\Delta G_c} OH* \quad \text{(S10)}$$

$$OH* + e^- + H^+ \xrightarrow{\Delta G_d} H_2O(l) + * \quad \text{(S11)}$$

The Gibbs free energy change (ΔG) for the elementary steps can be calculated as follows:

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S + \Delta G_U + \Delta G_{pH} + G_{solv} \quad \text{(S12)}$$

where ΔE, ΔZPE, and ΔS stand for the energy difference in adsorption energy, zero-point energy, and entropy between the product and reactant of each elemental step, respectively. $\Delta G_U = -eU$, of which U is the applied electrode potential, and e stands for the number of transferred electrons. $\Delta G_{pH} = -k_B T ln10\, pH$, of which k_B means the Boltzmann constant. The ZPE and TS can be defined as follows:

$$ZPE = \frac{1}{2}\sum_i h\nu_i \quad \text{(S13)}$$

$$-TS = k_B T \sum_i ln(1 - e^{-h\nu_i/k_B T}) - \sum_i h\nu_i \left(\frac{1}{e^{h\nu_i/k_B T} - 1}\right) \quad \text{(S14)}$$

where ν_i is the vibration frequency of the ith vibrational mode, and h is Planck's constant. The ZPE and TS of the reaction intermediates can be obtained from the vibration analysis using the VASPKIT code[8]. The ZPE and TS are calculated for the adsorbates only, as the contribution of the surface to the ZPE and entropy remains

almost constant under different adsorbed intermediates[9,10]. Moreover, G_{solv} means a solvation correction to the reaction intermediates, which was estimated to be 0.30 eV.[11] The correction accounts for the solvation of the OOH* and OH* by the solution surrounding the metal site. The reason for this correction is the following: the enthalpy difference between the gas and liquid phases of H_2O is ~0.45 eV at 298.15 K and 0.035 bar, but their free energies are identical. This principle behind this phenomenon can be ascribed to the presence of hydrogen bonds in the liquid phase, in which each H_2O creates three hydrogen bonds (include two donors and one acceptor) with adjacent molecules. Since OH* is able to create two hydrogen bonds, it will be stabilized by ~0.3 eV when solvated, and we expected OOH* to be stabilized in the same order of magnitude due to solvation effects.[12]

Generally, pH effects on electrochemical systems can be divided into three aspects[13]: i) change in the proton donor or acceptor with the electrolyte pH, ii) affect adsorbate dipolefiled interactions, and iii) induce solution-phase reactions. Since the solvation-induced adsorption free energy change is primarily associated with the formation of H-bonds with H_2O under the aqueous environment, and contribution of H-bonds might not be changed significantly with the variations of pH values. To this end, we did not consider more details about the pH effect just as many literatures[14-16] in terms of electrochemical catalysis in acidic conditions.

The overpotential (η) is adopted to evaluate the OER and ORR performance according to following equations:

$$\eta^{OER} = max\{\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4\}/e - 1.23 \quad \text{(S15)}$$

$$\eta^{OER} = max\{\Delta G_a, \Delta G_b, \Delta G_c, \Delta G_d\}/e + 1.23 \quad \text{(S16)}$$

Kinetic computations

The transition states (TS) are calculated by employing the climbing-image nudged elastic band (CI-NEB) method.[17] There are eight images between the initial state (IS) and final state (FS).

The Pt calculations are carried on a 3×3 two layers FCC(111) slab separated by

three equivalent layers of vacuum. The bottom three layers are fixed, and the top two layers are allowed to relax.

Table S1. The energies (*E*) and bond lengths for M-M and M-N in M_2/g-CN (M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Hf, Ta, W, Re, Os, Ir, Pt, Au).

M	*E* (eV)		The bond lengths (Å)			
	M-2N	M-3N	M-M	M-N1	M-N2	M-N3
Sc	-	-421.0724599	2.224	2.179	2.009	2.168
Ti	-	-424.5841186	1.975	2.187	2.031	2.148
V	-	-426.4234747	1.830	2.174	2.061	2.122
Cr	-	-425.8382477	2.078	2.098	2.007	2.071
Mn	-	-425.405069	2.395	2.056	1.906	2.005
Fe	-	-423.5734277	2.191	2.064	1.982	2.022
Co	-	-420.979397	2.253	2.032	1.935	1.998
Ni	-	-418.865846	2.403	2.011	1.888	1.978
Cu	-	-414.6877747	2.379	2.070	1.968	2.051
Zn	-410.6453237	-	2.243	2.069	2.031	-
Y	-	-423.5839285	3.095	2.435	2.147	2.365
Zr	-	-424.1222809	2.225	2.200	2.047	2.174
Nb	-	-427.8507333	2.060	2.183	2.063	2.146
Mo	-	-428.2043986	2.129	2.165	2.127	2.127
Ru	-424.1746241	-	2.193	-	1.988	1.950
Rh	-	-421.1317353	2.316	1.959	1.941	2.240
Pd	-	-417.7710435	2.407	2.077	1.979	2.055
Ag	-	-411.546058	2.633	2.406	2.234	2.420
Hf	-	-426.05604263	2.313	2.155	2.005	2.135

Ta	-	-429.3836541	2.157	2.156	2.023	2.123
W	-	-431.2287911	2.271	2.128	2.108	2.103
Re	-	-430.5398592	2.201	2.090	2.092	2.061
Os	-	-427.335763	2.250	2.057	2.040	2.053
Ir	-	-423.458621	2.345	1.952	1.970	2.155
Pt	-	-420.0054452	2.482	2.044	1.996	2.024
Au	-	-411.7909616	2.513	2.089	2.072	2.075

Table S2. The computed formation energy (E_f), dissolution potential (U_{diss}) of metals, the number of transferred electrons (N_e) during the dissolution, and the standard dissolution potential (U^0_{diss}) of metal atoms.

M	U^0_{diss} (V)	N_e	E_f (eV)	U_{diss} (eV)
Sc	-2.08	3	-4.81	-0.48
Ti	-1.63	2	-6.27	1.50
V	-1.18	2	-6.41	2.03
Cr	-0.91	2	-6.92	2.55
Mn	-1.19	2	-3.91	0.76
Fe	-0.45	2	-5.20	2.15
Co	-0.28	2	-5.72	2.58
Ni	-0.26	2	-5.53	2.51
Cu	0.34	2	-3.44	2.06
Zn	-0.76	2	-1.65	0.06
Y	-2.37	3	-6.00	-0.37
Zr	-1.45	4	-6.23	0.11
Nb	-1.10	3	-8.37	1.69
Mo	-0.20	3	-10.78	3.39
Ru	0.46	2	-6.26	3.59
Rh	0.60	2	-5.79	3.49

Pd	0.95	2	-3.76	2.83
Ag	0.80	1	-1.91	2.71
Hf	-1.55	4	-5.89	-0.08
Ta	-0.6	3	-7.58	1.93
W	0.1	3	-7.38	2.56
Re	0.3	3	-7.00	2.63
Os	0.84	8	-7.14	1.73
Ir	1.16	3	-6.95	3.48
Pt	1.18	2	-5.86	4.11
Au	1.50	3	-2.05	2.18

Table S3. The adsorption energies (E_{ad}) for H on possible sites in M_2/g-CN, the corresponding M-H bond lengths, the Gibbs free energy change for H adsorption (ΔG_{H^*}), and the charge transfer between H* and the M_2 atoms.

M	E_{ad}-T_I (eV)	E_{ad}-B_{II} (eV)	The bond length for M-H (Å)	ΔG_{H^*} (eV)	Q_e (|e|)
Ti	-	-1.01	1.859	-0.83	0.42
V	-	-0.72	1.808	-0.53	0.46
Cr	-	-1.56	1.742	-1.37	0.45
Mn	-	-1.05	1.676	-0.84	0.39
Fe	-	-0.82	1.603,1.667	-0.61	0.29
Co	-	-1.10	1.582	-0.87	0.27
Ni	-	-0.26	1.584	-0.05	0.22
Cu	-	-0.36	1.599	-0.16	0.29
Zn	-	-0.23	1.647	-0.03	0.30
Zr	-	-2.00	2.072	-1.85	0.63
Nb	-	-0.78	1.970	-0.62	0.48

Mo	-0.49	-	1.738	-0.35	0.32
Ru	-	-0.68	1.760	-0.47	0.21
Rh	-	-1.10	1.710	-0.88	0.18
Pd	-	-0.20	1.678	0.03	0.08
Ag	-	-0.63	1.747	-0.45	0.19
Ta	-	-1.63	1.937	-1.44	0.54
W	-0.52	-	1.739	-0.37	0.34
Re	-0.62	-	1.669	-0.44	0.20
Os	-	-0.63	1.838,1.741	-0.44	0.12
Ir	-	-1.22	1.733	-1.00	0.14
Pt	-	-0.38	1.695	-0.15	0.04
Au	-	-1.15	1.727	-0.94	0.07

Table S4. The adsorption energies (E_{ad}) for *I** (*I*=O, OH, OOH) on possible sites in M_2/g-CN, and the corresponding M-*I* bond lengths.

M	E_{ad}-T_I-*I** (eV)			E_{ad}-B_{II}-*I** (eV)			The bond length for M-*I* (Å)		
	I=OH	*I*=O	*I*=OOH	*I*=OH	*I*=O	*I*=OOH	*I*=OH	*I*=O	*I*=OOH
Ti	-	-	-	-2.46	-3.08	-4.97	1.992	1.828	1.817
V	-	-	-	-1.63	-1.52	-2.57	2.003	1.796	1.711,1.857
Cr	-	-	-	-2.27	-1.92	-2.10	1.953	1.780	1.784
Mn	-	-	-	-1.52	-1.39	-1.23	1.930	1.778	1.776,1.792
Fe	-	-	-	-0.88	-0.45	1.99	1.962	1.752	1.757

Co	-	-	-	- 1.28	- 0.40	1.84	1.855	1.720	1.792
Ni	-	-	-	0.20	1.12	3.38	1.903	1.751	1.875
Cu	-	-	-	- 0.21	1.26	3.02	1.917,1.860	1.787	1.876
Zn	-	-	3.56	- 0.43	0.35	-	1.942	1.804	1.955
Zr	-	-	-	- 3.72	- 4.30	-5.78	2.165	1.928,1.941	1.955
Nb	-	-		- 1.73	- 1.78	-3.01	2.144	1.953	2.423,1.769
Mo	- 1.30	-	1.83	-	- 1.10	-	1.922	1.854,2.067	1.899
Ru	-	-	-	- 0.53	0.12	2.40	2.044,2.076	1.874,1.923	1.938,1.884
Rh	-	-	-	- 0.77	0.33	2.34	2.010	1.881	1.970
Pd	-	-	-	1.07	1.94	4.21	2.040	1.914	2.145,2.282
Ag	-	-	3.12	- 0.12	2.08		2.437,2.053	1.995	2.043
Ta	-	-	-	- 2.71	- 3.21	-4.77	2.129	1.957	2.125,1.830
W	- 1.49	-	-2.64	-	- 1.35	-	1.910	1.864,2.086	1.745
Re	- 0.74	-	-	-	- 0.26	-0.32	1.929	1.952,1.972	2.029,1.880
Os	-	-	-	- 0.01	0.37	0.51	2.124,2.051	1.966,1.915	1.977,1.891

Ir	-	-	-	- 0.63	0.18	2.47	2.022	1.908	1.973
Pt	-	-	2.49	1.29	1.78		2.057	1.945	2.507
Au	- 0.12	-	3.34	-	- 1.08	-	1.953	1.961	1.964

Table S5. The Gibbs free energy change for oxygenated intermediate adsorption (ΔG_{O*}, ΔG_{OH*}, ΔG_{OOH*}) on M_2/g-CN, the overpotentials for OER (η^{OER}), and the overpotentials for ORR (η^{ORR}).

M	ΔG_{OH*} (eV)	ΔG_{OH*} under solvation correction (eV)	ΔG_{O*} (eV)	ΔG_{OOH*} (eV)	ΔG_{OOH*} (eV) under solvation correction	η^{OER} (V)	η^{ORR} (V)
Ti	-2.16	-2.46	-3.01	-4.64	-4.94	8.33	3.39
V	-1.29	-1.59	-1.47	-2.22	-2.52	5.92	2.52
Cr	-1.92	-2.22	-1.87	-1.75	-2.05	5.44	3.15
Mn	-1.18	-1.48	1.32	-0.87	-1.17	4.56	2.41
Fe	-0.54	-0.84	-0.38	2.28	1.98	1.43	1.77
Co	-0.90	-1.20	-0.33	2.20	1.90	1.49	2.13
Ni	0.56	0.26	1.20	3.74	3.44	1.31	0.67
Cu	0.14	-0.16	1.31	3.37	3.07	0.82	1.09
Zn	-0.07	-0.307	0.41	3.92	3.62	2.28	1.30
Zr	-3.42	-3.72	-4.23	-5.48	-5.78	9.17	4.65
Nb	-1.42	-1.72	-1.73	-2.68	-2.98	6.37	2.65
Mo	-0.99	-1.29	-1.05	2.16	1.86	1.97	2.22
Ru	-0.17	-0.47	0.18	2.72	2.42	1.31	1.40
Rh	-0.39	-0.69	0.40	2.70	2.40	1.07	1.62
Pd	1.44	1.14	2.00	4.54	4.24	1.31	0.85

Ag	0.17	-0.13	2.11	3.43	3.13	0.71	1.06
Ta	-2.38	-2.68	-3.16	-4.40	-4.70	8.09	3.61
W	-1.18	-1.48	-1.30	-2.26	-2.56	5.95	2.41
Re	-0.42	-0.72	-0.19	0.09	-0.21	3.60	1.65
Os	0.34	0.04	0.43	0.91	0.61	2.78	1.14
Ir	-0.25	-0.55	0.25	2.83	2.53	1.34	1.48
Pt	1.67	1.37	1.85	5.03	4.73	1.95	1.34
Au	0.18	-0.12	1.14	3.65	3.35	1.29	1.05

Table S6. The bond lengths for M_I-M_{II}, M_I-N, and M_{II}-N in M_IM_{II}/g-CN (M_I = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt, Au; M_{II} = V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt, Au; $M_I \neq M_{II}$).

M_IM_{II}/g-CN		The bond lengths (Å)						
M_I	M_{II}	M_I-M_{II}	M_I-N1	M_I-N2	M_I-N3	M_{II}-N1	M_{II}-N2	M_{II}-N3
Ti	Fe	1.958	2.207	2.177	2.164	2.046	2.020	2.092
Ti	Co	2.036	2.175	2.159	2.131	2.028	1.995	2.069
Ti	Ni	2.233	2.118	2.076	2.085	2.023	1.943	2.049
Ti	Cu	2.435	2.101	2.008	2.090	2.046	1.931	2.043
Ti	Pd	2.281	2.129	2.00	2.100	2.149	2.137	2.174
Ti	Pt	2.323	2.131	2.048	2.086	2.077	2.103	2.098
V	Ti	1.915	2.145	2.002	2.100	2.155	2.080	2.198
V	Fe	1.931	2.151	2.151	2.100	2.044	2.058	2.097
V	Co	2.110	2.130	2.084	2.099	2.027	1.981	2.063
V	Ni	2.220	2.052	2.042	2.120	2.062	1.928	1.979
V	Cu	2.455	2.085	1.960	2.083	2.023	1.930	2.046
V	Pd	2.281	2.093	1.967	2.100	2.125	2.100	2.123
V	Pt	2.320	2.086	2.011	2.108	2.076	2.121	2.063

Cr	Ti	1.835	2.122	1.982	2.071	2.181	2.142	2.228
Cr	V	1.877	2.148	2.063	2.098	2.125	2.091	2.168
Cr	Mn	2.001	2.120	2.078	2.082	2.055	2.051	2.101
Cr	Fe	2.424	2.068	1.945	2.048	1.995	1.853	2.008
Cr	Co	2.217	2.029	2.015	2.159	2.112	1.926	1.945
Cr	Ni	2.343	2.084	1.986	2.061	1.987	1.899	2.026
Cr	Cu	2.435	2.059	1.936	2.049	2.007	1.916	2.031
Cr	Zn	2.401	2.076	1.931	2.052	2.126	1.918	2.120
Cr	Zr	1.975	2.089	1.923	2.053	2.222	2.183	2.258
Cr	Nb	1.915	2.116	1.958	2.072	2.167	2.125	2.216
Cr	Mo	2.017	2.131	2.039	2.088	2.119	2.137	2.163
Cr	Ru	2.089	2.122	2.023	2.086	2.102	2.106	2.129
Cr	Rh	2.302	2.106	1.961	2.108	2.097	2.028	2.096
Cr	Pd	2.387	2.113	1.955	2.082	2.098	2.098	2.125
Cr	Ag	2.461	2.075	1.909	2.062	2.136	2.131	2.156
Cr	Ta	2.032	2.103	1.964	2.062	2.139	2.092	2.173
Cr	W	2.119	2.111	2.037	2.067	2.099	2.133	2.136
Cr	Re	2.107	2.121	2.046	2.079	2.064	2.125	2.097
Cr	Os	2.137	2.108	2.038	2.073	2.055	2.089	2.080
Cr	Ir	2.289	2.088	1.983	2.103	2.059	2.036	2.056
Cr	Pt	2.413	2.109	1.969	2.074	2.045	2.098	2.064
Cr	Au	2.466	2.036	1.871	2.004	2.071	2.150	2.093
Mn	Ti	1.911	2.111	2.010	2.071	2.172	2.159	2.216
Mn	V	2.000	2.124	2.055	2.082	2.114	2.102	2.157
Mn	Fe	2.291	2.071	1.980	2.039	2.002	1.927	2.038
Mn	Co	2.251	2.090	2.027	2.056	1.982	1.902	2.022
Mn	Ni	2.335	2.052	1.975	2.022	1.987	1.900	2.020
Mn	Cu	2.407	2.044	1.949	2.020	2.035	1.939	2.053
Mn	Pd	2.348	2.058	1.943	2.026	2.084	2.073	2.108

Mn	Pt	2.366	2.057	1.958	2.023	2.042	2.060	2.059
Fe	Co	2.206	2.064	2.003	2.021	1.991	1.927	2.032
Fe	Ni	2.327	2.033	1.946	2.005	1.989	1.898	2.015
Fe	Cu	2.361	2.052	1.952	2.028	2.050	1.950	2.062
Fe	Pd	2.315	2.026	1.911	2.006	2.072	2.033	2.089
Fe	Pt	2.343	2.023	1.927	1.997	2.040	2.034	2.055
Co	Ni	2.397	2.007	1.872	1.973	1.984	1.907	2.017
Cu	Co	2.456	2.038	1.947	2.003	1.964	1.808	1.973
Cu	Ni	2.389	2.076	1.963	2.043	2.003	1.874	2.024
Cu	Pd	2.409	2.069	1.923	2.043	2.074	2.016	2.088
Cu	Pt	2.425	2.051	1.917	2.020	2.041	1.986	2.049
Zn	Ti	2.556	2.344	2.137	-	2.245	2.026	2.108
Zn	V	2.403	2.103	1.906	2.153	2.089	1.945	2.069
Zn	Mn	2.369	2.209	1.987	2.245	2.038	1.944	2.060
Zn	Fe	2.309	2.093	1.984	2.246	2.105	1.898	1.966
Zn	Co	2.315	2.168	2.023	2.158	1.987	1.836	2.011
Zn	Ni	2.265	2.182	2.036	2.177	1.992	1.866	2.043
Zn	Cu	2.320	2.150	1.977	2.144	2.048	1.921	2.073
Zn	Pd	2.335	2.222	1.977	2.230	2.097	2.053	2.125
Zn	Pt	2.351	2.231	1.994	2.221	2.052	2.048	2.070
Zr	Ti	2.111	2.221	2.090	2.188	2.122	1.972	2.153
Zr	V	2.042	2.236	2.133	2.200	2.083	1.945	2.116
Zr	Mn	1.968	2.255	2.180	2.216	2.038	1.883	2.068
Zr	Fe	2.161	2.283	2.252	2.255	2.033	1.954	2.062
Zr	Co	2.182	2.257	2.242	2.230	2.021	1.935	2.050
Zr	Ni	2.325	2.209	2.188	2.187	2.025	1.921	2.047
Zr	Cu	2.498	2.209	2.211	2.376	-	2.034	2.074
Zr	Zn	2.722	2.266	2.252	2.399	-	-	-
Zr	Nb	2.151	2.219	2.087	2.186	2.130	2.018	2.163

Zr	Rh	2.284	2.273	2.200	2.258	2.129	2.086	2.141
Zr	Pd	2.393	2.222	2.136	2.202	2.139	2.116	2.158
Zr	Ag	2.677	2.277	2.257	2.415	-	-	-
Zr	Ta	2.190	2.211	2.074	2.181	2.116	2.003	2.146
Zr	Ir	2.359	2.270	2.203	2.250	2.064	2.065	2.080
Zr	Pt	2.444	2.232	2.151	2.205	2.073	2.106	2.091
Zr	Au	2.577	2.205	2.082	2.183	2.095	2.148	2.102
Nb	Ti	2.031	2.181	2.061	2.143	2.136	2.024	2.174
Nb	V	1.941	2.204	2.110	2.162	2.102	2.005	2.145
Nb	Mn	2.054	2.209	2.188	2.170	2.065	2.006	2.103
Nb	Fe	2.100	2.190	2.194	2.155	2.044	1.987	2.078
Nb	Co	2.151	2.157	2.175	2.125	2.025	1.950	2.057
Nb	Ni	2.287	2.131	2.125	2.110	2.033	1.921	2.041
Nb	Cu	2.432	2.136	2.102	2.254	-	2.010	2.026
Nb	Zn	2.606	2.136	2.111	2.233	-	2.164	-
Nb	Rh	2.229	2.161	2.118	2.130	2.115	2.068	2.139
Nb	Pd	2.354	2.132	2.067	2.120	2.140	2.100	2.146
Nb	Pt	2.392	2.135	2.081	2.110	2.075	2.081	2.092
Mo	Ti	1.962	2.154	2.042	2.112	2.153	2.071	2.194
Mo	V	1.926	2.171	2.064	2.127	2.103	2.015	2.154
Mo	Mn	2.080	2.148	2.156	2.113	2.073	2.015	2.108
Mo	Fe	2.070	2.134	2.157	2.102	2.029	1.988	2.072
Mo	Co	2.146	2.114	2.130	2.091	2.027	1.944	2.044
Mo	Ni	2.235	2.032	2.060	2.165	2.177	1.893	1.912
Mo	Cu	2.495	2.112	1.990	2.115	2.046	1.931	2.064
Mo	Zn	2.487	2.028	2.038	-	-	2.031	2.030
Mo	Zr	2.086	2.132	1.998	2.098	2.200	2.125	2.235
Mo	Nb	2.032	2.149	2.024	2.110	2.146	2.074	2.189
Mo	Ru	2.162	2.131	2.103	2.100	2.099	2.072	2.124

