Supporting Information for

Dual transition metal atoms embedded N-doped graphene for electrochemical nitrogen fixation under ambient conditions

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Figure S3. (a) The evolution curve of temperature and energy versus the simulation time for the Mo_2-TV catalyst. (b) The top and side views of the snapshots of Mo_2-TV catalyst before and after AIMD simulations. The simulations were performed at 600 K for 10 ps with a time step of 2 fs.
Figure S3. (a) The evolution curve of temperature and energy versus the simulation time for the Mo_2-TV catalyst. (b) The top and side views of the snapshots of Mo_2-TV catalyst before and after AIMD simulations. The simulations were performed at 600 K for 10 ps with a time step of 2 fs.
Figure S4. (a) The evolution curve of temperature and energy versus the simulation time for the Ir_2-TV catalyst. (b) The top and side views of the snapshots of Ir_2-TV catalyst before and after AIMD simulations. The simulations were performed at 600 K for 10 ps with a time step of 2 fs.
Table S19. The structure, lattice constant, space group and point group of catalysts.

Table S1. Gibbs free energy changes of N_2 adsorption on M_2-DV series.

ΔG (eV)	$(M^*\text{-}M^*)_S^L$	$(M^*\text{-}M^*)_S^R$	$(M^*\text{-}M)_S^L$	$(M\text{-}M^*)_S^R$	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$	$(M\text{-}M^*)_E^R$
Sc_2-DV	-1.42	/	/	/	/	/	/
Ti_2-DV	-2.23	/	/	/	/	/	/
V_2-DV	-1.83	/	/	/	/	/	/
Cr_2-DV	/	-1.11/	/	/	/	-1.24	/
Mn_2-DV	-0.28	/	/	/	/	-0.35	-0.23
Fe_2-DV	-0.11		/	/	-0.11	-0.30	/
Co_2-DV	/	/	/	/	/	-0.51	
Ni_2-DV	/	/	/	/	/	-0.13	/
Cu_2-DV	/	/	/	/	/	0.08	/
Zn_2-DV	/	/	/	/	/	0.06	/
Y_2-DV	-1.04	/	/	/	/	/	/
Zr_2-DV	/	-2.30	/	/	/	/	/
Nb_2-DV	-2.10	/	/	/	/	/	/
Mo_2-DV	-0.57	/	/	/	/	-0.73	/
Tc_2-DV	/	/	/	/	/	-0.24	/
Ru_2-DV	/	/		-0.19	/		-0.87
Rh_2-DV	/	/	-0.23		/	-0.73	
Pd_2-DV	/	/	/	/	/	-0.31	/
Ag_2-DV	/	/	/	/	0.38	-0.04	/
Cd_2-DV	/	/	/	/	0.28	/	/
Lu_2-DV	-0.81	/	/	/	/	-0.13	/
Hf_2-DV	-2.31	/	/	/	/	-0.66	/
Ta_2-DV	/	-2.35	/	/	/	/	/
W_2-DV	-1.49	/	/	/	/	-1.27	/
Re_2-DV	-0.58	/	/	-0.56	/	-0.93	/
Os_2-DV		/	/	/	-0.88	-1.17	/
Ir_2-DV	/	/	/	/	/	-0.92	/
Pt_2-DV	/	/	0.21	/	/	/	/
Au_2-DV	/	/	/	/	0.45	/	/

Notes: / means that the configuration of the N_2 adsorption doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively.

Table S2. The N−N bond lengths of N_2 adsorption on M_2-DV series.

ΔG (eV)	$(M^*\text{-}M^*)_S^L$	$(M^*\text{-}M^*)_S^R$	$(M^*\text{-}M)_S^L$	$(M\text{-}M^*)_S^R$	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$	$(M\text{-}M^*)_E^R$
Sc_2-DV	1.207	/	/	/	/	/	/
Ti_2-DV	1.225	/	/	/	/	/	/
V_2-DV	1.230	/	/	/	/	/	/
Cr_2-DV	/	1.199	/	/	/	1.157	/
Mn_2-DV	1.195	/	/	/	/	1.155	1.136
Fe_2-DV	1.175	/	/	/	1.194	1.137	/
Co_2-DV	/	/	/	/	/	1.139	/
Ni_2-DV	/	/	/	/	/	1.131	/
Cu_2-DV	/	/	/	/	/	1.124	/
Zn_2-DV	/	/	/	/	/	1.125	/
Y_2-DV	1.211		/	/	/	/	/
Zr_2-DV	/	1.238	/	/	/	/	/
Nb_2-DV	1.243	/	/	/	/	/	/
Mo_2-DV	1.302	/	/	/	/	1.155	/
Tc_2-DV	/	/	/	/	/	1.131	/
Ru_2-DV	/	/	/	1.159	/	/	1.137
Rh_2-DV	/	/	1.153	/	/	1.131	/
Pd_2-DV	/	/	/	/	/	1.126	/
Ag_2-DV	/	/	/	/	1.144	1.120	/
Cd_2-DV	/	/	/	/	1.158	/	/
Lu_2-DV	1.217	/	/	/	/	1.140	/
Hf_2-DV	1.252	/	/	/	/	1.150	/
Ta_2-DV	/	1.272	/	/	/	/	/
W_2-DV	1.374	/	/	/	/	1.155	/
Re_2-DV	1.281	/	/	1.190	/	1.147	/
Os_2-DV	/	/	/	/	1.217	1.144	/
Ir_2-DV	/	/	/	/	/	1.136	/
Pt_2-DV	/	/	1.162	/	/	/	/
Au_2-DV	/	/	/	/	1.173	/	/

Notes: / means that the configuration of the N_2 adsorption doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively.

Table S3. Gibbs free energy changes of N_2 adsorption on M_2-TV series.

ΔG (eV)	$(M^*\text{-}M^*)_S^L$	$(M^*\text{-}M^*)_S^R$	$(M^*\text{-}M)_S^L$	$(M\text{-}M^*)_S^R$	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$	$(M\text{-}M^*)_E^R$	$(M^*\text{-}M^*)_E$
Sc_2-TV	-1.70	-1.45	-0.52	/	/	/	/	/
Ti_2-TV	-1.92	-1.67	-0.73	/	/	/	/	/
V_2-TV	/	/	/	/	-0.08	/	-0.21	/
Cr_2-TV	/	-0.22	/	-0.30	/	-0.12	-0.55	/
Ni_2-TV	/	/	/	/	/	/	-0.84	/
Cu_2-TV	/	/	/	-0.39	/	/	-0.83	/
Y_2-TV	-1.10	-1.24	/	-0.35	/	/	-0.28	/
Zr_2-TV	-2.79	-2.95	/	-1.82	/	/	/	/
Nb_2-TV	/	-1.41	/	-0.58	/	/	-0.96	/
Mo_2-TV	-0.07	/	-0.29	/	/	/	-0.40	/
Tc_2-TV	/	/	/	/	/	-0.34	/	/
Ru_2-TV	/	/	/	-0.49	/	/	-0.91	0.45
Rh_2-TV	/	/	-0.25	/	/	-0.94	/	/
Pd_2-TV	/	/	-0.54	/	/	-0.86	/	/
Lu_2-TV	-0.72	-0.54	0.13	/	/	0.08	/	/
Hf_2-TV	-1.95	-1.70	-0.95	/	/	-0.88	/	/
Ta_2-TV	-2.08	-2.40	/	/	/	-0.57	/	/
W_2-TV	-1.52	-1.30	/	/	/	-1.01	-0.79	/
Re_2-TV	/	/	/	/	-0.11	-0.40	/	/
Os_2-TV	0.68	/	-0.62	/	/	-1.32	/	/
Ir_2-TV	/	/	/	-0.62	/	/	-1.00	/
Pt_2-TV	/	/	-0.90	/	/	-1.44	/	/

Notes: / means that the configuration of the N_2 adsorption doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively.

Table S4. The N−N bond lengths of N_2 adsorption on M_2-TV series.

Bond of length (Å)	$(M^*\text{-}M^*)_S^L$	$(M^*\text{-}M^*)_S^R$	$(M^*\text{-}M)_S^L$	$(M\text{-}M^*)_S^R$	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$	$(M\text{-}M^*)_E^R$	$(M^*\text{-}M^*)_E$
Sc_2-TV	1.224	1.216	1.173	/	/	/	/	/
Ti_2-TV	1.247	1.260	1.189	/	/	/	/	/
V_2-TV	/	/	/	/	1.215	/	1.139	/
Cr_2-TV	/	1.213	/	1.18	/	1.144	1.135	/
Ni_2-TV	/	/	/	/	/	/	1.138	/
Cu_2-TV	/	/	/	1.152	/	/	1.131	/
Y_2-TV	1.216	1.225	/	1.175	/	/	1.143	/
Zr_2-TV	1.272	1.267	/	1.188	/	/	/	/
Nb_2-TV	/	1.283	/	1.180	/	/	1.145	/
Mo_2-TV	1.239	/	1.156	/	/	/	1.133	/
Tc_2-TV	/	/	/	/	/	1.138	/	/
Ru_2-TV	/	/	/	1.187	/	/	1.139	1.178
Rh_2-TV	/	/	1.160	/	/	1.133	/	/
Pd_2-TV	/	/	1.159	/	/	1.130	/	/
Lu_2-TV	1.236	1.225	1.184	/	/	1.135	/	/
Hf_2-TV	1.284	1.279	1.197	/	/	1.152	/	/
Ta_2-TV	1.258	1.299	/	/	/	1.143	/	/
W_2-TV	1.346	1.300	/	/	/	1.146	1.147	/
Re_2-TV	/	/	/	/	1.259	1.145	/	/
Os_2-TV	1.244	/	1.195	/	/	1.142	/	/
Ir_2-TV	/	/	/	1.183	/	/	1.138	/
Pt_2-TV	/	/	1.182	/	/	1.133	/	/

Notes: / means that the configuration of the N_2 adsorption doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively.

Table S5. Gibbs free energy changes of N_2 adsorption on M_2-QV series.

ΔG (eV)	$(M^*\text{-}M^*)_S^L$	$(M^*\text{-}M^*)_S^R$	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$	$(M\text{-}M^*)_E^R$	$(M^*\text{-}M^*)_E$
V_2-QV	/	-0.33	/	/	0.20	/
Cr_2-QV	0.29	/	/	-0.27	/	/
Mn_2-QV	/	/	0.41	-0.63	/	/
Fe_2-QV	/	/	/	/	-0.20	-0.10
Co_2-QV	/	/	0.26	/	/	-0.32
Y_2-QV	/	-1.23	/	/	/	/
Nb_2-QV	-2.04	/	/	/	/	/
Mo_2-QV	/	/	/	0.19	0.10	/
Tc_2-QV	/	/	/	0.01	0.01	/
Lu_2-QV	-0.76	/	/	/	0.07	/
Hf_2-QV	/	-2.13	/	/	/	/
Ta_2-QV	-2.59	/	/	/	/	/
W_2-QV	/	-2.00	/	/	-1.15	/

Notes: / means that the configuration of the N_2 adsorption doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively.

Table S6. The N−N bond lengths of N_2 adsorption on M_2-QV series.

Bond of length (Å)	$(M^*\text{-}M^*)_S^L$	$(M^*\text{-}M^*)_S^R$	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$	$(M\text{-}M^*)_E^R$	$(M^*\text{-}M^*)_E$
V_2-QV	/	1.240	/	/	1.136	/
Cr_2-QV	1.227	/	/	1.141	/	/
Mn_2-QV	/	/	1.197	1.184	/	/
Fe_2-QV	/	/	/	/	1.140	1.159
Co_2-QV	/	/	1.166	/	/	1.156
Y_2-QV	/	1.212	/	/	/	/
Nb_2-QV	1.259	/	/	/	/	/
Mo_2-QV	/	/	/	1.135	1.126	/
Tc_2-QV	/	/	/	1.128	1.127	/
Lu_2-QV	1.217	/	/	/	1.137	/
Hf_2-QV	/	1.255	/	/	/	/
Ta_2-QV	1.283		/	/	/	/
W_2-QV	/	1.298	/	/	1.173	/

Notes: / means that the configuration of the N_2 adsorption doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively.

