Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electrocatalytic Reduction of CO_2 on Size-Selected Nanoclusters of First-Row Transition Metal Nanoclusters: A Comprehensive Mechanistic Investigation

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Energy Corrections:

Gas-phase corrections:

The free energy of a gaseous molecule is calculated using the following expression:

$U(T) = ZPE + \Delta U_{0->T}$

$H(T) = U(T) + PV = ZPE + \Delta U_{0->T} + PV$

$G(T) = H(T) - TS = ZPE + \Delta U_{0->T} + PV - TS$

Zero-point energy (ZPE) and entropy corrections for various gaseous species computed at 298.15 K and 1 atm are given in Table S1. All the molecules were optimized using PBE functional.

Table S1: Zero-point energy (ZPE, eV) and entropy corrections (TS*, eV) for various gaseous species computed at 298K.

Molecule	ZPE	TS	H(T)	G(T)
H_2O	0.568	0.584	0.671	0.087
CH_3OH	1.354	0.739	1.472	0.733
HCOOH	0.887	0.769	1.000	0.231
H_2	0.269	0.403	0.359	-0.044
CO	0.132	0.611	0.222	-0.389
CO_2	0.307	0.662	0.405	-0.258
CH_4	1.182	0.576	1.286	0.711

Gas-phase thermochemical reaction energies computed with PBE functional are inconsistent with experimental results. To accurately quantify these inconsistencies, we have compared the reaction enthalpies (ΔH_{PBE}) with the experimental reference reaction enthalpies (ΔH_{ref}) taken from the NIST database[1] for a dataset of nine reaction enthalpies that involve CO_2 and CO molecules. We have found an average error of +0.06 eV and -0.41 eV for reactions that involve CO_2 and CO respectively, and these corrections were added to the DFT energy values of CO_2 and CO. It can be seen that the errors of these nine reaction enthalpies reduced considerably after adding energy corrections to CO_2 and CO.

Table S2: Comparison of nine reaction enthalpies (eV) for reactions involving CO and CO_2: ΔH_{ref}, based on NIST database values; ΔH_{PBE}, computed DFT values using PBE functional without any corrections; ΔH_{corr}, DFT values corrected by adding energy corrections of +0.06 eV for CO_2 and -0.41 eV for CO.

Reaction	ΔH_{ref}	ΔH_{PBE}	$\Delta H_{PBE} - \Delta H_{ref}$	ΔH_{corr}	$\Delta H_{corr} - \Delta H_{ref}$
$CO_2 + H_2 \rightarrow CO + H_2O$	0.43	0.86	0.43	0.39	-0.04
$4H_2 + CO_2 \rightarrow CH_4 + H_2O$	-1.71	-1.66	0.05	-1.72	-0.01
$3H_2 + CO \rightarrow CH + H_2O$	-2.14	-2.52	-0.38	-2.11	0.03
$CO_2 + H_2 \rightarrow HCOOH$	0.15	0.07	-0.08	0.01	-0.14
$CO + H_2O \rightarrow HCOOH$	-0.27	-0.79	-0.51	-0.38	-0.10
$3H_2 + CO_2 \rightarrow CH_3OH + H_2O$	-0.55	-0.52	0.04	-0.58	-0.02
$2H_2 + CO \rightarrow CH_3OH$	-0.98	-1.38	-0.40	-0.97	0.01
$3H_2 + CO_2 \rightarrow 1/2C_2H_4 + 2H_2O$	-0.66	-0.57	0.09	-0.63	0.03
$2H_2 + CO \rightarrow ½\ C_2H_4 + H_2O$	-1.09	1.43	-0.35	-1.03	0.06

Liquid-phase corrections:

CO_2 electron reduction reaction results in the release of **H_2O**, HCOOH, and CH_3OH which are formed in the liquid-phase. As it is difficult to calculate the liquid-phase free energies for H_2O, HCOOH, and CH_3OH with the DFT method, we applied an empirical correction based on the free energy difference between the formations of liquid and gas phases using the NIST database values. Based on this, liquid free energy corrections of -0.09 eV ad -0.12 eV were applied to **H_2O** and HCOOH respectively.

Table S3: Empirical liquid-phase free energy corrections (eV) from the free energy difference between the formations of liquid and gas phases using the NIST database values.

	$\Delta_f G°$(l)/kJ mol^{-1}	$\Delta_f G°$(g)/kJ mol^{-2}	ΔfG°(l) eV	ΔfG°(g) eV	Difference
H_2O	-237.126	-228.5457418	-2.4576	-2.3687	-0.0889
CH_3OH	-166.148	-166.3493248	-1.7220	-1.7241	0.0021
HCOOH	-362.589	-350.9525505	-3.7579	-3.6373	-0.1206

Solvent Corrections:

We have used an empirical solvent correction based on previously reported literature values. An empirical solvation correction of -0.5 eV was applied to OH* species and for hydroxyl species that are indirectly bound to the nanocluster surface through other atoms such as COH* and COOH*, a solvent correction of -0.38 eV was applied. For other species that contain C-O bonds, a correction of -0.1 eV was applied.[2,3]

Table S4: Coefficient of determination (R^2) for the linear free energy scaling relationship between the adsorption energies of CO_2*, O* and C* with other CO_2RR adsorbates.

