

Supporting Information

How the Balance between *CO and *H Intermediates in Dual Atom Catalysts Boosts Selectivity for Hydrocarbons

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Calculation details

The Gibbs free energy change (ΔG) was defined as [1]:

$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S + \Delta G_{pH} + \Delta G_U \quad (1)$$

where ΔE is the electronic energy difference directly obtained from DFT calculations, ΔE_{ZPE} is the change in zero-point energy, T is the temperature (298.15 k), and ΔS is the entropy change. $\Delta G_U = -neU$, where n is the number of transferred electrons and U is the electrode potential. ΔG_{pH} is the correction of the H^+ free energy by the concentration; $\Delta G_{pH} = k_B T \times \ln 10 \times pH$, where k_B is the Boltzmann constant, and the value of pH was set to be zero for acidic conditions. Zero-point energies and total entropies of molecules were computed from the vibrational frequencies. The vibrational modes of the adsorbate were computed explicitly, while the catalyst sheet was fixed (assuming that the vibrations of the substrate were negligible).

The adsorption energies (E_{ads}) were calculated by the following equation:

$$E_{ads} = E_{A-S} - E_S - E_A \quad (2)$$

where E_{A-S} , E_S , and E_A are the total energies of the adsorbate–substrate (A–S) complex, the substrate (S), and the adsorbate (A), respectively.

Support Pictures

Figure S1.

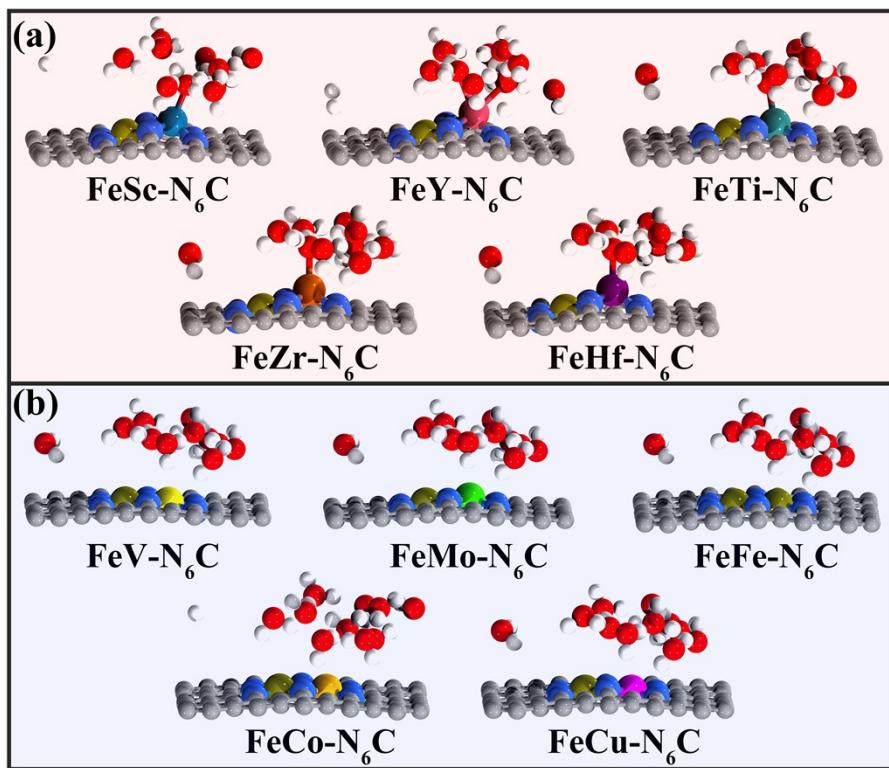


Figure S1. Initial optimized structures: (a) FeM₁-N₆C, (b) FeM₂-N₆C.

Figure S2.

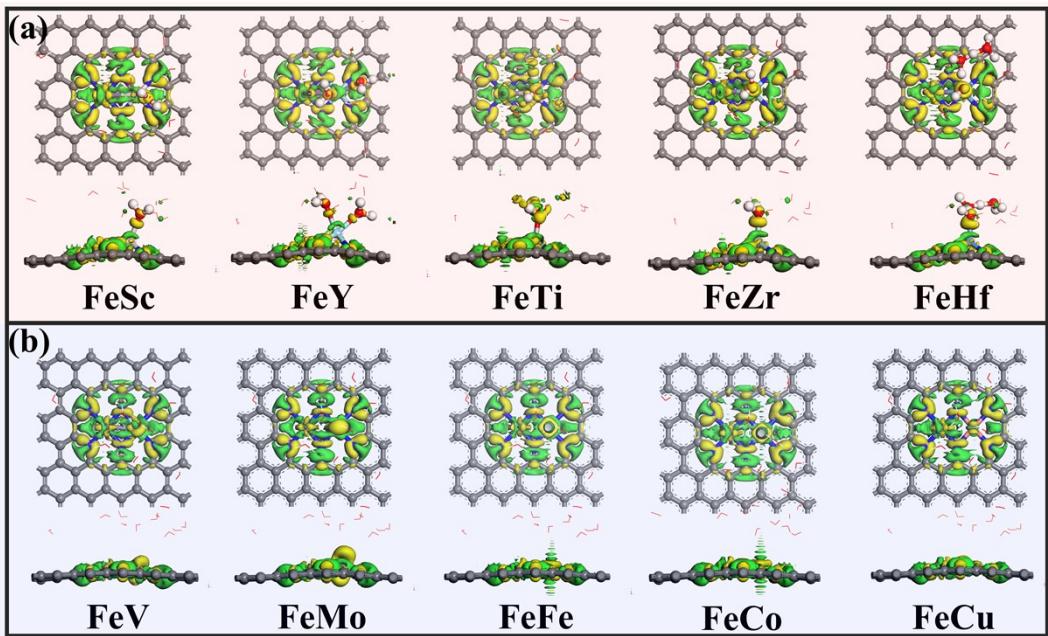


Figure S2. Charge density difference plots for the initial structure of FeM-N₆C: (a) FeM₁-N₆C, (b) FeM₂-N₆C. Yellow color represents an increase in electron density and green color represents a decrease in electron density.

Figure S3.