ΔG (eV)	$(M^*\text{-}M^*)_S^L$-a	$(M^*\text{-}M^*)_S^L$-b	$(M^*\text{-}M^*)_S^R$-a	$(M^*\text{-}M^*)_S^R$-b	$(M^*\text{-}M)_S^L$-a	$(M^*\text{-}M)_S^L$-b	$(M\text{-}M^*)_S^R$-a	$(M\text{-}M^*)_S^R$-b	$(M^*\text{-}M^*)_S$	$(M^*\text{-}M)_E^L$-c	$(M\text{-}M^*)_E^R$-c
Sc_2-DV	-0.14	0.85	/	/	/	/	/	/	/	/	/
Ti_2-DV	0.10	0.91	/	/	/	/	/	/	/	/	/
V_2-DV	0.37	0.08	/	/	/	/	/	/	/	/	/
Cr_2-DV	/	/	0.51	0.38	/	/	/	/	/	0.69	/
Mn_2-DV	0.30	0.36	/	/	/	/	/	/	/	0.44	0.32
Fe_2-DV	0.50	0.48	/	/	/	/	/	/	0.47	0.92	/
Co_2-DV	/	/	/	/	/	/	/	/	/	0.95	/
Ni_2-DV	/	/	/	/	/	/	/	/	/	0.64	/
Y_2-DV	-0.30	0.72	/	/	/	/	/	/	/	/	/
Zr_2-DV	/	/	0.20	-0.10	/	/	/	/	/	/	/
Nb_2-DV	0.02	0.55	/	/	/	/	/	/	/	/	/
Mo_2-DV	-0.05	-0.11	/	/	/	/	/	/	/	-0.06	/
Tc_2-DV	/	/	/	/	/	/	/	/	/	1.10	/
Ru_2-DV	/	/	/	/	/	/	0.77	0.89	/	/	1.06
Rh_2-DV	/	/	/	/	0.87	0.95	/	/	/	1.34	/
Pd_2-DV	/	/	/	/	/	/	/	/	/	0.99	/
Ag_2-DV	/	/	/	/	/	/	/	/	/	1.71	/
Lu_2-DV	-0.38	0.68	/	/	/	/	/	/	/	-1.06	/
Hf_2-DV	-0.43	0.12	/	/	/	/	/	/	/	-2.07	/
Ta_2-DV	/	/	0.60	-0.24	/	/	/	/	/	/	/
W_2-DV	-0.31	-1.63	/	/	/	/	/	/	/	-0.23	/
Re_2-DV	-0.35	-0.49	/	/	/	/	0.86	0.38	/	0.43	
Os_2-DV	/	/	/	/	/	/	/	/	-0.36	0.46	/
Ir_2-DV	/	/	/	/	/	/	/	/	/	1.03	/

Table S7. Gibbs free energy changes of the first protonation step for M_2-DV series.

Notes: / means that the configuration of the first protonation step doesn't exit. An asterisk * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively. -a and -b mean that the first proton−electron pair attacks different N atom of adsorbed N_2 molecule for side-on configuration, -c shows that the first proton-electron pair attacks distal N atom of adsorbed N_2 molecule for end-on configuration.

Table S8. Gibbs free energy changes of the last (sixth) protonation step for M_2-DV series.

ΔG (eV)	C-S	S_1-S_1	S_2-S_2
Sc_2-DV	1.34	/	/
Ti_2-DV	1.34	/	/
V_2-DV	1.32	/	/
Cr_2-DV	1.07	0.42	/
Mn_2-DV	0.63	-0.34	/
Fe_2-DV	0.90	/	/
Co_2-DV	/	/	/
Ni_2-DV	/	/	/
Y_2-DV	1.76	/	/
Zr_2-DV	1.53	1.03	/
Nb_2-DV	1.55	/	/
Mo_2-DV	1.24	0.33	/
Tc_2-DV	/	/	/
Ru_2-DV	/	/	/
Rh_2-DV	/	/	/
Pd_2-DV	/	/	/
Ag_2-DV	/	/	/
Lu_2-DV	1.22	0.33	/
Hf_2-DV	/	/	/
Ta_2-DV	1.10	0.91	/
W_2-DV	2.07	0.56	/
Re_2-DV	0.67	/	/
Os_2-DV	0.95	0.34	0.47
Ir_2-DV	/	/	/

Notes: / means that the configuration of the last protonation step doesn't exit. C and S mean that the adsorbates are located in the center and side of M_2. When adsorbates have two different configurations in two transition metal atoms, S_1 and S_2 are used to distinguish them.

Table S9. Gibbs free energy changes of the first protonation step for M_2-TV series

ΔG (eV)	$(M^*\text{-}M^*)_S^L$-a	$(M^*\text{-}M^*)_S^L$-b	$(M^*\text{-}M^*)_S^R$-a	$(M^*\text{-}M^*)_S^R$-b	$(M^*\text{-}M)_S^L$-a	$(M^*\text{-}M)_S^L$-b	$(M\text{-}M^*)_S^R$-a	$(M\text{-}M^*)_S^R$-b	$(M^*\text{-}M^*)_S$-a	$(M^*\text{-}M^*)_S$-b	$(M^*\text{-}M)_E^L$-c	$(M\text{-}M^*)_E^R$-c
Sc_2-TV	/	/	-0.18	0.15	0.31	-0.30	-1.37	/	/	/	/	/
Ti_2-TV	/	/	0.04	0.28	0.09	-0.09	0.34	0.44	/	/	/	/
V_2-TV	/	/	/	/	/	/	/	/	-0.62	-0.50	/	0.47
Cr_2-TV	/	/	/	/	0.55	0.29	/	/	0.76	1.04	0.14	0.97
Ni_2-TV	/	/	/	/	/	/	/	/	/	/	1.20	/
Cu_2-TV	/	/	/	/	/	/	1.64	1.68	/	/	1.62	/
Y_2-TV	-0.40	0.84	-0.17	-0.32	/	/	0.32	0.35	/	/	/	0.70
Zr_2-TV	-0.25	0.07	0.14	-0.28	/	/	0.01		/	/	/	/
Nb_2-TV	/	/	0.02	-0.11	/	/	0.48	0.29	/	/	/	0.39
Mo_2-TV	0.19	0.08	/	/	1.00	0.18	/	/	/	/	/	0.41
Tc_2-TV	/	/	/	/	/	/	/	/	/	/	0.94	/
Ru_2-TV	/	/	/	/	/	/	0.52	0.55	/	/	/	0.91
Rh_2-TV	/	/	/	/	0.44	0.43	/	/	/	/	1.03	/
Pd_2-TV	/	/	/	/	1.48	1.53	/	/	/	/	1.57	/
Lu_2-TV	-0.41	-0.02	0.80	-0.49	/	/	/	/	/	/	/	/
Hf_2-TV	-0.42	0.77	-0.05	-0.49	-0.03	/	/	/	/	/	0.45	/
Ta_2-TV	-0.25	0.44	0.69	0.05	/	/	/	/	/	/	-1.80	/
W_2-TV	0.60	0.32	-0.02	0.45	/	/	/	/	/	/	0.58	0.23
Re_2-TV	/	/	/	/	/	/	/	/	-0.17	-0.59	0.60	/
Os_2-TV	/	/	/	/	0.46	0.58	/	/	/	/	0.68	/
Ir_2-TV	/	/	/	/	/	/	0.40	0.39	/	/	/	0.54
Pt_2-TV	/	/	/	/	1.20	1.21	/	/	/	/	1.48	/

Notes: / means that the configuration of the first protonation step doesn't exit. * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively. -a and -b mean that the first proton-electron pair attacks different N atom of adsorbed N_2 molecule for side-on configuration, -c shows that the first proton-electron pair attacks distal N atom of adsorbed N_2 molecule for end-on configuration.

Table S10. Gibbs free energy changes of the last (sixth) protonation step for M_2-TV series.

ΔG (eV)	C-S	C-S_1	C-S_2	S_1-S_1	S_2-S_2
Sc_2-TV	1.76	/	/	0.52	/
Ti_2-TV	/	1.58	/	/	1.23
V_2-TV	/	0.40	/	-0.18	/
Cr_2-TV	/	0.79	0.24	/	/
Ni_2-TV	/	/	/	/	/
Cu_2-TV	/	/	/	/	/
Y_2-TV	/	1.31	/	/	0.62
Zr_2-TV	/	1.25	/	/	/
Nb_2-TV	/	1.36	/	/	0.82
Mo_2-TV	/	0.40	/	-0.03	/
Tc_2-TV	/	/	/	/	/
Ru_2-TV	/	/	/	/	/
Rh_2-TV	/	-1.04	/	-0.18	/
Pd_2-TV	/		/	/	/
Lu_2-TV	/	1.06	/	0.37	/
Hf_2-TV	/	/	/	1.12	/
Ta_2-TV	/	/	/	0.84	/
W_2-TV	/	/	/	0.83	0.70
Re_2-TV	/	/	/	0.47	/
Os_2-TV	/	/	/	/	/
Ir_2-TV	/	/	/	0.24	/
Pt_2-TV	/	/	/	/	/

Notes: / means that the configuration of the last protonation step doesn't exit. C and S mean that the adsorbates are located in the center and side of M_2. When adsorbates have two different configurations in two transition metal atoms, S_1 and S_2 are used to distinguish them.

Table S11. Gibbs free energy changes of the first protonation step for M_2-QV series.

ΔG (eV)	$(M^*\text{-}M^*)_S^L$-a	$(M^*\text{-}M^*)_S^L$-b	$(M^*\text{-}M^*)_S^R$-a	$(M^*\text{-}M^*)_S^R$-b	$(M^*\text{-}M^*)_E$-c	$(M^*\text{-}M)_E^L$-c	$(M\text{-}M^*)_E^R$-c
V_2-QV	/	/	0.53	0.17	/	/	/
Cr_2-QV	/	/	/	/	/	0.34	/
Mn_2-QV	/	/	/	/	/	0.35	/
Fe_2-QV	/	/	/	/	0.28	/	1.01
Co_2-QV	/	/	/	/	0.45	/	/
Y_2-QV	/	/	0.81	-0.18	/	/	/
Nb_2-QV	0.06	0.91	/	/	/	/	/
Lu_2-QV	-0.26	0.78	/	/	/	/	/
Hf_2-QV	/	/	0.81	-0.51	/	/	/
Ta_2-QV	0.00	0.80	/	/	/	/	/
W_2-QV	/	/	0.19	0.26	/	/	-0.32

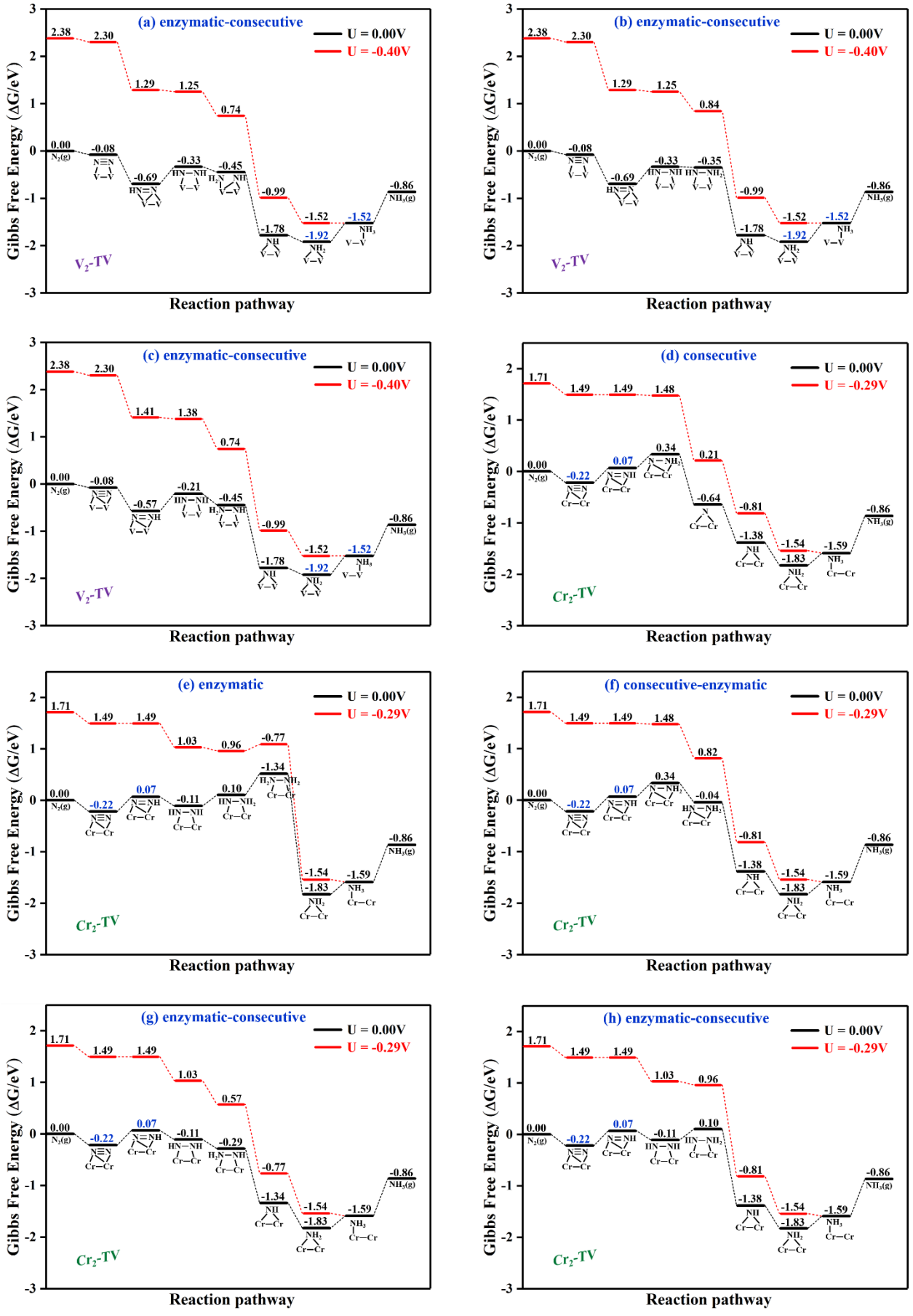
Notes: / means that the configuration of the first protonation step doesn't exit. * denotes the active site on the surface of catalysts that the adsorbed N_2 connected to. The M means the transition metal atom (3d, 4d and 5d series). The subscripts E and S represent the end-on and side-on configurations, respectively. The

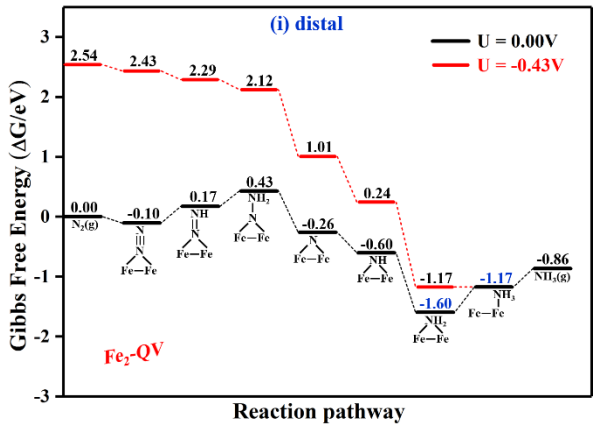
superscripts L and R mean that adsorbed N_2 molecules are closer to the left and right sides of M_2, respectively. -a and -b mean that the first proton-electron pair attacks different N atom of adsorbed N_2 molecule for side-on configuration, -c shows that the first proton-electron pair attacks distal N atom of adsorbed N_2 molecule for end-on configuration.