CO_2*	CHO*	0.93	O	CH_2O*	0.92	C	CH*	0.85
CO_2*	CH_2O*	0.92	O	OH*	0.91	C	CH_2O*	0.82
CO_2*	OOCH*	0.91	O	CHO*	0.90	C	COH*	0.82
CO_2*	COOH*	0.91	O	CH_3O*	0.90	C	CHOH*	0.82
CO_2*	O*	0.89	O	CO_2*	0.89	C	CO*	0.80
CO_2*	CO*	0.85	O	CH_2*	0.84	C	CHO*	0.80
CO_2*	CH_3O*	0.85	O	OOCH*	0.84	C	CO_2*	0.80
CO_2*	OH*	0.85	O	COOH*	0.83	C	CH_2*	0.79
CO_2*	CH_2*	0.82	O	CHOH*	0.78	C	COOH*	0.76
CO_2*	CHOH	0.82	O	C*	0.75	C	O*	0.75
CO_2*	C*	0.80	O	CH*	0.75	C	CH_3O*	0.72
CO_2*	CH*	0.71	O	CO*	0.68	C	OOCH*	0.72
CO_2*	CH_2OH*	0.63	O	COH*	0.66	C	OH*	0.71
CO_2*	COH*	0.62	O	CH_2OH*	0.66	C	CH_2OH*	0.62
CO_2*	CH_3*	0.38	O	CH_3*	0.40	C	H*	0.45
CO_2*	H*	0.35	O	H*	0.35	C	CH_3*	0.39

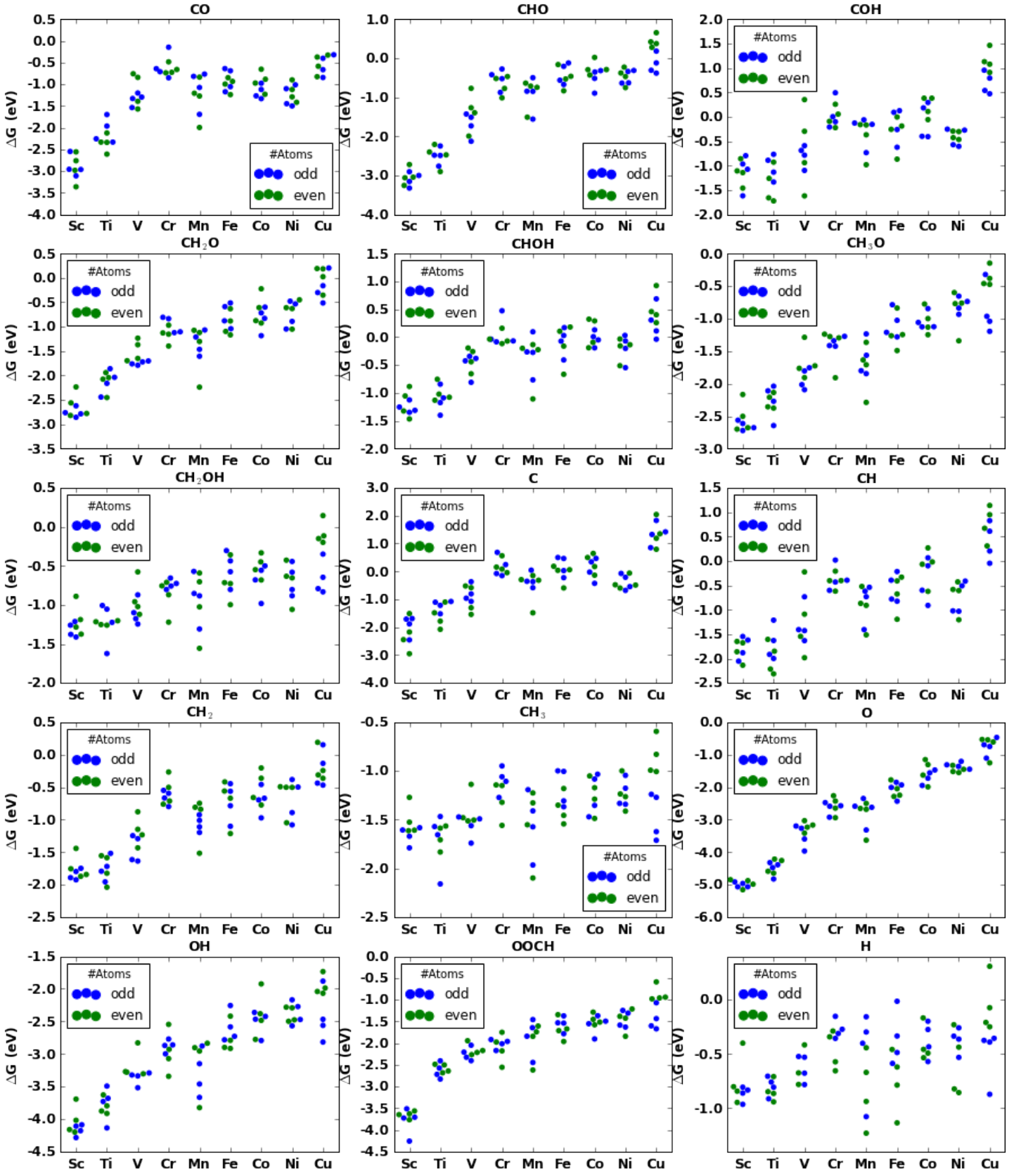

Figure S1: Adsorption free energies (ΔG, eV) of various adsorbates on first-row transition metal nanoclusters.