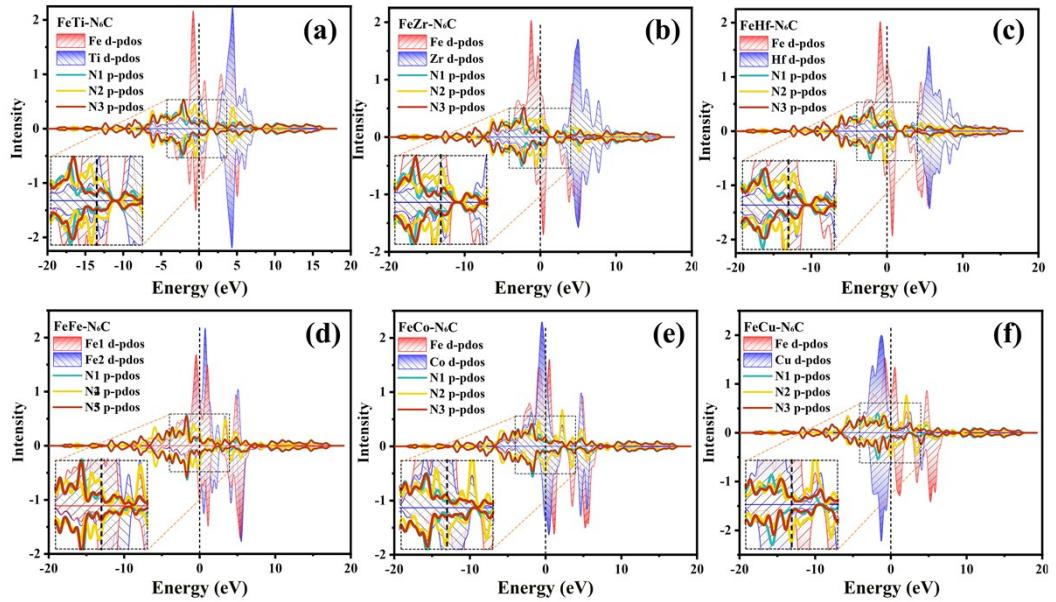


Figure S3. PDOS maps of each atom in the initial structure of FeM-N₆C: (a) FeTi-N₆C, (b) FeZr-N₆C, (c) FeHf-N₆C, (d) FeFe-N₆C, (e) FeCo-N₆C, (f) FeCu-N₆C. (The illustration in the bottom left corner is an enlarged view of the vicinity of the Fermi level)

Figure S4.

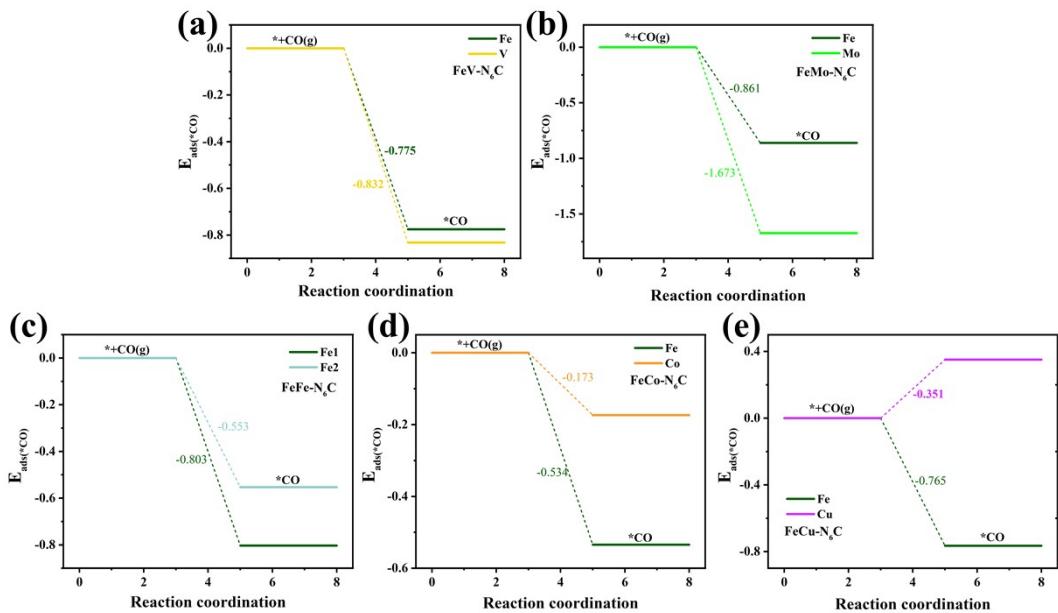


Figure S4. Calculated adsorption energies of ${}^*\text{CO}$ in $\text{FeM}_2\text{-N}_6\text{C}$ catalysts: (a) $\text{FeV-N}_6\text{C}$, (b) $\text{FeMo-N}_6\text{C}$, (c) $\text{FeFe-N}_6\text{C}$, (d) $\text{FeCo-N}_6\text{C}$, (e) $\text{FeCu-N}_6\text{C}$.

Figure S5.