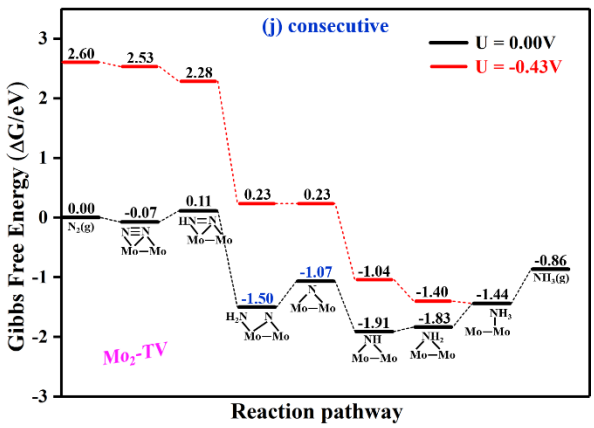
Table S12. Gibbs free energy changes of the last (sixth) protonation step for M_2-QV series.

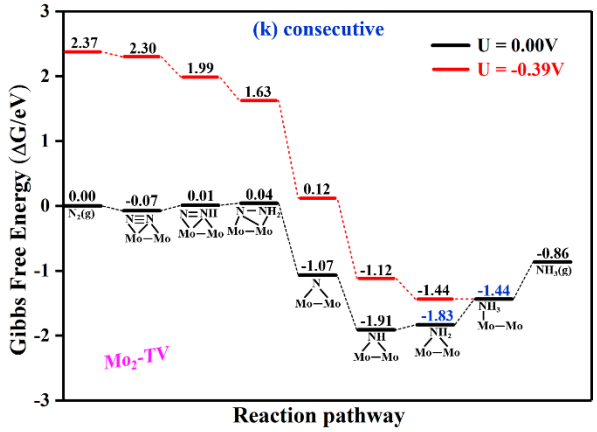
ΔG (eV)	C-S	S-S
V_2-QV	0.64	-0.19
Cr_2-QV	0.91	/
Mn_2-QV	0.95	/
Fe_2-QV	0.42	/
Co_2-QV	/	/
Y_2-QV	1.26	/
Nb_2-QV	/	/
Lu_2-QV	0.94	/
Hf_2-QV	-0.43	/
Ta_2-QV	1.68	0.67
W_2-QV	0.88	-0.12

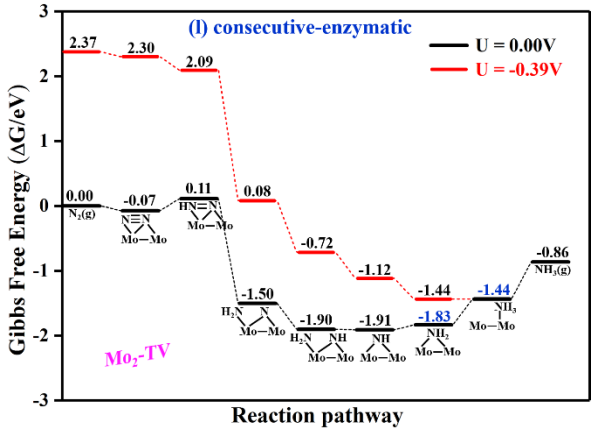
Notes: / means that the configuration of the last protonation step doesn't exit. C and S mean that the adsorbates are located in the center and side of M_2. The Nb_2-QV catalyst can't adsorb $*NH_2$.

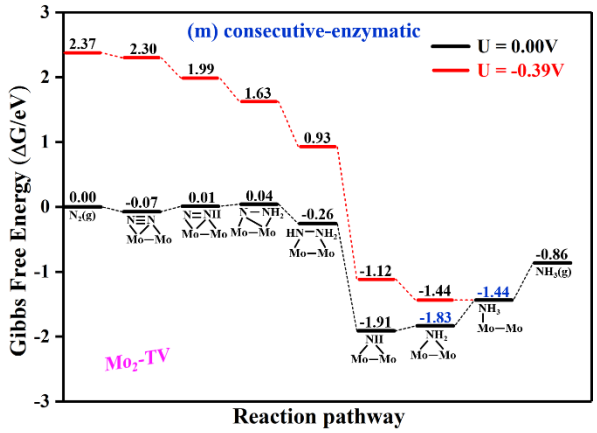

(a) enzymatic-consecutive
U = 0.00V
U = -0.40V
V2-TV
(b) enzymatic-consecutive
U = 0.00V
U = -0.40V
V2-TV
(c) enzymatic-consecutive
U = 0.00V
U = -0.40V
V2-TV
(d) consecutive
U = 0.00V
U = -0.29V
Cr2-TV
(e) enzymatic
U = 0.00V
U = -0.29V
Cr2-TV
(f) consecutive-enzymatic
U = 0.00V
U = -0.29V
Cr2-TV
(g) enzymatic-consecutive
U = 0.00V
U = -0.29V
Cr2-TV
(h) enzymatic-consecutive
U = 0.00V
U = -0.29V
Cr2-TV
Gibbs Free Energy (ΔG/eV)
Reaction pathway

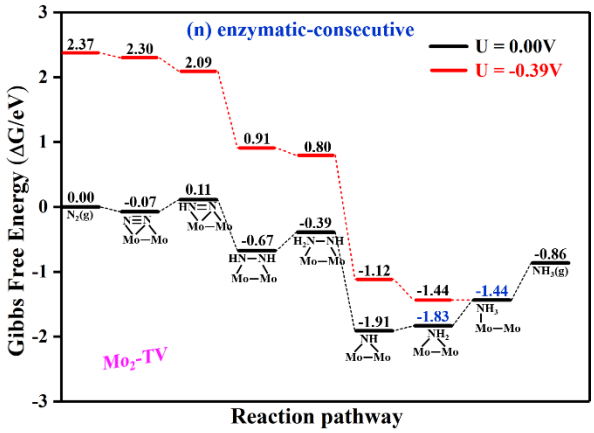

(i) distal
U = 0.00V
U = -0.43V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Fe2-QV

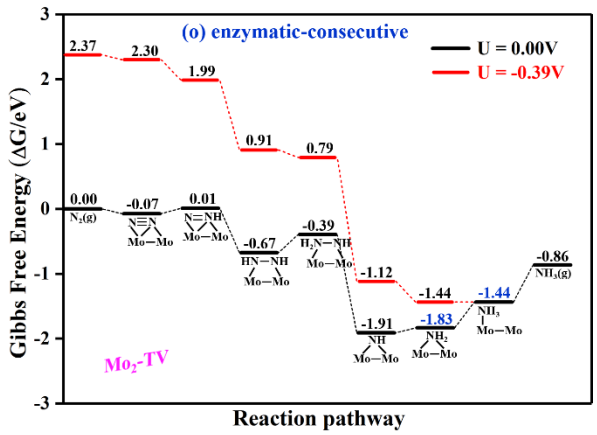

(j) consecutive
U = 0.00V
U = -0.43V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Mo2-TV

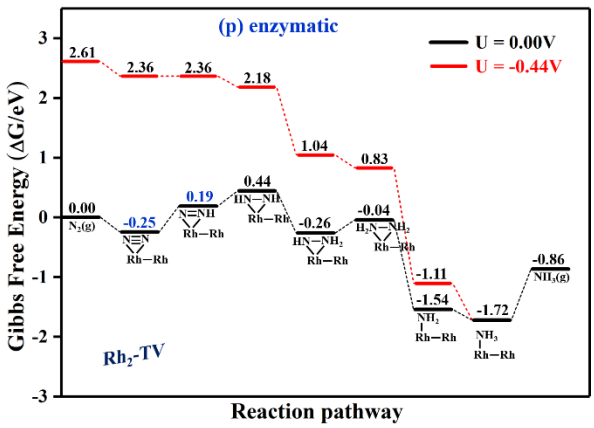

(k) consecutive
U = 0.00V
U = -0.39V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Mo2-TV


(l) consecutive-enzymatic
U = 0.00V
U = -0.39V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Mo2-TV


(m) consecutive-enzymatic
U = 0.00V
U = -0.39V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Mo2-TV


(n) enzymatic-consecutive
U = 0.00V
U = -0.39V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Mo2-TV


(o) enzymatic-consecutive
U = 0.00V
U = -0.39V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Mo2-TV


(p) enzymatic
U = 0.00V
U = -0.44V
Gibbs Free Energy (ΔG/eV)
Reaction pathway
Rh2-TV

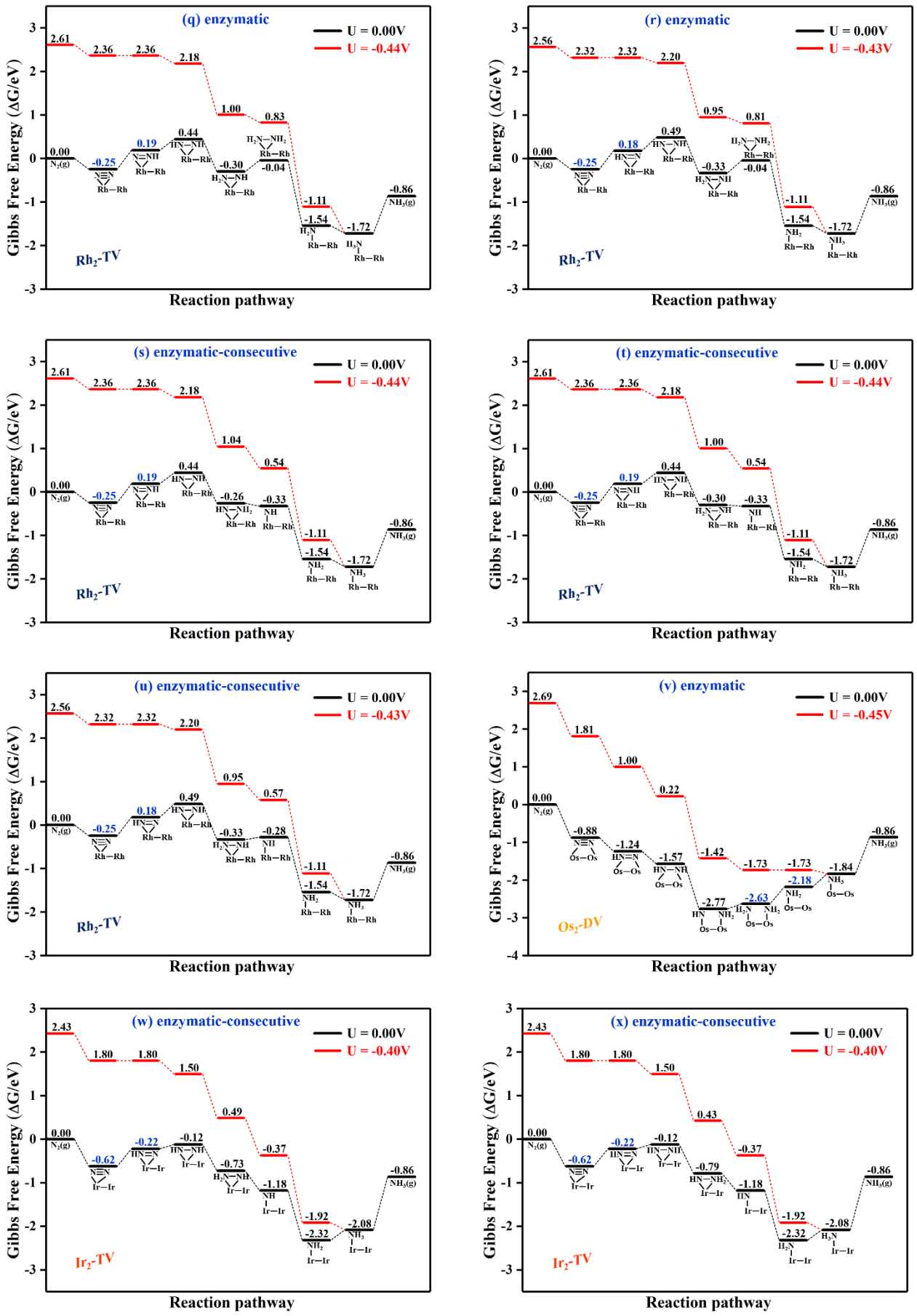


Figure S1. Gibbs free energy diagrams for NRR onV_2-TV, Cr_2-TV, Fe_2-QV, Mo_2-TV, Rh_2-TV, Os_2-DV and Ir_2-TV.