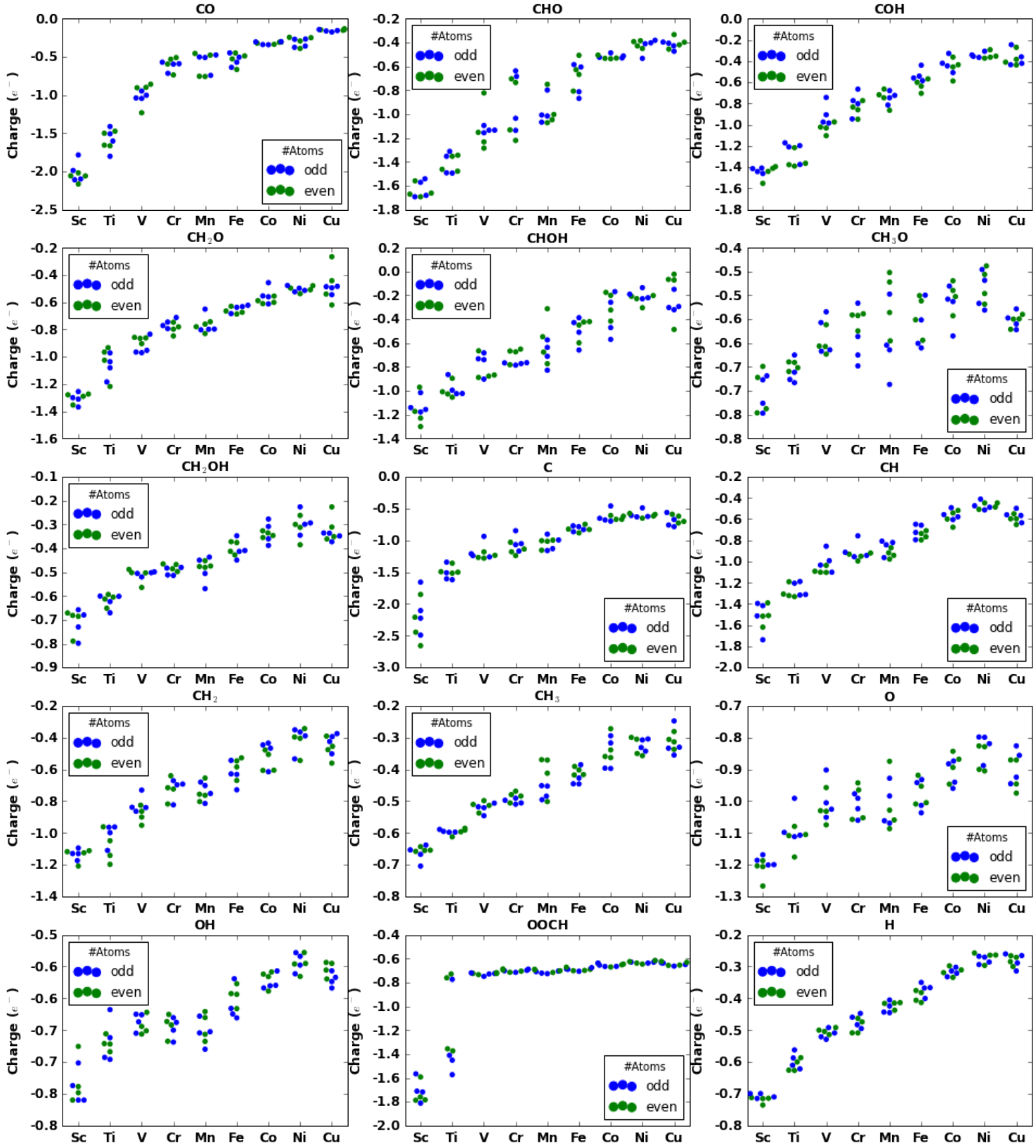

Figure S2: Residual changes (e^-) on various adsorbed species on binding with first-row transition metal nanoclusters.