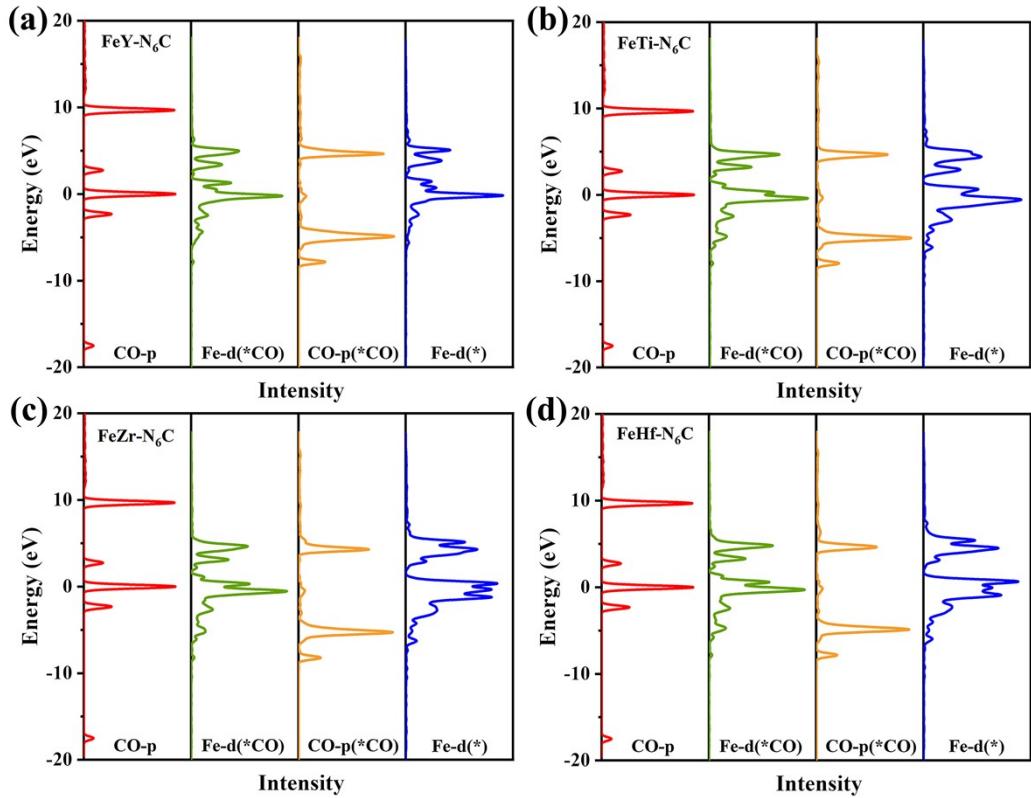


Figure S5. PDOS plots of each atom before and after adsorption of $^*\text{CO}$ intermediates on $\text{FeM}_1\text{-N}_6\text{C}$ catalysts: (a) $\text{FeY-N}_6\text{C}$, (b) $\text{FeTi-N}_6\text{C}$, (c) $\text{FeZr-N}_6\text{C}$, (d) $\text{FeHf-N}_6\text{C}$.

Figure S6.

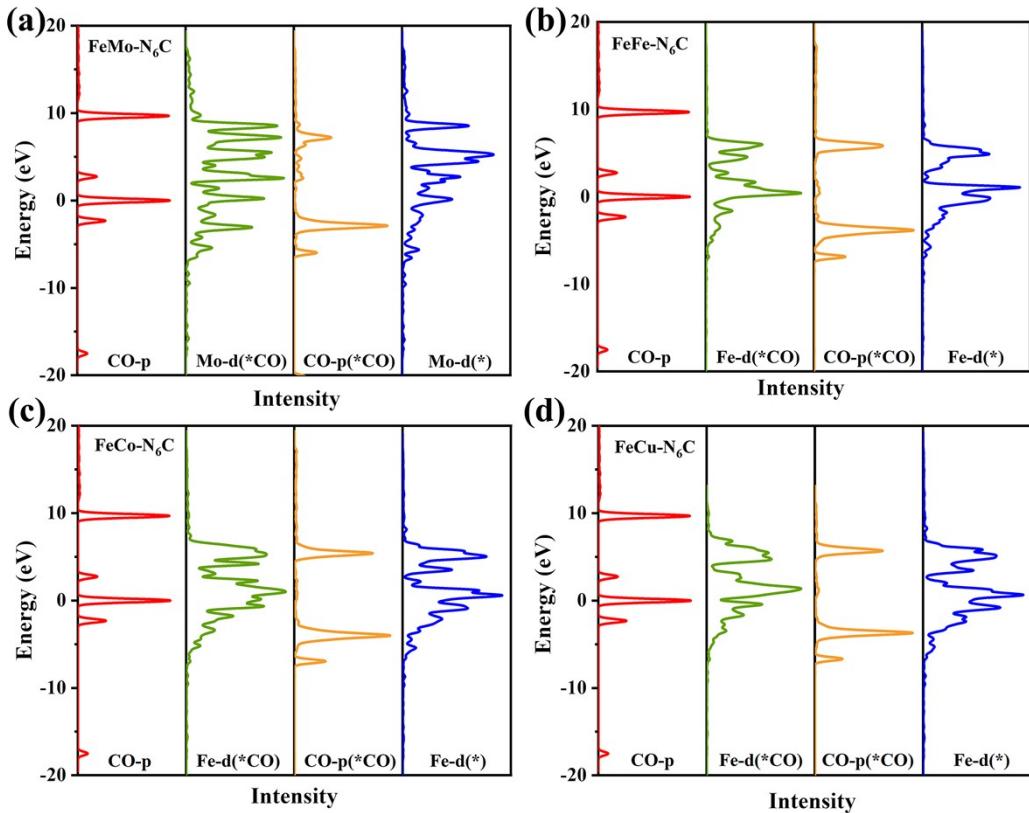


Figure S6. PDOS plots of each atom before and after adsorption of *CO intermediates on $\text{FeM}_2\text{-N}_6\text{C}$ catalysts: (a) $\text{FeMo-N}_6\text{C}$, (b) $\text{FeFe-N}_6\text{C}$, (c) $\text{FeCo-N}_6\text{C}$, (d) $\text{FeCu-N}_6\text{C}$.

Figure S7.