Table S13. On Cr_2-TV, Mo_2-TV and Ir_2-TV catalysts, the evolution length of N-N bond through eight different reaction pathways.

catalyst	Cr_2-TV		Mo_2-TV			Ir_2-TV		
pathway	distal	distal-alternating	consecutive	distal	enzymatic-consecutive	consecutive	enzymatic-consecutive	enzymatic-consecutive
N_2	1.144	1.144	1.114	1.114	1.114	1.114	1.114	1.114
first	1.252	1.252	1.156	1.133	1.239	1.183	1.183	1.183
second	1.331	1.331	1.364	1.262	1.337	1.253	1.253	1.253
third	/	1.444	1.459	1.356	1.410	1.430	1.416	1.416

Notes: / means that the corresponding configuration doesn't exit. First, second and third means that they are first, second and third protonation step.

Table S14. Onset potential of NRR and the corresponding magnetic moment for Cr_2-, Mo_2, Ir_2-TV catalysts that meet four screening criterias.

catalyst	magnetic moment (μ_B)	onset potential (V)
Cr_2-TV	0.53	0.24
Mo_2-TV	0.00	0.39
Ir_2-TV	0.00	0.39

Table S15. The charge variations (the Bader charge variation of each intermediate between two adjacent steps) on the Cr_2-TV catalyst for NRR through (a) distal and (b) distal-alternating pathway.

(a) distal				(b) distal-alternating			
intermediate	Part A	Part B	Part C	intermediate	Part A	Part B	Part C
*N-N	0.39	-0.36	-0.04	*N-N	0.39	-0.36	-0.04
*N-NH	0.29	-0.24	-0.04	*N-NH	0.29	-0.24	-0.04
*N-NH_2	-0.11	0.01	0.10	*N-NH_2	-0.11	0.01	0.10
*N	0.30	-0.22	-0.08	*NH-NH_2	-0.14	0.07	0.08
*NH	-0.09	0.11	-0.01	*NH	0.34	-0.17	-0.17
*NH_2	-0.29	0.17	0.11	*NH_2	-0.29	0.17	0.11
*NH_3	-0.59	0.29	0.29	*NH_3	-0.59	0.29	0.29

Notes: * denotes the active site on the surface of catalysts that the adsorbed intermediate connected to.

Table S16. The charge variations (the Bader charge variation of each intermediate between two adjacent steps) on the Mo_2-TV catalyst for NRR through (c) consecutive pathway, (d) distal pathways, (e) enzymatic-consecutive pathway.

(c) consecutive				(d) distal				(e) enzymatic-consecutive			
intermediate	Part A	Part B	Part C	intermediate	Part A	Part B	Part C	intermediate	Part A	Part B	Part C
*N-*N	0.37	0.00	-0.38	*N-*N	0.28	-0.16	-0.12	*N-*N	0.85	-0.92	0.06
*N-*NH	0.57	-0.82	0.25	*N-*NH	0.46	-0.62	0.16	*N-*NH	-0.01	0.14	-0.13
N-NH_2	-0.24	0.17	0.07	*N-*NH_2	-0.08	0.09	-0.01	*N-*NH_2	-0.07	-0.05	0.12
*N	0.24	-0.17	-0.07	*NH-*NH_2	0.28	-0.12	-0.16	*NH-*NH_2	-0.34	0.32	0.01
*NH	-0.12	-0.08	0.20	*NH	-0.12	-0.08	0.20	*NH	0.39	-0.38	0.00
*NH_2	-0.31	0.35	-0.04	*NH_2	-0.31	0.35	-0.04	*NH_2	-0.31	0.35	-0.04
*NH_3	-0.60	0.49	0.11	*NH_3	-0.60	0.49	0.11	*NH_3	-0.60	0.49	0.11

Notes: * denotes the active site on the surface of catalysts that the adsorbed intermediate connected to.

Table S17. The charge variations (the Bader charge variation of each intermediate between two adjacent steps) on the Ir_2-TV catalyst for NRR through (f) consecutive-enzymatic pathway, (g) enzymatic-consecutive pathway and (h) consecutive-enzymatic pathway.

(f) consecutive				(g) enzymatic-consecutive				(h) enzymatic-consecutive			
intermediate	Part A	Part B	Part C	intermediate	Part A	Part B	Part C	intermediate	Part A	Part B	Part C
*N-*N	0.41	-0.22	-0.18	*N-*N	0.41	-0.22	-0.18	*N-*N	0.41	-0.22	-0.18
*N-*NH	-0.07	-0.10	0.17	*NH-*N	-0.07	-0.10	0.17	*N-*NH	-0.07	-0.10	0.17
N-NH_2	0.04	0.02	-0.06	*NH-*NH	0.16	-0.03	-0.13	*NH-*NH	0.16	-0.03	-0.13
*N	0.17	-0.10	-0.07	*NH-*NH_2	-0.32	0.10	0.22	*NH_2-*NH	-0.31	0.01	0.29
*NH	-0.03	0.01	0.02	*NH	0.35	-0.15	-0.20	*NH	0.31	0.06	-0.38
*NH_2	-0.25	0.20	0.05	*NH_2	-0.26	0.20	0.06	*NH_2	-0.23	0.08	0.15
*NH_3	-0.46	0.19	0.26	*NH_3	-0.46	0.19	0.26	*NH_3	-0.46	0.19	0.26

Notes: * denotes the active site on the surface of catalysts that the adsorbed intermediate connected to.

Table S18. The comparison of the catalytic performance between U_{onset}-HER and U_{onset}-NRR.

Catalyst	U_{onset}-HER (V)	U_{onset}-NRR (V)
Cr_2-TV	-0.26	-0.24
Mo_2-TV	-0.58	-0.39
Ir_2-TV	-0.01	-0.38

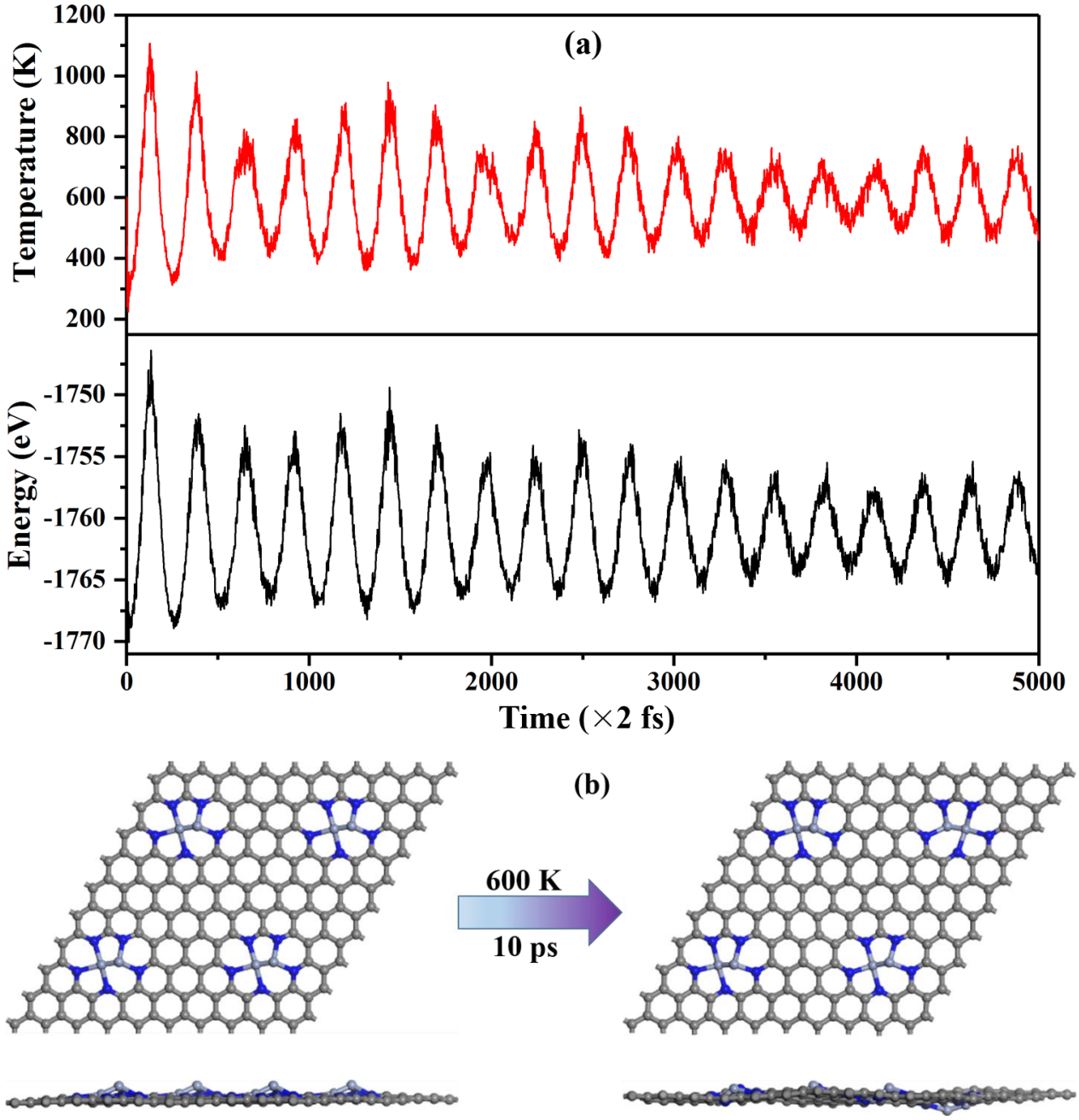


Figure S2. (a) The evolution curve of temperature and energy versus the simulation time for the Cr_2-TV catalyst. (b) The top and side views of the snapshots of Cr_2-TV catalyst before and after AIMD simulations. The simulations were performed at 600 K for 10 ps with a time step of 2 fs.

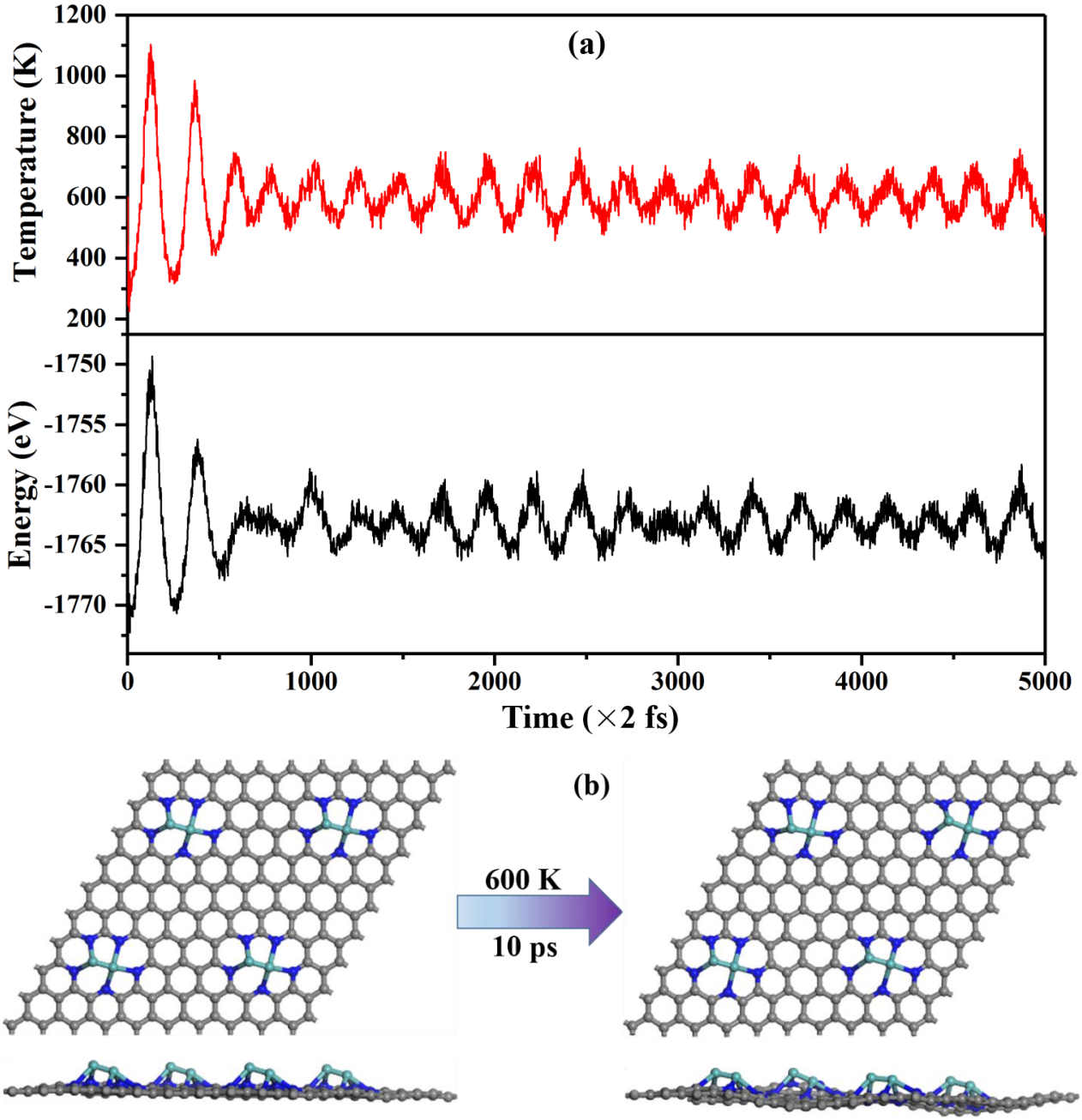


Figure S3. (a) The evolution curve of temperature and energy versus the simulation time for the Mo_2-TV catalyst. (b) The top and side views of the snapshots of Mo_2-TV catalyst before and after AIMD simulations. The simulations were performed at 600 K for 10 ps with a time step of 2 fs.