Mo	Rh	2.221	2.114	2.065	2.092	2.111	2.053	2.125
Mo	Pd	2.439	2.138	1.996	2.127	2.131	2.071	2.144
Mo	Ag	2.670	2.128	1.991	2.232	-	2.392	-
Mo	Ta	2.089	2.140	2.006	2.103	2.130	2.039	2.166
Mo	W	2.223	2.154	2.127	2.131	2.105	2.120	2.131
Mo	Re	2.201	2.147	2.125	2.112	2.065	2.094	2.099
Mo	Os	2.222	2.124	2.108	2.092	2.058	2.066	2.083
Mo	Ir	2.271	2.109	2.078	2.083	2.063	2.048	2.081
Mo	Pt	2.455	2.138	2.011	2.111	2.075	2.044	2.097
Mo	Au	2.560	2.137	1.982	2.115	2.084	2.136	2.097
Ru	Ti	2.051	2.118	2.091	2.094	2.157	2.113	2.196
Ru	V	2.050	2.132	2.125	2.103	2.098	2.073	2.139
Ru	Mn	2.275	2.101	2.004	2.090	2.082	1.973	2.110
Ru	Fe	2.146	2.003	2.028	2.221	2.234	1.921	1.916
Ru	Co	2.205	1.991	2.005	2.219	2.228	1.873	1.887
Ru	Ni	2.311	2.030	1.998	2.096	2.050	1.901	1.981
Ru	Cu	2.484	2.050	1.904	2.058	2.040	1.948	2.079
Ru	Zn	2.454	2.065	1.903	2.123	-	2.020	2.189
Ru	Zr	2.264	2.103	2.023	2.114	2.273	2.234	2.285
Ru	Nb	2.170	2.123	2.080	2.103	2.167	2.159	2.197
Ru	Rh	2.333	1.994	1.937	2.214	2.222	1.959	2.009
Ru	Pd	2.496	2.103	1.910	2.082	2.116	2.048	2.145
Ru	Ag	2.590	2.080	1.875	2.104	2.537	2.285	2.518
Ru	Ta	2.230	2.112	2.065	2.083	2.138	2.143	2.169
Ru	Ir	2.432	2.059	1.944	2.120	2.080	1.966	2.060
Ru	Pt	2.502	2.096	1.920	2.068	2.068	2.003	2.090
Ru	Au	2.535	2.070	1.906	2.047	2.076	2.134	2.098
Rh	Ti	2.115	2.138	2.117	2.114	2.132	2.089	2.170
Rh	V	2.123	2.140	2.107	2.116	2.089	2.033	2.122

Rh	Mn	2.312	2.095	2.015	2.075	2.071	1.996	2.114
Rh	Fe	2.256	2.068	2.017	2.065	2.022	1.966	2.043
Rh	Co	2.295	2.023	1.991	2.121	2.082	1.903	1.964
Rh	Ni	2.391	2.055	1.959	2.041	1.982	1.885	2.031
Rh	Cu	2.446	2.041	1.917	2.042	2.006	1.921	2.042
Rh	Zn	2.378	2.046	1.925	2.055	2.142	1.944	2.127
Rh	Pd	2.475	2.086	1.937	2.060	2.093	2.046	2.126
Rh	Pt	2.494	2.087	1.952	2.052	2.049	2.029	2.072
Pd	Co	2.364	2.098	2.041	2.070	1.973	1.846	2.009
Pd	Ni	2.374	2.088	2.013	2.067	1.982	1.858	2.020
Pd	Pt	2.464	2.086	2.006	2.062	2.036	1.993	2.052
Ag	Ti	2.594	-	-	-	2.273	2.053	2.195
Ag	V	2.604	2.478	2.256	-	2.176	1.946	2.123
Ag	Mn	2.395	2.117	2.070	2.096	2.001	1.860	2.016
Ag	Fe	2.397	2.128	2.089	2.100	1.986	1.818	1.998
Ag	Co	2.389	2.137	2.106	2.107	1.967	1.782	1.979
Ag	Ni	2.360	2.157	2.110	2.133	2.007	1.825	2.024
Ag	Cu	2.386	2.160	2.174	2.150	2.056	1.909	2.059
Ag	Zn	2.367	2.193	2.122	2.170	2.157	1.916	2.140
Ag	Nb	2.638	-	-	-	2.257	2.099	2.181
Ag	Rh	2.432	2.123	2.058	2.093	2.033	1.889	2.036
Ag	Pd	2.474	2.181	2.117	2.159	2.078	1.992	2.087
Ag	Pt	2.486	2.143	2.090	2.119	2.039	1.969	2.046
Ta	Ti	2.078	2.160	2.037	2.126	2.130	2.012	2.166
Ta	V	2.003	2.179	2.072	2.139	2.092	1.986	2.136
Ta	Mn	2.180	2.183	2.160	2.151	2.054	1.995	2.090
Ta	Fe	2.169	2.157	2.168	2.125	2.025	1.977	2.064
Ta	Co	2.209	2.132	2.150	2.102	2.012	1.940	2.050
Ta	Ni	2.301	2.110	2.110	2.082	2.013	1.918	2.039

Ta	Cu	2.411	2.118	2.073	2.214	-	2.031	2.029
Ta	Zn	2.557	2.094	2.084	2.243	-	2.083	2.173
Ta	Nb	2.111	2.163	2.035	2.130	2.139	2.044	2.175
Ta	Rh	2.276	2.135	2.103	2.106	2.100	2.058	2.128
Ta	Pd	2.368	2.114	2.062	2.092	2.130	2.102	2.144
Ta	Ag	2.622	2.157	2.070	2.217	-	-	-
Ta	Pt	2.402	2.116	2.080	2.087	2.067	2.080	2.090
W	Ti	2.025	2.129	2.011	2.094	2.144	2.050	2.184
W	V	1.994	2.139	2.021	2.104	2.094	1.994	2.144
W	Mn	2.150	2.112	2.133	2.079	2.057	2.011	2.096
W	Fe	2.162	2.099	2.125	2.068	2.022	1.981	2.063
W	Co	2.189	2.083	2.113	2.056	2.009	1.948	2.043
W	Ni	2.257	2.038	2.076	2.054	2.049	1.913	1.974
W	Cu	2.441	2.062	1.986	2.063	2.059	1.927	2.068
W	Zn	2.482	2.016	2.024	-	-	2.023	2.019
W	Zr	2.139	2.114	1.980	2.083	2.192	2.103	2.225
W	Nb	2.091	2.126	1.996	2.092	2.140	2.053	2.178
W	Ru	2.215	2.095	2.093	2.066	2.085	2.065	2.114
W	Rh	2.259	2.086	2.057	2.056	2.095	2.052	2.117
W	Pd	2.353	2.044	2.013	2.077	2.161	2.093	2.091
W	Ag	2.609	2.104	2.002	2.176	-	-	-
W	Ta	2.142	2.117	1.986	2.085	2.123	2.027	2.156
W	Re	2.242	2.119	2.112	2.087	2.066	2.087	2.092
W	Os	2.257	2.093	2.097	2.063	2.055	2.063	2.082
W	Ir	2.297	2.076	2.075	2.050	2.054	2.051	2.074
W	Pt	2.378	2.051	2.040	2.056	2.079	2.077	2.065
W	Au	2.545	2.091	1.974	2.073	2.085	2.122	2.094
Re	Ti	2.032	2.102	2.008	2.074	2.141	2.066	2.182
Re	V	2.095	2.104	2.116	2.072	2.096	2.084	2.145

Re	Mn	2.141	2.089	2.094	2.063	2.049	2.016	2.091
Re	Fe	2.105	2.076	2.106	2.053	2.023	2.003	2.061
Re	Co	2.156	2.020	2.061	2.115	2.179	1.938	1.916
Re	Ni	2.308	2.048	2.028	2.044	2.003	1.909	2.015
Re	Cu	2.436	2.051	1.963	2.046	2.043	1.930	2.063
Re	Zn	2.336	1.956	1.971	-	-	1.908	1.899
Re	Zr	2.136	2.090	1.955	2.066	2.186	2.098	2.222
Re	Nb	2.253	2.093	2.082	2.076	2.189	2.174	2.213
Re	Ru	2.210	2.080	2.053	2.058	2.089	2.056	2.111
Re	Rh	2.246	1.985	1.994	2.153	2.247	2.024	1.977
Re	Pd	2.423	2.078	1.977	2.061	2.108	2.075	2.134
Re	Ag	2.587	2.074	1.934	2.108	-	2.315	-
Re	Ta	2.287	2.093	2.073	2.072	2.159	2.151	2.190
Re	Os	2.227	2.076	2.073	2.053	2.053	2.063	2.077
Re	Ir	2.278	2.055	2.039	2.054	2.065	2.039	2.063
Re	Pt	2.446	2.076	1.993	2.058	2.062	2.051	2.084
Re	Au	2.505	2.054	1.963	2.039	2.069	2.100	2.085
Os	Ti	2.156	2.074	2.077	2.051	2.151	2.113	2.188
Os	V	2.122	2.083	2.108	2.057	2.080	2.080	2.125
Os	Mn	2.236	2.041	2.022	2.080	2.146	1.988	2.030
Os	Fe	2.164	1.999	2.032	2.129	2.206	1.958	1.918
Os	Co	2.211	1.990	2.005	2.138	2.211	1.904	1.891
Os	Ni	2.319	2.027	1.995	2.036	2.013	1.915	2.009
Os	Cu	2.471	2.032	1.907	2.036	2.039	1.948	2.088
Os	Zn	2.432	1.968	1.924	-	-	2.024	2.031
Os	Zr	2.349	2.071	2.026	2.072	2.276	2.230	2.290
Os	Nb	2.246	2.080	2.073	2.058	2.158	2.160	2.189
Os	Ru	2.272	2.045	2.001	2.090	2.140	2.010	2.057
Os	Rh	2.348	1.996	1.942	2.138	2.219	1.979	2.007

Os	Pd	2.482	2.061	1.924	2.057	2.126	2.057	2.125
Os	Ag	2.585	2.058	1.883	2.073	2.518	2.280	2.507
Os	Ta	2.277	2.079	2.062	2.052	2.133	2.147	2.159
Os	Ir	2.368	2.000	1.963	2.125	2.129	1.980	2.013
Os	Pt	2.497	2.069	1.934	2.045	2.063	2.008	2.091
Os	Au	2.534	2.042	1.911	2.026	2.078	2.118	2.099
Ir	Ti	2.199	2.078	2.096	2.057	2.123	2.099	2.159
Ir	V	2.189	2.081	2.087	2.062	2.072	2.045	2.113
Ir	Mn	2.330	2.053	2.005	2.035	2.063	1.995	2.103
Ir	Fe	2.282	2.042	2.014	2.031	2.006	1.975	2.046
Ir	Co	2.294	2.026	2.004	2.046	2.025	1.932	2.000
Ir	Ni	2.403	2.031	1.961	2.019	1.977	1.889	2.027
Ir	Cu	2.449	2.023	1.923	2.023	2.000	1.915	2.041
Ir	Zn	2.386	2.028	1.935	2.029	2.138	1.949	2.133
Ir	Nb	2.290	2.086	2.059	2.066	2.123	2.130	2.155
Ir	Rh	2.330	1.960	1.942	2.167	2.242	1.963	1.948
Ir	Pd	2.484	2.053	1.939	2.033	2.087	2.045	2.123
Ir	Ag	2.497	2.032	1.907	2.026	2.119	2.103	2.147
Ir	Ta	2.317	2.084	2.053	2.062	2.100	2.115	2.128
Ir	Pt	2.505	2.051	1.953	2.026	2.044	2.029	2.069
Pt	Co	2.388	2.053	2.031	2.035	1.967	1.866	2.004
Pt	Ni	2.399	2.050	2.007	2.035	1.971	1.867	2.015
Au	Ti	2.483	2.095	2.150	2.082	2.085	1.978	2.107
Au	V	2.407	2.075	2.082	2.059	2.038	1.939	2.051
Au	Mn	2.410	2.074	2.074	2.056	1.991	1.885	2.016
Au	Fe	2.414	2.076	2.086	2.058	1.973	1.845	1.998
Au	Co	2.412	2.087	2.101	2.059	1.953	1.803	1.978
Au	Ni	2.403	2.082	2.073	2.062	1.979	1.837	2.008
Au	Cu	2.419	2.089	2.171	2.079	2.052	1.920	2.062

Au	Zn	2.338	2.101	2.066	2.075	2.148	1.929	2.137
Au	Nb	2.519	2.096	2.136	2.109	2.113	2.028	2.113
Au	Rh	2.464	2.072	2.061	2.048	2.014	1.906	2.029
Au	Pd	2.450	2.069	2.035	2.047	2.041	1.949	2.058
Au	Ag	2.604	2.141	2.209	2.126	2.477	2.213	2.491
Au	Ta	2.512	2.096	2.129	2.099	2.079	2.020	2.095
Au	Ir	2.483	2.066	2.048	2.042	2.001	1.919	2.013
Au	Pt	2.475	2.062	2.038	2.046	2.022	1.954	2.035

Table S7. The adsorption energies (E_{ad}) for H on possible sites in M_IM_{II}/g-CN (M_I = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt, Au; M_{II} = V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt, Au; $M_I \neq M_{II}$), the corresponding M_I-H and M_{II}-H bond lengths, and ΔG_{H^*}.

M_IM_{II}/g-CN		The bond length for M_I-H (Å)	The bond length for M_{II}-H (Å)	ΔG_{H^*} (eV)	E_{ad} (eV)
M_I	M_{II}				
Ti	Fe	1.868	1.706	-0.35	-0.53
Ti	Co	1.869	1.635	-0.19	-0.38
Ti	Ni	1.831	1.606	-0.49	-0.69
Ti	Cu	1.908	1.573	-0.92	-1.11
Ti	Pd	1.724	-	-0.26	-0.38
Ti	Pt	1.930	1.644	-0.28	-0.50
V	Ti	1.759	1.913	-0.74	-0.92
V	Fe	1.765	1.756	-0.50	-0.68
V	Co	1.801	1.558	-0.49	-0.71
V	Ni	1.777	1.591	-0.41	-0.62
V	Cu	1.816	1.591	-0.55	-0.55
V	Pd	1.646	-	-0.15	-0.35

V	Pt	1.869	1.636	-0.42	-0.65
Cr	Ti	1.724	1.880	-0.61	-0.80
Cr	V	1.745	1.762	-0.68	-0.86
Cr	Mn	1.746	1.683	-0.92	-1.12
Cr	Fe	1.735	1.616	-0.80	-1.01
Cr	Co	1.760	1.554	-0.92	-1.14
Cr	Ni	1.745	1.567	-0.50	-0.71
Cr	Cu	1.770	1.593	-0.44	-0.64
Cr	Zn	1.788	1.609	-0.83	-1.03
Cr	Zr	1.706	-	-0.62	-0.80
Cr	Nb	1.745	1.895	-0.66	-0.85
Cr	Mo	1.812	1.785	-0.58	-0.78
Cr	Ru	1.911	1.681	-0.68	-0.88
Cr	Rh	1.841	1.649	-0.96	-1.18
Cr	Pd	1.778	1.639	-0.16	-0.38
Cr	Ag	1.874	1.697	-0.54	-0.71
Cr	Ta	1.789	1.812	-1.04	-1.25
Cr	W	1.860	1.740	-0.73	-0.93
Cr	Re	-	1.676	-0.28	-0.47
Cr	Os	-	1.667	-0.86	-1.06
Cr	Ir	1.893	1.656	-1.14	-1.36
Cr	Pt	1.825	1.627	-0.53	-0.77
Cr	Au	-	1.584	-1.74	-1.94
Mn	Ti	1.658	1.874	-0.78	-0.98
Mn	V	1.752	1.779	-0.48	-0.67
Mn	Fe	1.714	1.605	-0.82	-1.04
Mn	Co	1.740	1.546	-0.69	-0.91
Mn	Ni	1.690	1.588	-0.41	-0.61
Mn	Cu	1.691	1.613	-0.38	-0.58

Mn	Pd	1.683	1.699	-0.20	-0.40
Mn	Pt	1.746	1.642	-0.33	-0.55
Fe	Co	1.653	1.565	-0.62	-0.84
Fe	Ni	1.621	1.588	-0.39	-0.61
Fe	Cu	1.632	1.622	-0.39	-0.60
Fe	Pd	1.616	1.689	-0.24	-0.46
Fe	Pt	1.657	1.656	-0.27	-0.50
Co	Ni	1.571	1.602	-0.77	-0.99
Cu	Co	1.632	1.575	-0.37	-0.59
Cu	Ni	1.603	1.575	-0.16	-0.37
Cu	Pd	1.621	1.655	-0.02	-0.24
Cu	Pt	1.666	1.652	-0.29	-0.52
Zn	Ti	1.587	-	-0.46	-0.65
Zn	V	1.591	-	-1.26	-1.46
Zn	Mn	1.621	1.779	-0.35	-0.54
Zn	Fe	1.658	1.622	-0.68	-0.89
Zn	Co	1.672	1.559	-0.85	-1.07
Zn	Ni	1.665	1.574	-0.26	-0.47
Zn	Cu	1.657	1.602	-0.43	-0.63
Zn	Pd	1.702	1.664	-0.06	-0.26
Zn	Pt	1.791	1.621	-0.31	-0.54
Zr	Ti	1.954	1.857	-1.05	-1.24
Zr	V	2.056	1.767	-0.88	-1.06
Zr	Mn	1.977	1.665	-1.07	-1.27
Zr	Fe	2.060	1.663	-0.32	-0.48
Zr	Co	2.063	1.627	-0.05	-0.23
Zr	Ni	1.875	-	-0.40	-0.54
Zr	Cu	2.042	1.581	-1.20	-1.39
Zr	Zn	-	1.569	0.24	0.10

Zr	Nb	-	1.889	-1.21	-1.37
Zr	Rh	-	1.648	0.26	0.08
Zr	Pd	1.882	-	-0.33	-0.54
Zr	Ag	1.847	-	0.36	-0.04
Zr	Ta	-	1.886	-1.65	-1.82
Zr	Ir	-	1.643	0.14	-0.08
Zr	Pt	2.050	1.655	-0.18	-0.40
Zr	Au	1.876	-	-0.44	-0.69
Nb	Ti	1.862	-	-0.85	-1.03
Nb	V	1.958	1.816	-0.49	-0.67
Nb	Mn	1.927	1.776	-0.45	-0.61
Nb	Fe	1.913	1.781	-0.32	-0.49
Nb	Co	1.935	1.684	-0.10	-0.28
Nb	Ni	1.769	-	-0.69	-0.85
Nb	Cu	1.909	1.613	-1.06	-1.25
Nb	Zn	1.729	-	-0.33	-0.51
Nb	Rh	1.789	-	-0.24	-0.38
Nb	Pd	1.779	-	-0.60	-0.76
Nb	Pt	1.911	1.705	-0.12	-0.33
Mo	Ti	1.841	-	-0.53	-0.70
Mo	V	1.887	1.770	-0.70	-0.89
Mo	Mn	1.793	-	-0.51	-0.67
Mo	Fe	1.809	1.859	-0.48	-0.65
Mo	Co	1.829	1.667	-0.31	-0.50
Mo	Ni	1.750	1.770	-0.58	-0.79
Mo	Cu	1.799	1.658	-0.61	-0.80
Mo	Zn	1.732	-	-0.24	-0.41
Mo	Zr	1.812	-	-0.79	-0.95
Mo	Nb	1.899	1.874	-0.63	-0.83

Mo	Ru	-	1.662	0.09	-0.08
Mo	Rh	1.699	-	-0.62	-0.79
Mo	Pd	1.686	-	-0.56	-0.74
Mo	Ag	1.677	-	-0.45	-0.63
Mo	Ta	1.935	1.815	-1.19	-1.40
Mo	W	-	1.736	-0.61	-0.81
Mo	Re	-	1.671	-0.31	-0.50
Mo	Os	-	1.650	0.05	-0.13
Mo	Ir	1.701	-	-0.62	-0.80
Mo	Pt	1.878	1.685	-0.25	-0.46
Mo	Au	1.701	-	-0.44	-0.60
Ru	Ti	1.628	-	-0.08	-0.26
Ru	V	1.644	-	0	-0.18
Ru	Mn	1.690	1.854	-0.92	-1.13
Ru	Fe	1.693	1.795	-0.93	-1.12
Ru	Co	1.705	1.643	-0.76	-0.97
Ru	Ni	1.660	1.694	-0.76	-0.97
Ru	Cu	1.634	-	-0.68	-0.87
Ru	Zn	1.731	1.740	-0.81	-1.03
Ru	Zr	1.618	-	-0.18	-0.38
Ru	Nb	1.619	-	0.06	-0.13
Ru	Rh	1.695	1.814	-0.36	-0.55
Ru	Pd	1.709	1.770	-0.30	-0.50
Ru	Ag	1.588	-	-0.37	-0.56
Ru	Ta	1.650	-	0.03	-0.16
Ru	Ir	1.783	1.736	-0.47	-0.67
Ru	Pt	1.697	1.741	-0.62	-0.84
Ru	Au	1.577	-	-0.53	-0.72
Rh	Ti	1.671	1.904	-0.59	-0.80

Rh	V	1.659	-	-0.51	-0.72
Rh	Mn	1.639	1.809	-0.80	-1.02
Rh	Fe	1.658	1.683	-0.64	-0.85
Rh	Co	1.673	1.618	-0.90	-1.13
Rh	Ni	1.658	1.626	-0.85	-1.07
Rh	Cu	1.670	1.666	-0.32	-0.53
Rh	Zn	1.655	1.743	-1.12	-1.33
Rh	Pd	1.653	1.732	-0.53	-0.74
Rh	Pt	1.693	1.694	-0.75	-0.98
Pd	Co	1.698	1.567	-0.66	-0.88
Pd	Ni	1.676	1.582	0	-0.22
Pd	Pt	1.731	1.657	-0.08	-0.30
Ag	Ti	1.719	-	-0.51	-0.68
Ag	V	1.717	-	-0.70	-0.87
Ag	Mn	1.696	1.906	-0.68	-0.84
Ag	Fe	1.732	1.683	-0.35	-0.54
Ag	Co	1.780	1.582	-0.20	-0.40
Ag	Ni	1.721	1.651	-0.20	-0.39
Ag	Cu	1.722	1.630	-0.29	-0.48
Ag	Zn	1.709	1.710	-0.62	-0.81
Ag	Nb	-	1.755	-0.05	-0.21
Ag	Rh	1.759	1.711	-0.38	-0.57
Ag	Pd	2.070	1.571	0.13	-0.09
Ag	Pt	1.766	1.673	0	-0.21
Ta	Ti	1.850	-	-1.18	-1.36
Ta	V	1.893	1.853	-0.96	-1.15
Ta	Mn	1.880	1.850	-0.67	-0.84
Ta	Fe	1.867	1.901	-0.51	-0.67
Ta	Co	1.881	1.789	-0.31	-0.47

Ta	Ni	1.767	-	-0.96	-1.13
Ta	Cu	1.900	1.609	-1.05	-1.24
Ta	Zn	1.720	-	-0.36	-0.56
Ta	Nb	1.893	-	-1.08	-1.26
Ta	Rh	1.785	-	-0.50	-0.66
Ta	Pd	1.777	-	-0.94	-1.10
Ta	Ag	1.759	-	-0.37	-0.54
Ta	Pt	1.925	1.694	-0.10	-0.30
W	Ti	1.817	-	-1.00	-1.19
W	V	1.846	1.802	-1.36	-1.56
W	Mn	1.743	1.822	-0.38	-0.57
W	Fe	1.712	-	-0.71	-0.88
W	Co	1.790	1.665	-0.43	-0.62
W	Ni	1.689	-	-0.92	-1.10
W	Cu	1.812	1.672	-0.79	-0.98
W	Zn	1.677	-	-0.56	-0.75
W	Zr	1.801	-	-1.25	-1.44
W	Nb	-	1.898	-1.31	-1.50
W	Ru	1.712	-	-0.41	-0.58
W	Rh	1.850	1.724	-0.31	-0.51
W	Pd	1.699	-	-0.92	-1.10
W	Ag	1.702	-	-0.79	-0.98
W	Ta	-	1.838	-1.66	-1.87
W	Re	-	1.718	-0.23	-0.40
W	Os	-	1.705	-0.05	-0.23
W	Ir	1.711	-	-0.90	-1.09
W	Pt	1.707	-	-0.97	-1.16
W	Au	1.696	-	-0.99	-1.17
Re	Ti	1.674	-	-0.67	-0.86