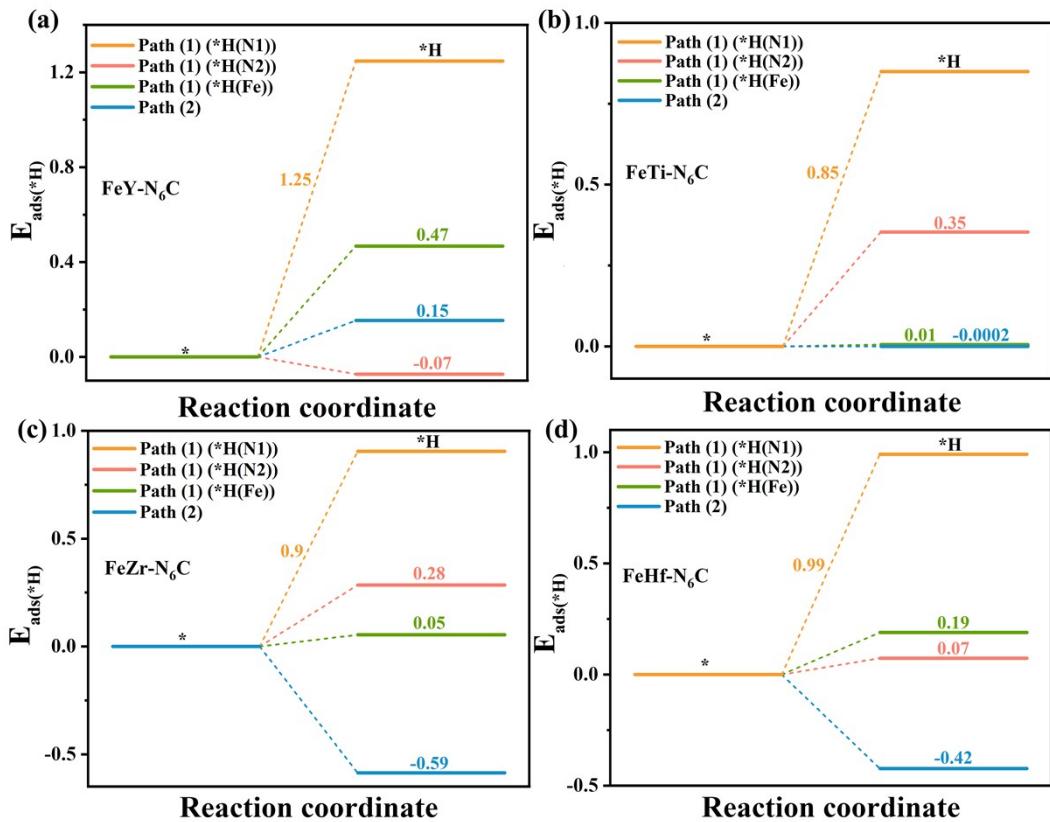


Figure S7. Adsorption energy calculations for ${}^*\text{H}$ intermediates: (a) $\text{FeY-N}_6\text{C}$, (b) $\text{FeTi-N}_6\text{C}$, (c) $\text{FeZr-N}_6\text{C}$, (d) $\text{FeHf-N}_6\text{C}$.

Figure S8.

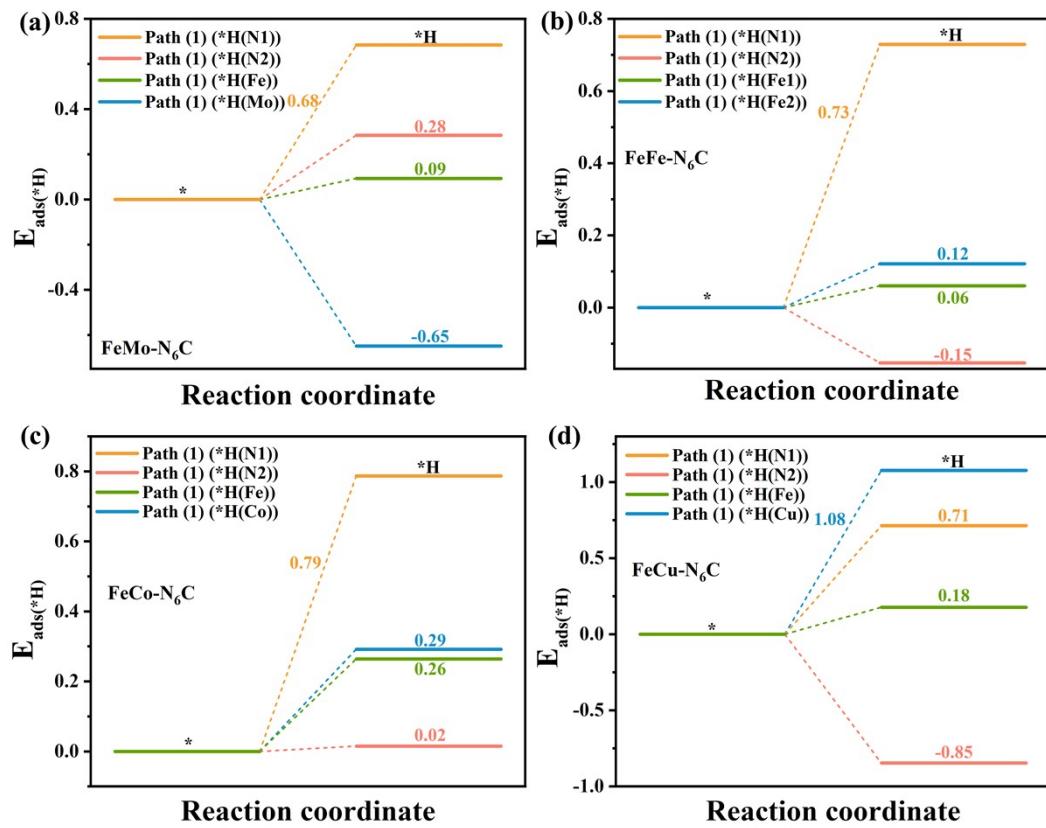


Figure S8. Adsorption energy calculations for *H intermediates: (a) FeMo-N₆C, (b) FeFe-N₆C, (c) FeCo-N₆C, (d) FeCu-N₆C.

Figure S9.

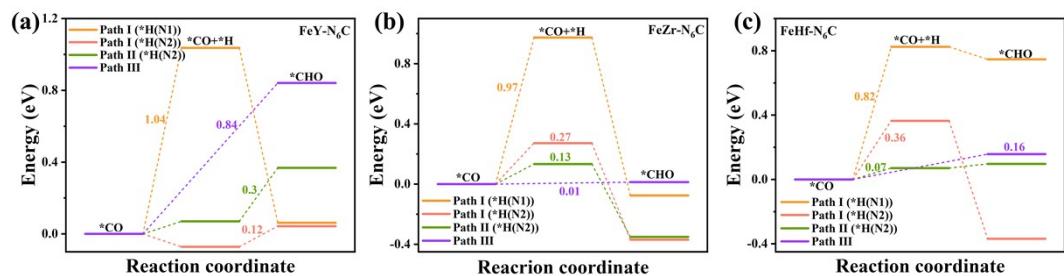


Figure S9. Free energy calculations for the $\text{*CO} \rightarrow \text{*CHO}$ reaction processes: (a) FeY-N₆C, (b) FeZr-N₆C, (c) FeHf-N₆C.

Figure S10.