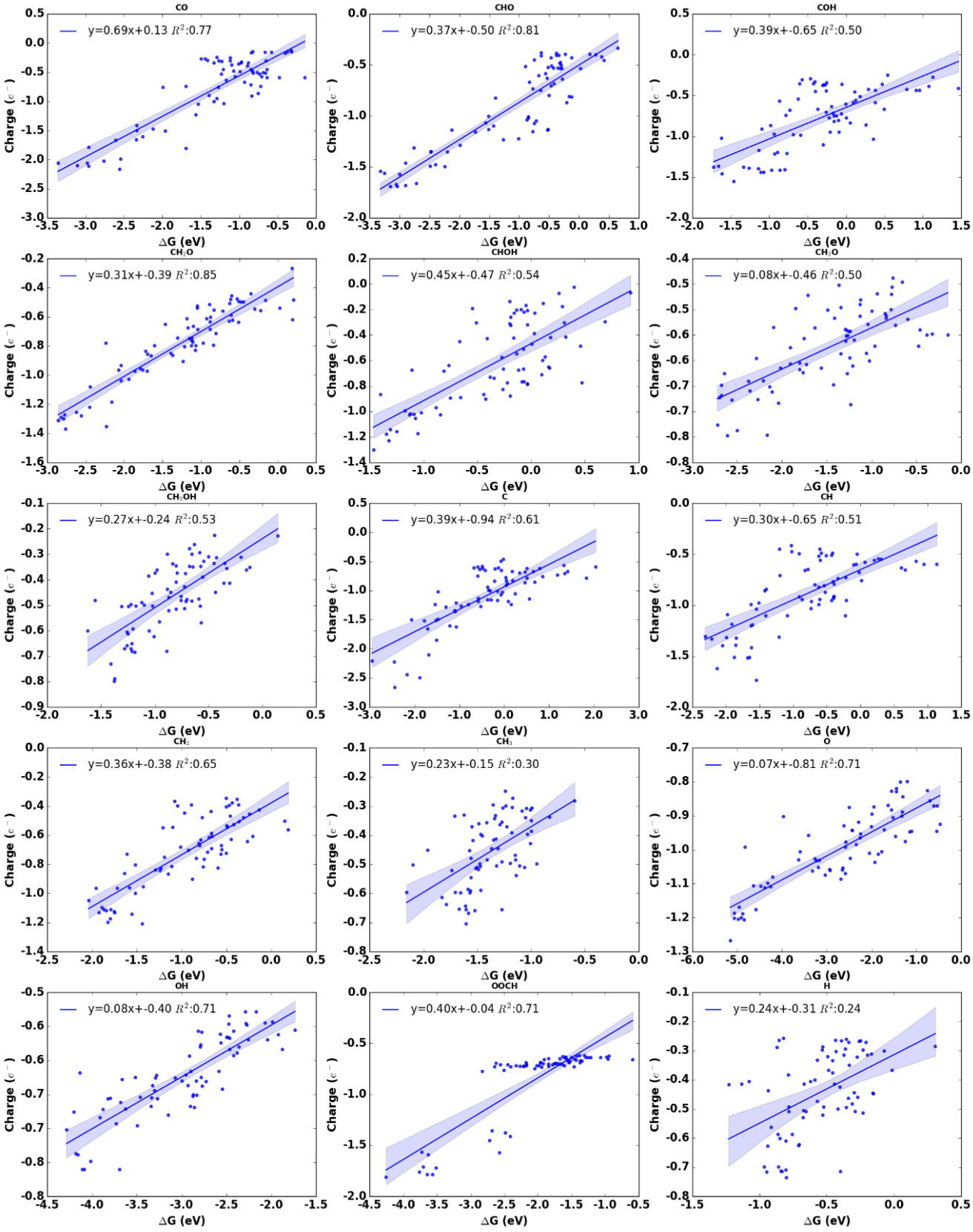

Figure S3: Correlation between residual charges (e^-) on adsorbates and adsorption free energies (eV) for various adsorbates.