Re	V	1.674	-	-0.44	-0.64
Re	Mn	1.645	-	-0.44	-0.60
Re	Fe	1.720	-	-0.69	-0.84
Re	Co	1.745	1.710	-0.78	-0.97
Re	Ni	1.635	-	-1.01	-1.21
Re	Cu	1.644	-	-0.90	-1.09
Re	Zn	1.641	-	-1.23	-1.43
Re	Zr	1.773	2.046	-1.74	-1.95
Re	Nb	1.670	-	-0.37	-0.57
Re	Ru	1.790	1.799	-0.30	-0.48
Re	Rh	1.655	-	-1.04	-1.23
Re	Pd	1.651	-	-0.78	-0.96
Re	Ag	1.656	-	-0.78	-0.97
Re	Ta	1.679	-	-0.36	-0.56
Re	Os	1.659	-	-0.82	-1.02
Re	Ir	1.787	1.775	-0.30	-0.50
Re	Pt	1.742	1.788	-0.37	-0.56
Re	Au	1.632	-	-0.60	-0.81
Os	Ti	1.624	-	-0.22	-0.41
Os	V	1.637	-	-0.08	-0.26
Os	Mn	1.690	-	-1.02	-1.22
Os	Fe	1.692	1.864	-1.07	-1.27
Os	Co	1.702	1.709	-0.99	-1.20
Os	Ni	1.674	1.747	-0.88	-1.08
Os	Cu	1.685	1.797	-0.83	-1.03
Os	Zn	1.711	-	-0.99	-1.19
Os	Zr	1.710	2.086	-1.28	-1.48
Os	Nb	1.735	1.977	-0.83	-1.02
Os	Ru	1.620	-	-0.63	-0.82

Os	Rh	1.715	1.848	-0.59	-0.79
Os	Pd	1.604	-	-0.71	-0.90
Os	Ag	1.619	-	-0.67	-0.85
Os	Ta	1.635	-	0.05	-0.14
Os	Ir	1.745	1.773	-0.66	-0.87
Os	Pt	1.701	1.777	-0.69	-0.91
Os	Au	1.607	-	-0.88	-1.06
Ir	Ti	1.665	-	-0.85	-1.07
Ir	V	1.657	-	-0.78	-1.00
Ir	Mn	1.646	1.874	-0.97	-1.19
Ir	Fe	1.655	1.743	-0.81	-1.02
Ir	Co	1.681	1.648	-0.98	-1.20
Ir	Ni	1.665	1.663	-0.98	-1.20
Ir	Cu	1.671	1.713	-0.48	-0.70
Ir	Zn	1.655	1.823	-1.30	-1.52
Ir	Nb	1.693	-	0.26	0.07
Ir	Rh	1.707	1.752	-1.00	-1.21
Ir	Pd	1.660	1.766	-0.65	-0.87
Ir	Ag	1.632	-	-0.21	-0.41
Ir	Ta	1.739	-	0.19	0.02
Ir	Pt	1.693	1.726	-0.80	-1.02
Pt	Co	1.668	1.608	-0.87	-1.10
Pt	Ni	1.656	1.626	-0.19	-0.42
Au	Ti	-	1.718	-0.13	-0.45
Au	V	1.580	-	-1.18	-1.38
Au	Mn	1.579	-	-0.51	-0.71
Au	Fe	-	1.542	0.02	-0.16
Au	Co	1.797	1.565	0.05	-0.15
Au	Ni	1.615	-	0.08	-0.12

Au	Cu	1.628	1.812	-0.43	-0.63
Au	Zn	1.599	-	-0.68	-0.88
Au	Nb	-	1.772	-0.63	-0.78
Au	Rh	1.843	1.640	-0.09	-0.29
Au	Pd	1.569	-	0.19	-0.01
Au	Ag	1.568	-	-1.15	-1.36
Au	Ta	-	1.770	-0.97	-1.14
Au	Ir	-	1.586	-0.13	-0.30
Au	Pt	1.812	1.664	0.56	0.35

Table S8. The adsorption energies (E_{ad}) for OH on possible sites in M_IM_{II}/g-CN (M_I = Fe, Co, Ni, Cu, Zn, Mo, Ru, Rh, Pd, Ag, Re, Os, Ir, Pt, Au; M_{II} = Co, Ni, Cu, Zn, Mo, Ru, Rh, Pd, Ag, Re, Os, Ir, Pt, Au; $M_I \neq M_{II}$), the corresponding M_I-OH and M_{II}-OH bond lengths, and the Gibbs free energy change for OH adsorption (ΔG_{OH*}).

M_IM_{II}/g-CN		E_{ad} (eV)	The bond length for M_I-OH (Å)	The bond length for M_{II}-OH (Å)	ΔG_{OH*} (eV)	ΔG_{OH*} under solvation correction (eV)
M_I	M_{II}					
Fe	Co	-0.85	1.921	1.930	-0.51	-0.81
Fe	Ni	-0.59	1.883	1.965	-0.24	-0.54
Fe	Cu	-0.49	1.867	1.998	-0.14	-0.44
Fe	Pd	0.00	1.816	-	0.25	-0.05
Fe	Pt	0.03	1.906	2.064	0.41	0.11
Co	Ni	-0.69	1.858	1.910	-0.31	-0.61
Cu	Co	-0.45	1.968	1.863	-0.09	-0.39
Cu	Ni	0.06	1.936	1.892	0.41	0.11
Cu	Pd	0.48	1.917	2.073	0.82	0.52

Cu	Pt	0.33	2.012	2.053	0.67	0.37
Zn	Fe	-0.80	2.059	1.897	-0.46	-0.76
Zn	Co	-1.14	1.994	1.869	-0.78	-1.08
Zn	Ni	-0.29	1.948	1.929	0.01	-0.29
Zn	Cu	-0.63	1.950	1.888	-0.16	-0.46
Zn	Pd	0.25	1.971	2.139	0.70	0.40
Zn	Pt	0.13	2.012	2.065	0.43	0.13
Mo	Fe	-1.32	1.989	2.220	-1.02	-1.32
Mo	Co	-1.43	1.898	-	-1.15	-1.45
Mo	Ni	-1.49	1.866	-	-1.22	-1.52
Mo	Cu	-1.49	1.870	-	-1.21	-1.51
Mo	Zn	-1.26	1.905	-	-0.98	-1.28
Mo	Ru	-1.02	1.918	-	-0.73	-1.03
Mo	Rh	-1.39	1.909	-	-1.11	-1.41
Mo	Pd	-1.62	1.894	-	-1.33	-1.63
Mo	Ag	-1.41	1.878	-	-1.11	-1.41
Mo	Re	-0.77	2.146	2.055	-1.02	-1.32
Mo	Os	-1.23	1.904	-	-0.92	-1.22
Mo	Ir	-1.44	1.905	-	-1.14	-1.44
Mo	Pt	-0.10	2.029	2.065	0.27	-0.03
Mo	Au	-1.55	1.865	-	-1.27	-1.57
Ru	Fe	-1.21	2.039	2.014	-0.85	-1.15
Ru	Co	-0.97	2.010	1.956	-0.61	-0.91
Ru	Ni	-0.77	1.998	2.008	-0.42	-0.72
Ru	Cu	-0.61	2.007	2.033	-0.26	-0.56
Ru	Zn	-1.23	2.034	2.111	-0.88	-1.18
Ru	Rh	-0.48	2.031	2.027	-0.11	-0.41
Ru	Pd	-0.62	1.915	-	-0.31	-0.61
Ru	Ag	-0.61	1.925	-	-0.30	-0.60

Ru	Ir	-0.45	2.041	2.035	-0.08	-0.38
Ru	Pt	-0.11	2.044	2.037	0.26	-0.04
Ru	Au	-0.12	1.931	-	0.19	-0.11
Rh	Fe	-0.74	2.039	1.910	-0.37	-0.67
Rh	Co	-1.00	2.013	1.860	-0.62	-0.92
Rh	Ni	-0.49	2.018	1.927	-0.13	-0.43
Rh	Cu	-0.10	2.030	1.971	0.25	-0.05
Rh	Zn	-1.20	2.046	2.014	-0.85	-1.15
Rh	Pd	0.24	1.991	2.227	0.59	0.29
Rh	Pt	0.09	2.023	2.039	0.46	0.16
Pd	Co	-0.26	2.046	1.840	0.12	-0.18
Pd	Ni	0.68	2.046	1.891	1.04	0.74
Pd	Pt	1.15	2.215	2.039	1.50	1.20
Ag	Fe	-0.57	-	1.816	-0.25	-0.55
Ag	Co	-0.28	-	1.797	0.05	-0.25
Ag	Ni	-0.20	-	1.787	0.08	-0.22
Ag	Cu	-0.37	2.405	1.815	-0.06	-0.36
Ag	Zn	-0.65	2.116	1.967	-0.31	-0.61
Ag	Rh	-0.29	-	1.957	0.04	-0.26
Ag	Pd	0.42	-	1.973	0.75	0.45
Ag	Pt	0.80	2.069	2.122	1.15	0.85
Re	Fe	-1.03	1.993	2.199	-0.74	-1.04
Re	Co	-1.27	1.913	-	-0.99	-1.29
Re	Ni	-1.26	1.904	-	-0.95	-1.25
Re	Cu	-1.39	1.918	-	-1.09	-1.39
Re	Zn	-1.82	1.913	-	-1.53	-1.83
Re	Ru	-0.13	2.040	2.086	0.23	-0.07
Re	Rh	-1.54	1.922	-	-1.24	-1.54
Re	Pd	-1.31	1.906	-	-1.00	-1.30

Re	Ag	-1.40	1.918	-	-1.11	-1.41
Re	Os	-1.06	1.937	-	-1.06	-1.36
Re	Ir	-0.12	2.048	2.068	0.25	-0.05
Re	Pt	-1.40	1.909	-	-1.08	-1.38
Re	Au	-1.12	1.901	-	-0.81	-1.11
Os	Fe	-1.23	2.042	2.046	-0.88	-1.18
Os	Co	-0.97	2.012	1.995	-0.62	-0.92
Os	Ni	-0.79	1.997	2.066	-0.45	-0.75
Os	Cu	-0.85	1.995	2.113	-0.51	-0.81
Os	Zn	-1.41	2.012	2.252	-1.07	-1.37
Os	Ru	-0.43	2.035	2.126	-0.08	-0.38
Os	Rh	-0.86	1.926	-	-0.54	-0.84
Os	Pd	-0.91	1.922	-	-0.59	-0.89
Os	Ag	-0.99	1.935	-	-0.66	-0.96
Os	Ir	-0.81	1.928	-	-0.49	-0.79
Os	Pt	-1.05	1.919	-	-0.72	-1.02
Os	Au	-0.73	1.933	-	-0.41	-0.71
Ir	Fe	-0.64	2.043	1.932	-0.27	-0.57
Ir	Co	-0.89	2.014	1.895	-0.51	-0.81
Ir	Ni	-0.52	2.023	1.956	-0.15	-0.45
Ir	Cu	-0.18	2.028	2.020	0.17	-0.13
Ir	Zn	-1.26	2.051	2.059	-0.90	-1.20
Ir	Rh	-0.75	2.004	2.046	-0.37	-0.67
Ir	Pd	0.16	1.999	2.351	0.50	0.20
Ir	Ag	-0.26	1.969	-	0.07	-0.23
Ir	Pt	0.17	2.018	2.074	0.55	0.25
Pt	Co	-0.33	2.040	1.859	0.05	-0.25
Pt	Ni	0.64	2.048	1.932	1.01	0.71
Au	Fe	0.08	-	1.829	0.24	-0.06

Au	Co	0.46	-	1.844	0.75	0.45
Au	Ni	1.02	-	1.912	1.33	1.03
Au	Cu	-0.14	2.038	1.963	0.21	-0.09
Au	Zn	0.20	-	1.843	0.48	0.18
Au	Rh	0.58	-	1.974	0.90	0.60
Au	Pd	1.39	-	2.009	1.71	1.41
Au	Ag	-0.73	1.961	-	-0.44	-0.74
Au	Ir	0.47	-	1.991	0.79	0.49
Au	Pt	1.34	-	2.041	1.64	1.34

Table S9. The adsorption energies (E_{ad}) for *I** (*I*=O, OH, OOH) on possible sites in M_IM_{II}/g-CN (M_IM_{II} = FePd, FePt, CuNi, CuPd, CuPt, ZnNi, ZnPd, ZnPt, MoPt, RuPt, RuAu, RhCu, RhPd, RhPt, PdCo, PdNi, PdPt, AgCo, AgNi, AgCu, AgRh, AgPd, AgPt, ReIr, IrCu, IrPd, IrAg, IrPt, PtCo, PtNi, AuFe, AuCo, AuNi, AuCu, AuZn, AuRh, AuPd, AuIr, AuPt), and the corresponding M_I-*I* and M_{II}-*I* bond lengths.

M_IM_{II}/g-CN		E_{ad}-*I** (eV)			The bond length for M_I-*I* (Å)			The bond length for M_{II}-*I* (Å)		
M_I	M_{II}	*I*=OH	*I*=O	*I*=OOH	*I*=OH	*I*=O	*I*=OOH	*I*=OH	*I*=O	*I*=OOH
Fe	Pd	0.70	0.00	3.01	1.816	1.701	1.705	-	1.993	-
Fe	Pt	0.03	0.70	1.46	1.906	1.723	1.743	2.064	1.985	1.986
Cu	Ni	0.06	1.35	3.13	1.936	1.804	1.940	1.892	1.729	1.875
Cu	Pd	0.48	1.81	3.83	1.917	1.783	1.832	2.073	1.918	-
Cu	Pt	0.33	1.59	3.47	2.012	1.850	2.070	2.053	1.923	2.034
Zn	Ni	-0.29	0.82	3.03	1.948	1.847	1.999	1.929	1.746	1.881
Zn	Pd	0.25	1.55	3.46	1.971	1.828	2.029	2.139	1.932	2.121
Zn	Pt	0.13	1.36	3.37	2.012	1.860	2.064	2.065	1.945	2.049
Mo	Pt	-0.10	-1.90	-1.99	2.029	1.693	1.700	2.065	-	-

Ru	Pt	-0.11	0.51	1.26	2.044	1.861	1.873	2.037	1.970	1.982
Ru	Au	-0.12	0.88	2.48	1.931	1.867	1.840	-	2.009	-
Rh	Cu	-0.10	1.21	3.03	2.030	1.857	1.981	1.971	1.873	1.999
Rh	Pd	0.23	1.28	3.38	1.991	1.877	1.948	2.227	1.930	-
Rh	Pt	0.09	1.01	1.94	2.023	1.895	1.882	2.039	1.938	1.932
Pd	Co	-0.26	0.83	2.92	2.046	1.939	2.043	1.840	1.723	1.792
Pd	Ni	0.68	1.64	3.84	2.046	1.916	2.037	1.891	1.751	1.887
Pd	Pt	1.15	1.89	4.44	2.215	1.933	-	2.039	1.927	2.038
Ag	Co	-0.28	1.04	2.73	-	2.072	-	1.797	1.717	1.757
Ag	Ni	-0.20	1.34	2.89	-	2.078	-	1.787	1.705	1.779
Ag	Cu	-0.37	1.70	2.91	2.405	2.022	-	1.815	1.773	1.811
Ag	Rh	-0.29	1.36	2.64	-	2.035	-	1.957	1.858	1.913
Ag	Pd	0.42	2.37	3.47	-	2.392	-	1.973	1.851	1.964
Ag	Pt	0.80	2.05	4.10	2.069	2.000	2.066	2.122	1.916	-
Re	Ir	-0.12	-1.12	-0.45	2.048	1.721	1.843	2.068	-	2.048
Ir	Cu	-0.18	0.85	2.94	2.028	1.863	1.976	2.020	1.920	2.055
Ir	Pd	0.16	1.10	3.31	1.999	1.881	1.936	2.351	1.960	-
Ir	Ag	-0.26	1.06	2.68	1.969	1.796	1.921	-	-	-
Ir	Pt	0.17	0.93	1.72	2.018	1.898	1.947	2.074	1.963	1.948
Pt	Co	-0.33	0.66	2.87	2.040	1.947	2.024	1.859	1.734	1.809
Pt	Ni	0.64	1.49	3.82	2.048	1.927	2.032	1.932	1.766	1.917
Au	Fe	0.01	1.18	2.92	-	-	-	1.829	1.656	1.770
Au	Co	0.46	1.94	3.44	-	2.104	-	1.844	1.722	1.838
Au	Ni	1.02	2.28	4.02	-	1.961	-	1.912	1.753	1.876
Au	Cu	-0.14	1.46	3.89	2.038	1.949	-	1.963	1.814	1.807
Au	Zn	0.20	0.83	3.52	-	1.955	-	1.843	1.846	1.884
Au	Rh	0.58	1.72	3.54	-	1.960	-	1.974	1.926	1.949
Au	Pd	1.39	2.74	3.99	-	1.959	1.974	2.009	1.918	-
Au	Ir	0.47	1.81	3.46	-	2.258	-	1.991	1.856	1.953

Au	Pt	1.34	2.74	4.74	-	1.973	2.709	2.041	1.934	-

Table S10. The Gibbs free energy change for oxygenated intermediates adsorption (ΔG_{O*}, ΔG_{OH*}, ΔG_{OOH*}) on M_IM_{II}/g-CN (M_IM_{II} = FePd, FePt, CuNi, CuPd, CuPt, ZnNi, ZnPd, ZnPt, MoPt, RuPt, RuAu, RhCu, RhPd, RhPt, PdCo, PdNi, PdPt, AgCo, AgNi, AgCu, AgRh, AgPd, AgPt, ReIr, IrCu, IrPd, IrAg, IrPt, PtCo, PtNi, AuFe, AuCo, AuNi, AuCu, AuZn, AuRh, AuPd, AuIr, AuPt), the overpotentials for OER (η^{OER}), and the overpotentials for ORR (η^{ORR}).

M_IM_{II}/g-CN		ΔG_{OH*} (eV)	ΔG_{O*} (eV)	ΔG_{OOH*} (eV)	η^{OER} (V)	η^{ORR} (V)
M_I	M_{II}					
Fe	Pd	0.25	0.77	3.32	1.33	0.98
Fe	Pt	0.41	0.77	1.92	1.77	0.87
Cu	Ni	0.41	1.41	3.47	0.83	0.82
Cu	Pd	0.82	1.87	4.16	1.06	0.47
Cu	Pt	0.67	1.64	3.85	0.97	0.56
Zn	Ni	0.06	0.88	3.38	1.28	1.17
Zn	Pd	0.70	1.61	3.83	0.99	0.53
Zn	Pt	0.49	1.42	3.76	1.11	0.74
Mo	Pt	0.27	-1.87	-1.61	5.30	3.37
Ru	Pt	0.26	0.58	1.72	1.97	0.97
Ru	Au	0.19	0.94	2.78	0.91	1.04
Rh	Cu	0.25	1.27	3.39	0.89	0.98
Rh	Pd	0.59	1.35	3.72	1.14	0.64
Rh	Pt	0.46	1.08	2.37	1.32	0.77
Pd	Co	0.12	0.90	3.30	1.17	1.11

Pd	Ni	1.04	1.71	4.22	1.28	0.56
Pd	Pt	1.50	1.96	4.80	1.61	1.11
Ag	Co	0.05	1.09	3.08	0.77	1.18
Ag	Ni	0.08	1.37	3.21	0.61	1.15
Ag	Cu	-0.06	1.73	3.25	0.56	1.29
Ag	Rh	0.04	1.41	2.98	0.71	1.19
Ag	Pd	0.75	2.41	3.83	0.43	0.48
Ag	Pt	1.15	2.10	4.40	1.06	0.71
Re	Ir	0.25	-1.07	-0.05	3.74	2.55
Ir	Cu	0.17	0.91	3.26	1.16	1.06
Ir	Pd	0.50	1.17	3.63	1.23	0.73
Ir	Ag	0.07	1.09	3.03	0.71	1.16
Ir	Pt	0.55	1.00	2.11	1.58	0.78
Pt	Co	0.05	0.73	3.24	1.28	1.18
Pt	Ni	1.01	1.57	4.20	1.40	0.67
Au	Fe	0.24	1.22	3.22	0.78	0.99
Au	Co	0.75	2.00	3.75	0.52	0.48
Au	Ni	1.33	2.35	4.35	0.76	0.66
Au	Cu	0.21	1.51	4.21	1.47	1.02
Au	Zn	0.48	0.88	3.83	1.72	0.83
Au	Rh	0.90	1.78	3.86	0.85	0.35
Au	Pd	1.71	2.81	4.32	0.48	0.63
Au	Ir	0.78	1.86	3.79	0.70	0.44
Au	Pt	1.64	2.81	4.99	0.95	1.30

Table S11. The initial data set of intrinsic descriptors including the distance of two metal atoms (L, Å), the average bond lengths between the surrounding N atoms and metal atoms ($\bar{d}$, Å), the covalent radius ($R_{cov\text{-}ul}$, $R_{cov\text{-}lr}$, Å), the number of valance electrons ($N_{va\text{-}ul}$, $N_{va\text{-}lr}$), the number of d electrons ($N_{d\text{-}ul}$, $N_{d\text{-}lr}$), the Pauling electronegativity ($E_{p\text{-}ul}$, $E_{p\text{-}dr}$), the first ionization energy ($E_{I\text{-}ul}$, $E_{Id\text{-}r}$, eV), the electron affinity ($A_{e\text{-}ul}$, $A_{e\text{-}dr}$, eV), and the d-band center ($\varepsilon_{d\text{-}ul}$, $\varepsilon_{d\text{-}dr}$, eV) for 23 homonuclear and 253 heteronuclear metal dimers adsorbed on g-CN. Herein, -ul and -lr denote the characteristis for metal atoms situated at the upper left and the down right sites of g-CN, respectively.