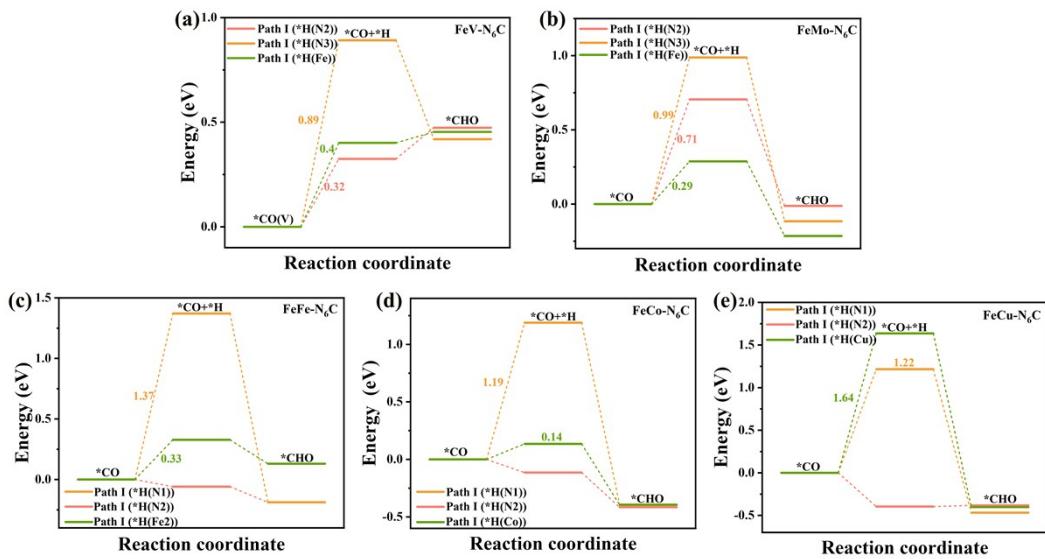


Figure S10. Free energy calculations for the $*\text{CO} \rightarrow *\text{CHO}$ reaction processes: (a) FeV-N₆C, (b) FeMo-N₆C, (c) FeFe-N₆C, (d) FeCo-N₆C, (e) FeCu-N₆C.

Figure S11.

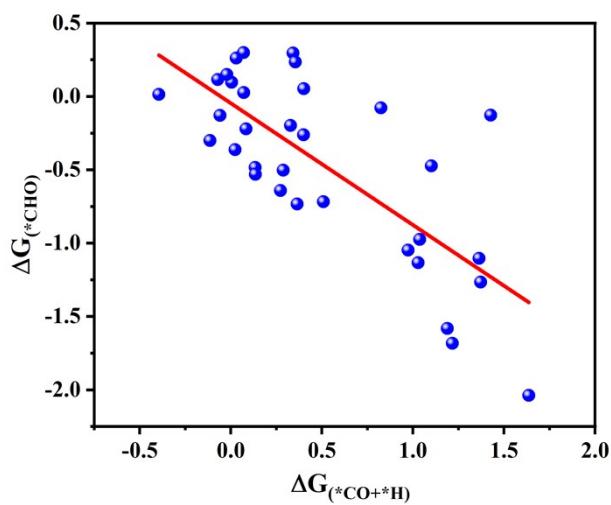


Figure S11. Relationship between $\Delta G_{(*\text{CO}+\text{*H})}$ and $\Delta G_{(*\text{CHO})}$.

Figure S12.

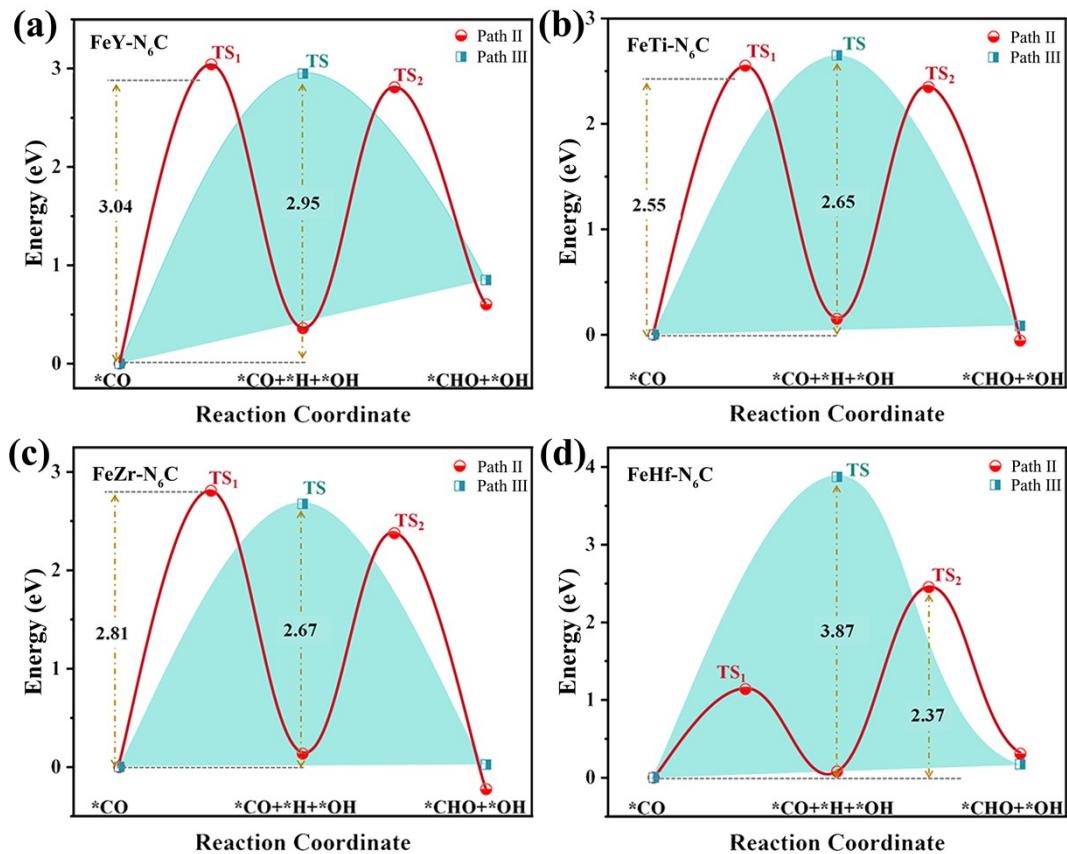


Figure S12. Transition state calculations. (a) FeY-N₆C, (b) FeTi-N₆C, (c) FeZr-N₆C, (d) FeHf-N₆C.