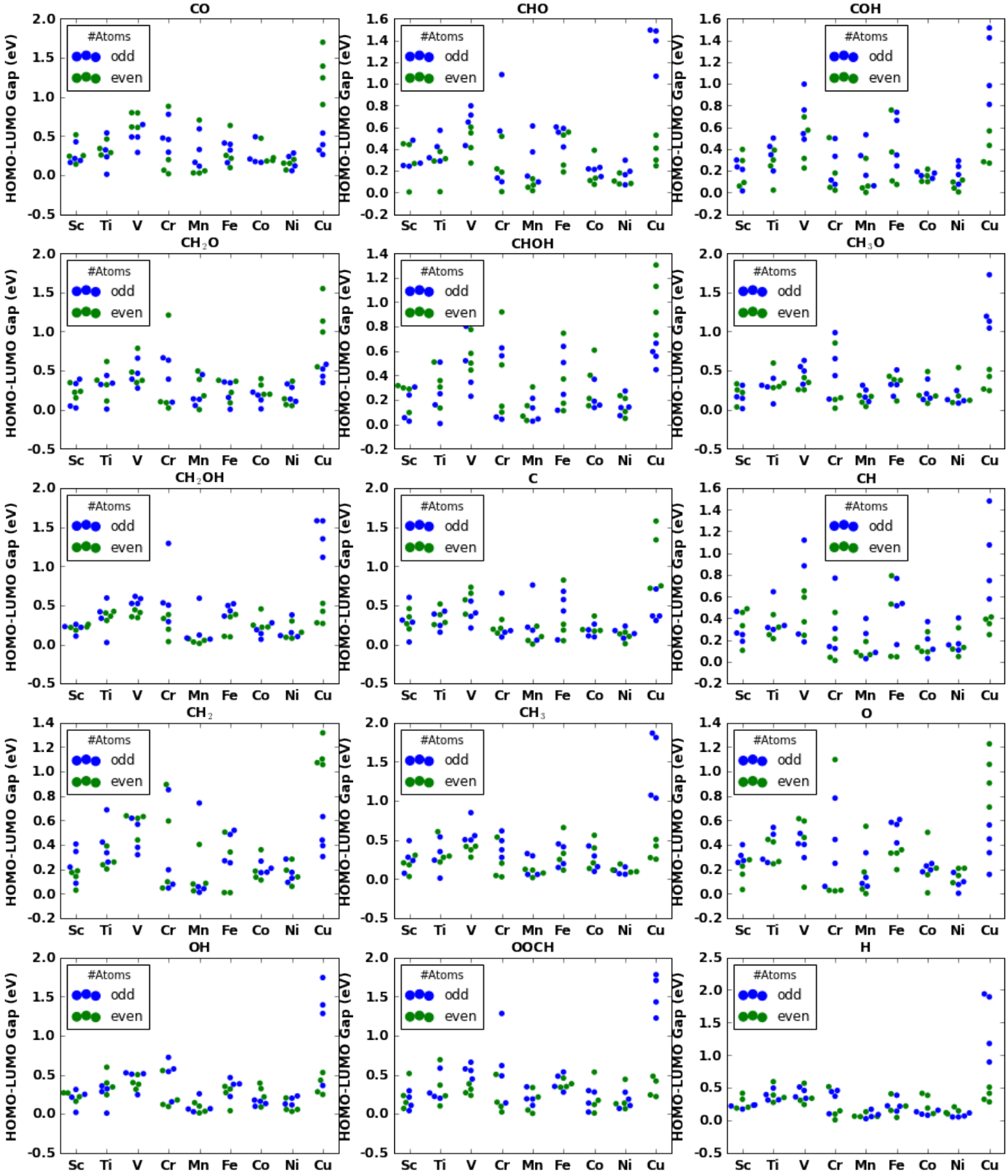

Figure S4: HOMO-LUMO gaps (eV) of various adsorbates bound on first-row transition metal nanoclusters.

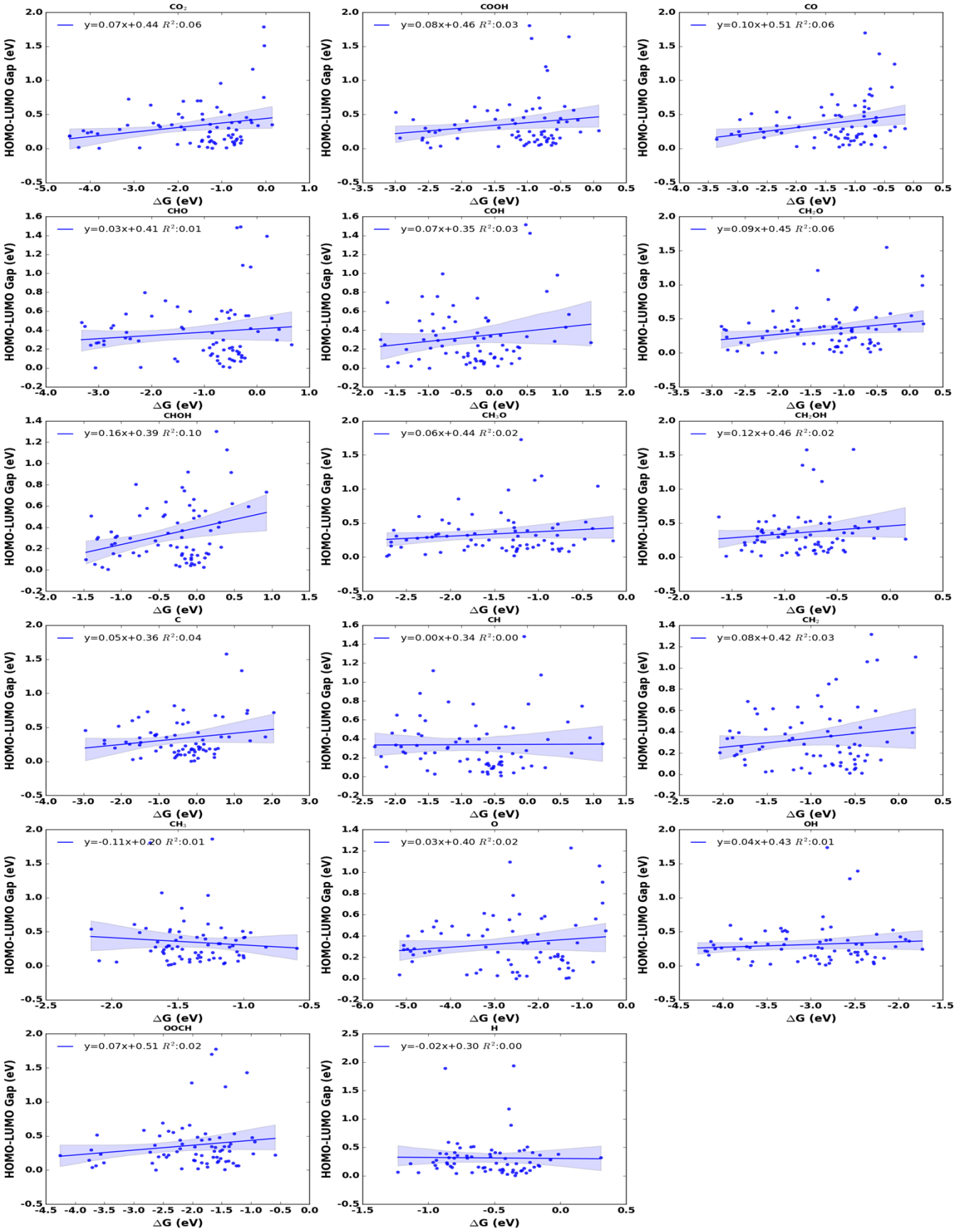

Figure S5: correlation between HOMO-LUMO gaps (eV) and adsorption free energies (eV) for various adsorbates.