Metal dimers	L	$\bar{d}$	$R_{cov\text{-}ul}$	$R_{cov\text{-}lr}$	$N_{va\text{-}ul}$	$N_{va\text{-}lr}$	$N_{d\text{-}ul}$	$N_{d\text{-}lr}$	$E_{P\text{-}ul}$	$E_{P\text{-}lr}$	$E_{I\text{-}ul}$	$E_{I\text{-}lr}$	$A_{e\text{-}ul}$	$A_{e\text{-}lr}$	$\varepsilon_{d\text{-}ul}$	$\varepsilon_{d\text{-}lr}$	$E_{p\text{-}ul}+E_{p\text{-}lr}$	$\lvert E_{p\text{-}ul}-E_{p\text{-}lr}\rvert$	$R_{cov\text{-}ul}+R_{cov\text{-}lr}$	$\lvert R_{cov\text{-}ul}-R_{cov\text{-}lr}\rvert$
Ti_2	1.975	2.123	1.6	1.6	4	4	2	2	1.54	1.54	6.827	6.827	0.079	0.079	2.323	2.324	3.08	0	3.2	0

V_2	1.83	2.1119	1.53	1.53	5	5	3	3	1.663	1.663	6.7466	6.7466	0.5255	0.5255	0.921−0	0.919−0	3.26	0	3.06	0
Cr_2	2.0788	2.0599	1.39	1.39	6	6	5	5	1.666	1.666	6.7666	6.7666	0.6666	0.6666	0.891−0	0.893−0	3.32	0	2.78	0
Mn_2	2.3955	1.9889	1.39	1.39	7	7	5	5	1.555	1.555	7.4344	7.4344	0	0	0.607−0	0.620−0	3.1	0	2.78	0
Fe_2	2.1911	2.0233	1.32	1.32	8	8	6	6	1.883	1.883	7.9022	7.9022	0.1511	0.1511	0.823−1	0.823−1	3.66	0	2.64	0
Co_2	2.2533	1.9888	1.26	1.26	9	9	7	7	1.888	1.888	7.888	7.888	0.6622	0.6622	1.178−1	1.178−1	3.76	0	2.52	0
Ni_2	2.4033	1.9599	1.24	1.24	10	10	8	8	1.991	1.991	7.6399	7.6399	1.1556	1.1556	1.778−1	1.777−1	3.82	0	2.48	0
Cu_2	2.3799	2.0300	1.32	1.32	11	11	10	10	1.99	1.99	7.7266	7.7266	1.2355	1.2355	1.336−2	1.319−2	3.8	0	2.64	0
Z	2.2	2.3	1.2	1.2	12	12	10	10	1.6	1.6	9.3	9.3	0	0	6.	6.	3.3	0	2.44	0

n_2	43	20	2	2					5	5	94	94			192	192						
Z_{r_2}	2.2255	2.1400	1.75	1.75	4	4	2	2	1.33	1.33	66.6334	66.6334	0.4266	0.4266	0.9932	0.995	2.66	0	3.5	0		
N_{b_2}	2.06	2.1311	1.64	1.64	5	5	4	4	1.6	1.6	66.7588	66.7588	0.8933	0.8933	0.473	0.410	3.2	0	3.28	0		
Mo_2	2.1299	2.1399	1.54	1.54	6	6	5	5	2.166	2.16	7.0922	7.0922	0.7488	0.7488	0.755	0.757	4.32	0	3.08	0		
Ru_2	2.1933	2.0800	1.42	1.42	8	8	7	7	2.22	2.22	7.3611	7.3611	1.05	1.05	−1.734	−1.735	4.4	0	2.84	0		
Rh_2	2.3166	2.0477	1.42	1.42	9	9	8	8	2.288	2.288	7.4599	7.4599	1.1377	1.1377	−2.505	−2.507	4.56	0	2.84	0		
Pd_2	2.4077	2.0377	1.39	1.39	10	10	10	10	2.22	2.22	8.3377	8.3377	0.5622	0.5622	−2.478	−2.479	4.4	0	2.78	0		
Ag	2.6333	2.3566	1.45	1.45	11	11	10	10	1.93	1.93	7.5766	7.5766	1.3022	1.3022	−3.75	−3.75	3.86	0	2.9	0		

$_2$															5	1						
Ta_2	2.1572	2.10121	1.7	1.7	55	53	15	15	7.8887	7.8887	0.32220	0.32200	0.7080	0.7050	3	0	3.4	0				
We_2	2.2713	2.1123	1.62	1.62	66	44	2.36	2.36	7.98	7.98	0.8155	0.8155	0.488−0	0.488−0	4.72	0	3.24	0				
Re_2	2.2001	2.0081	1.51	1.51	77	55	1.9	1.9	7.8777	7.8777	0.155	0.155	0.357−2	0.360−2	3.8	0	3.02	0				
Os_2	2.25	2.0500	1.44	1.44	88	66	2.2	2.2	8.7006	8.7006	1.1	1.1	0.031−2	0.031−2	4.4	0	2.88	0				
Ir_2	2.3455	2.0266	1.41	1.41	99	77	2.2	2.2	9.1211	9.1211	1.5655	1.5655	0.749−2	0.750−2	4.4	0	2.82	0				
Pt_2	2.4822	2.0211	1.36	1.36	1010	99	2.28	2.28	9.0177	9.0177	2.1288	2.1288	0.414−4	0.412−4	4.56	0	2.72	0				
Au_2	2.5133	2.0799	1.36	1.36	1111	1010	2.54	2.54	9.2255	9.2255	2.3099	2.3099	0.6255	0.6266	5.08	0	2.72	0				
Ti	1.	2.	1.	1.	4	8	2	6	1.	1.	6.	7.	0.	0.	-1.	-1.	3.37	0.29	2.92	0.28		

Fe	958	1182	6	32					54	83	8276	9027	0790	1510	7133	4188						
TiCo	82.0362	.0932	1.6	1.26	4	9	2	7	1.54	1.88	.8276	.88	.0790	.6621	-3.5111	-2.7733	3.42	0.34	2.86	0.34		
TiNi	2.2332	.0492	1.6	1.24	4	10	2	8	1.54	1.91	.8276	.63977	.0790	.1561	-2.7764	-1.6443	3.45	0.37	2.84	0.36		
TiCu	2.4352	.0372	1.6	1.32	4	11	2	10	1.54	1.9	.8276	.72768	.0790	.2350	-1.5766	-2.9300	3.44	0.36	2.92	0.28		
TiPd	2.2812	.1152	1.6	1.39	4	10	2	10	1.54	2.2	.8276	.33790	.0790	.5622	-4.3223	-3.5944	3.74	0.66	2.99	0.21		
TiPt	2.3231	.0912	1.6	1.36	4	10	2	9	1.54	2.28	.8276	.01766	.0790	.1280	-1.5622	-3.3244	3.82	0.74	2.96	0.24		
VTi	1.9151	.1132	1.53	1.6	5	4	3	2	1.63	1.54	.7466	.82776	.5250	.0790	-2.2333	-2.3866	3.17	0.09	3.13	0.07		
VFe	1.9312	.1002	1.53	1.32	5	8	3	6	1.63	1.83	.7466	.90277	.5250	.1510	-3.1799	-2.9885	3.46	0.2	2.85	0.21		
VCo	2.112	.0642	1.53	1.26	5	9	3	7	1.63	1.88	.7466	.887	.5250	.6621	-2.4900	-2.4999	3.51	0.25	2.79	0.27		
V					5	1	3	8	1	1	6		0		-	-	3.	0.	2.	0.2		

Ni	.22	.0312	.53	.24		0			.63	.91	.74666	.63967	.52500	.15611	1.9888	1.7922	54	28	77	9
VCu	2.4555	.02122	1.53	1.32	5	11	3	10	1.63	.9	.74666	.72668	.52500	.23500	1.187	3.7554	3.53	0.27	2.85	0.21
VPd	2.28122	.08522	1.53	1.39	5	10	3	10	1.63	.2	.74666	.33379	.52500	.56222	3.003	3.1331	3.83	0.57	2.92	0.14
VPt	2.322	.07822	1.53	1.36	5	10	3	9	1.63	.28	.74666	.01766	.52500	.12800	3.2559	4.6811	3.91	0.65	2.89	0.17
CrTi	1.83511	.12122	1.39	1.6	6	4	5	2	1.66	.54	.76666	.82766	.66600	.07900	1.8433	2.3444	3.2	0.12	2.99	0.21
CrV	1.87722	.11622	1.39	1.53	6	5	5	3	1.66	.63	.76666	.74667	.66600	.5255	2.9211	2.532	3.29	0.03	2.92	0.14
CrMn	2.00122	.08111	1.39	1.39	6	7	5	5	1.66	.55	.76666	.43470	.66600	0	1.511	1.887	3.21	0.11	2.78	0
CrFe	2.42422	.98622	1.39	1.32	6	8	5	6	1.66	.83	.76666	.90027	.66600	.15100	3.334	3.192	3.49	0.17	2.71	0.07
CrCo	2.217	.031	1.39	1.26	6	9	5	7	1.66	.88	.76666	.88	.66600	.66622	1.759	1.112	3.54	0.22	2.65	0.13

CrNi	2.3432	2.0072	1.39	1.24	6	10	5	8	1.666	1.91	67.7663	70.6397	0.6660	1.1561	-2.220	-1.661	3.57	0.25	2.63	0.15
CrCu	2.4352	2.0002	1.39	1.32	6	11	5	10	1.666	1.9	67.7666	72.697	0.6660	1.235	-2.647	-3.499	3.56	0.24	2.71	0.07
CrZn	2.4011	2.0372	1.39	1.22	6	12	5	10	1.666	1.65	67.7666	69.3946	0.6660	0	-2.151	-7.134	3.31	0.01	2.61	0.17
CrZr	1.9751	2.1212	1.39	1.75	6	4	5	2	1.666	1.33	67.7666	63.4660	0.6660	0.4260	-2.388	-3.040	2.99	0.33	3.14	0.36
CrNb	1.9152	2.1092	1.39	1.64	6	5	5	5	1.666	1.6	67.7666	75.8760	0.6660	0.8930	-2.929	-3.510	3.26	0.06	3.03	0.25
CrMo	2.0172	2.1132	1.39	1.54	6	6	5	5	1.666	1.16	67.7666	70.9267	0.6660	0.7488	-1.9888	-2.5596	3.82	0.5	2.93	0.15
CrRu	2.0892	2.0952	1.39	1.42	6	8	5	7	1.666	1.22	67.7666	36.1760	0.6660	1.05	-3.010	-3.277	3.86	0.54	2.81	0.03
CrRh	2.3022	2.0662	1.39	1.42	6	9	5	8	1.666	1.28	67.7666	45.9860	0.6660	1.1370	-3.327	-2.980	3.94	0.62	2.81	0.03
CrPd	2.38	2.07	1.39	1.39	6	10	5	10	1.666	1.22	67.766	33.666	0.6660	0.556	-2.889	-2.441	3.86	0.54	2.78	0

CrAg	72.4612	92.0782	1.39	1.45	6	11	5	10	1.666	1.93	66.7766	77.5767	60.6660	21.3020	7-2.9991	3-5.0339	3.59	0.27	2.84	0.06
CrTa	12.0322	1.39	1.7	6	5	5	3	1.666	1.5	66.7666	87.8767	60.6660	20.3220	2.3155	3.4669	3.16	0.16	3.09	0.31
CrW	22.1192	1.39	1.62	6	6	5	4	1.666	2.36	66.7666	7.98	60.6660	20.8150	1.9931	2.7887	4.02	0.7	3.01	0.23
CrRe	2.1072	1.39	1.51	6	7	5	5	1.666	1.9	66.7666	87.8780	60.6660	0.15	2.5711	3.7006	3.56	0.24	2.9	0.12
CrOs	2.1372	1.39	1.44	6	8	5	6	1.666	2.2	66.7666	70.6960	60.6660	1.1	2.6400	2.8544	3.86	0.54	2.83	0.05
CrIr	2.2892	1.39	1.41	6	9	5	7	1.666	2.2	66.7666	12.1969	60.6660	1.5652	2.1500	3.1744	3.86	0.54	2.8	0.02
CrPt	2.4132	2.0602	1.39	1.36	6	10	5	9	1.666	2.28	66.7666	01.7966	60.6660	12.8820	1.3988	3.5775	3.94	0.62	2.75	0.03
CrAu	2.4661	2.0382	1.39	1.36	6	11	5	10	1.666	2.54	66.7667	22.5668	60.6660	30.9000	2.8341	5.0300	4.2	0.88	2.75	0.03
MnT	19.1	1.3	1.6	7	4	5	5	2	1.5	1.5	4.4	8.0	0	.0	1.7	1.7	3.09	0.01	2.99	0.21

i	1	2	9						5	4	3	2		7	0	8	2					
MnV	12	32.1062	1.39	1.53	7	5	5	3	1.555	1.63	47.4347	76.7467	0	90.5250	-2.4611	3.682-	3.18	0.08	2.92	0.14
MnFe	2.2912	2.01102	1.39	1.32	7	8	5	6	1.555	1.83	47.4347	.9902	0	.15100	-2.8011	-2.782	3.38	0.28	2.71	0.07
MnCo	2.2512	1.90132	1.39	1.26	7	9	5	7	1.555	1.88	47.4347	7.88	0	.66621	-3.2488	-2.217	3.43	0.33	2.65	0.13
MnNi	2.3352	1.99322	1.39	1.24	7	10	5	8	1.555	1.91	47.4347	7.6397	0	1.15610	-2.8874	-2.7223	3.46	0.36	2.63	0.15
MnCu	2.4072	2.00722	1.39	1.32	7	11	5	10	1.555	1.9	47.4347	7.7268	0	.23500	-2.6355	-3.2556	3.45	0.35	2.71	0.07
MnPd	2.3482	2.04922	1.39	1.39	7	10	5	10	1.555	1.22	47.4347	.3379	0	.56222	-3.1855	-2.9188	3.75	0.65	2.78	0
MnPt	2.3662	2.03322	1.39	1.36	7	10	5	9	1.555	1.28	47.4347	.0177	0	.12800	-3.3255	-3.9933	3.83	0.73	2.75	0.03
FeCo	2.2062	2.00612	1.32	1.26	8	9	6	7	1.883	1.88	47.4347	7.8887	0.15110	.66621	-2.4833	-2.1220	3.71	0.05	2.58	0.06
Fe	2.	1.	1.	1.	8	10	6	8	1.	1.	47.	7.	0.	1.	-2.	-2.	3.74	0.08	2.56	0.08

Ni	32	98	32	24					83	91	90	63	15	15	67	08						
FeCu	72.36	12.0162	1.32	1.32	8	11	6	10	1.83	1.9	9027	9726	1510	1561	74--2.250	84--3.276	3.73	0.07	2.64	0		
FePd	1512.3152	1232.0233	1.32	1.39	8	10	6	10	1.83	12.2	9027	6879	1510	1562	74--1.874	66--3.266	4.03	0.37	2.71	0.07		
FePt	1512.3432	1232.0133	1.32	1.36	8	10	6	9	1.83	12.28	9027	7701	1510	1281	74--2.942	02--3.7022	4.11	0.45	2.68	0.04		
CoNi	1512.3972	1160.9601	1.26	1.24	9	10	7	8	1.888	1.91	7.888	7.6639	1.6623	1.1560	1.6223	2.4442	3.79	0.03	2.5	0.02		
CuCo	1512.4562	1160.9561	1.32	1.26	11	9	10	7	1.9	1.888	7.7267	7.888	1.2351	1.6621	1.8623	1.8088	3.78	0.02	2.58	0.06		
CuNi	1512.3892	1160.9972	1.32	1.24	11	10	10	8	1.9	1.91	1.7267	1.6398	1.2351	1.1560	1.3426	2.6599	3.81	0.01	2.56	0.08		
CuPd	1512.4092	1162.0362	1.32	1.39	11	10	10	10	1.9	12.2	1.7267	1.3379	1.2351	1.5622	1.3535	3.2277	4.1	0.3	2.71	0.07		
CuPt	1512.4252	1162.0112	1.32	1.36	11	10	10	9	1.9	12.28	1.7269	1.0176	1.2350	1.1280	1.3694	3.7556	4.18	0.38	2.68	0.04		
Z	21	11	14	11	12	11											3.	0.	2.	0.3		

nTi	.556203	.291244	.22	.6	2		0		.65	.54	.394949	.827676		.0790	6.5099-7.0211	3.1029--1.9599	19	11	82	8
ZnV	.403232	.044281	1.22	1.53	12	5	10	3	1.65	1.63	.394949	.746767	0	.525			3.28	0.02	2.75	0.31
ZnMn	.369292	.081249	1.22	1.39	12	7	10	5	1.65	1.55	.394949	.434747	0	0	6.6664--6.6298	3.4022--2.0441	3.2	0.1	2.61	0.17
ZnFe	.309292	.049231	1.22	1.32	12	8	10	6	1.65	1.83	.394949	.90227	0	.1510			3.48	0.18	2.54	0.1
ZnCo	.315292	.031249	1.22	1.26	12	9	10	7	1.65	1.88	.394949	.887	0	.66221	6.4800--6.2398	2.7500--3.0441	3.53	0.23	2.48	0.04
ZnNi	.265292	.049231	1.22	1.24	12	10	10	8	1.65	1.91	.394949	.639707	0	.15611			3.56	0.26	2.46	0.02
ZnCu	.32	.052292	1.22	1.32	12	11	10	10	1.65	1.9	.394949	.726808	0	.23500	6.5103--7.0039	3.6077--3.5911	3.55	0.25	2.54	0.1
ZnPd	2.335292	.117292	1.22	1.39	12	10	10	10	1.65	1.2	.394949	.337979	0	.56222			3.85	0.55	2.61	0.17
ZnPt	.351103		1.22	1.36	12	10	10	9	1.65	1.28	.394947	.0177	0	.128	4.9588--2.1992		3.93	0.63	2.58	0.14

ZrTi	2.1112	2.1242	1.75	1.6	4	4	2	2	1.33	1.54	66.6346	66.8276	0.42600	0.0790	-3.039	-2.533	2.87	0.21	3.35	0.15
ZrV	2.0421	2.1192	1.75	1.53	4	5	2	3	1.33	1.63	66.6346	66.7467	0.42600	0.5225	-1.017	-0.848	2.96	0.3	3.28	0.22
ZrMn	1.9682	2.1072	1.75	1.39	4	7	2	5	1.33	1.55	66.6346	66.4347	0.42600	0	-4.374	-3.512	2.88	0.22	3.14	0.36
ZrFe	2.1612	2.1402	1.75	1.32	4	8	2	6	1.33	1.83	66.6346	66.9027	0.42600	0.1510	-3.6322	-2.7336	3.16	0.5	3.07	0.43
ZrCo	2.1822	2.1232	1.75	1.26	4	9	2	7	1.33	1.88	66.6346	7.887	0.42600	0.6621	-1.1752	-1.0688	3.21	0.55	3.01	0.49
ZrNi	2.3252	2.0962	1.75	1.24	4	10	2	8	1.33	1.91	66.6346	66.3397	0.42600	0.1561	-3.5275	-2.1644	3.24	0.58	2.99	0.51
ZrCu	2.4982	2.3323	1.75	1.32	4	11	2	10	1.33	1.9	66.6346	66.7269	0.42600	0.2355	-4.1752	-2.1266	3.23	0.57	3.07	0.43
ZrZn	2.7222	2.1402	1.75	1.22	4	12	2	10	1.33	1.65	66.6346	66.3946	0.42600	0	-2.210	-7.378	2.98	0.32	2.97	0.53
ZrNb	2.15	2.13	1.75	1.64	4	5	2	5	1.33	1.63	66.6346	66.7546	0.42600	0.890	-2.911	-2.544	2.93	0.27	3.39	0.11

ZrRh	12.2842.393	42.1812.162	1.75	1.42	4	9	2	8	1.33	2.28	46.63446	87.45998	60.42600	31.13700	1-4.4436	4-3.8200	3.61	0.95	3.17	0.33
ZrPd	12.3932.677	42.1623.194	1.75	1.39	4	10	2	10	1.33	2.2	46.63446	33.37700	60.42600	56.2210	3.9222-2.5005	4.3449-3.3844	3.53	0.87	3.14	0.36
ZrAg	22.1942	42.1222	1.75	1.45	4	11	2	10	1.33	1.93	46.63446	57.67067	60.42600	30.2200	2.505-2.156	3.384-2.2277	3.26	0.6	3.2	0.3
ZrTa	23.5922	42.1552	1.75	1.41	4	9	2	7	1.33	2.2	46.63446	88.12179	60.42600	56.5221	4.2846-4.2669	3.7729-3.9599	3.53	0.87	3.16	0.34
ZrPt	22.4442	42.1432	1.75	1.36	4	10	2	9	1.33	2.28	46.63446	0.01779	60.42600	12.2822	4.2669-3.4555	5.2556-0.919	3.61	0.95	3.11	0.39
ZrAu	22.5772	42.1362	1.75	1.36	4	11	2	10	1.33	2.54	46.63446	22.25666	60.42600	30.2900	3.455-0.905	5.256-0.919	3.87	1.21	3.11	0.39
NbTi	23.1119	42.1202	1.64	1.6	5	4	5	2	1.6	1.54	46.75866	82.76676	60.89300	0.0790	1-2.9	4-2.6	3.14	0.06	3.24	0.04
NbV	23.9	42.1	1.6	1.5	5	5	5	3	1.6	1.6	46.7	87.7	60.8	31.5	1-4.4436	4-3.8200	3.23	0.03	3.17	0.11

NbMn	412.0542.1	212.1242.1082	1.64	1.39	5	7	5	5	1.6	3 1.55	586.7586	467.4347	930.8930	25	82-2.401	25--2.158	3.15	0.05	3.03	0.25
NbFe	2.1512.2822	2.0822.0602	1.64	1.26	5	9	5	7	1.6	1 1.88	586.7586	7.88	930.8930	0	82-2.7035	25--2.1888	3.48	0.28	2.9	0.38
NbNi	2.2872.4322	2.2332.3492	1.64	1.24	5	10	5	8	1.6	1 1.91	586.7586	637.7269	930.8930	10.1561	82-4.3400	25--2.7825	3.51	0.31	2.88	0.4
NbCu	2.6062.2292	2.1222.1182	1.64	1.32	5	11	5	10	1.6	1 1.9	586.7586	7.3947	930.8930	0.2355	82-2.6633	25--2.7822	3.5	0.3	2.96	0.32
NbZn	2.2922.3542	2.1222.1182	1.64	1.22	5	12	5	10	1.6	1 1.65	586.7586	7.3947	930.8930	0	82-2.1944	25--6.7337	3.25	0.05	2.86	0.42
NbRh	2.2292.3542	2.1222.1182	1.64	1.42	5	9	5	8	1.6	1 2.28	586.7586	459.3398	930.8930	1.1370	82-3.5225	25--3.1777	3.88	0.68	3.06	0.22
NbPd	2.3542	2.1182	1.64	1.39	5	10	5	10	1.6	1 2.2	586.7586	3.3379	930.8930	0.5622	82-4.2223	25--4.5539	3.8	0.6	3.03	0.25
Nb	1.	1.	1.	1.	5	10	5	9	1.	1 2.	586.	3.	930.	0.	82-3.	25--4.	3.88	0.68	3	0.28

Pt	392	0962	64	36					6	28	7587	0176	8930	1280	706	105						
MoTi	21.962	1212.106	1.54	1.6	6	4	5	2	2.16	1.54	.0927	.8276	.7480	.0790	-3.491	--3.109	3.7	0.62	3.14	0.06		
MoV	21.926	2212.102	1.54	1.53	6	5	5	3	2.16	1.63	.0927	.7467	.7480	.5255	-3.713	--3.156	3.79	0.53	3.07	0.01		
MoMn	22.08	2202.080	1.54	1.39	6	7	5	5	2.16	1.55	.0927	.4347	.7480	0	-2.442	--2.279	3.71	0.61	2.93	0.15		
MoFe	22.07	2202.058	1.54	1.32	6	8	5	6	2.16	1.83	.0927	.9022	.7480	.1510	-3.428	--2.751	3.99	0.33	2.86	0.22		
MoCo	22.146	2202.040	1.54	1.26	6	9	5	7	2.16	1.88	.0927	7.88	.7480	.6621	-2.608	--2.562	4.04	0.28	2.8	0.28		
MoNi	22.235	2202.043	1.54	1.24	6	10	5	8	2.16	1.91	.0927	.6397	.7480	.1561	-3.173	--2.374	4.07	0.25	2.78	0.3		
MoCu	22.495	2202.043	1.54	1.32	6	11	5	10	2.16	1.9	.0927	.7269	.7480	.2355	-2.535	--3.061	4.06	0.26	2.86	0.22		
MoZn	22.487	2202.472	1.54	1.22	6	12	5	10	2.16	1.65	.0927	.3946	.7480	0	-1.977	--6.676	3.81	0.51	2.76	0.32		
M	2	2	1	1	6	4	5	2	2	1	2	7	0	0	-	-	3.	0.	3.	0.2		

oZr	.0862	.13122	.54	.75					.16	.133	.09227	.63466	.74800	.4260	3.0448	3.0794	49	83	29	1
MoNb	.0322	.11522	1.54	1.64	6	5	5	5	2.16	1.16	.09227	.75887	.74800	.8933	3.2900	3.2944	3.76	0.56	3.18	0.1
MoRu	.16222	.10522	1.54	1.42	6	8	5	7	2.16	2.12	.09227	.36177	.74800	1.05	3.5299	3.2966	4.36	0.04	2.96	0.12
MoRh	.22122	.09322	1.54	1.42	6	9	5	8	2.16	2.28	.09227	.45988	.74800	1.1370	3.5188	3.8955	4.44	0.12	2.96	0.12
MoPd	.43922	.10122	1.54	1.39	6	10	5	10	2.16	2.12	.09227	.33777	.74800	.56221	4.8842	3.8661	4.36	0.04	2.93	0.15
MoAg	.6722	.39322	1.54	1.45	6	11	5	10	2.16	1.93	.09227	.57667	.74800	.30200	5.5022	3.7544	4.09	0.23	2.99	0.09
MoTa	.08922	.09722	1.54	1.7	6	5	5	3	2.16	1.5	.09227	.88774	.74800	.32200	4.4082	4.8566	3.66	0.66	3.24	0.16
MoW	.22322	.12822	1.54	1.62	6	6	5	4	2.16	2.36	.09227	7.98	.74800	.81500	3.0511	3.2566	4.52	0.2	3.16	0.08
MoRe	.2012	.1072	1.54	1.51	6	7	5	5	2.16	1.9	.0922	.8777	.7488	0.15	3.0077	2.9700	4.06	0.26	3.05	0.03