Support Forms

Catalyst	Metal element	Atomic populations (Mulliken) charge (e)	Catalyst	Metal element	Atomic populations (Mulliken) charge (e)
FeSc-N ₆ C	Sc	1.81	FeV-N ₆ C	V	1.51
FeY-N ₆ C	Y	1.94	FeMo-N ₆ C	Mo	1.39
FeTi-N ₆ C	Ti	1.68	FeFe-N ₆ C	Fe	1.22
FeZr-N ₆ C	Zr	1.89	FeCo-N ₆ C	Co	1.22
FeHf-N ₆ C	Hf	1.8	FeCu-N ₆ C	Cu	1.3

Table S1. Atomic populations (Mulliken) charge of the M metal in FeM-N₆C.

Table S2. Orbital Populations of the d orbitals of the metal atoms of the initial structure of FeM-N₆C.

Catalyst	Atom	Orbital	Up	Down	Spin
Fe-N-C	Fe	d _{z²}	0.949	0.136	0.813
		d _{zy}	0.981	0.057	0.924
		d _{zx}	0.948	0.858	0.091
		d _{x²-y²}	0.984	0.889	0.095
		d _{xy}	0.43	0.33	0.101

Catalyst	Ion	Orbital	Up	Down	Spin
FeSc-N ₆ C	Sc	d _{z²}	0.093	0.093	-0.001
		d _{zy}	0.101	0.099	0.002
		d _{zx}	0.116	0.121	-0.005
		d _{x²-y²}	0.127	0.094	0.033
		d _{xy}	0.222	0.222	0
		d _{z²}	0.941	0.05	0.891
		d _{zy}	0.925	0.804	0.121
		d _{zx}	0.948	0.833	0.115
		d _{x²-y²}	0.97	0.222	0.748
		d _{xy}	0.476	0.43	0.046

Catalyst	Ion	Orbital	Up	Down	Spin
FeY-N ₆ C	Y	d _{z²}	0.089	0.09	-0.001
		d _{zy}	0.114	0.114	0
		d _{zx}	0.129	0.13	-0.001
		d _{x²-y²}	0.102	0.105	-0.003
		d _{xy}	0.174	0.175	0
		d _{z²}	0.921	0.641	0.28
		d _{zy}	0.118	0.899	-0.781
		d _{zx}	0.944	0.35	0.594
		d _{x²-y²}	0.955	0.946	0.009
		d _{xy}	0.352	0.449	-0.097

Catalyst	Ion	Orbital	Up	Down	Spin
FeTi-N ₆ C	Ti	d _{z²}	0.197	0.201	-0.004
		d _{zy}	0.152	0.176	-0.023
		d _{zx}	0.18	0.177	0.004
		d _{x²-y²}	0.306	0.349	-0.043
		d _{xy}	0.299	0.301	-0.002
		d _{z²}	0.937	0.135	0.803
		d _{zy}	0.18	0.968	-0.788
		d _{zx}	0.918	0.857	0.061
		d _{x²-y²}	0.909	0.874	0.034
		d _{xy}	0.418	0.399	0.019

Catalyst	Ion	Orbital	Up	Down	Spin
FeZr-N ₆ C	Zr	d _{z²}	0.192	0.202	-0.009
		d _{zy}	0.197	0.191	0.005
	Fe	d _{zx}	0.183	0.184	-0.001
		d _{x²-y²}	0.258	0.288	-0.03
	FeZr	d _{xy}	0.271	0.271	0
N ₆ C	N ₆ C	d _{z²}	0.92	0.881	0.038
		d _{zy}	0.955	0.091	0.864
	Fe	d _{zx}	0.962	0.089	0.873
		d _{x²-y²}	0.938	0.907	0.031
		d _{xy}	0.488	0.342	0.147

Catalyst	Ion	Orbital	Up	Down	Spin
FeHf-N ₆ C	Hf	d _{z²}	0.197	0.203	-0.006
		d _{zy}	0.189	0.184	0.004
	Fe	d _{zx}	0.185	0.186	-0.001
		d _{x²-y²}	0.23	0.251	-0.021
	FeHf-N ₆ C	d _{xy}	0.256	0.255	0
N ₆ C	N ₆ C	d _{z²}	0.921	0.905	0.016
		d _{zy}	0.943	0.091	0.852
	Fe	d _{zx}	0.964	0.067	0.897
		d _{x²-y²}	0.942	0.911	0.031
		d _{xy}	0.494	0.329	0.165

Catalyst	Ion	Orbital	Up	Down	Spin
FeV-N ₆ C	V	d _{z²}	0.195	0.06	0.135
		d _{zy}	0.753	0.096	0.656
	Fe	d _{zx}	0.915	0.07	0.845
		d _{x²-y²}	0.418	0.279	0.139
	FeV	d _{xy}	0.368	0.293	0.075
N ₆ C	N ₆ C	d _{z²}	0.928	0.933	-0.005
		d _{zy}	0.972	0.07	0.902
	Fe	d _{zx}	0.969	0.074	0.895
		d _{x²-y²}	0.894	0.904	-0.011
		d _{xy}	0.468	0.359	0.109

Catalyst	Ion	Orbital	Up	Down	Spin
FeMo-N ₆ C	Mo	d _{z²}	0.856	0.127	0.729
		d _{zy}	0.432	0.233	0.199
		d _{zx}	0.684	0.54	0.145
		d _{x²-y²}	0.498	0.452	0.046
		d _{xy}	0.395	0.369	0.025
FeFe-N ₆ C	Fe	d _{z²}	0.937	0.869	0.069
		d _{zy}	0.962	0.062	0.899
		d _{zx}	0.953	0.328	0.625
		d _{x²-y²}	0.883	0.816	0.068
		d _{xy}	0.465	0.346	0.118

Catalyst	Ion	Atom	Orbital	Up	Down	Spin
FeFe-N ₆ C	Fe	2	d _{z²}	0.931	0.047	0.884
			d _{zy}	0.933	0.929	0.005
			d _{zx}	0.942	0.875	0.067
			d _{x²-y²}	0.737	0.477	0.26
			d _{xy}	0.443	0.372	0.071
FeCo-N ₆ C	Fe	1	d _{z²}	0.935	0.938	-0.002
			d _{zy}	0.974	0.108	0.866
			d _{zx}	0.971	0.149	0.822
			d _{x²-y²}	0.805	0.82	-0.016
			d _{xy}	0.488	0.384	0.104