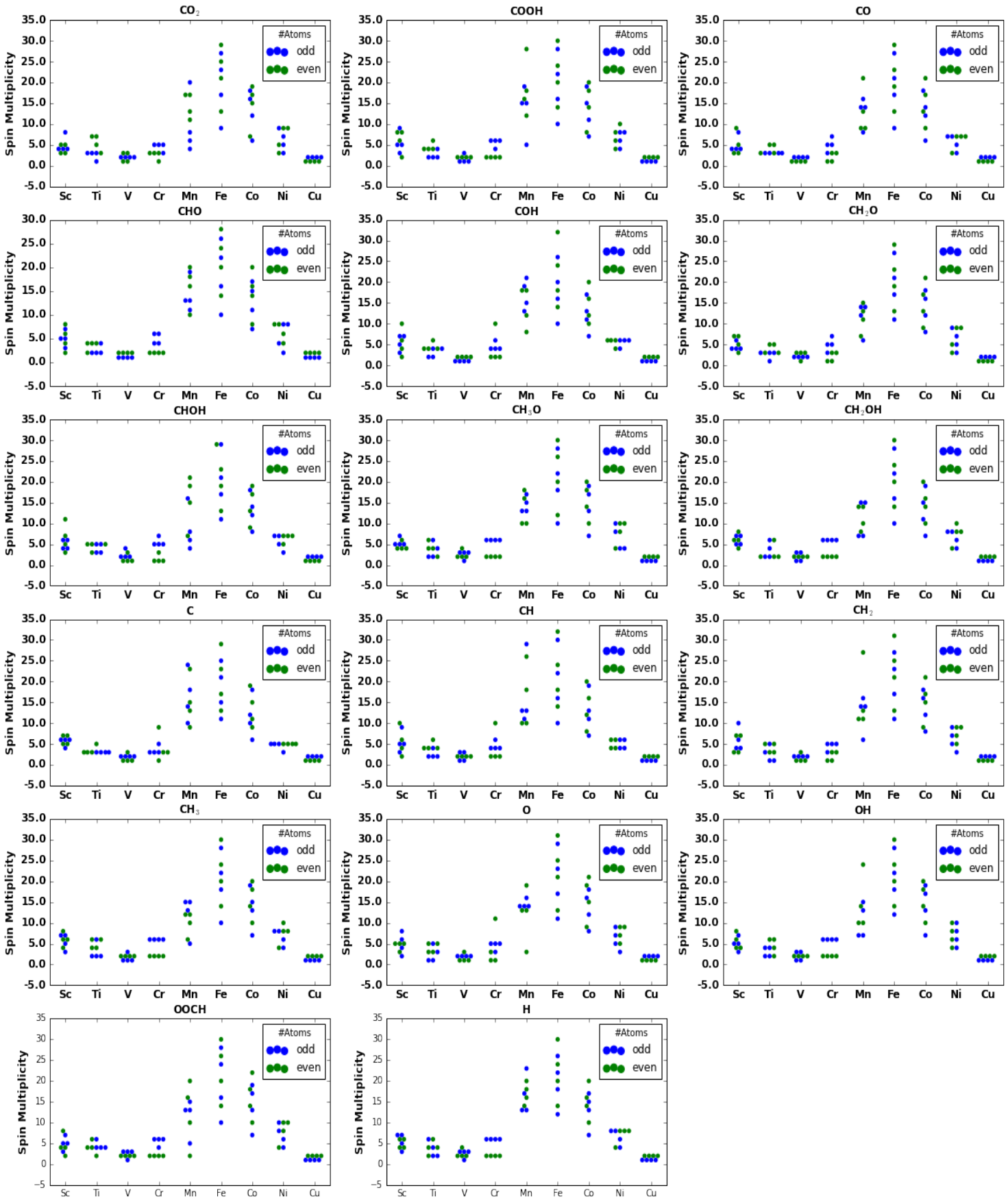

Figure S6: Spin multiplicities of various adsorbates bound on first-row transition metal nanoclusters.