MoOs	2.222	2.089	1.54	1.44	6	8	5	6	2.16	2.2	7.09	8.706	0.748	1.1	-3.672	-4.941	4.36	0.04	2.98	0.1
MoIr	2.271	2.077	1.54	1.41	6	9	5	7	2.16	2.2	7.092	9.121	0.748	1.565	-2.686	-4.464	4.36	0.04	2.95	0.13
MoPt	2.455	2.079	1.54	1.36	6	10	5	9	2.16	2.28	7.092	9.017	0.748	1.282	-2.458	-3.891	4.44	0.12	2.9	0.18
MoAu	2.56	2.092	1.54	1.36	6	11	5	10	2.16	2.54	7.092	9.225	0.748	1.309	-3.352	-5.046	4.7	0.38	2.9	0.18
RuTi	2.051	2.1282	1.42	1.6	8	4	7	2	2.2	1.54	7.361	8.276	1.05	1.079	-2.962	-3.211	3.74	0.66	3.02	0.18
RuV	2.05	2.1122	1.42	1.53	8	5	7	3	2.2	1.63	7.361	7.467	1.05	1.525	-3.075	-2.740	3.83	0.57	2.95	0.11
RuMn	2.275	2.0602	1.42	1.39	8	7	7	5	2.2	1.55	7.361	8.434	1.05	0	-2.050	-2.424	3.75	0.65	2.81	0.03
RuFe	2.1462	2.0542	1.42	1.32	8	8	7	6	2.2	1.83	7.361	9.027	1.05	0.151	-3.155	-2.378	4.03	0.37	2.74	0.1
RuCo	2.20	2.03	1.42	1.26	8	9	7	7	2.2	1.88	7.361	8.88	1.05	0.66	-3.12	-2.68	4.08	0.32	2.68	0.16

RuNi	52.3111	42.0092	1.42	1.24	8	10	7	8	2.2	1.91	17.3617	7.6397	1.05	21.1561	9-4.2111	4-3.1599	4.11	0.29	2.66	0.18
RuCu	12.4842	2.0132	1.42	1.32	8	11	7	10	2.2	1.9	17.3617	7.7269	1.05	1.2355	-3.3044	-3.4445	4.1	0.3	2.74	0.1
RuZn	42.4542	2.1092	1.42	1.22	8	12	7	10	2.2	1.65	17.3617	9.3946	1.05	0	-4.2622	-6.7900	3.85	0.55	2.64	0.2
RuZr	42.2642	2.1722	1.42	1.75	8	4	7	2	2.2	1.33	17.3617	6.6346	1.05	0.4260	-3.2559	-3.6442	3.53	0.87	3.17	0.33
RuNb	42.17	2.1382	1.42	1.64	8	5	7	5	2.2	1.6	17.3617	6.7587	1.05	0.8931	-2.9966	-3.1779	3.8	0.6	3.06	0.22
RuRh	22.3332	2.0562	1.42	1.42	8	9	7	8	2.2	2.28	17.3617	4.5598	1.05	1.1370	-2.6665	-2.9299	4.48	0.08	2.84	0
RuPd	22.4962	2.0672	1.42	1.39	8	10	7	10	2.2	2.2	17.3617	8.3377	1.05	0.5621	-2.3988	-2.4445	4.4	0	2.81	0.03
RuAg	22.59	2.2332	1.42	1.45	8	11	7	10	2.2	1.93	17.3617	7.5767	1.05	1.3020	-5.2044	-3.6445	4.13	0.27	2.87	0.03
RuT	22.2	2.1	1.4	1.7	8	5	7	3	2.2	1.5	17.3	8.8	10.3	1	-3.0	-4.2	3.7	0.7	3.12	0.28

a	3	182.0382	2									617.361	879.121	5	221.565	33-2.6033	71--3.4377					
RuIr	2.4322		1.42	1.41	8	9	7	7	2.2	2.2		7	9	1.05	2			4.44	0	2.83	0.01	
RuPt	2.5022	182.0412	1.42	1.36	8	10	7	9	2.2	2.28		7	9	1.05	2	-1.4722	-3.4599	4.48	0.08	2.78	0.06	
RuAu	2.5352	182.0552	1.42	1.36	8	11	7	10	2.2	2.54		7	9	1.05	2	-2.9889	-4.7722	4.74	0.34	2.78	0.06	
RhTi	2.1152	182.1272	1.42	1.6	9	4	8	2	2.28	1.54		7	6	1.05	1	-3.5777	-3.4655	3.82	0.74	3.02	0.18	
RhV	2.1232	182.1012	1.42	1.53	9	5	8	3	2.28	1.63		7	6	1.05	1	-3.5499	-3.3199	3.91	0.65	2.95	0.11	
RhMn	2.3122	182.0612	1.42	1.39	9	7	8	5	2.28	1.55		7	7	1.05	0	-3.0005	-3.7399	3.83	0.73	2.81	0.03	
RhFe	2.2562	182.0302	1.42	1.32	9	8	8	6	2.28	1.83		7	9027	1.05	0	-2.4449	-2.8400	4.11	0.45	2.74	0.1	
RhCo	2.2952	182.0141	1.42	1.26	9	9	8	7	2.28	1.88		7	.887	1.05	1	-3.2280	-2.3300	4.16	0.4	2.68	0.16	
Rh	2.	1.	1.	1.	9	10	8	8	2.	1.		7	7	1.	1	-0.	-0.	4.19	0.37	2.66	0.18	

Ni	39	992	42	24					28	91	459	639	137	156	464	517					
RhCu	12.446	1.995	1.42	1.32	9	11	8	10	2.28	1.9	.4597	.7269	.1371	.2355	-3.102	-3.211	4.18	0.38	2.74	0.1	
RhZn	2.378	2.0402	1.42	1.22	9	12	8	10	2.28	1.65	.4597	.3948	.1371	0	-3.052	-6.762	3.93	0.63	2.64	0.2	
RhPd	2.475	2.0582	1.42	1.39	9	10	8	10	2.28	2.2	.4597	.3379	.1371	.5622	-2.372	-3.024	4.48	0.08	2.81	0.03	
RhPt	2.494	2.0402	1.42	1.36	9	10	8	9	2.28	2.28	.4597	.0177	.1371	.1280	-2.706	-2.992	4.56	0	2.78	0.06	
PdCo	2.364	2.0062	1.39	1.26	10	9	10	7	2.2	1.88	.3378	.887	.5620	.6621	-3.540	-2.157	4.08	0.32	2.65	0.13	
PdNi	2.374	2.0052	1.39	1.24	10	10	10	8	2.2	1.91	.3378	.6399	.5620	.1562	-3.488	-3.052	4.11	0.29	2.63	0.15	
PdPt	2.464	2.0393	1.39	1.36	10	10	10	9	2.2	2.28	.3377	.0176	.5621	.1280	-3.286	-3.707	4.48	0.08	2.75	0.03	
AgTi	2.594	3.1712	1.451	1.6	11	4	10	2	1.93	1.54	.5767	.8276	.3021	.0790	-2.575	-1.138	3.47	0.39	3.05	0.15	
A	2	2	1	1	1	5	1	3	1	1	7	6	1	0	-	-	3.	0.	2.	0.0	

gV	.6042	.2652	.45	.53	1		0		.93	.63	.57676	.74667	.30211	.525	4.1777	2.7378	56	3	98	8
AgMn	.39522	.02722	1.45	1.39	11	7	10	5	1.93	1.55	.57676	.43447	.30211	0	5.6697	3.302	3.48	0.38	2.84	0.06
AgFe	.39722	.02022	1.45	1.32	11	8	10	6	1.93	1.83	.57676	.90202	.30211	.1510	5.0884	2.1887	3.76	0.1	2.77	0.13
AgCo	.38922	.01322	1.45	1.26	11	9	10	7	1.93	1.88	.57676	.887	.30211	.66211	4.8897	1.7441	3.81	0.05	2.71	0.19
AgNi	.36	.04332	1.45	1.24	11	10	10	8	1.93	1.91	.57676	.63977	.30211	.15611	4.5564	2.0600	3.84	0.02	2.69	0.21
AgCu	2.3862	.08522	1.45	1.32	11	11	10	10	1.93	1.9	.57676	.72669	.30211	.2355	4.5164	2.9449	3.83	0.03	2.77	0.13
AgZn	.36722	.11632	1.45	1.22	11	12	10	10	1.93	1.65	.57676	.39466	.30211	0	5.0433	7.1744	3.58	0.28	2.67	0.23
AgNb	.63822	.14622	1.45	1.64	11	5	10	5	1.93	1.6	.57676	.75887	.30211	.8931	3.2554	3.7277	3.53	0.33	3.09	0.19
AgRh	.43239	.0239	1.45	1.42	11	9	10	8	1.93	1.28	.5766	.4599	.3022	.1377	4.8203	2.7003	4.21	0.35	2.87	0.03

AgPd	2.474	2.1022	1.45	1.39	11	10	10	10	1.93	2.2	7.5767	8.3379	1.3021	0.5622	-4.747	-3.469	4.13	0.27	2.84	0.06
AgPt	2.4862	2.0682	1.45	1.36	11	10	10	9	1.93	2.28	7.5767	0.0176	1.3020	0.1280	-5.252	-4.216	4.21	0.35	2.81	0.09
TaTi	2.0782	2.1052	1.7	1.6	5	4	3	2	1.5	1.54	8.8877	8.2776	1.3220	0.0790	-3.459	-2.568	3.04	0.04	3.3	0.1
TaV	2.0032	2.1012	1.7	1.53	5	5	3	3	1.5	1.63	8.8877	7.4667	1.3220	0.5225	-3.316	-2.484	3.13	0.13	3.23	0.17
TaMn	2.182	2.1062	1.7	1.39	5	7	3	5	1.5	1.55	8.8877	8.4347	1.3220	0	-2.909	-2.477	3.05	0.05	3.09	0.31
TaFe	2.1692	2.0862	1.7	1.32	5	8	3	6	1.5	1.83	8.8877	9.0227	1.3220	0.1510	-3.209	-2.285	3.33	0.33	3.02	0.38
TaCo	2.2092	2.0642	1.7	1.26	5	9	3	7	1.5	1.88	8.8877	7.88	1.3220	0.6621	-4.333	-2.663	3.38	0.38	2.96	0.44
TaNi	2.3012	2.0452	1.7	1.24	5	10	3	8	1.5	1.91	8.8877	6.3977	1.3220	0.1561	-3.262	-2.995	3.41	0.41	2.94	0.46
TaCu	2.412	2.222	1.7	1.32	5	11	3	10	1.5	1.9	8.888	7.722	1.322	0.233	-3.955	-2.766	3.4	0.4	3.02	0.38

TaZn	12.557	12.2722	1.7	1.22	5	12	3	10	1.5	1.65	77.887	69.396	20.320	0	5-3.205	0-6.738	3.15	0.15	2.92	0.48
TaNb	12.1112	12.1142	1.7	1.64	5	5	3	5	1.5	1.6	77.887	69.4587	20.3220	0.8931	3.107-4.480	2.897-3.691	3.1	0.1	3.34	0.06
TaRh	12.2762	12.1052	1.7	1.42	5	9	3	8	1.5	1.28	77.887	69.4598	20.3220	0.1370	3.256-3.595	3.595-3.491	3.78	0.78	3.12	0.28
TaPd	12.3682	12.1073	1.7	1.39	5	10	3	10	1.5	1.2	77.887	69.3377	20.3220	0.5622	3.330-3.493	3.493-3.189	3.7	0.7	3.09	0.31
TaAg	12.6222	12.1522	1.7	1.45	5	11	3	10	1.5	1.93	77.887	69.5769	20.3220	0.3022	3.683-3.889	3.889-3.406	3.43	0.43	3.15	0.25
TaPt	12.4022	12.0872	1.7	1.36	5	10	3	9	1.5	1.28	77.887	69.0176	20.3220	0.1280	3.683-3.889	3.889-3.406	3.78	0.78	3.06	0.34
WTi	12.0251	12.1022	1.62	1.6	6	4	4	2	2.36	1.54	77.98	76.8276	20.8150	0.0790	2.219-1.973		3.9	0.82	3.22	0.02
WV	11.9942	12.0832	1.62	1.53	6	5	4	3	2.36	1.63	77.98	76.7467	20.8150	0.5250	3.358-3.190		3.99	0.73	3.15	0.09
WMn	12.1	12.0	1.6	1.3	6	7	4	5	2.3	1.5	77.9	76.4	20.8	0	3.1-2.3		3.91	0.81	3.01	0.23

WFe	52.1622	812.0602	2 1.662	9 1.32	6	8	4	6	6 2.236	5 1.883	8 7.98	347.9022	150.8150	0 0.1510	65 -2.8777	00 -1.9958	4.19	0.53	2.94	0.3
WCo	22.1892	2.0422	1 1.662	1 1.26	6	9	4	7	2 2.336	1 1.888	7 7.98	7.888	0.8150	0 0.6621	-3.6996	-2.8622	4.24	0.48	2.88	0.36
WNi	2 2.2572	2.0172	1 1.662	1 1.24	6	10	4	8	2 2.336	1 1.911	7 7.98	7.639	0.8150	0 0.1561	-3.6683	-2.1112	4.27	0.45	2.86	0.38
WCu	2 2.4412	2.0282	1 1.662	1 1.32	6	11	4	10	2 2.336	1 1.99	7 7.98	7.726	0.8150	0 0.2355	-2.4442	-3.4600	4.26	0.46	2.94	0.3
WZn	2 2.4822	2.2262	1 1.662	1 1.22	6	12	4	10	2 2.336	1 1.655	7 7.98	7.394	0.8150	0	-2.1777	-6.5001	4.01	0.71	2.84	0.4
WZr	2 2.1392	2.1162	1 1.662	1 1.75	6	4	4	2	2 2.336	1 1.333	7 7.98	7.634	0.8150	0 0.4260	-3.7722	-3.9336	3.69	1.03	3.37	0.13
WNb	2 2.0912	2.0982	1 1.662	1 1.64	6	5	4	5	2 2.336	1 1.66	7 7.98	7.758	0.8150	0 0.8933	-2.3441	-2.5611	3.96	0.76	3.26	0.02
WRu	2 2.2152	2.0862	1 1.662	1 1.42	6	8	4	7	2 2.336	2 2.22	7 7.98	7.361	0.8150	1 1.05	-4.2008	-4.4408	4.56	0.16	3.04	0.2
WR	2.	2.	1.	1.	6	9	4	8	2.	2.	7.	7.	0.	1.	-4.	-4.	4.64	0.08	3.04	0.2

h	259	0772	62	42					36	28	98	4598	8150	1370	223	005				
WPd	2.353	.0803	1.62	1.39	6	10	4	10	2.36	2.2	7.98	.3377	.8150	.5621	-3.728	-4.256	4.56	0.16	3.01	0.23
WAg	2.6092	.0002	1.62	1.45	6	11	4	10	2.36	1.93	7.98	.5767	.8150	.3020	-2.170	-3.400	4.29	0.43	3.07	0.17
WTa	2.1422	.0822	1.62	1.7	6	5	4	3	2.36	1.5	7.98	.8877	.8150	.3222	-2.9644	-3.3557	3.86	0.86	3.32	0.08
WRe	2.2422	.0942	1.62	1.51	6	7	4	5	2.36	1.9	7.98	.8777	.8150	0.15	-3.2744	-3.1332	4.26	0.46	3.13	0.11
WOs	2.2572	.0762	1.62	1.44	6	8	4	6	2.36	2.2	7.98	.8706	.8150	1.1	-4.0488	-4.4188	4.56	0.16	3.06	0.18
WIr	2.2972	.0632	1.62	1.41	6	9	4	7	2.36	2.2	7.98	.1219	.8150	.5652	-4.2248	-3.7388	4.56	0.16	3.03	0.21
WPt	2.3782	.0612	1.62	1.36	6	10	4	9	2.36	2.28	7.98	.0179	.8150	.1282	-4.3488	-4.4244	4.64	0.08	2.98	0.26
WAu	2.5452	.0732	1.621	1.361	67	11	45	102	2.361	2.541	7.987	.2256	.8150	.3090	-2.5970	-4.9500	4.9	0.18	2.98	0.26
R															-	-	3.	0.	3.	0.0

eTi	.032	.0962	.51	.6					.9	.54	.8777	.8276	.15	.0790	3.792	2.685	44	36	11	9
ReV	.0952	.1032	1.51	1.53	7	5	5	3	1.9	1.63	.8777	.7466	0.15	.5255	-3.749	-2.647	3.53	0.27	3.04	0.02
ReMn	.1412	.0672	1.51	1.39	7	7	5	5	1.9	1.55	.8777	.4347	0.15	0	-3.326	-3.042	3.45	0.35	2.9	0.12
ReFe	.1052	.0542	1.51	1.32	7	8	5	6	1.9	1.83	.8777	.9027	0.15	.1510	-3.342	-2.577	3.73	0.07	2.83	0.19
ReCo	.1562	.0382	1.51	1.26	7	9	5	7	1.9	1.88	.8777	7.88	0.15	.6621	-2.981	-2.312	3.78	0.02	2.77	0.25
ReNi	.3082	.0082	1.51	1.24	7	10	5	8	1.9	1.91	.8777	.6397	0.15	1.1561	-3.923	-1.971	3.81	0.01	2.75	0.27
ReCu	.4362	.0162	1.51	1.32	7	11	5	10	1.9	1.9	.8777	.7269	0.15	1.235	-3.196	-3.461	3.8	0	2.83	0.19
ReZn	.3362	.1402	1.51	1.22	7	12	5	10	1.9	1.65	.8777	.3946	0.15	0	-3.080	-6.677	3.55	0.25	2.73	0.29
ReZr	.1362	.1032	1.51	1.75	7	4	5	2	1.9	1.33	.8777	.6344	0.15	.4260	-4.630	-4.880	3.23	0.57	3.26	0.24

ReNb	2.2532	2.13825	1.511	1.642	7	5	5	5	1.9	1.6	7.8777	6.75871	0.15	0.893	-2.6000	-2.0399	3.5	0.3	3.15	0.13
ReRu	2.21	2.07522	1.511	1.422	7	8	5	7	1.9	2.2	7.8777	7.36177	0.15	1.05	-3.3833	-2.9799	4.1	0.3	2.93	0.09
ReRh	2.2462	2.06322	1.511	1.422	7	9	5	8	1.9	2.28	7.8777	7.45987	0.15	1.137	-3.6225	-2.9551	4.18	0.38	2.93	0.09
RePd	2.4232	2.07222	1.511	1.39	7	10	5	10	1.9	2.2	7.8777	8.33777	0.15	0.562	-2.4335	-3.4333	4.1	0.3	2.9	0.12
ReAg	2.5872	2.29322	1.511	1.445	7	11	5	10	1.9	1.93	7.8777	8.57677	0.15	1.3020	-4.5335	-3.6044	3.83	0.03	2.96	0.06
ReTa	2.2872	2.12332	1.511	1.7	7	5	5	3	1.9	1.15	7.8777	8.88778	0.15	0.322	-3.1955	-3.4441	3.4	0.4	3.21	0.19
ReOs	2.2272	2.06622	1.511	1.444	7	8	5	6	1.9	2.2	7.8777	7.07069	0.15	1.1	-3.7266	-3.6977	4.1	0.3	2.95	0.07
ReIr	2.2782	2.05322	1.511	1.411	7	9	5	7	1.9	2.2	7.8777	8.12190	0.15	1.5652	-4.7866	-4.2666	4.1	0.3	2.92	0.1
RePt	2.44	2.05	1.511	1.366	7	10	5	9	1.9	2.28	7.887	8.0115	0.15	0.112	-2.543	-3.633	4.18	0.38	2.87	0.15

ReAu	62.5052	42.0522	1.51	1.36	7	11	5	10	1.9	2.54	77.8778	79.2256	0.15	82.3090	5-2.7500	1--5.2388	4.44	0.64	2.87	0.15
OsTi	2.15622	1.0922	1.44	1.6	8	4	6	2	2.2	1.54	.7068	.8276	1.1	.0790	3.0573	2.4333	3.74	0.66	3.04	0.16
OsV	2.12222	2.0892	1.44	1.53	8	5	6	3	2.2	1.63	.7068	.7467	1.1	.5255	3.2887	2.7733	3.83	0.57	2.97	0.09
OsMn	2.23622	2.0512	1.44	1.39	8	7	6	5	2.2	1.55	.7068	.4347	1.1	0	2.3223	1.8089	3.75	0.65	2.83	0.05
OsFe	2.16422	2.0402	1.44	1.32	8	8	6	6	2.2	1.83	.7068	.9027	1.1	0.15103	3.5530	2.3000	4.03	0.37	2.76	0.12
OsCo	2.21122	2.0231	1.44	1.26	8	9	6	7	2.2	1.88	.7068	7.88	1.1	0.66221	3.1330	2.0885	4.08	0.32	2.7	0.18
OsNi	2.31922	1.99922	1.44	1.24	8	10	6	8	2.2	1.91	.7068	.6397	1.1	1.15615	2.8688	1.8807	4.11	0.29	2.68	0.2
OsCu	2.47122	2.0082	1.44	1.32	8	11	6	10	2.2	1.9	.7068	.7269	1.1	1.2355	3.7216	3.1466	4.1	0.3	2.76	0.12
OsZ	2.4	1	1.4	1.2	8	12	6	10	2.2	1.6	.7	.3	1.1	0	3.4	6.7	3.85	0.55	2.66	0.22

n	3	5	4	2						5	0	9			0	0	5					
	2	7									6	4			4	8	8					
Os	2	2	1	1					2	1	8	6	1	0	-	-	-	3.	0.	3.	0.	0.
Zr	3	.	.	.	8	4	6	2	.	.	.	.	.	4	2.	3.	3.	53	87	19	3	31
	4	2	4	7					2	3	7	6	1	6	9	6	6					
	9	.	4	5						3	0	3			3	4	8					
	2	1									6	4										
	2	6									8	6										
Os	2	1	1	1					2	1	7	7	1	0	-	-	-	3.	0.	3.	0.	
Nb	.	.	.	.	8	5	6	5	.	.	.	.	.	.	3.	3.	3.	8	6	08	2	
	2	2	4	6					2	6	8	7	1	3	1	5	5					
	4	0									6	8			3	4	5					
	6	2									8	7										
Os	2	2	1	1					2	2	7	3	1	1	-	-	-	4.		2.	0.	
Ru	.	.	.	.	8	8	6	7	.	.	.	.	.	.	3.	2.	2.	4	0	86	0	
	2	2	4	4					2	2	7	6	1	0	3	9	7				2	
	7	0									8	1			0	5	1					
	2	5									6	7										
Os	2	2	1	1					2	2	7	4	1	1	-	-	-	4.	0.	2.	0.	
Rh	.	.	.	.	8	9	6	8	.	.	.	.	.	.	3.	3.	3.	48	08	86	0	
	3	2	4	4					2	2	7	5	1	1	3	2	2				2	
	4	8									6	9			4	5	5					
	8	2									8	8			1	6	6					
Os	2	2	1	1					2	2	7	3	1	1	-	-	-	4.		2.	0.	
Pd	.	.	.	.	8	1	6	1	.	.	.	.	.	.	3.	3.	3.	4	0	83	0	
	4	2	4	3		0		0	2	2	7	7	1	1	6	0	8				5	
	8	2									6	8			9	7	7					
	2	0									8	7			5	0	7					
Os	2	2	1	1					2	1	7	3	1	1	-	-	-	4.	0.	2.	0.	
Ag	.	.	.	.	8	1	6	1	.	.	.	.	.	.	3.	3.	3.	13	27	89	0	
	5	5	4	4		1		0	2	9	7	6	1	1	5	0	6				1	
	8	2									6	8			1	2	4					
	5	0									8	7			0	0	7					
Os	2	2	1	1					2	1	7	8	1	1	-	-	-	3.	0.	3.	0.	
Ta	.	.	.	.	8	5	6	3	.	.	.	.	.	.	2.	3.	3.	7	7	14	2	
	2	2	4	7					2	5	7	6	1	0	9	5	2				6	
	7	0									6	8			2	9	9					
	7	2									8	7			2	2	2					
OsIr	2	2	1	1					2	2	7	9	1	1	-	-	-	4.	0	2.	0.	
	.	.	.	.	8	9	6	7	.	.	.	.	.	.	3.	3.	3.	4		85	0	
	3	6	4	4					2	2	7	0	1	1	0	3	4				3	
	8	0									6	8			0	6	4					
	2	3									8	9			5	5	4					
Os	2	1	1	1					2	2	7	9	1	1	-	-	-	4.	0.	2.	0.	
	.	.	.	.	8	1	6	9	.	.	.	.	.	.	1.	3.	3.	48	08	8	0	
	4	2	4	1		0			2	2	7	8	1	1	1	2	4				8	
	8	2									6	8			2	2	4					
	2	0									8	9			5	5	4					