Catalyst	Ion	Orbital	Up	Down	Spin	
FeCo-N ₆ C	Co	2	d _{z²}	0.964	0.114	0.85
			d _{zy}	0.97	0.92	0.05
			d _{zx}	0.968	0.931	0.037
			d _{x²-y²}	0.99	0.834	0.156
			d _{xy}	0.471	0.406	0.065
FeCo-N ₆ C	Fe	1	d _{z²}	0.95	0.895	0.056
			d _{zy}	0.976	0.109	0.866
			d _{zx}	0.968	0.139	0.829
			d _{x²-y²}	0.99	0.562	0.428
			d _{xy}	0.485	0.403	0.082

Catalyst	Ion	Orbital	Up	Down	Spin
FeCu- N ₆ C	Cu	d _{z²}	0.984	0.985	0
		d _{z_y}	0.993	0.984	0.009
	Fe	d _{z_x}	0.987	0.984	0.004
		d _{x²-y²}	0.996	0.971	0.025
	N ₆ C	d _{x_y}	0.993	0.591	0.402
		d _{z²}	0.949	0.92	0.029
		d _{z_y}	0.971	0.114	0.857
	Fe	d _{z_x}	0.97	0.107	0.862
		d _{x²-y²}	0.989	0.54	0.449
		d _{x_y}	0.518	0.388	0.13

Table S3. Orbital Populations of metal active sites after adsorption of *CO by FeM-N₆C.

Catalyst	Ion	Orbital	Up	Down	Spin
Fe-N-C *CO(Fe)	Fe	d _{z²}	0.421	0.421	0
		d _{z_y}	0.847	0.847	0
		d _{z_x}	0.817	0.817	0
		d _{x²-y²}	0.975	0.975	0
		d _{x_y}	0.344	0.344	0

Catalyst	Ion	Orbital	Up	Down	Spin
FeSc- N ₆ C *CO(Fe)	Fe	d _{z²}	0.52	0.518	0.001
		d _{z_y}	0.824	0.823	0.001
		d _{z_x}	0.726	0.713	0.013
		d _{x²-y²}	0.93	0.928	0.002
		d _{x_y}	0.399	0.399	0

Catalyst	Ion	Orbital	Up	Down	Spin
FeY-N ₆ C *CO(Fe)	Fe	d _{z²}	0.639	0.454	0.185
		d _{z_y}	0.842	0.837	0.005
		d _{z_x}	0.864	0.667	0.197
		d _{x²-y²}	0.764	0.908	-0.145
		d _{x_y}	0.419	0.39	0.029

Catalyst	Ion	Orbital	Up	Down	Spin
FeTi-N ₆ C *CO(Fe)	Fe	d _{z²}	0.532	0.532	0
		d _{z_y}	0.823	0.823	0
		d _{z_x}	0.735	0.735	0
		d _{x²-y²}	0.891	0.891	0
		d _{x_y}	0.417	0.417	0

Catalyst	Ion	Orbital	Up	Down	Spin
FeZr-N ₆ C *CO(Fe)	Fe	d _{z²}	0.52	0.52	0
		d _{z_y}	0.835	0.835	0
		d _{z_x}	0.741	0.741	0
		d _{x²-y²}	0.9	0.9	0
		d _{x_y}	0.407	0.407	0

Catalyst	Ion	Orbital	Up	Down	Spin
FeHf- N ₆ C *CO(Fe)	Fe	d _{z²}	0.518	0.518	0
		d _{z_y}	0.828	0.828	0
		d _{z_x}	0.741	0.741	0
		d _{x²-y²}	0.908	0.908	0
		d _{x_y}	0.405	0.405	0

Catalyst	Ion	Orbital	Up	Down	Spin
FeV-N ₆ C *CO(V)	V	d _{z²}	0.259	0.22	0.04
		d _{zy}	0.646	0.122	0.524
		d _{zx}	0.574	0.53	0.044
		d _{x²-y²}	0.348	0.322	0.026
		d _{xy}	0.336	0.304	0.032

Catalyst	Ion	Orbital	Up	Down	Spin
FeMo- N ₆ C *CO(Mo)	Mo	d _{z²}	0.461	0.472	-0.011
		d _{zy}	0.549	0.593	-0.044
		d _{zx}	0.537	0.532	0.006
		d _{x²-y²}	0.426	0.473	-0.047
		d _{xy}	0.372	0.375	-0.002

Catalyst	Ion	Orbital	Up	Down	Spin
FeFe- N ₆ C *CO(Fe)	Fe	d _{z²}	0.603	0.456	0.147
		d _{zy}	0.859	0.831	0.028
		d _{zx}	0.835	0.685	0.15
		d _{x²-y²}	0.825	0.847	-0.022
		d _{xy}	0.399	0.399	0.001

Catalyst	Ion	Orbital	Up	Down	Spin
FeCo- N ₆ C *CO(Fe)	Fe	d _{z²}	0.82	0.248	0.572
		d _{zy}	0.895	0.853	0.042
		d _{zx}	0.881	0.781	0.1
		d _{x²-y²}	0.97	0.387	0.583
		d _{xy}	0.438	0.392	0.046

Catalyst	Ion	Orbital	Up	Down	Spin
FeCu- N ₆ C *CO(Fe)	Fe	d _{z²}	0.891	0.384	0.507
		d _{zy}	0.871	0.822	0.049
		d _{zx}	0.897	0.543	0.354
		d _{x²-y²}	0.979	0.392	0.587
		d _{xy}	0.459	0.386	0.073

Table S4 Hubbard U value test

Fe(FeCo-N ₆ C) without aqueous solvent layer	
Hubbard U (eV)	Energy (eV)
2	-11481.4085
2.5	-11481.4091
3	-11481.1429
3.5	-11480.9033

Table S5 Calculation data for E_{ads}(*CO)