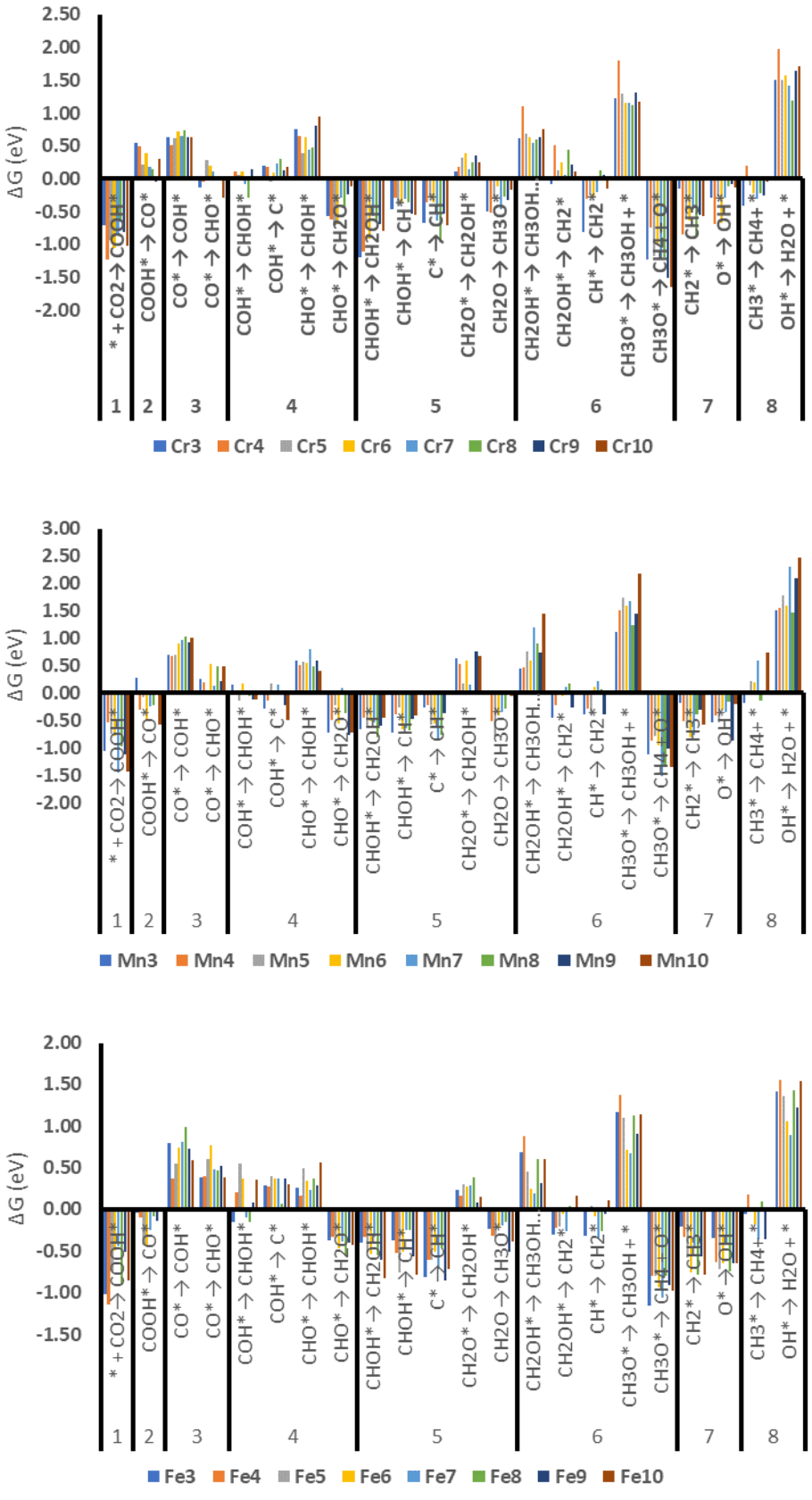

Figure S7: Free energy changes (eV) for various electrochemical steps in the CO_2RR process on Cr, Mn and Fe clusters. Step numbers 1-8 show the total number of (H^+ + e^-) pairs transferred.