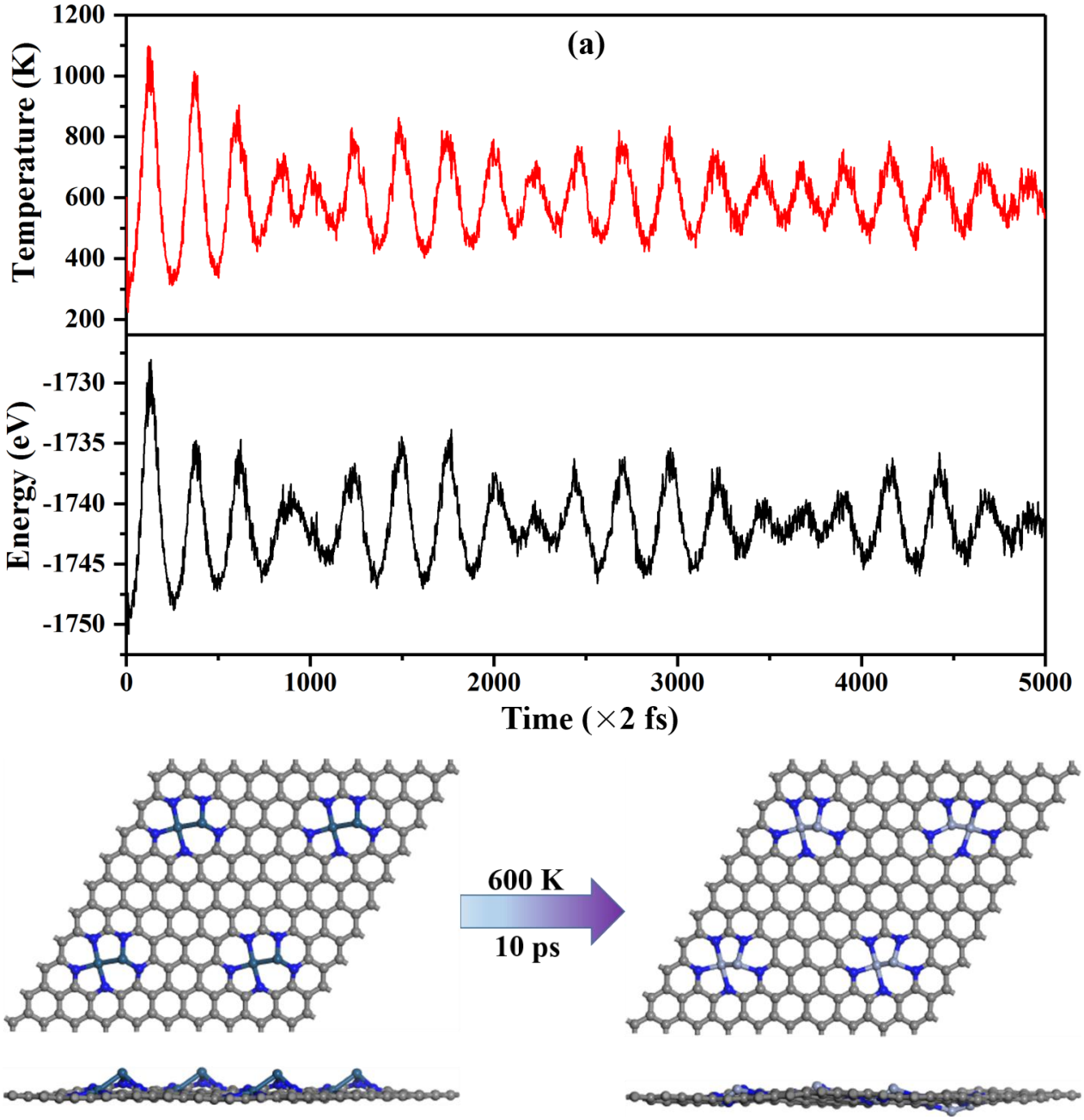
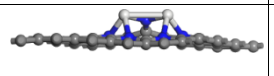
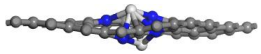
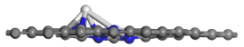
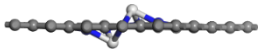
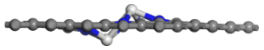
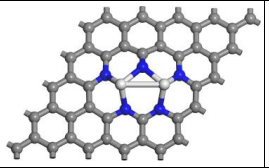
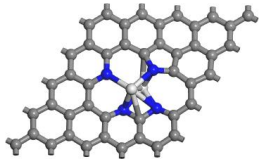
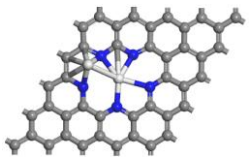
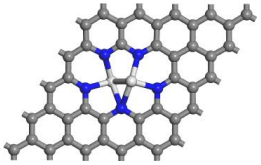
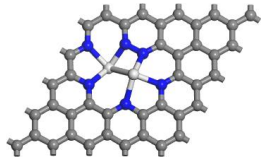
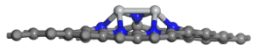
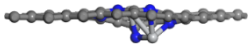
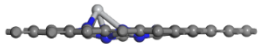
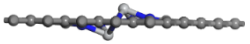
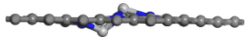
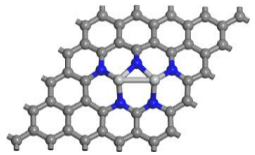
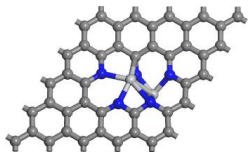
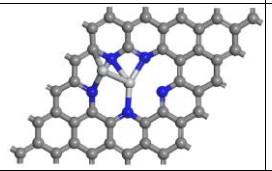
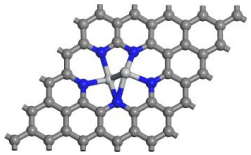
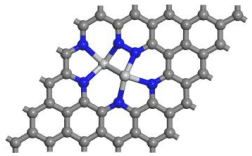


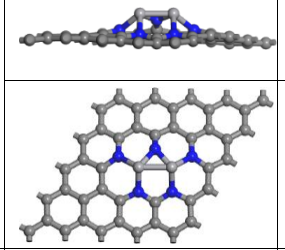
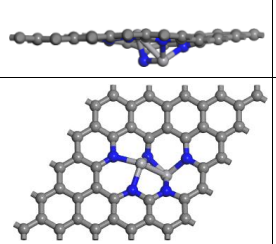
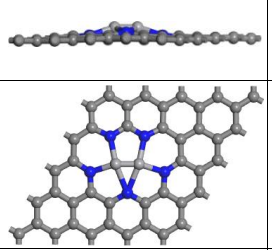
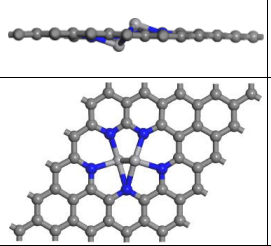
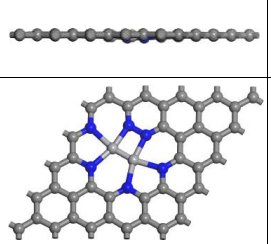
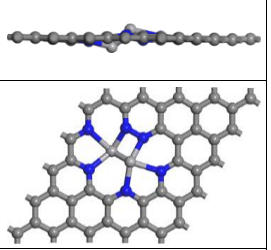
Figure S4. (a) The evolution curve of temperature and energy versus the simulation time for the Ir_2-TV catalyst. (b) The top and side views of the snapshots of Ir_2-TV catalyst before and after AIMD simulations. The simulations were performed at 600 K for 10 ps with a time step of 2 fs.

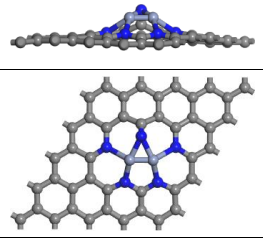
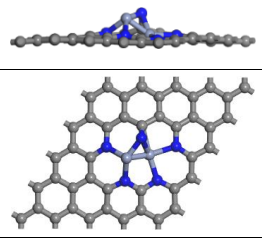
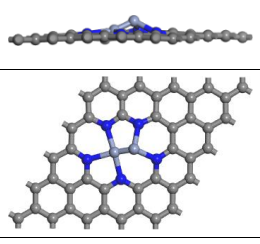
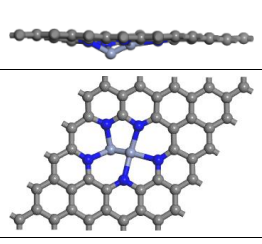
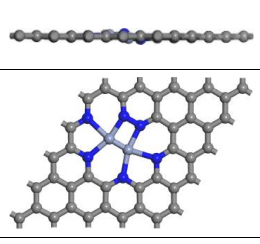
Table S19. The structure, lattice constant, space group and point group of catalysts.

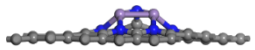
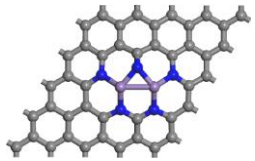
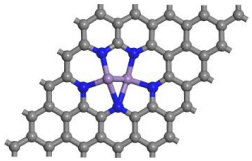
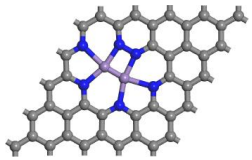
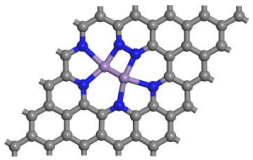
Notes: / means that the corresponding configuration doesn't exit.

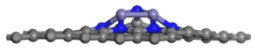
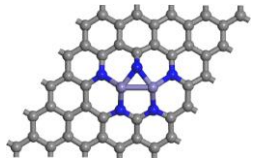
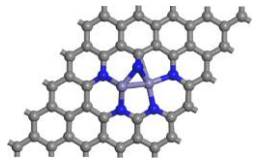
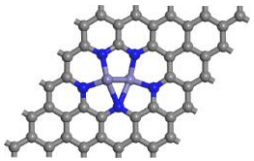
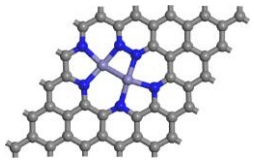
Catalysts	Sc_2-DV-A	Sc_2-DV-B	Sc_2-TV-A	Sc_2-TV-B	Sc_2-QV-A	Sc_2-QV-B
Crystal structure						/
						/
Lattice constant	a = 12.36 Å b = 12.29 Å c = 16.82 Å	a = 12.42 Å b = 12.08 Å c = 17.07 Å	a = 12.28 Å b = 12.28 Å c = 16.98 Å	a = 12.36 Å b = 12.26 Å c = 16.86 Å	a = 12.25 Å b = 12.31 Å c = 16.94 Å	/
Space group	Cm (#8)	P1 (#1)	P1 (#1)	C2 (#5)	C2 (#5)	/
Point group	Cs-3	C1-1	C1-1	C2-3	C2-3	/

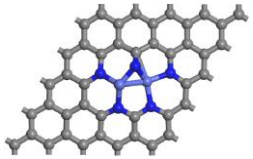
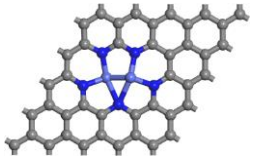
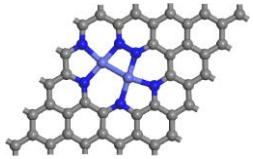
Catalysts	Ti_2-DV-A	Ti_2-DV-B	Ti_2-TV-A	Ti_2-TV-B	Ti_2-QV-A	Ti_2-QV-B
Crystal structure						/
						/
Lattice constant	a = 12.35 Å b = 12.28 Å c = 16.83 Å	a = 12.36 Å b = 12.23 Å c = 16.92 Å	a = 12.32 Å b = 12.29 Å c = 16.87 Å	a = 12.36 Å b = 12.24 Å c = 16.87 Å	a = 12.25 Å b = 12.30 Å c = 16.97 Å	/
Space group	Cm (#8)	P1 (#1)	P1 (#1)	C2 (#5)	C2 (#5)	/
Point group	Cs-3	C1-1	C1-1	C2-3	C2-3	/