Pt	49	03	44	36					2	28	70	01	1	12	72	60						
Os	72	52	1	1					2	2	68	79		82	4-	4-						
Au	.53	.04	.44	.36	8	11	6	10	.2	.54	.70	.22	1	.30	1.2	4.5	4.74	0.34	2.8	0.08		
Ir	42	62	1	1					2	1	69	56	1	90	40	53						
Ti	.19	.10	.41	.6	9	4	7	2	.2	.54	.12	.82	.56	.07	3.9	2.6	3.74	0.66	3.01	0.19		
Ir	92	22	1	1					2	1	19	76	51	90	95	60						
V	.18	.07	.41	.53	9	5	7	3	.2	.63	.12	.74	.56	.52	-3.	-3.	3.83	0.57	2.94	0.12		
Ir	92	72	1	1					2	1	19	67	51		90	16						
Mn	.33	.04	.41	.39	9	7	7	5	.2	.55	.12	.43	.56	0	6-	5-	3.75	0.65	2.8	0.02		
Ir	2.	22	1	1					2	1	19	.9	51	0	4.3	3.1						
Fe	282	.01	.41	.32	9	8	7	6	.2	.83	.12	02	.56	.15	12	30						
Ir	2.	92	1	1					2	1	19	7	51	10	-2.	-2.	4.03	0.37	2.73	0.09		
Co	294	.00	.41	.26	9	9	7	7	.2	.88	.12	.88	.56	.66	8548	3729						
Ir	2.	1.	1	1					2	1	19	7	51	21	-3.	-2.						
Ni	403	984	.41	.24	9	10	7	8	.2	.91	.12	.63	.56	.15	2.44	1.51	4.11	0.29	2.65	0.17		
Ir	2.	1.	1	1					2	1	19	7	51	61	-2.	-3.						
Cu	449	982	.41	.32	9	11	7	10	.2	.9	.12	.72	.56	.23	7082	2372	4.1	0.3	2.73	0.09		
Ir	2	2	1	1	9	1	7	1	2	1	19	69	51	50	-	-	3.	0.	2.	0.1		

Zn	.386	.0352	.41	.22		2		0	.2	.65	.1219	.3946	.5651		3.858	6.501	85	55	63	9
IrNb	2.29	.1032	1.41	1.64	9	5	7	5	2.2	1.6	.1219	.7587	.5651	.8931	-5.181	-4.941	3.8	0.6	3.05	0.23
IrRh	2.33	.0372	1.41	1.42	9	9	7	8	2.2	2.28	.1219	.4598	.5651	.1370	-3.727	-3.142	4.48	0.08	2.83	0.01
IrPd	2.4842	.0472	1.41	1.39	9	10	7	10	2.2	2.2	.1219	.3377	.5651	.5621	-4.439	-3.540	4.4	0	2.8	0.02
IrAg	2.4972	.0562	1.41	1.45	9	11	7	10	2.2	1.93	.1219	.5767	.5651	.3020	-3.810	-4.973	4.13	0.27	2.86	0.04
IrTa	2.3172	.0902	1.41	1.7	9	5	7	3	2.2	2.5	.1219	.8879	.5651	.3222	-3.516	-3.868	3.7	0.7	3.11	0.29
IrPt	2.5052	.0291	1.41	1.36	9	10	7	9	2.2	2.28	.1219	.0177	.5651	.1280	-2.848	-2.776	4.48	0.08	2.77	0.05
PtCo	2.3882	.9931	1.36	1.26	10	9	9	7	2.28	1.88	.0179	7.88	2.1282	.6621	-3.076	-2.188	4.16	0.4	2.62	0.1
PtNi	2.399	.9911	1.36	1.24	10	10	9	8	2.28	1.91	.0179	.6399	.1288	.1156	-4.098	-3.417	4.19	0.37	2.6	0.12

AuTi	2.4832	2.0832	1.36	1.6	11	4	10	2	2.54	1.54	9.2259	6.8276	2.3092	0.0790	-4.6477	-2.2299	4.08	1	2.96	0.24
AuV	2.4072	2.0412	1.36	1.53	11	5	10	3	2.54	1.63	2.2259	7.4677	3.0922	0.525	-4.7555	-2.3511	4.17	0.91	2.89	0.17
AuMn	2.41	2.0162	1.36	1.39	11	7	10	5	2.54	1.55	2.2259	4.3477	3.0920	0	-5.0779	-2.2443	4.09	0.99	2.75	0.03
AuFe	2.4142	2.0061	1.36	1.32	11	8	10	6	2.54	1.83	2.2259	9.0227	3.0920	0.1510	-4.9822	-2.1822	4.37	0.71	2.68	0.04
AuCo	2.41222	1.99722	1.36	1.26	11	9	10	7	2.54	1.88	2.2259	7.887	3.0920	0.66210	-4.6700	-2.0644	4.42	0.66	2.62	0.1
AuNi	2.40322	2.00722	1.36	1.24	11	10	10	8	2.54	1.91	2.2259	6.3997	3.0920	0.15610	-5.3199	-3.5222	4.45	0.63	2.6	0.12
AuCu	2.41922	2.06222	1.36	1.32	11	11	10	10	2.54	1.9	2.2259	7.2269	3.0920	0.2350	-4.5444	-2.8999	4.44	0.64	2.68	0.04
AuZn	2.33822	2.07622	1.36	1.22	11	12	10	10	2.54	1.65	2.2259	3.9466	3.0920	0	-5.0622	-6.6355	4.19	0.89	2.58	0.14
AuNb	2.51	2.09	1.36	1.64	11	5	10	5	2.54	1.6	2.22	7.75	3.030	0.89	-5.887	-3.336	4.14	0.94	3	0.28

AuRh	92.4642	92.0222	1.36	1.42	11	9	10	8	2.54	2.28	59.22559	87.45598	92.30920	31.13700	0-5.0755	8-3.6466	4.82	0.26	2.78	0.06
AuPd	2.45	2.0332	1.36	1.39	11	10	10	10	2.54	2.2	.22559	.33377	.30920	.56210	5.249	3.917	4.74	0.34	2.75	0.03
AuAg	2.6042	2.2762	1.36	1.45	11	11	10	10	2.54	1.93	.22559	.57767	.30920	.30220	-4.6223	-3.7669	4.47	0.61	2.81	0.09
AuTa	2.5122	2.0862	1.36	1.7	11	5	10	3	2.54	1.5	.22559	.88879	.30920	.32210	-5.5582	-4.0331	4.04	1.04	3.06	0.34
AuIr	2.4832	2.0152	1.36	1.41	11	9	10	7	2.54	2.2	.22559	.12199	.30920	.56522	-4.7388	-1.9688	4.74	0.34	2.77	0.05
AuPt	2.4752	2.0266	1.36	1.36	11	10	10	9	2.54	2.28	.2225	.0177	.3099	.1288	-5.2399	-3.6722	4.82	0.26	2.72	0

Table S12. The calculated coefficient of determination (R^2) and the root-mean-square-error (RMSE) values for training samples and testing samples.

DFT calculated vs predicted values	Training samples		Testing samples	
	R^2	RMSE	R^2	RMSE
ΔG_{H^*} (eV)	0.978	0.333	0.965	0.012
η^{OER} (V)	0.987	0.243	0.982	0.007
η^{ORR} (V)	0.982	0.245	0.977	0.012

Table S13. The calculated ΔG_{H^*}, η^{OER} and η^{ORR} values for Ni_2/g-CN, Pd_2/g-CN, CuPd/g-CN, PdNi/g-CN, AgPt/g-CN, AuFe/g-CN, AuCo/g-CN, AuNi/g-CN, AuRh/g-CN, AgPd/g-CN, AuPd/g-CN, and AuIr/g-CN after considering solvation correction via Vaspsol.

Systems	ΔG_{H^*}		η^{OER}		η^{OER}	
	vaspsol	vasp	vaspsol	vasp	vaspsol	vasp
Ni_2/g-CN	-0.07	-0.05	-	-	-	-
Pd_2/g-CN	-0.01	0.03	-	-	-	-
CuPd/g-CN	-0.03	-0.02	-	-	0.56	0.47
PdNi/g-CN	-0.03	0	-	-	-	-
AgPt/g-CN	0.05	0	-	-	-	-

AuFe/g-CN	0.11	0.02	-	-	-	-
AuCo/g-CN	0.02	0.05	0.44	0.52	0.62	0.48
AuNi/g-CN	0.11	0.08	-	-	-	-
AuRh/g-CN	-0.11	-0.09	-	-	0.47	0.35
AgPd/g-CN	-	-	0.46	0.43	0.67	0.48
AuPd/g-CN	-	-	0.39	0.48	-	-
AuIr/g-CN	-	-	-	-	0.57	0.44

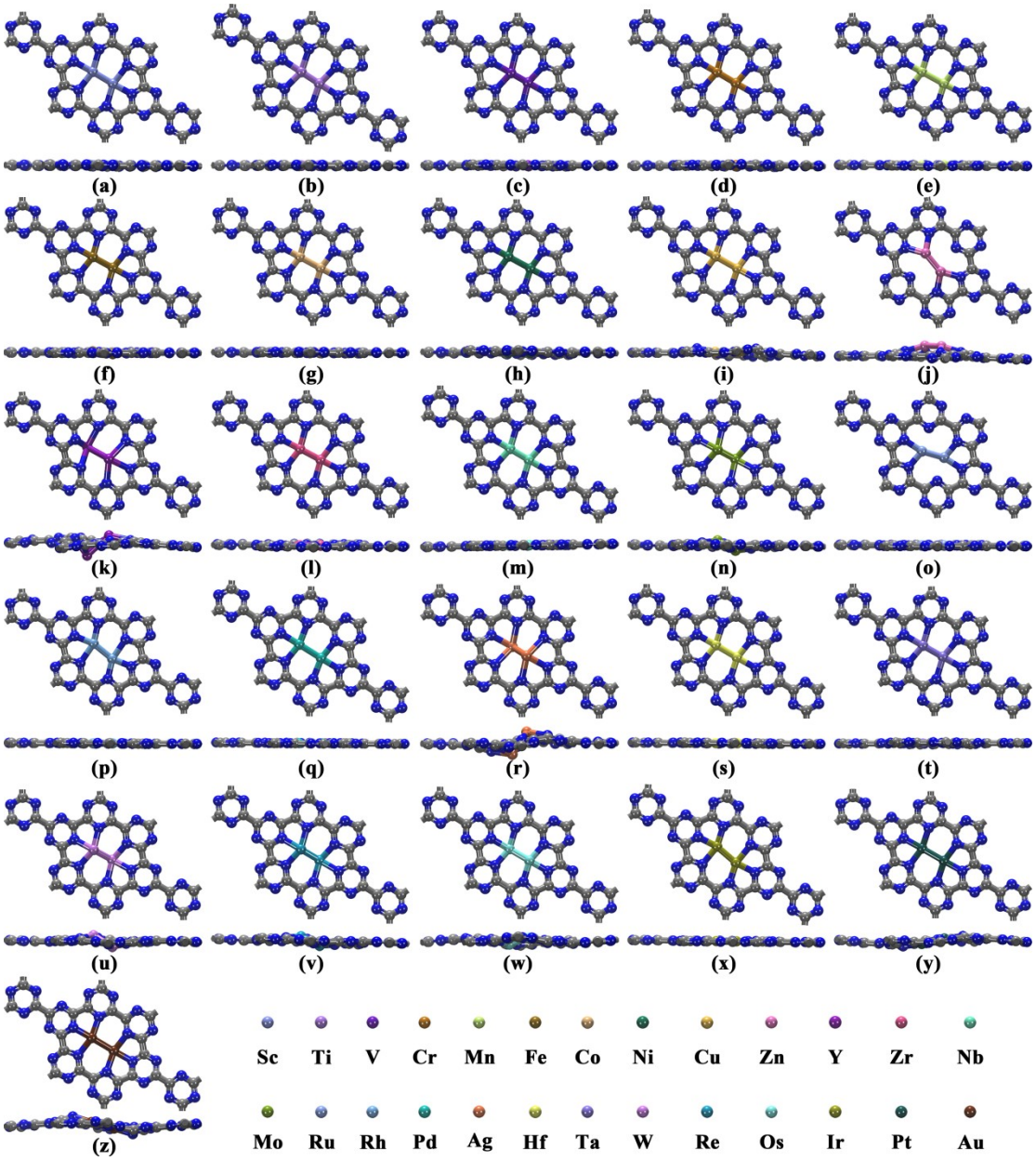

Fig. S1. The stable configurations for (a) Sc_2/g-CN, (b) Ti_2/g-CN, (c) V_2/g-CN, (d)

Cr_2/g-CN, (e) Mn_2/g-CN, (f) Fe_2/g-CN, (g) Co_2/g-CN, (h) Ni_2/g-CN, (i) Cu_2/g-CN, (j) Zn_2/g-CN, (k) Y_2/g-CN, (l) Zr_2/g-CN, (m) Nb_2/g-CN, (n) Mo_2/g-CN, (o) Ru_2/g-CN, (p) Rh_2/g-CN, (q) Pd_2/g-CN, (r) Ag_2/g-CN, (s) Hf_2/g-CN, (t) Ta_2/g-CN, (u) W_2/g-CN, (v) Re_2/g-CN, (w) Os_2/g-CN, (x) Ir_2/g-CN, (y) Pt_2/g-CN, and (z) Au_2/g-CN.

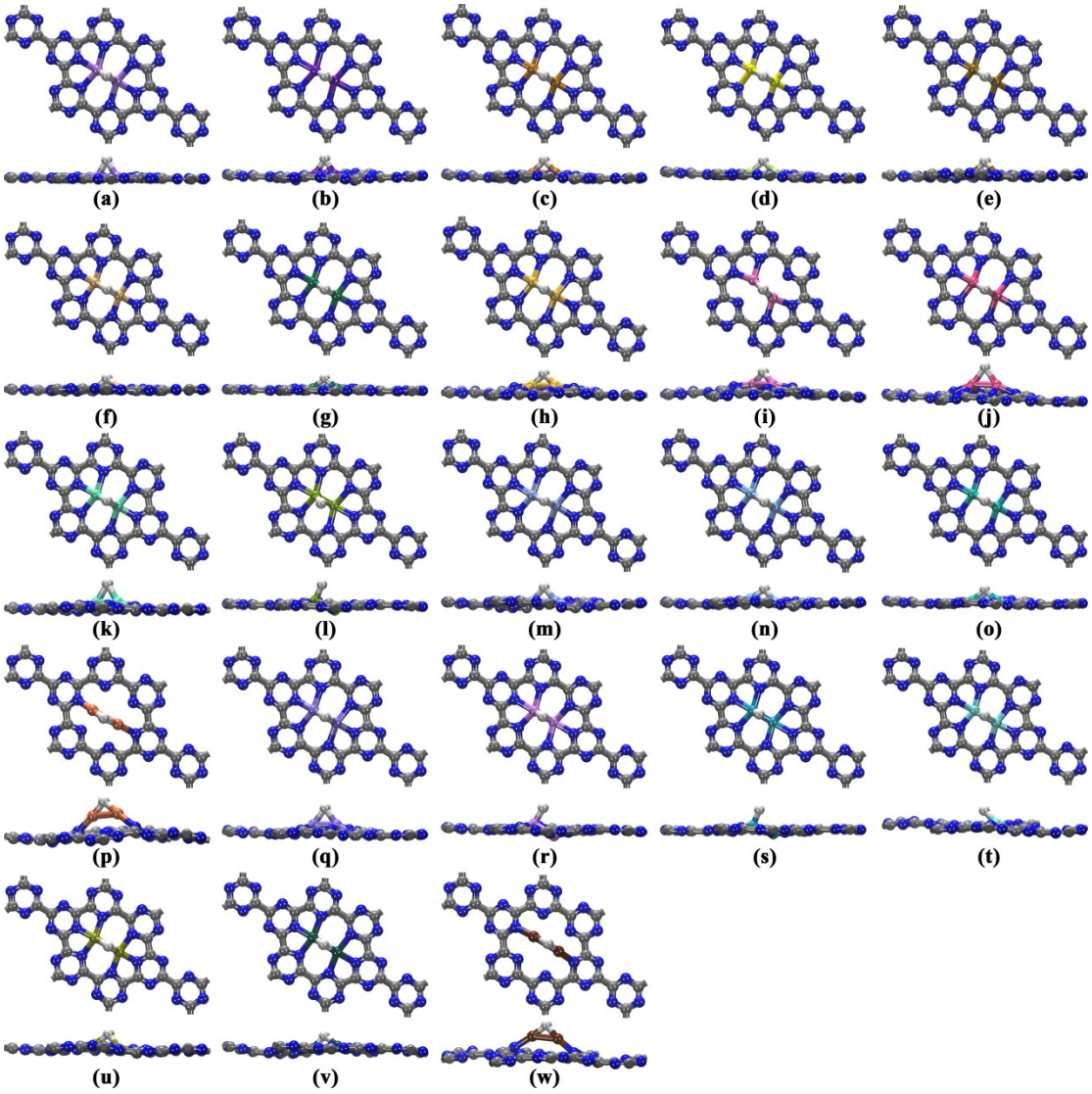

Fig. S2. The stable configurations for H adsorption on (a) Ti_2/g-CN, (b) V_2/g-CN, (c) Cr_2/g-CN, (d) Mn_2/g-CN, (e) Fe_2/g-CN, (f) Co_2/g-CN, (g) Ni_2/g-CN, (h) Cu_2/g-CN, (i) Zn_2/g-CN, (j) Zr_2/g-CN, (k) Nb_2/g-CN, (l) Mo_2/g-CN, (m) Ru_2/g-CN, (n) Rh_2/g-CN, (o) Pd_2/g-CN, (p) Ag_2/g-CN, (q) Ta_2/g-CN, (r) W_2/g-CN, (s) Re_2/g-CN, (t) Os_2/g-CN, (u) Ir_2/g-CN, (v) Pt_2/g-CN, and (w) Au_2/g-CN.

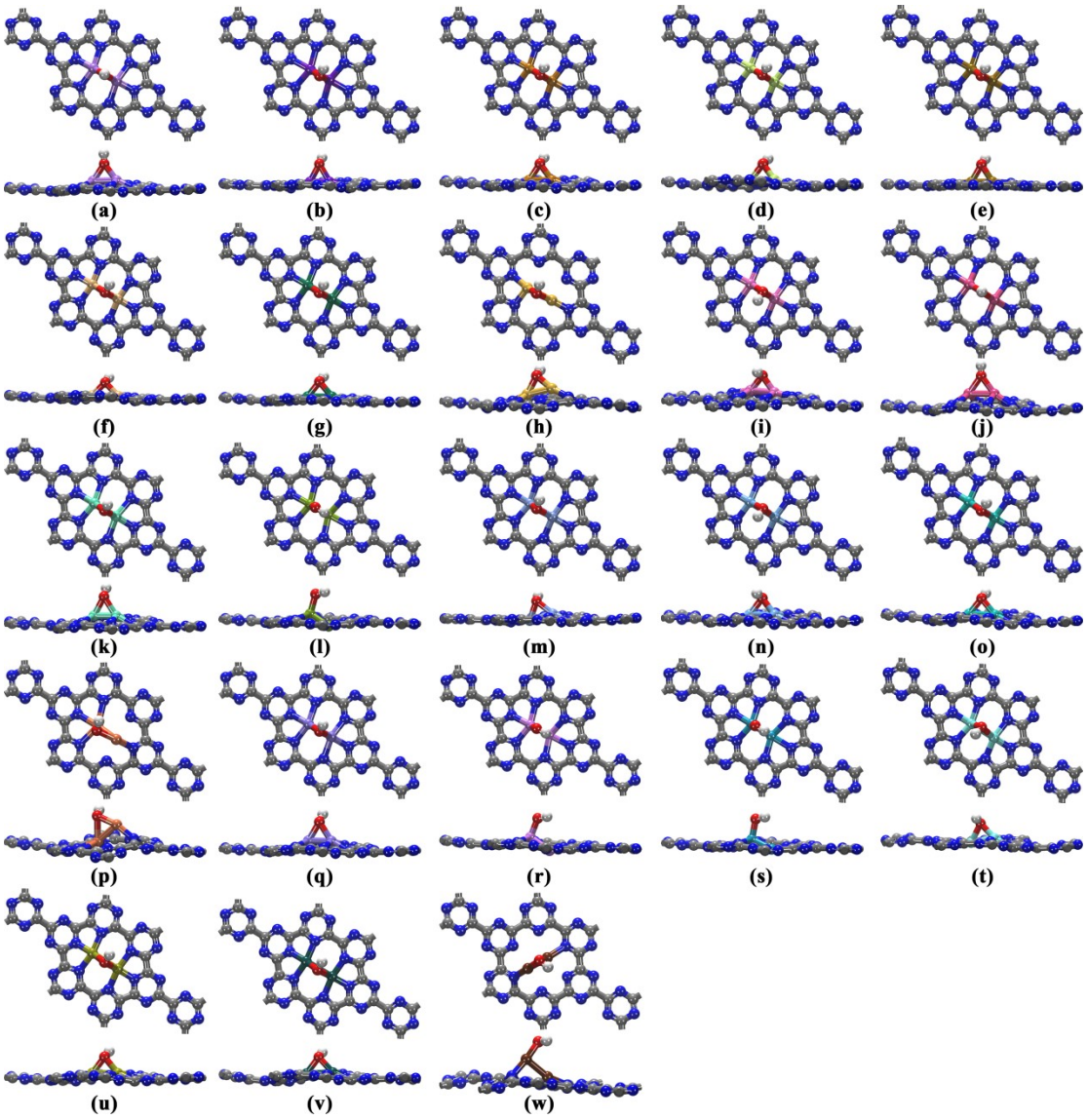

Fig. S3. The stable configurations for OH adsorption on (a) Ti_2/g-CN, (b) V_2/g-CN, (c) Cr_2/g-CN, (d) Mn_2/g-CN, (e) Fe_2/g-CN, (f) Co_2/g-CN, (g) Ni_2/g-CN, (h) Cu_2/g-CN, (i) Zn_2/g-CN, (j) Zr_2/g-CN, (k) Nb_2/g-CN, (l) Mo_2/g-CN, (m) Ru_2/g-CN, (n) Rh_2/g-CN, (o) Pd_2/g-CN, (p) Ag_2/g-CN, (q) Ta_2/g-CN, (r) W_2/g-CN, (s) Re_2/g-CN, (t) Os_2/g-CN, (u) Ir_2/g-CN, (v) Pt_2/g-CN, and (w) Au_2/g-CN.