Catalyst	E* (eV)	E* _{CO(Fe)} (eV)	E* _{CO(M)} (eV)
H ₂	-31.1850392		
CO	-594.083018		
Fe-N ₄ C	-15203.2525	-15800.9361	
FeSc-N ₆ C	-16372.9073	-16967.7628	
FeY-N ₆ C	-16172.6574	-16767.3274	
FeTi-N ₆ C	-16692.6075	-17287.4291	
FeZr-N ₆ C	-16392.3184	-16987.4195	
FeHf-N ₆ C	-22968.094	-23563.3161	
FeV-N ₆ C	-17049.3603	-17644.2186	-17644.2753
FeMo-N ₆ C	-17031.7814	-17626.7259	-17627.4129
FeFe-N ₆ C	-15959.8801	-16554.7662	-16554.5161
FeCo-N ₆ C	-16791.0328	-16791.5984	-16791.2373
FeCu-N ₆ C	-16777.4508	-17372.2989	-17371.1829

Table S6 Calculation data for $E_{\text{ads}}(^*\text{H})$

Catalyst	E^* (eV)	$E^*_{\text{H(Fe)}}$ (eV)	$E^*_{\text{H(M)}}$ (eV)	$E^*_{\text{H(N1)}}$ (eV)	$E^*_{\text{H(N2)}}$ (eV)	$E^*_{\text{H(N2)}}$ $(^*\text{H}_2\text{O} \rightarrow ^*\text{H}(\text{N2}) + ^*\text{OH})$
FeSc-N ₆ C	-16372.9073	-16388.1061		-16386.9852	-16388.5737	-16372.9254
FeY-N ₆ C	-16172.6574	-16187.79		-16187.01	-16188.33	-16172.5036
FeTi-N ₆ C	-16692.6075	-16708.1944		-16707.3504	-16707.8465	-16692.6077
FeZr-N ₆ C	-16392.3184	-16407.857		-16407.006	-16407.626	-16392.905
FeHf-N ₆ C	-22968.094	-22983.4976		-22982.6955	-22968.5167	-22968.5167
FeV-N ₆ C	-17049.3603	-17064.6079	-17064.7239	-17064.3497	-17064.7488	
FeMo-N ₆ C	-17031.7814	-17047.2806	-17048.0224	-17046.6895	-17047.0891	
FeFe-N ₆ C	-15959.8801	-15975.4126	-15975.3516	-15974.7435	-15975.626	
FeCo-N ₆ C	-16196.9809	-16212.3093	-16212.2815	-16211.7863	-16212.5583	
FeCu-N ₆ C	-16777.4508	-16792.8657	-16791.9672	-16792.3306	-16793.8899	

Table S7 Calculation data for $E_{\text{CO}+\text{H}}$ and E_{CHO}

Catalyst	Path	E_{CO} (eV)	$E_{\text{CO}+\text{H}}$ (eV)	E_{CHO} (eV)
FeSc-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-16967.7628	-16982.3269	-16983.4605
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-16967.7628	-16983.332	-16983.6956
	*CO+*H ₂ O(Sc)=*CO+*H(N2)+*OH(Sc)=*CHO+*OH(Sc)	-16967.7628	-16967.7335	-16967.4723
	*CO+*H ₂ O(Sc)=*CHO+*OH(Sc)	-16967.7628		-16966.8806
FeY-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-16767.3274	-16781.8907	-16782.8657
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-16767.3274	-16782.9996	-16782.8842
	*CO+*H ₂ O(Y)=*CO+*H(N2)+*OH(Y)=*CHO+*OH(Y)	-16767.3274	-16767.2575	-16766.9592
	*CO+*H ₂ O(Y)=*CHO+*OH(Y)	-16767.3274		-16766.4864
FeTi-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-17287.4291	-17302.0918	-17302.22
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-17287.4291	-17302.5976	-17302.8599
	*CO+*H ₂ O(Ti)=*CO+*H(N2)+*OH(Ti)=*CHO+*OH(Ti)	-17287.4291	-17287.2903	-17287.5108
	*CO+*H ₂ O(Ti)=*CHO+*OH(Ti)	-17287.4291		-17287.4764
FeZr-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-16987.4195	-17002.0384	-17003.0869
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-16987.4195	-17002.7397	-17003.3808
	*CO+*H ₂ O(Zr)=*CO+*H(N2)+*OH(Zr)=*CHO+*OH(Zr)	-16987.4195	-16987.286	-16987.77
	*CO+*H ₂ O(Zr)=*CHO+*OH(Zr)	-16987.4195		-16987.4062
FeHf-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-16987.4195	-17002.0384	-17003.0869
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-16987.4195	-17002.7397	-23579.2775
	*CO+*H ₂ O(Hf)=*CO+*H(N2)+*OH(Hf)=*CHO+*OH(Hf)	-16987.4195	-23563.2453	-23563.2196
	*CO+*H ₂ O(Hf)=*CHO+*OH(Hf)	-16987.4195		-23563.1589
FeV-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-17644.2753	-17658.9761	-17659.449
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-17644.2753	-17659.5432	-17659.3942
	*CO+H ⁺ +e-=*CO+*H(Fe)=*CHO	-17644.2753	-17659.4668	-17659.414
FeMo-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-17627.4129	-17642.0176	-17643.1212
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-17627.4129	-17642.2998	-17643.0177
	*CO+H ⁺ +e-=*CO+*H(Mo)=*CHO	-17627.4129	-17642.7174	-17643.2203
FeFe-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-16554.7662	-16568.9874	-16570.2532
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-16554.7662	-16570.4175	-16570.547
	*CO+H ⁺ +e-=*CO+*H(Fe2)=*CHO	-16554.7662	-16570.031	-16570.2281
FeCo-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-16791.5984	-16806.002	-16807.5837
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-16791.5984	-16807.3053	-16807.6062
	*CO+H ⁺ +e-=*CO+*H(Co)=*CHO	-16791.5984	-16807.0559	-16807.5862
FeCu-N ₆ C	*CO+H ⁺ +e-=*CO+*H(N1)=*CHO	-17372.2989	-17386.6752	-17388.3584
	*CO+H ⁺ +e-=*CO+*H(N2)=*CHO	-17372.2989	-17388.287	-17388.2737
	*CO+H ⁺ +e-=*CO+*H(Cu)=*CHO	-17372.2989	-17386.2548	-17388.2934

Notes and references:

1 Y. L. Wang, Y. Tian, Z. L. Lang, W. Guan and L. K. Yan, *J. Mater. Chem. A*, 2018, **6**, 21056–21063.