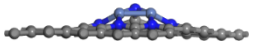
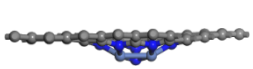
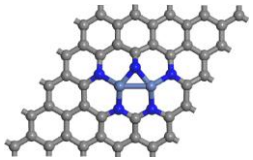
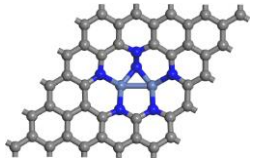
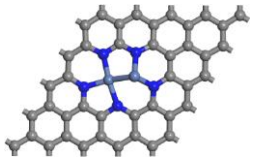
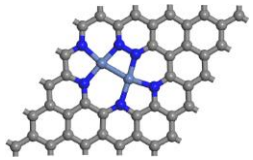
Catalysts	V_2-DV-A	V_2-DV-B	V_2-TV-A	V_2-TV-B	V_2-QV-A	V_2-QV-B
Crystal structure						
Lattice constant	a = 12.35 Å b = 12.27 Å c = 16.86 Å	a = 12.37 Å b = 12.27 Å c = 16.81 Å	a = 12.70 Å b = 12.29 Å c = 16.76 Å	a = 12.38 Å b = 12.22 Å c = 16.84 Å	a = 12.33 Å b = 12.30 Å c = 16.90 Å	a = 12.24 Å b = 12.30 Å c = 16.98 Å
Space group	Cm (#8)	P1 (#1)	Cm (#8)	C2 (#5)	Amm2 (#38)	C2 (#5)
Point group	Cs-3	C1-1	Cs-3	C2-3	C2V-14	C2-3

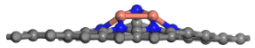
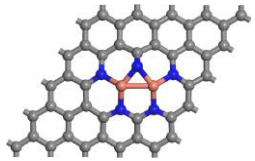
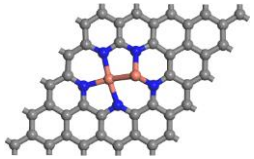
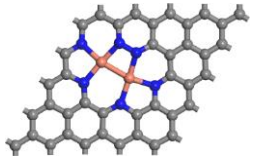
Catalysts	Cr_2-DV-A	Cr_2-DV-B	Cr_2-TV-A	Cr_2-TV-B	Cr_2-QV-A	Cr_2-QV-B
Crystal structure						/
Lattice constant	a = 12.36 Å b = 12.21 Å c = 16.89 Å	a = 12.42 Å b = 12.26 Å c = 16.81 Å	a = 12.43 Å b = 12.24 Å c = 16.81 Å	a = 12.35 Å b = 12.24 Å c = 16.81 Å	a = 12.29 Å b = 12.29 Å c = 16.94 Å	/
Space group	Cm (#8)	P1 (#1)	P1 (#1)	P1 (#1)	C2 (#5)	/
Point group	Cs-3	C1-1	C1-1	C1-1	C2-3	/

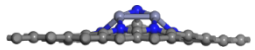
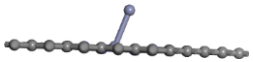
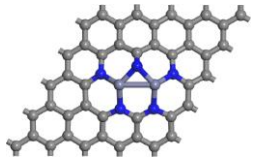
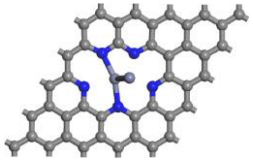
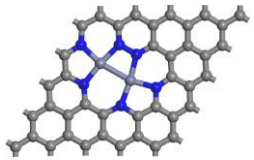
Catalysts	Mn_2-DV-A	Mn_2-DV-B	Mn_2-TV-A	Mn_2-TV-B	Mn_2-QV-A	Mn_2-QV-B
Crystal structure		/		/		
		/		/		
Lattice constant	a = 12.37 Å b = 12.27 Å c = 16.83 Å	/	a = 12.38 Å b = 12.23 Å c = 16.73 Å	/	a = 12.26 Å b = 12.33 Å c = 16.91 Å	a = 12.25 Å b = 12.31 Å c = 16.95 Å
Space group	Cm (#8)	/	C2 (#5)	/	Amm2 (#38)	C2 (#5)
Point group	Cs-3	/	C2-3	/	C2v-14	C2-3

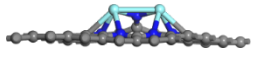
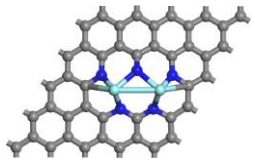
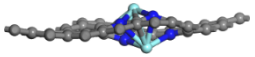
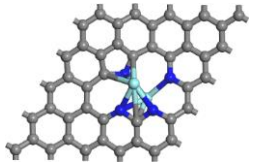
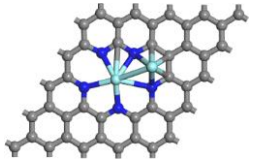
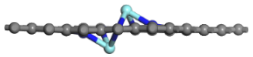
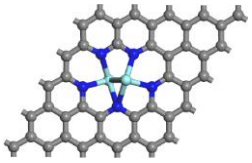
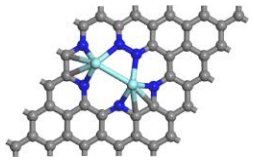
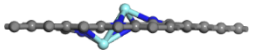
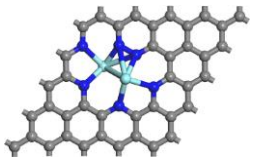
Catalysts	Fe_2-DV-A	Fe_2-DV-B	Fe_2-TV-A	Fe_2-TV-B	Fe_2-QV-A	Fe_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.38 Å b = 12.26 Å c = 16.82 Å	a = 12.43 Å b = 12.26 Å c = 16.80 Å	a = 12.36 Å b = 12.26 Å c = 16.85 Å	/	a = 12.22 Å b = 12.34 Å c = 16.92 Å	/
Space group	Cm (#8)	P1 (#1)	C2 (#5)	/	C2 (#5)	/
Point group	Cs-3	C1-1	C2-3	/	C2-3	/

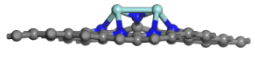
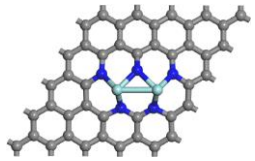
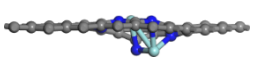
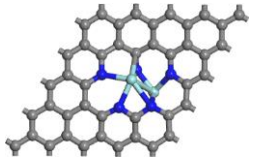
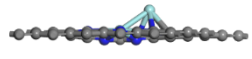
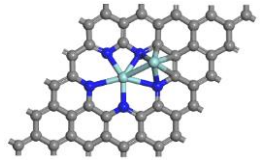
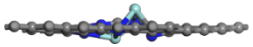
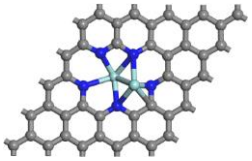
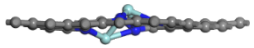
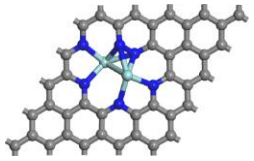
Catalysts	Co_2-DV-A	Co_2-DV-B	Co_2-TV-A	Co_2-TV-B	Co_2-QV-A	Co_2-QV-B
Crystal structure		/		/		/
		/		/		/
Lattice constant	a = 12.42 Å b = 12.27 Å c = 16.80Å	/	a = 12.34 Å b = 12.26 Å c = 16.88 Å	/	a = 12.20 Å b = 12.33 Å c = 16.96 Å	/
Space group	P1 (#1)	/	C2 (#5)	/	Amm2 (#38)	/
Point group	C1-1	/	C2-3	/	C2v-14	/

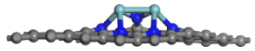
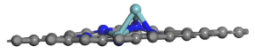
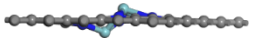
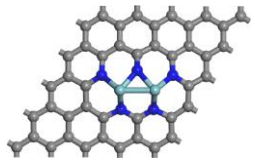
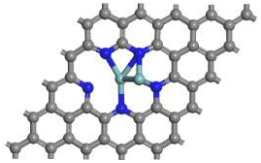
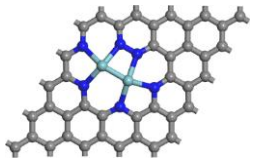
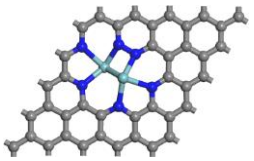
Catalysts	Ni_2-DV-A	Ni_2-DV-B	Ni_2-TV-A	Ni_2-TV-B	Ni_2-QV-A	Ni_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.37 Å b = 12.28 Å c = 16.81 Å	a = 12.37 Å b = 12.26 Å c = 16.83 Å	a = 12.39 Å b = 12.24 Å c = 16.90 Å	/	a = 12.12 Å b = 12.33 Å c = 16.97 Å	/
Space group	Cm (#8)	Cm (#8)	P1 (#1)	/	Amm2 (#38)	/
Point group	Cs-3	Cs-3	C1-1	/	C2v-14	/

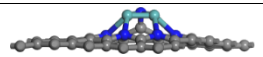
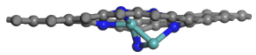
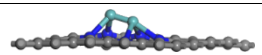
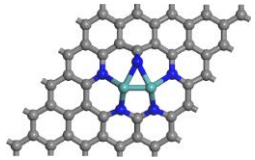
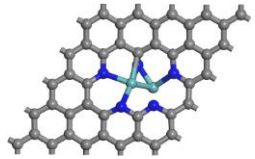
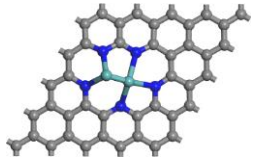
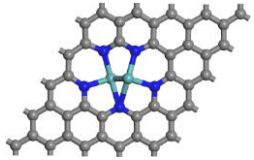
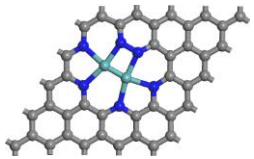
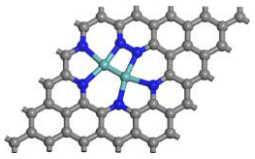
Catalysts	Cu_2-DV-A	Cu_2-DV-B	Cu_2-TV-A	Cu_2-TV-B	Cu_2-QV-A	Cu_2-QV-B
Crystal structure		/		/		/
		/		/		/
Lattice constant	a = 12.37 Å b = 12.28 Å c = 16.81 Å	/	a = 12.40 Å b = 12.25 Å c = 16.87 Å	/	a = 12.20 Å b = 12.35 Å c = 16.93 Å	/
Space group	Cm (#8)	/	P1 (#1)	/	Cm (#8)	/
Point group	Cs-3	/	C1-1	/	Cs-3	/

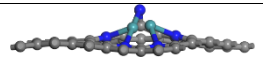
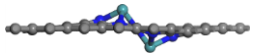
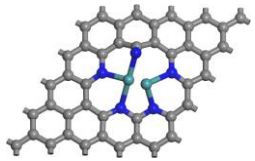
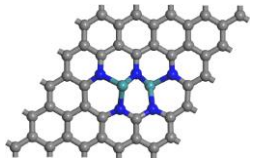
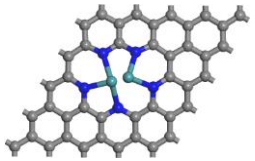
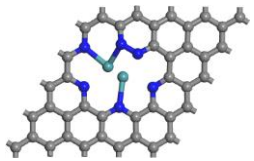
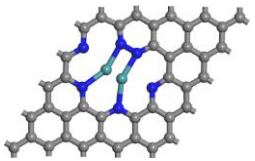
Catalysts	Zn_2-DV-A	Zn_2-DV-B	Zn_2-TV-A	Zn_2-TV-B	Zn_2-QV-A	Zn_2-QV-B
Crystal structure		/		/		/
		/		/		/
Lattice constant	a = 12.38 Å b = 12.29 Å c = 16.78 Å	/	a = 12.36 Å b = 12.21 Å c = 16.92 Å	/	a = 12.22 Å b = 12.42 Å c = 16.78 Å	/
Space group	Cm (#8)	/	P1 (#1)	/	Amm2 (#38)	/
Point group	Cs-3	/	C1-1	/	C2v-14	/

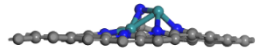
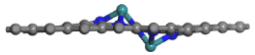
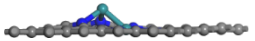
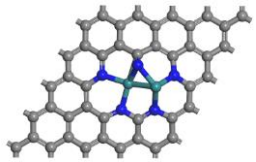
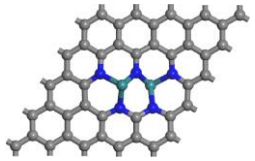
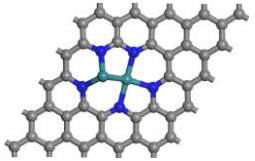
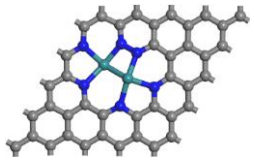
Catalysts	Y_2-DV-A	Y_2-DV-B	Y_2-TV-A	Y_2-TV-B	Y_2-QV-A	Y_2-QV-B
Crystal structure	 	 	 	 	 	 
Lattice constant	a = 12.36 Å b = 12.29 Å c = 16.82 Å	a = 12.25 Å b = 12.07 Å c = 17.09 Å	a = 12.41 Å b = 12.23 Å c = 16.83 Å	a = 12.37 Å b = 12.26 Å c = 16.83 Å	a = 12.25 Å b = 12.33 Å c = 16.92 Å	a = 12.27 Å b = 12.32 Å c = 16.91 Å
Space group	Cm (#8)	P1 (#1)	P1 (#1)	C2 (#5)	Cm (#8)	C2 (#5)
Point group	Cs-3	C1-1	C1-1	C2-3	Cs-3	C2-3