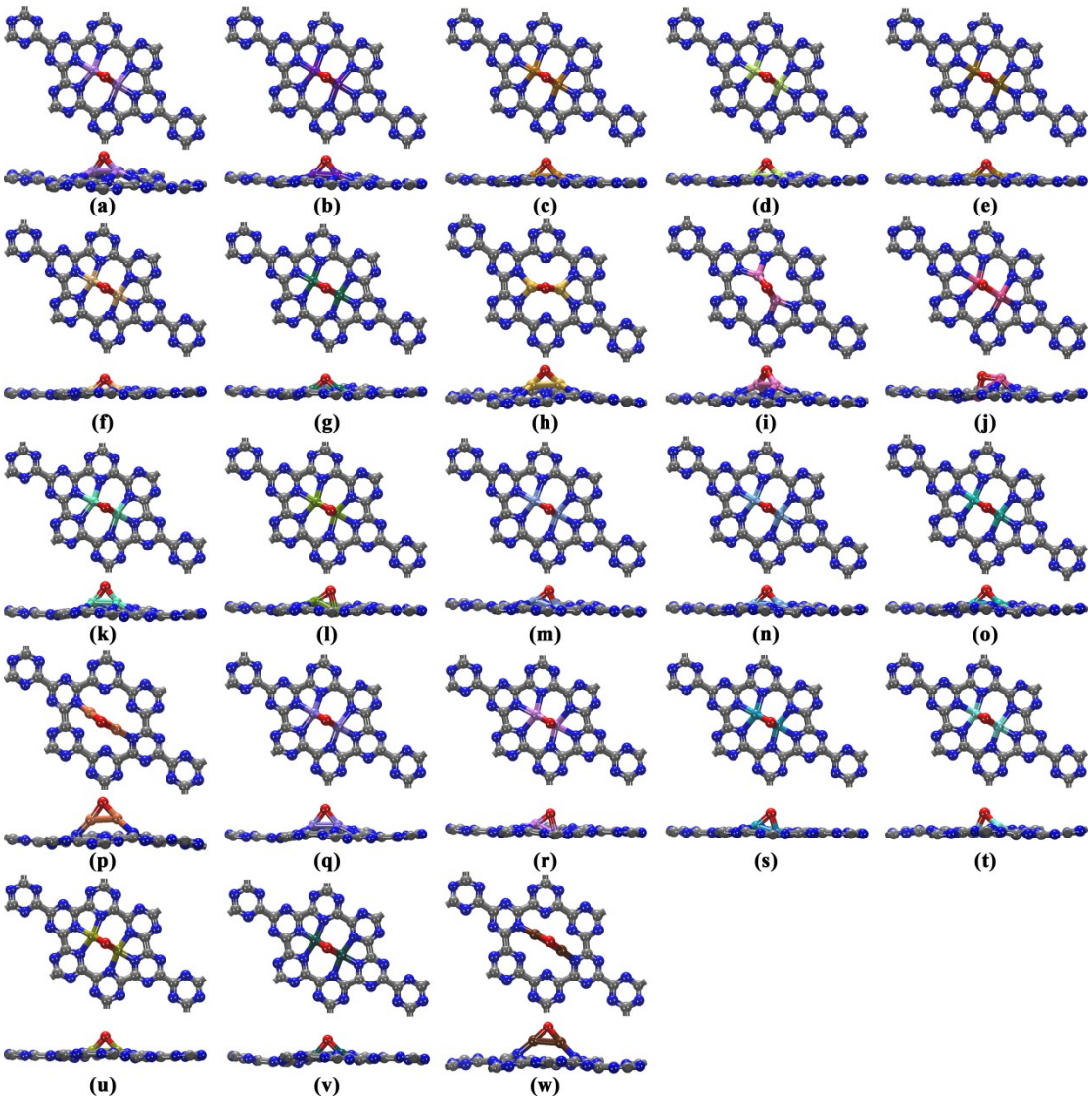

Fig. S4. The stable configurations for O adsorption on (a) Ti_2/g-CN, (b) V_2/g-CN, (c) Cr_2/g-CN, (d) Mn_2/g-CN, (e) Fe_2/g-CN, (f) Co_2/g-CN, (g) Ni_2/g-CN, (h) Cu_2/g-CN, (i) Zn_2/g-CN, (j) Zr_2/g-CN, (k) Nb_2/g-CN, (l) Mo_2/g-CN, (m) Ru_2/g-CN, (n) Rh_2/g-CN, (o) Pd_2/g-CN, (p) Ag_2/g-CN, (q) Ta_2/g-CN, (r) W_2/g-CN, (s) Re_2/g-CN, (t) Os_2/g-CN, (u) Ir_2/g-CN, (v) Pt_2/g-CN, and (w) Au_2/g-CN.

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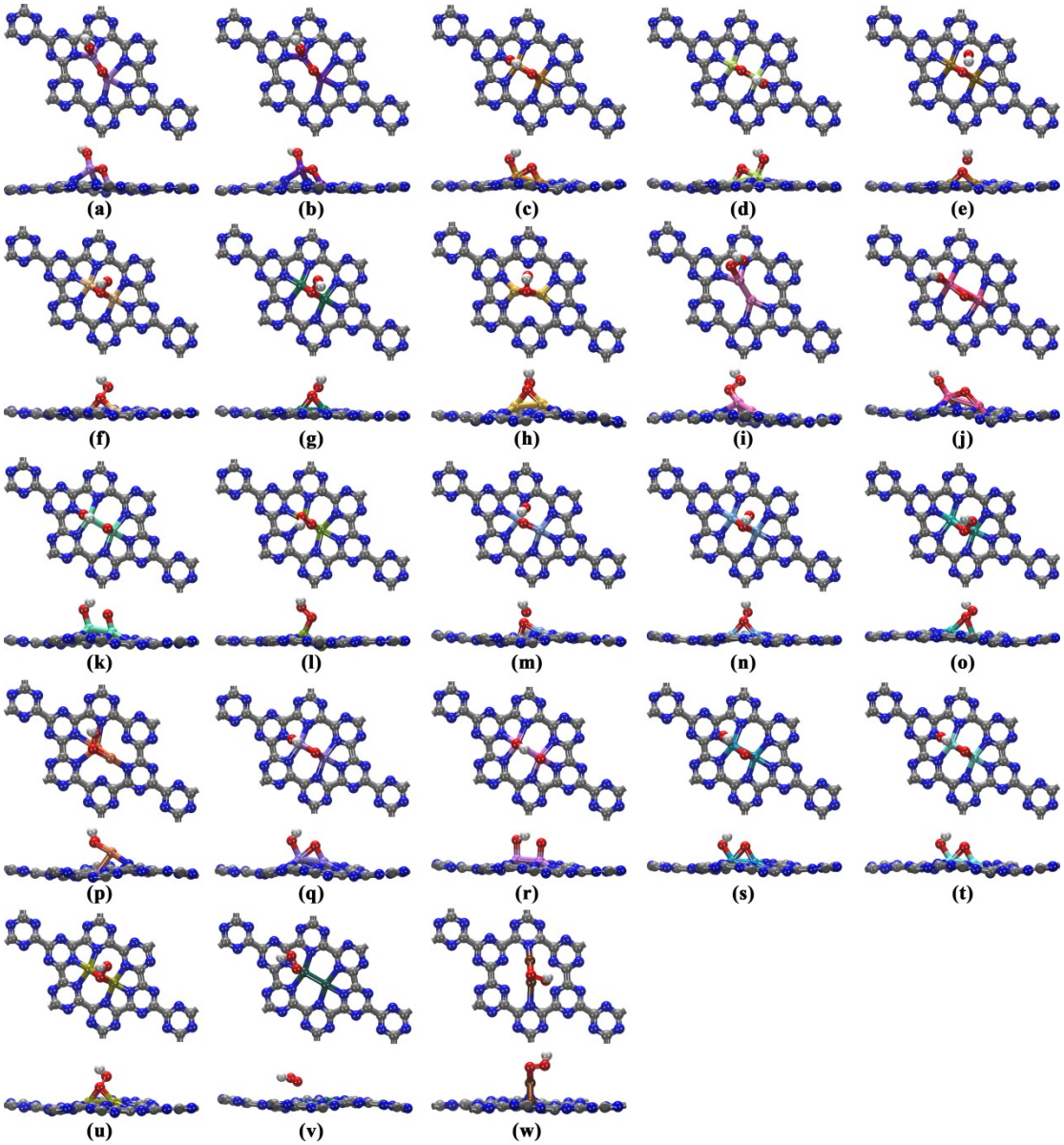

Fig. S5. The stable configurations for OOH adsorption on (a) Ti_2/g-CN, (b) V_2/g-CN, (c) Cr_2/g-CN, (d) Mn_2/g-CN, (e) Fe_2/g-CN, (f) Co_2/g-CN, (g) Ni_2/g-CN, (h) Cu_2/g-CN, (i) Zn_2/g-CN, (j) Zr_2/g-CN, (k) Nb_2/g-CN, (l) Mo_2/g-CN, (m) Ru_2/g-CN, (n) Rh_2/g-CN, (o) Pd_2/g-CN, (p) Ag_2/g-CN, (q) Ta_2/g-CN, (r) W_2/g-CN, (s) Re_2/g-CN, (t) Os_2/g-CN,

(u) Ir_2/g-CN, (v) Pt_2/g-CN, and (w) Au_2/g-CN.

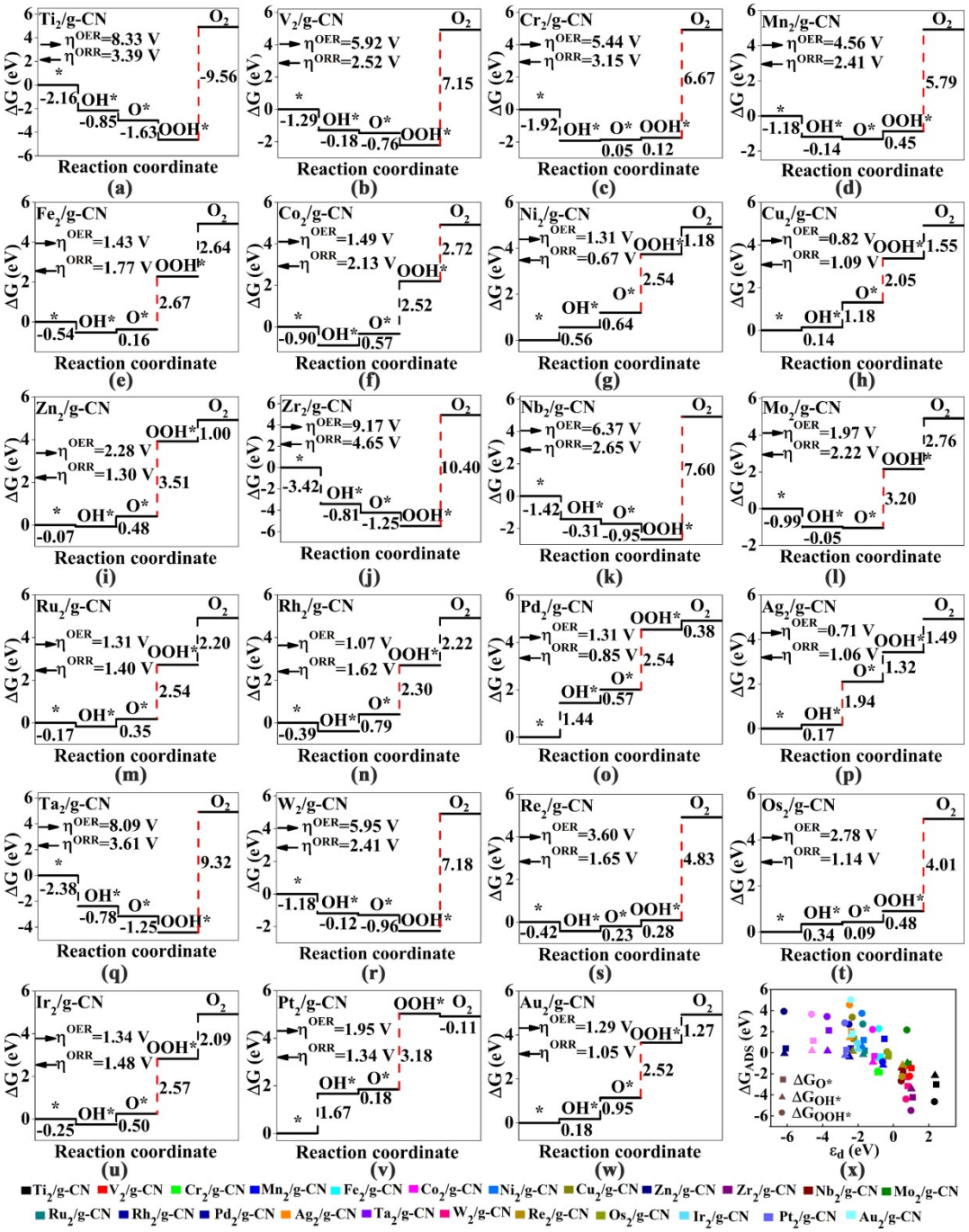

Fig. S6. (a)-(w) The Gibbs free energy for O/OH/OOH adsorption on M_2/g-CN (M = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt,

Au). (x) The relations between the d band center (ε_d) and $\Delta G_{O*}/\Delta G_{OH*}/\Delta G_{OOH*}$.

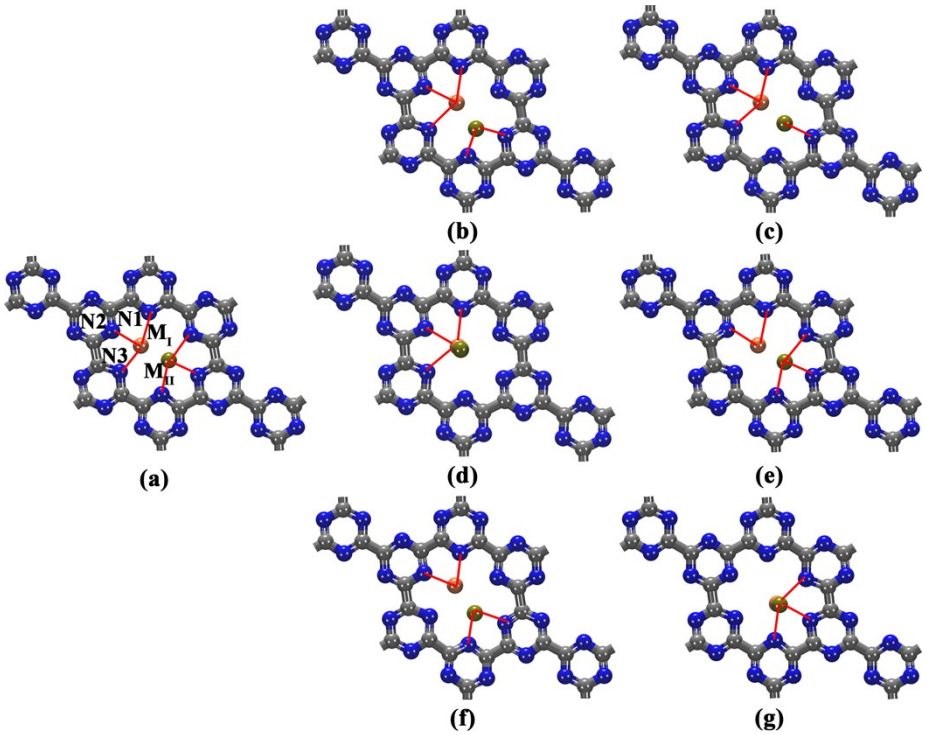

Fig. S7. The stable configurations for (a) M_IM_{II}/g-CN (M_I = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt, Au; M_{II} = V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Os, Ir, Pt, Au; $M_I \neq M_{II}$; $M_IM_{II} \neq$ ZrCu, NbCu, TaCu, RuZn, TaZn, ZnTi, NbZn, MoAg, ReAg, AgTi, ZrZn, ZrAg, AgNb, TaAg, WAg, MoZn, WZn, ReZn, OsZn), (b) M_IM_{II}/g-CN (M_IM_{II} = ZrCu, NbCu, RuZn, TaCu, TaZn), (c) M_IM_{II}/g-CN (M_IM_{II} = NbZn, MoAg, ReAg), (d) M_IM_{II}/g-CN (M_IM_{II} =ZrZn, ZrAg, TaAg, WAg), (e) M_IM_{II}/g-CN (M_IM_{II} = ZnTi, AgV), (f) M_IM_{II}/g-CN (M_IM_{II} = MoZn, WZn, ReZn, OsZn), and (g) M_IM_{II}/g-CN (M_IM_{II} = AgTi, AgNb).

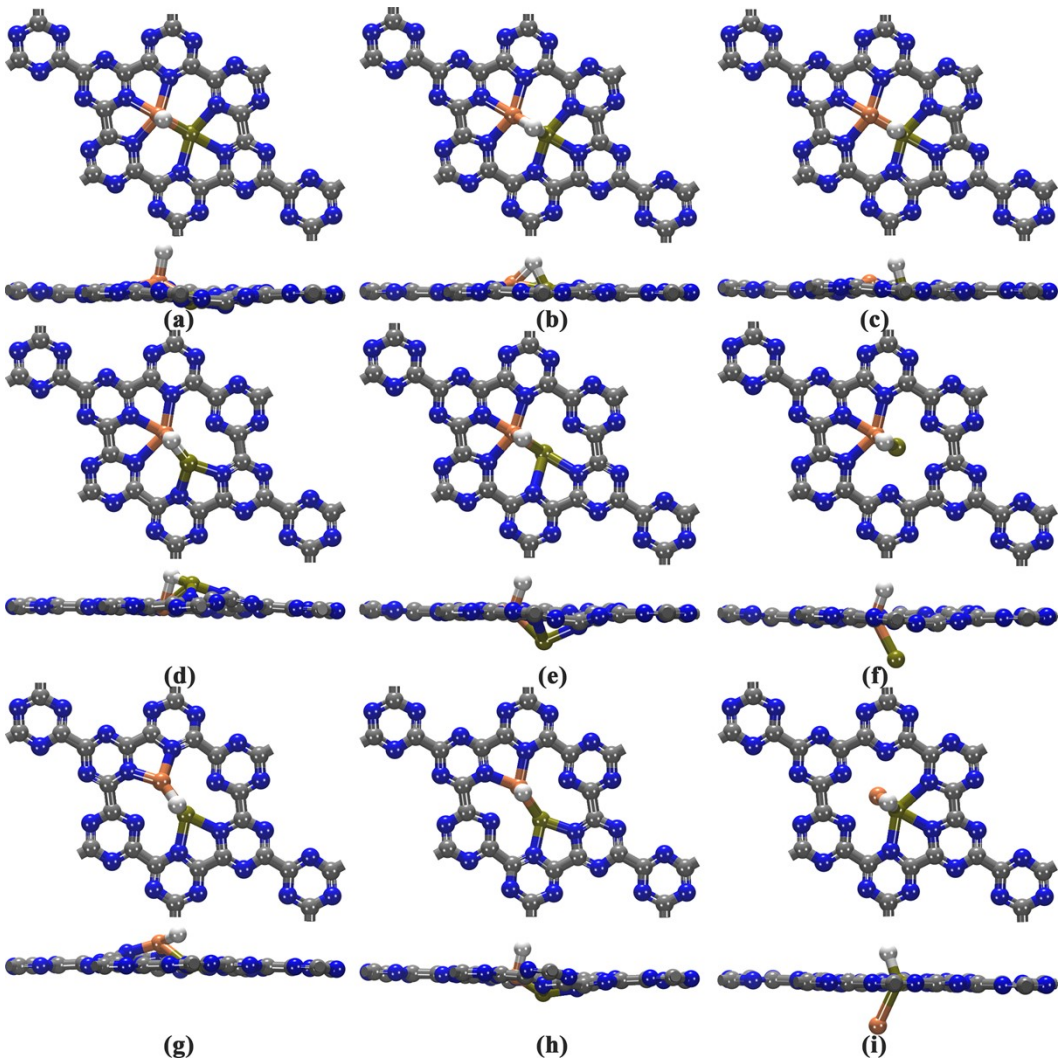

Fig. S8. The stable configurations for H adsorption on (a) M_IM_{II}/g-CN (M_IM_{II} = TiPd, VPd, CrZr, ZnV, ZrNi, ZrPd, ZrAu, NbTi, NbNi, NbRh, NbPd, MoTi, MoMn, MoZr, MoRh, MoPd, MoIr, MoAu, RuTi, RuV, RuCu, RuZr, RuNb, RuAg, RuTa, RuAu, RhV, TaTi, TaNi, TaNb, TaRh, TaPd, WTi, WFe, WNi, WZr, WRu, WPd, WIr, WPt, WAu, ReTi, ReV, ReMn, ReFe, ReNi, ReCu, ReNb, ReRh, RePd, ReTa, ReOs, ReAu, OsTi, OsV, OsMn, OsRu, OsPd, OsAg, OsTa, OsAu, IrTi, IrV, IrNb, IrAg, IrTa, AuV,

AuMn, AuNi, AuZn, AuPd, AuAg), (b) M_IM_{II}/g-CN (M_IM_{II} = TiFe, TiCo, TiNi, TiCu, TiPt, VTi, VFe, VCo, VNi, VCu, VPt, CrTi, CrV, CrMn, CrFe, CrCo, CrNi, CrCu, CrZn, CrNb, CrMo, CrRu, CrRh, CrPd, CrAg, CrTa, CrW, CrIr, CrPt, MnTi, MnV, MnFe, MnCo, MnNi, MnCu, MnPd, MnPt, FeCo, FeNi, FeCu, FePd, FePt, CoNi, CuCo, CuNi, CuPd, CuPt, ZnMn, ZnTi, ZnCo, ZnNi, ZnCu, ZnPd, ZnPt, ZrTi, ZrV, ZrMn, ZrFe, ZrCo, ZrPt, NbV, NbMn, NbFe, NbCo, NbPt, MoV, MoFe, MoCo, MoNi, MoCu, MoNb, MoTa, MoPt, RuMn, RuFe, RuCo, RuNi, RuRh, RuPd, RuIr, RuPt, RhTi, RhMn, RhFe, RhCo, RhNi, RHCu, RhZn, RhPd, RhPt, PdCo, PdNi, PdPt, AgMn, AgFe, AgCo, AgNi, AgCu, AgZn, AgRh, AgPd, AgPt, TaV, TaMn, TaFe, TaCo, TaPt, WV, WMn, WCo, WCu, WRh, ReCo, ReZr, ReRu, ReIr, RePt, OsFe, OsCo, OsNi, OsCu, OsZr, OsNb, OsRh, OsIr, OsPt, IrMn, IrFe, IrCo, IrNi, IrCu, IrZn, IrRh, IrPd, IrPt, PtCo, PtNi, AuPt), (c) M_IM_{II}/g-CN (M_IM_{II} = CrRe, CrOs, CrAu, ZrNb, ZrRh, ZrTa, ZrIr, MoRu, MoW, MoRe, MoOs, AgNb, WNb, WTa, WRe, WOs, AuTi, AuFe, AuNb, AuTa, AuIr), (d) M_IM_{II}/g-CN (M_IM_{II} = ZrCu, NbCu, RuZn, TaCu, TaZn), (e) M_IM_{II}/g-CN (M_IM_{II} = NbZn, MoAg, ReAg), (f) M_IM_{II}/g-CN (M_IM_{II} = ZrZn, ZrAg, TaAg, WAg), (g) M_IM_{II}/g-CN (M_IM_{II} = ZnTi, AgV), (h) M_IM_{II}/g-CN (M_IM_{II} = MoZn, WZn, ReZn, OsZn), and (i) M_IM_{II}/g-CN (M_IM_{II} = AgTi, AgNb).