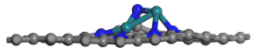
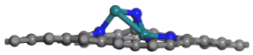
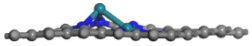
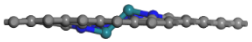
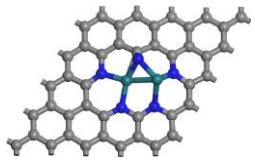
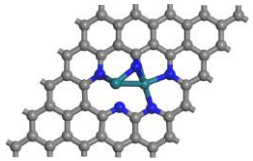
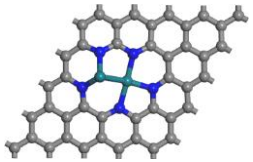
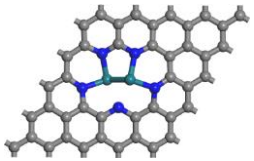
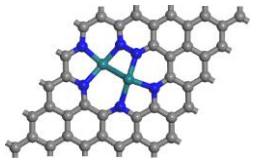
Catalysts	Zr_2-DV-A	Zr_2-DV-B	Zr_2-TV-A	Zr_2-TV-B	Zr_2-QV-A	Zr_2-QV-B
Crystal structure	 	 	 	 	 	/ /
Lattice constant	a = 12.36 Å b = 12.28 Å c = 16.83 Å	a = 12.36 Å b = 12.24 Å c = 16.92 Å	a = 12.29 Å b = 12.27 Å c = 16.97 Å	a = 12.32 Å b = 12.21 Å c = 16.96 Å	a = 12.19 Å b = 12.28 Å c = 17.06 Å	/
Space group	Cm (#8)	P1 (#1)	P1 (#1)	P1 (#1)	C2 (#5)	/
Point group	Cs-3	C1-1	C1-1	C1-1	C2-3	/

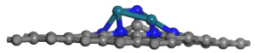
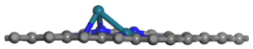
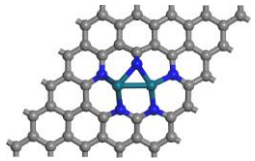
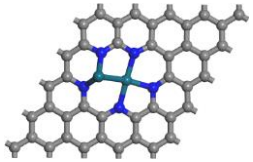
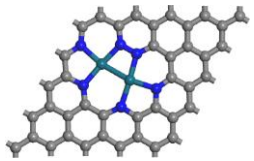
Catalysts	Nb_2-DV-A	Nb_2-DV-B	Nb_2-TV-A	Nb_2-TV-B	Nb_2-QV-A	Nb_2-QV-B
Crystal structure		/		/		
		/		/		
Lattice constant	a = 12.35 Å b = 12.29 Å c = 16.83 Å	/	a = 12.37 Å b = 12.25 Å c = 16.93 Å	/	a = 12.29 Å b = 12.35 Å c = 16.84 Å	a = 12.30 Å b = 12.32 Å c = 16.89 Å
Space group	Cm (#8)	/	P1 (#1)	/	Cm (#8)	C2 (#5)
Point group	Cs-3	/	C1-1	/	Cs-3	C2-3

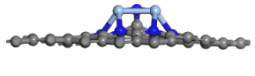
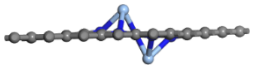
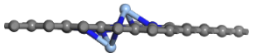
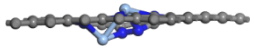
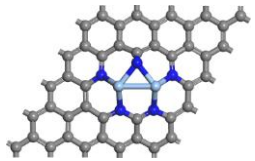
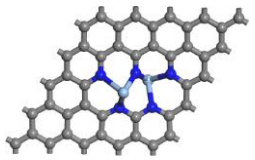
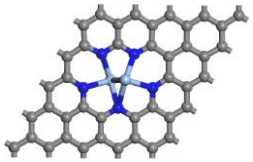
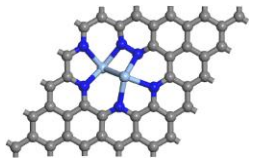
Catalysts	Mo_2-DV-A	Mo_2-DV-B	Mo_2-TV-A	Mo_2-TV-B	Mo_2-QV-A	Mo_2-QV-B
Crystal structure						
						
Lattice constant	a = 12.35 Å b = 12.22 Å c = 16.91 Å	a = 12.34 Å b = 12.25 Å c = 16.89 Å	a = 12.32 Å b = 12.23 Å c = 16.90 Å	a = 12.46 Å b = 12.26 Å c = 16.67 Å	a = 12.36 Å b = 12.34 Å c = 16.79 Å	a = 12.40 Å b = 12.38 Å c = 16.69 Å
Space group	Cm (#8)	P1 (#1)	P1 (#1)	C2 (#5)	Cm (#8)	Amm2 (#38)
Point group	Cs-3	C1-1	C1-1	C2-3	Cs-3	C2v-14

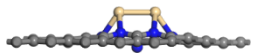
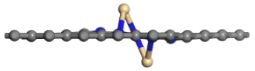
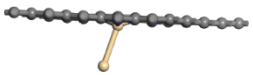
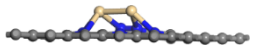
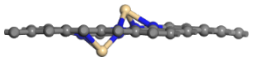
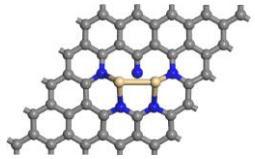
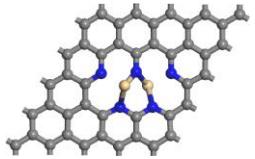
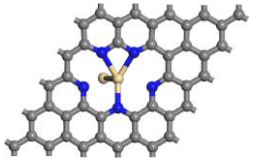
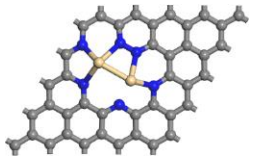
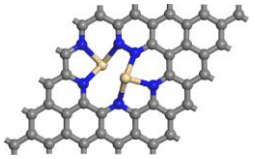
Catalysts	Tc_2-DV-A	Tc_2-DV-B	Tc_2-TV-A	Tc_2-TV-B	Tc_2-QV-A	Tc_2-QV-B
Crystal structure				/		
				/		
Lattice constant	a = 12.37 Å b = 12.20 Å c = 16.88 Å	a = 12.42 Å b = 12.31 Å c = 16.69 Å	a = 12.42 Å b = 12.23 Å c = 16.82 Å	/	a = 12.33 Å b = 12.28 Å c = 16.93 Å	a = 12.24 Å b = 12.35 Å c = 16.72 Å
Space group	P1 (#1)	C2 (#5)	Cm (#8)	/	Cm (#8)	C2 (#5)
Point group	C1-1	C2-3	Cs-3	/	Cs-3	C2-3

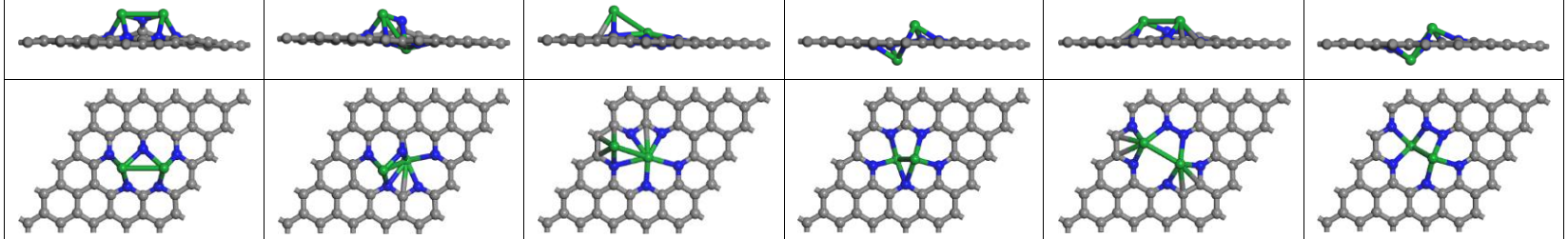
Catalysts	Ru_2-DV-A	Ru_2-DV-B	Ru_2-TV-A	Ru_2-TV-B	Ru_2-QV-A	Ru_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.33 Å b = 12.28 Å c = 16.88 Å	a = 12.42 Å b = 12.32 Å c = 16.69 Å	a = 12.35 Å b = 12.24 Å c = 16.78 Å	/	a = 12.31 Å b = 12.34 Å c = 16.85 Å	/
Space group	P1 (#1)	C2 (#5)	P1 (#1)	/	C2 (#5)	/
Point group	C1-1	C2-3	C1-1	/	C2-3	/

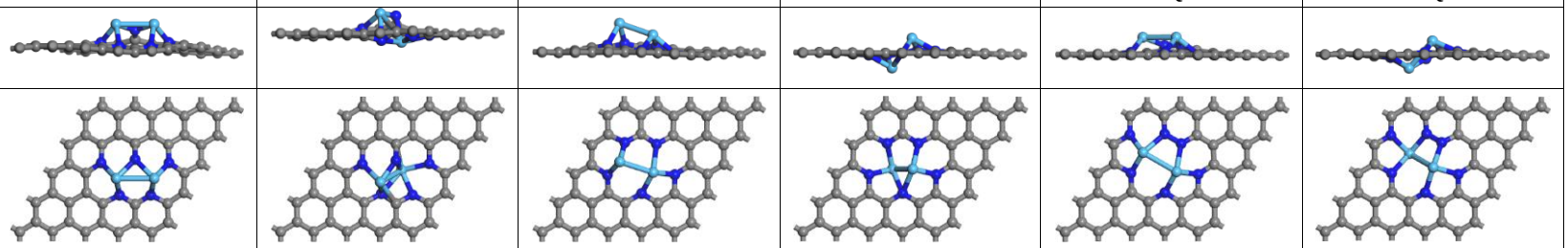
Catalysts	Rh_2-DV-A	Rh_2-DV-B	Rh_2-TV-A	Rh_2-TV-B	Rh_2-QV-A	Rh_2-QV-B
Crystal structure						/
						/
Lattice constant	a = 12.33 Å b = 12.28 Å c = 16.81 Å	a = 12.36 Å b = 12.23 Å c = 16.90 Å	a = 12.30 Å b = 12.24 Å c = 16.86 Å	a = 12.39 Å b = 12.28 Å c = 16.77 Å	a = 12.28 Å b = 12.34 Å c = 16.86 Å	/
Space group	P1 (#1)	P1 (#1)	P1 (#1)	C2 (#5)	C2 (#5)	/
Point group	C1-1	C1-1	C1-1	C2-3	C2-3	/

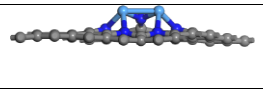
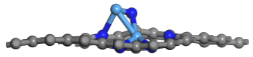
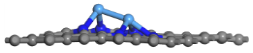
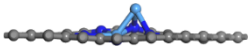
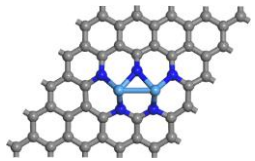
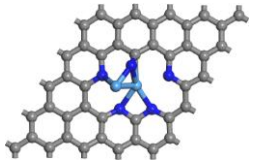
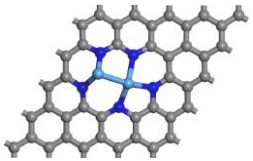
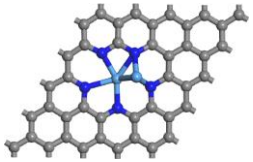
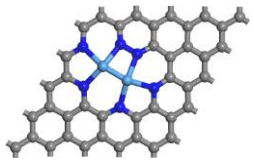
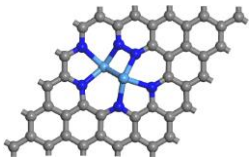
Catalysts	Pd_2-DV-A	Pd_2-DV-B	Pd_2-TV-A	Pd_2-TV-B	Pd_2-QV-A	Pd_2-QV-B
Crystal structure		/		/		/
		/		/		/
Lattice constant	a = 12.37 Å b = 12.26 Å c = 16.84 Å	/	a = 12.33 Å b = 12.22 Å c = 16.87 Å	/	a = 12.28 Å b = 12.45 Å c = 16.67 Å	/
Space group	P1 (#1)	/	P1 (#1)	/	C2 (#5)	/
Point group	C1-1	/	C1-1	/	C2-3	/

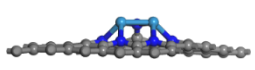
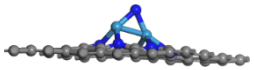
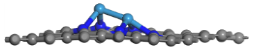
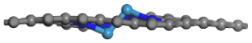
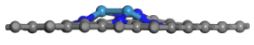
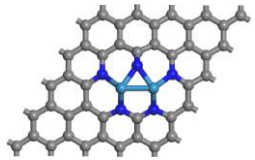
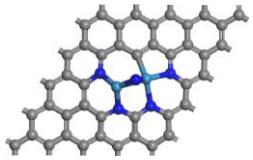
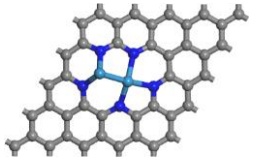
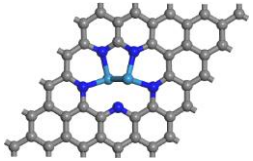
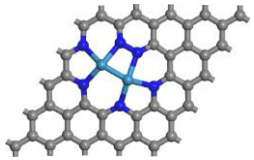
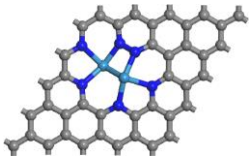
Catalysts	Ag_2-DV-A	Ag_2-DV-B	Ag_2-TV-A	Ag_2-TV-B	Ag_2-QV-A	Ag_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.35 Å b = 12.25 Å c = 16.88 Å	a = 12.42 Å b = 12.29 Å c = 16.71 Å	a = 12.38 Å b = 12.23 Å c = 16.84 Å	/	a = 12.29 Å b = 12.31 Å c = 16.92 Å	/
Space group	Cm (#8)	C2 (#5)	C2 (#5)	/	P1 (#1)	/
Point group	Cs-3	C2-3	C2-3	/	C1-1	/

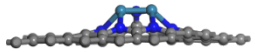
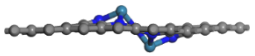
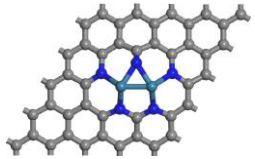
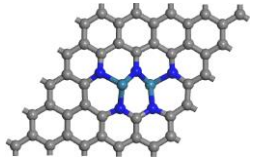
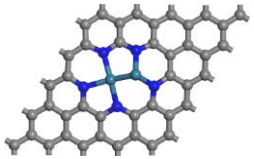
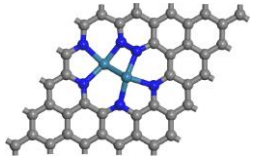
Catalysts	Cd_2-DV-A	Cd_2-DV-B	Cd_2-TV-A	Cd_2-TV-B	Cd_2-QV-A	Cd_2-QV-B
Crystal structure				/		
				/		
Lattice constant	a = 12.35 Å b = 12.30 Å c = 16.84 Å	a = 12.41 Å b = 12.28 Å c = 16.74 Å	a = 12.41 Å b = 12.21 Å c = 16.81 Å	/	a = 12.28 Å b = 12.32 Å c = 16.90 Å	a = 12.25 Å b = 12.31 Å c = 16.96 Å
Space group	Cm (#8)	C2 (#5)	P1 (#1)	/	Cm (#8)	C2 (#5)
Point group	Cs-3	C2-3	C1-1	/	Cs-3	C2-3

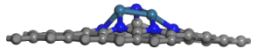
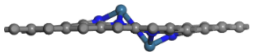
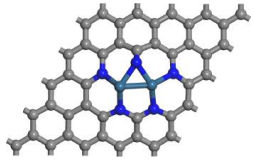
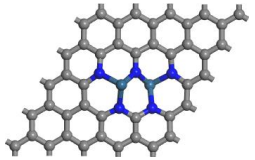
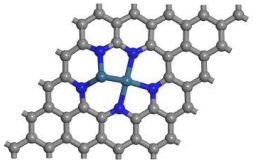
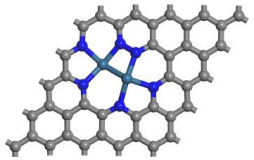
Catalysts	Lu_2-DV-A	Lu_2-DV-B	Lu_2-TV-A	Lu_2-TV-B	Lu_2-QV-A	Lu_2-QV-B
Crystal structure						
Lattice constant	a = 12.35 Å b = 12.28 Å c = 16.86 Å	a = 12.35 Å b = 12.28 Å c = 16.83 Å	a = 12.40 Å b = 12.22 Å c = 16.83 Å	a = 12.38 Å b = 12.26 Å c = 16.82 Å	a = 12.24 Å b = 12.32 Å c = 16.94 Å	a = 12.28 Å b = 12.33 Å c = 16.88 Å
Space group	Cm (#8)	P1 (#1)	Cm (#8)	C2 (#5)	Cm (#8)	C2 (#5)
Point group	Cs-3	C1-1	Cs-3	C2-3	Cs-3	C2-3

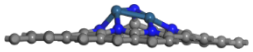
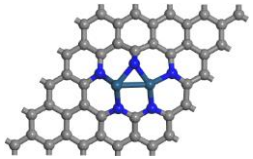
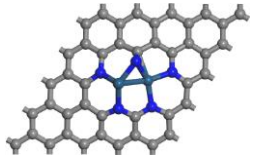
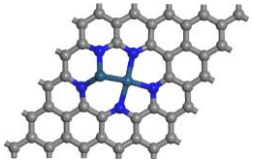
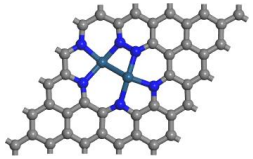
Catalysts	Hf_2-DV-A	Hf_2-DV-B	Hf_2-TV-A	Hf_2-TV-B	Hf_2-QV-A	Hf_2-QV-B
Crystal structure						
Lattice constant	a = 12.35 Å b = 12.27 Å c = 16.86 Å	a = 12.30 Å b = 12.26 Å c = 16.94 Å	a = 12.30 Å b = 12.28 Å c = 16.89 Å	a = 12.37 Å b = 12.28 Å c = 16.80 Å	a = 12.24 Å b = 12.33 Å c = 16.93 Å	a = 12.30 Å b = 12.31 Å c = 16.89 Å
Space group	Cm (#8)	P1 (#1)	P1 (#1)	C2 (#5)	Cm (#8)	C2 (#5)
Point group	Cs-3	C1-1	C1-1	C2-3	Cs-3	C2-3

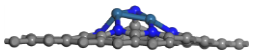
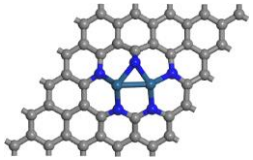
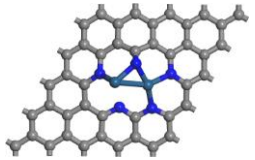
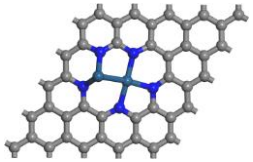
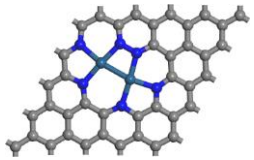
Catalysts	Ta_2-DV-A	Ta_2-DV-B	Ta_2-TV-A	Ta_2-TV-B	Ta_2-QV-A	Ta_2-QV-B
Crystal structure						
						
Lattice constant	a = 12.36 Å b = 12.29 Å c = 16.82 Å	a = 12.35 Å b = 12.15 Å c = 16.97 Å	a = 12.27 Å b = 12.26 Å c = 16.92 Å	a = 12.40 Å b = 12.17 Å c = 16.91 Å	a = 12.32 Å b = 12.36 Å c = 16.79 Å	a = 12.30 Å b = 12.33 Å c = 16.88 Å
Space group	Cm (#8)	P1 (#1)	P1 (#1)	P1 (#1)	Cm (#8)	C2 (#5)
Point group	Cs-3	C1-1	C1-1	C1-1	Cs-3	C2-3

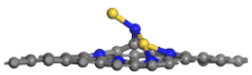
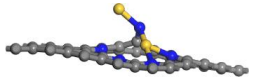
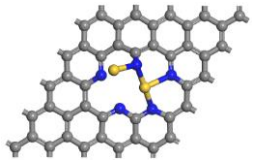
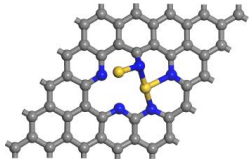
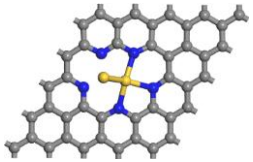
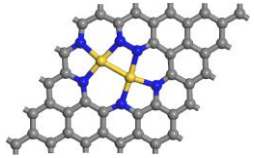
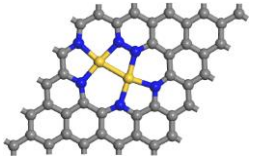
Catalysts	W_2-DV-A	W_2-DV-B	W_2-TV-A	W_2-TV-B	W_2-QV-A	W_2-QV-B
Crystal structure						
						
Lattice constant	a = 12.35 Å b = 12.25 Å c = 16.88 Å	a = 12.39 Å b = 12.27 Å c = 16.90 Å	a = 12.26 Å b = 12.26 Å c = 16.72 Å	a = 12.44 Å b = 12.24 Å c = 16.72 Å	a = 12.27 Å b = 12.32 Å c = 16.90 Å	a = 12.31 Å b = 12.32 Å c = 16.88 Å
Space group	Cm (#8)	P1 (#1)	P1 (#1)	C2 (#5)	Cm (#8)	C2 (#5)
Point group	Cs-3	C1-1	C1-1	C2-3	Cs-3	C2-3

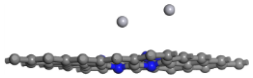
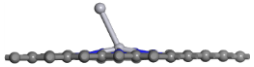
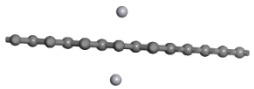
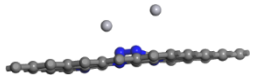
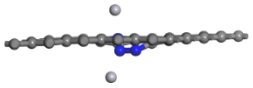
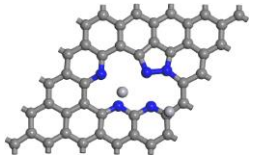
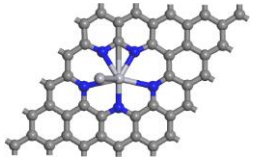
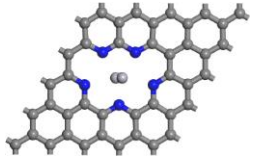
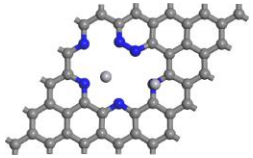
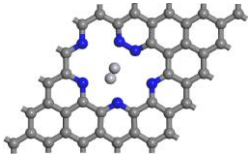
Catalysts	Re_2-DV-A	Re_2-DV-B	Re_2-TV-A	Re_2-TV-B	Re_2-QV-A	Re_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.34 Å b = 12.26 Å c = 16.88 Å	a = 12.48 Å b = 12.33 Å c = 16.58 Å	a = 12.47 Å b = 12.27 Å c = 16.78 Å	/	a = 12.33 Å b = 12.34 Å c = 16.82 Å	/
Space group	Cm (#8)	C2 (#5)	P1 (#1)	/	C2 (#5)	/
Point group	Cs-3	C2-3	C1-1	/	C2-3	/

Catalysts	Os_2-DV-A	Os_2-DV-B	Os_2-TV-A	Os_2-TV-B	Os_2-QV-A	Os_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.38 Å b = 12.25 Å c = 16.85 Å	a = 12.43 Å b = 12.33 Å c = 16.65 Å	a = 12.33 Å b = 12.25 Å c = 16.78 Å	/	a = 12.29 Å b = 12.35 Å c = 16.83 Å	/
Space group	Cm (#8)	C2 (#5)	P1 (#1)	/	C2 (#5)	/
Point group	Cs-3	C2-3	C1-1	/	C2-3	/

Catalysts	Ir_2-DV-A	Ir_2-DV-B	Ir_2-TV-A	Ir_2-TV-B	Ir_2-QV-A	Ir_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.39 Å b = 12.27 Å c = 16.82 Å	a = 12.45 Å b = 12.29 Å c = 16.79 Å	a = 12.29 Å b = 12.24 Å c = 16.85 Å	/	a = 12.27 Å b = 12.37 Å c = 16.83 Å	/
Space group	P1 (#1)	P1 (#1)	P1 (#1)	/	C2 (#5)	/
Point group	C1-1	C1-1	C1-1	/	C2-3	/

Catalysts	Pt_2-DV-A	Pt_2-DV-B	Pt_2-TV-A	Pt_2-TV-B	Pt_2-QV-A	Pt_2-QV-B
Crystal structure				/		/
				/		/
Lattice constant	a = 12.38 Å b = 12.27 Å c = 16.82 Å	a = 12.36 Å b = 12.23 Å c = 16.86 Å	a = 12.31 Å b = 12.23 Å c = 16.86 Å	/	a = 12.26 Å b = 12.47 Å c = 16.65 Å	/
Space group	Cm (#8)	P1 (#1)	Cm (#8)	/	Cm (#8)	/
Point group	Cs-3	C1-1	Cs-3	/	Cs-3	/

Catalysts	Au_2-DV-A	Au_2-DV-B	Au_2-TV-A	Au_2-TV-B	Au_2-QV-A	Au_2-QV-B
Crystal structure				/		
				/		
Lattice constant	a = 12.36 Å b = 12.27 Å c = 16.84 Å	a = 12.34 Å b = 12.20 Å c = 17.02 Å	a = 12.35 Å b = 12.21 Å c = 16.86 Å	/	a = 12.25 Å b = 12.44 Å c = 16.71 Å	a = 12.28 Å b = 12.49 Å c = 16.60 Å
Space group	P1 (#1)	P1 (#1)	P1 (#1)	/	Cm (#8)	Amm2 (#38)
Point group	C1-1	C1-1	C1-1	/	Cs-3	C2v-14

Catalysts	Hg_2-DV-A	Hg_2-DV-B	Hg_2-TV-A	Hg_2-TV-B	Hg_2-QV-A	Hg_2-QV-B
Crystal structure		/				
		/				
Lattice constant	a = 12.40 Å b = 12.13 Å c = 16.18 Å	/	a = 12.42 Å b = 12.23 Å c = 16.77 Å	a = 12.33 Å b = 12.21 Å c = 16.96 Å	a = 12.23 Å b = 12.26 Å c = 16.15 Å	a = 12.23 Å b = 12.26 Å c = 16.07 Å
Space group	P1 (#1)	/	P1 (#1)	C2 (#5)	P1 (#1)	Amm2 (#38)
Point group	C1-1	/	C1-1	C2-3	C1-1	C2v-14