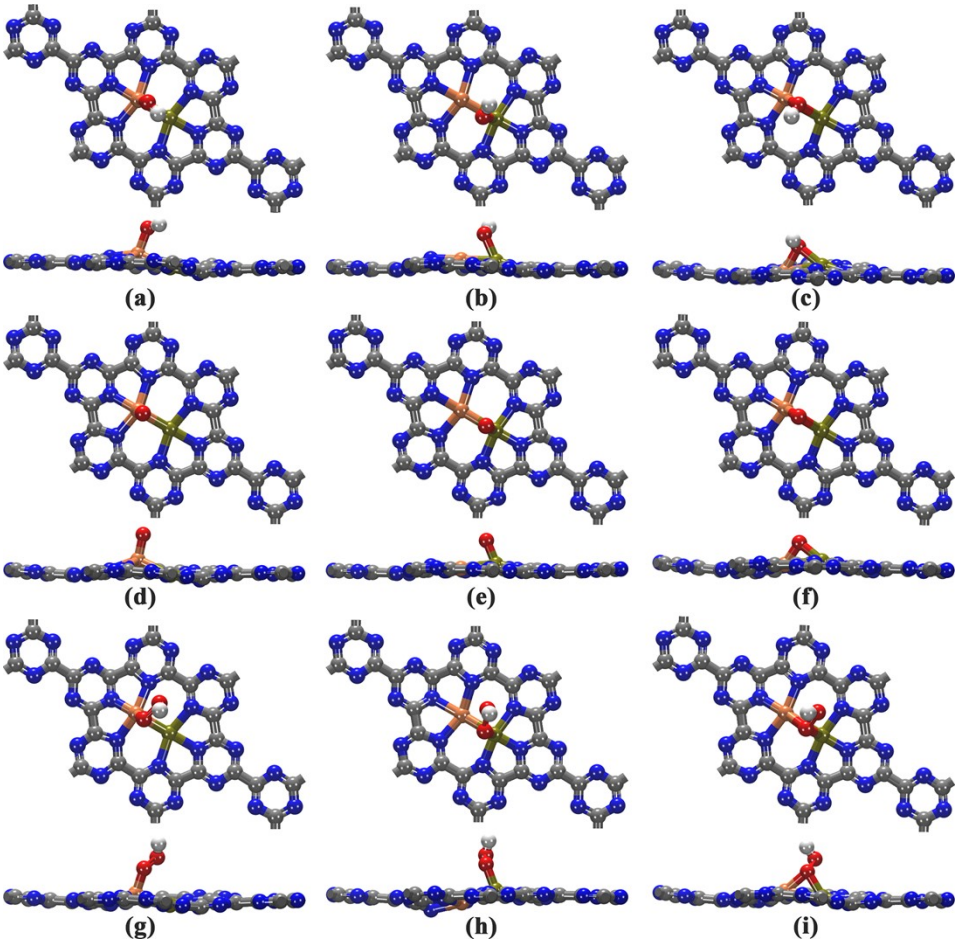

Fig. S9. The stable configurations for OH adsorption on (a) M_IM_{II}/g-CN (M_IM_{II} = FePd, RuAu, IrAg), (b) M_IM_{II}/g-CN (M_IM_{II} = AgCo, AgNi, AgRh, AgPd, AuFe, AuCo, AuNi, AuZn, AuRh, AuPd, AuIr, AuPt), and (c) M_IM_{II}/g-CN (FePt, CuNi, CuPd, CuPt, ZnNi, ZnPd, ZnPt, MoPt, RuPt, RhCu, RhPd, RhPt, PdCo, PdNi, PdPt, AgCu, AgPt, ReIr, IrCu, IrPd, IrPt, PtCo, PtNi, AuCu). The stable configurations for O adsorption on (d) M_IM_{II}/g-CN (M_IM_{II} = MoPt, ReIr, IrAg), (e) AuFe/g-CN, and (f) M_IM_{II}/g-CN (M_IM_{II} = FePd, FePt, CuNi, CuPd, CuPt, ZnNi, ZnPd, ZnPt, RuPt, RuAu, RhCu, RhPd, RhPt, PdCo, PdNi, PdPt, AgCo, AgNi, AgCu, AgRh, AgPd, AgPt, IrCu, IrPd, IrPt, PtCo, PtNi, AuFe, AuCo, AuNi, AuCu, AuZn, AuRh, AuPd, AuIr, AuPt). The stable configurations for OOH adsorption on (g) M_IM_{II}/g-CN (M_IM_{II} = FePd, CuPd, MoPt, RuAu, RhPd, AgPt, IrPd, IrAg, AuPd, AuPt), (h) M_IM_{II}/g-CN (M_IM_{II} = PdPt, AgCo, AgNi, AgCu, AgRh, AgPd, AuFe, AuCo, AuNi, AuCu, AuZn, AuRh, AuIr), and (i) (FePt, CuNi, CuPt, ZnNi, ZnPd, ZnPt, RuPt, RhCu, RhPt, PdCo, PdNi, ReIr, IrCu, IrPt, PtCo, PtNi).

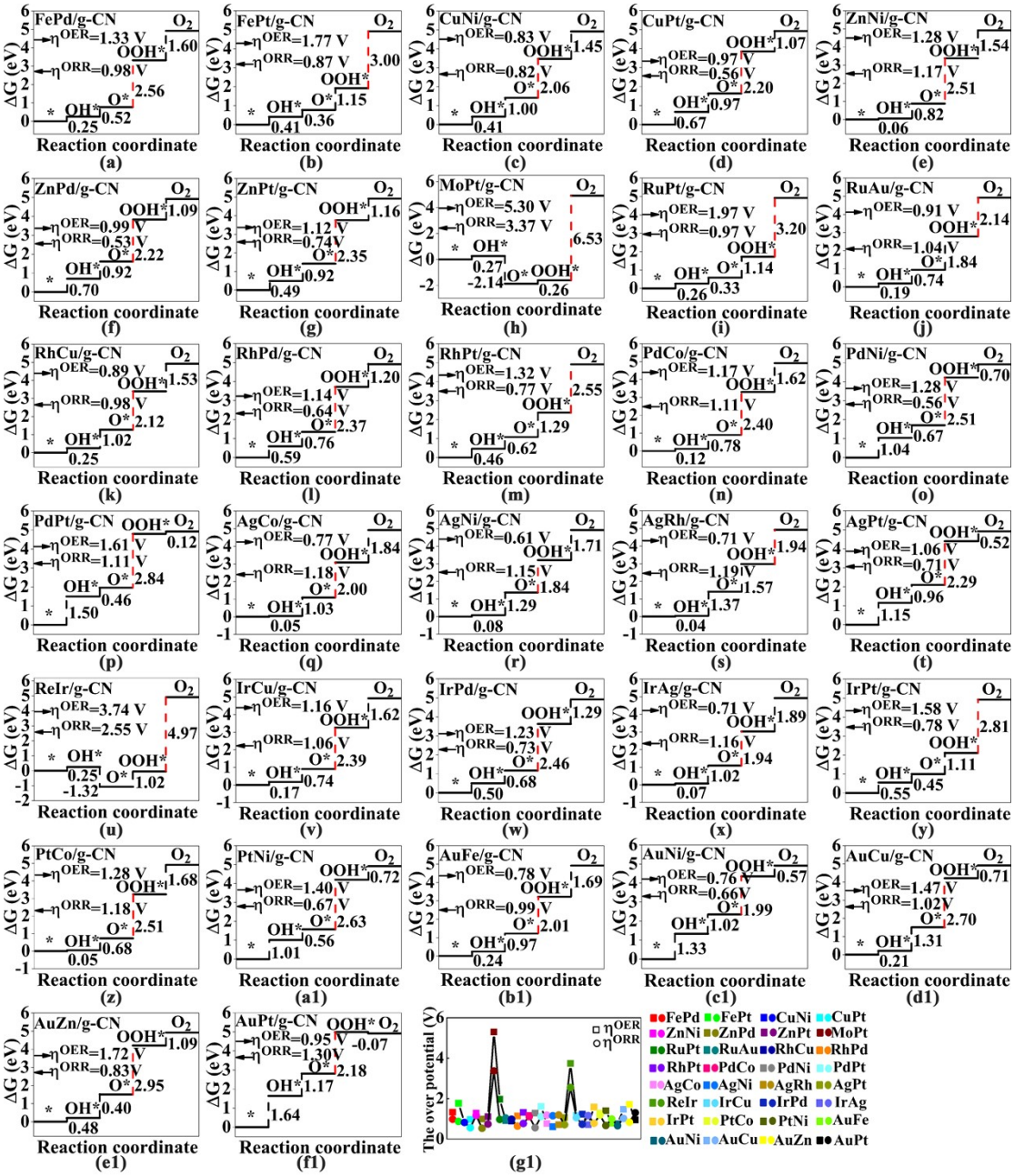

Fig. S10. Calculated free energy diagram of OER/ORR on (a) FePd/g-CN, (b) FePt/g-CN, (c) CuNi/g-CN, (d) CuPt/g-CN, (e) ZnNi/g-CN, (f) ZnPd/g-CN, (g) ZnPt/g-CN, (h) MoPt/g-CN, (i) RuPt/g-CN, (j) RuAu/g-CN, (k) RhCu/g-CN, (l) RhPd/g-CN, (m) RhPt/g-CN, (n) PdCo/g-CN, (o) PdNi/g-CN, (p) PdPt/g-CN, (q) AgCo/g-CN, (r) AgNi/g-CN, (s) AgRh/g-CN, (t) AgPt/g-CN, (u) ReIr/g-CN, (v) IrCu/g-CN, (w) IrPd/g-CN, (x) IrAg/g-CN, (y) IrPt/g-CN, (z) PtCo/g-CN, (a1) PtNi/g-CN, (b1) AuFe/g-CN, (c1) AuNi/g-CN, (d1) AuCu/g-CN, (e1) AuZn/g-CN, and (f1) AuPt/g-CN under U=0 V, wherein the PDS of the elementary reactions are denoted as red lines. (g1) The overpotentials of OER/ORR for M_IM_{II}/g-CN (M_IM_{II} = FePd, FePt,

CuNi, CuPt, ZnNi, ZnPd, ZnPt, MoPt, RuPt, RuAu, RhCu, RhPd, RhPt, PdCo, PdNi, PdPt, AgCo, AgNi, AgRh, AgPt, ReIr, IrCu, IrPd, IrAg, IrPt, PtCo, PtNi, AuFe, AuNi, AuCu, AuZn, AuPt).

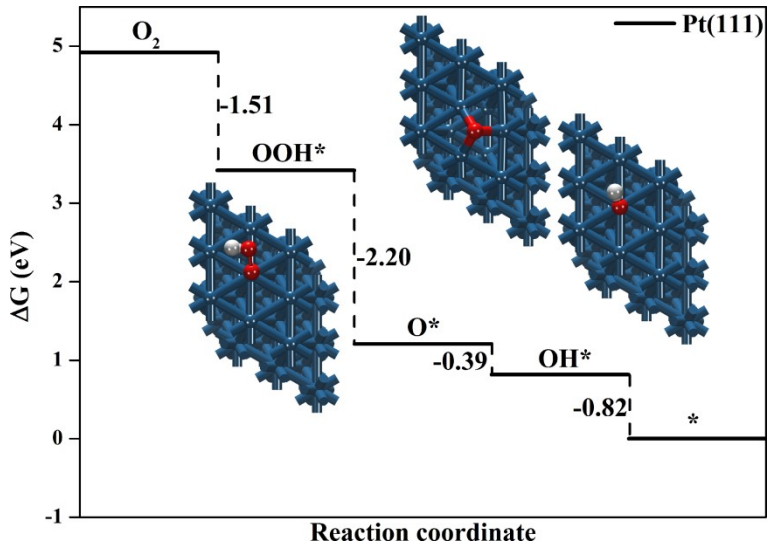

Fig. S11. Calculated free energy diagram of ORR on the benchmark catalyst Pt(111).

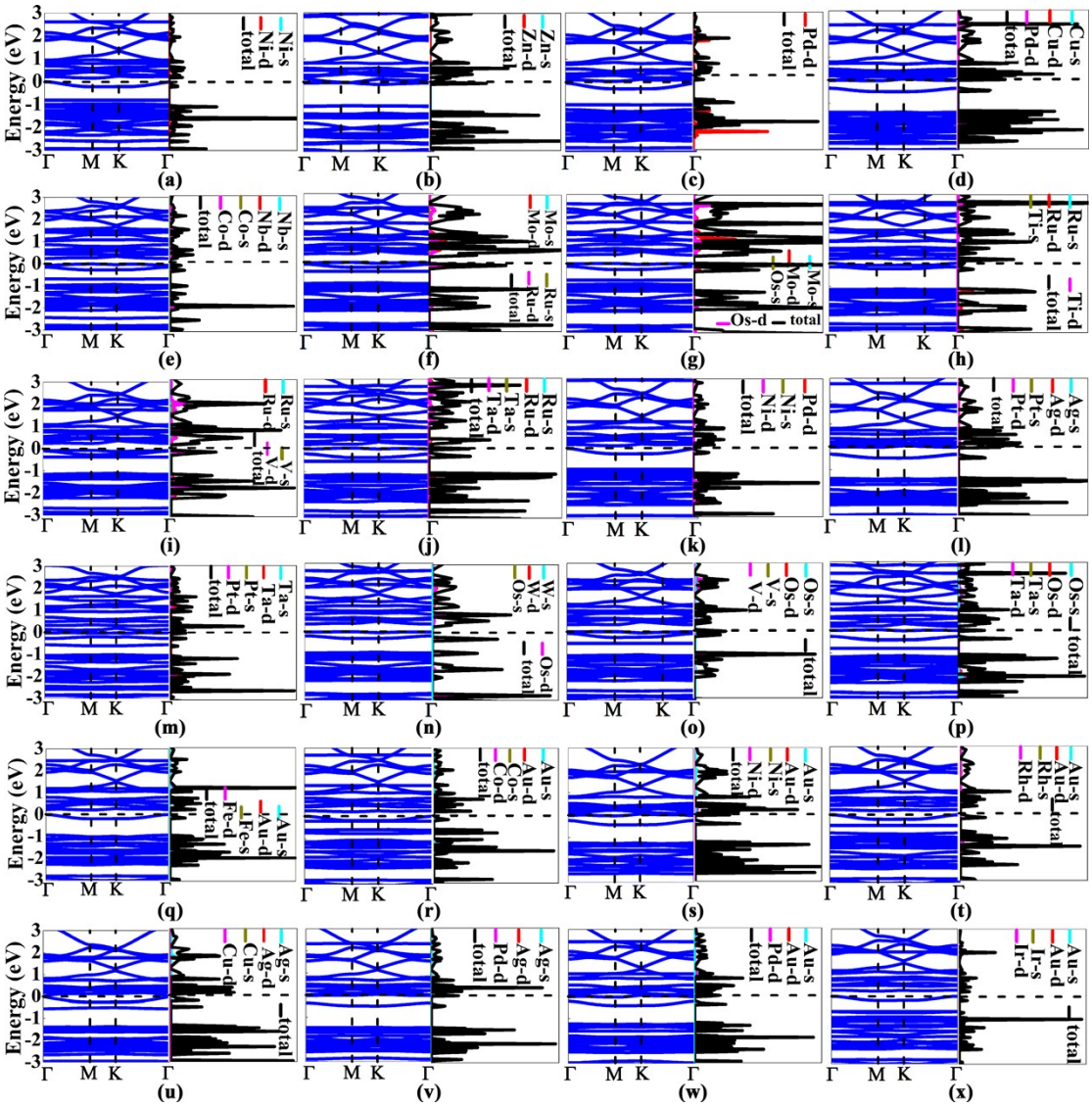

Fig. S12. The band structures and DOS for (a) Ni_2/g-CN, (b) Zn_2/g-CN, (c) Pd_2/g-CN, (d) CuPd/g-CN, (e) NbCo/g-CN, (f) MoRu/g-CN, (g) MoOs/g-CN, (h) RuTi/g-CN, (i) RuV/g-CN, (j) RuTa/g-CN, (k) PdNi/g-CN, (l) AgPt/g-CN, (m) TaPt/g-CN, (n) WOs/g-CN, (o) OsV/g-CN, (p) OsTa/g-CN, (q) AuFe/g-CN, (r) AuCo/g-CN, (s) AuNi/g-CN, (t) AuRh/g-CN, (u) AgCu/g-CN, (v) AgPd/g-CN, (w) AuPd/g-CN, and (x) AuIr/g-CN.

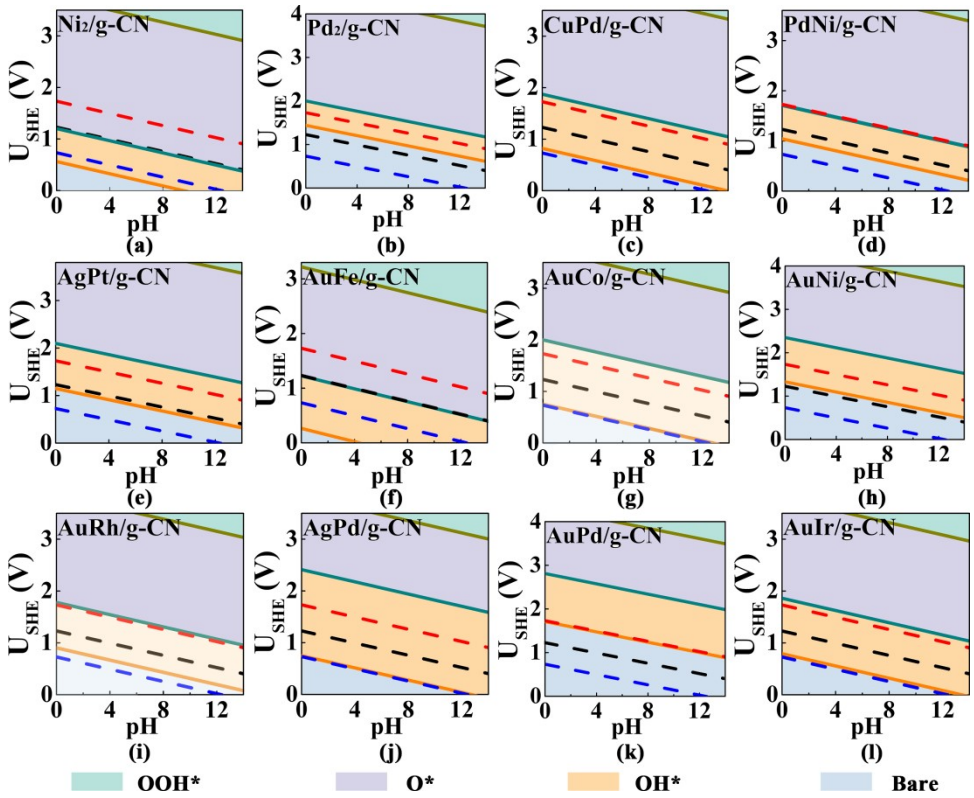

Fig. S13. The surface pourbaix diagrams of (a) Ni_2/g-CN, (b) Pd_2/g-CN, (c) CuPd/g-CN, (d) PdNi/g-CN, (e) AgPt/g-CN, (f) AuFe/g-CN, (g) AuCo/g-CN, (h) AuNi/g-CN, (i) AuRh/g-CN, (j) AgPd/g-CN, (k) AuPd/g-CN, and (l) AuIr/g-CN. The black dashed lines represent the HER/OER/ORR at equilibrium ($U_{eq} = 1.23\ V - 0.059\ pH$). The red and blue dashed lines denote the oxidizing state for OER and ORR, respectively at an overpotential 0.5 V. The other solid lines represent the phase boundary of two oxidizing states.

References

1 S. Grimme, J. Antony, S. Ehrlich, and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.

2 A. M. Patel, S. Ringe, S. Siahrostami, ,M. Bajdich, J. K. Nørskov, and A. R. Kulkarni, *J. Phys. Chem. C*, 2018, **122**, 29307-29318.

3 Y. Ying, K. Fan, X. Luo, and H. Huang, *J. Mater. Chem. A*, 2019, **7**, 11444-11451.

4 Y. Cui, L. Peng, L. Sun, Q. Qian, and T. Huang, *J. Mater. Chem. A*, 2018, **6**, 22768-22777.

5 J. K. Nørskov, T. Bligaard, A. Logadottir, J. Kitchin, J. G. Chen, S. Pandelov, and U. Stimming, *J. Am. Chem. Soc.*, 2005, **152**, J23.

6 J. Rossmeisl, Z.-W. Qu, H. Zhu, G.-J. Kroes, and J. K. Nørskov, *J. Electroanal. Chem.*, 2007, **607**, 83-89.

7 J. K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J. R. Kitchin, T. Bligaard, and H. Jonsson, *J. Phys. Chem. B*, 2004, **108**, 17886-17892.

8 V. Wang, N. Xu, J C Liu, G. Tang, and W. T. Geng, *Comput. Phys. Commun.*, 2021, **267**, 108033.

9 C. Ling, X. Niu, Q. Li, A. Du, and J. Wang, *J. Am. Chem. Soc.*, 2018, **140**, 14161-14168.

10 P. Roy, A. Pramanik, and P. Sarkar, *J. Phys. Chem. Lett.*, 2021, **12**, 10837-10844.

11 F. Calle-Vallejo, J. I. Martínez, and J. Rossmeisl, *Phys.Chem.Chem.Phys.*, 2011, **13**, 15639-15643.

12 X. Guo, S. Lin, J. Gu, S. Zhang, Z. Chen, and S. Huang, *ACS Catal.*, 2019, **9**, 11042-11054.

13 N. Govindarajan, A. Xu, K. *Science*, 2022, **375**, 379-380.

14 D. A. Kitchaev, G. Ceder, *Nat. Commun*., 2016, **7**, 1-7.

15 G. A. Kamat, J. A. Zamora Zeledón, G. T. Gunasooriya, S. M. Dull, J. T. Perryman, J. K. Nørskov, M. B. Stevens, and T. F. Jaramillo, *Commun. Chem*., 2022, **5**, 1-10.

16 K. Holst Olesen, M. Reda, H. A. Hansen, V. Tejs, and A. Matthias, *ACS Catal.*, 2018, **8**, 7104-7112.

17 G. Henkelman, B. P. Uberuaga, and H. Jónsson, *J. Chem. Phys.*, 2000, **113**, 9901-9904.