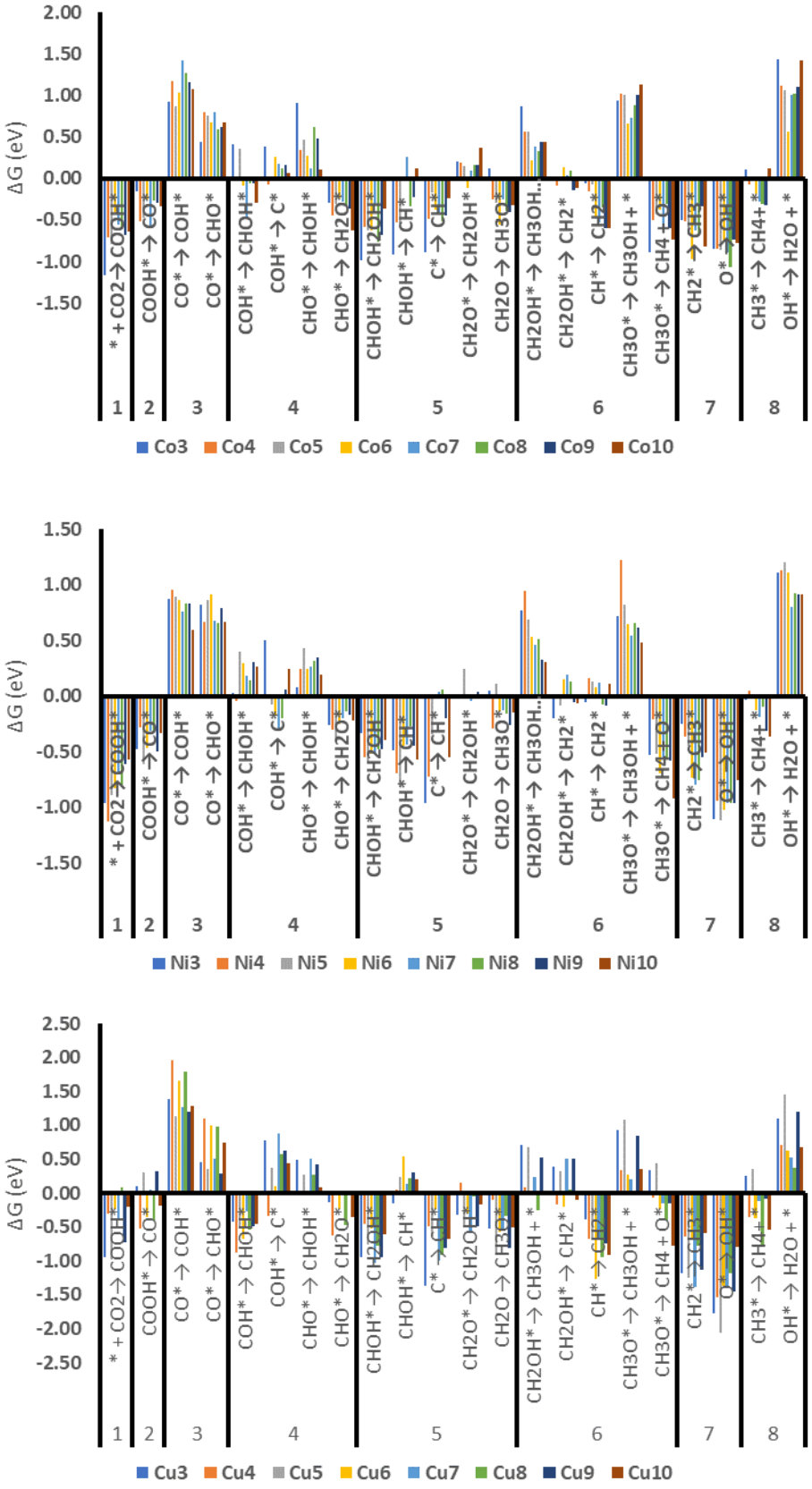

Figure S8: Free energy changes (eV) for various electrochemical steps in the CO_2RR process on Co, Ni and Cu clusters. Step numbers 1-8 show the total number of ($H^+ + e^-$) pairs transferred.

Table S5: Adsorption free energies (ΔG, eV) of CO_2RR adsorbates on various first-row transition metal nanoclusters (Sc_n-Cu_n; n = 3-10)

Adsorb	Sc3	Sc4	Sc5	Sc6	Sc7	Sc8	Sc9	Sc10	Ti3	Ti4	Ti5	Ti6	Ti7	Ti8	Ti9	Ti10	V3	V4	V5	V6	V7	V8	V9	V10
CO_2	-3.83	-3.79	-4.46	-3.97	-4.25	-4.05	-4.15	-4.46	-3.12	-2.62	-2.40	-2.56	-2.43	-2.87	-3.14	-3.33	-1.88	-1.48	-2.14	-1.93	-1.90	-1.98	-1.85	-1.55
H	-0.81	-0.80	-0.86	-0.40	-0.83	-0.84	-0.96	-0.95	-0.91	-0.85	-0.76	-0.86	-0.71	-0.71	-0.81	-0.94	-0.52	-0.42	-0.78	-0.78	-0.53	-0.68	-0.68	-0.23
COOH	-3.00	-2.73	-2.49	-2.55	-2.40	-2.59	-2.93	-2.47	-2.60	-2.03	-2.06	-2.10	-1.92	-2.34	-2.32	-2.51	-1.23	-1.18	-1.60	-1.80	-1.28	-1.49	-1.46	-0.75
OOCH	-3.73	-3.63	-3.51	-3.56	-3.71	-3.65	-4.26	-3.77	-2.83	-2.50	-2.41	-2.68	-2.58	-2.49	-2.72	-2.64	-2.05	-2.22	-2.33	-2.17	-2.21	-2.27	-2.41	-1.95
CO	-2.96	-2.76	-2.55	-2.56	-2.96	-2.98	-3.11	-3.36	-2.33	-2.12	-1.96	-2.33	-1.70	-2.34	-2.26	-2.61	-1.30	-0.84	-1.54	-1.57	-1.33	-1.39	-1.20	-0.76
COHOH	-0.88	-0.65	-0.84	-0.63	-0.67	-0.85	-0.84	-0.89	-0.64	-0.43	-0.46	-0.64	-0.59	-0.60	-0.72	-0.64	-0.14	0.09	-0.37	-0.08	-0.02	-0.04	-0.07	0.15
CHO	-3.33	-3.26	-3.00	-2.72	-2.91	-3.05	-3.16	-3.06	-2.76	-2.47	-2.48	-2.40	-2.25	-2.21	-2.49	-2.90	-1.51	-1.27	-2.13	-1.99	-1.73	-1.40	-1.43	-0.77
COH	-1.62	-1.14	-0.97	-0.86	-0.80	-1.11	-1.07	-1.46	-1.13	-0.93	-0.89	-1.72	-0.77	-1.26	-1.34	-1.66	-0.79	-0.94	-1.10	-1.62	-0.69	-0.30	-0.59	0.35
CH_2O	-2.86	-2.82	-2.79	-2.23	-2.62	-2.56	-2.76	-2.78	-2.44	-2.08	-1.86	-1.94	-2.04	-2.04	-2.16	-2.45	-1.72	-1.37	-1.79	-1.70	-1.76	-1.65	-1.70	-1.23
C	-1.71	-1.51	-1.69	-2.45	-1.88	-2.17	-2.46	-2.95	-1.11	-1.10	-1.22	-2.08	-1.08	-1.48	-1.52	-1.78	-0.37	-0.58	-1.07	-1.54	-0.81	-1.30	-0.96	-0.52
CHOH	-1.13	-0.88	-1.31	-1.05	-1.25	-1.32	-1.35	-1.47	-1.40	-0.75	-0.84	-1.13	-1.09	-1.08	-1.17	-1.02	-0.81	-0.26	-0.34	-0.66	-0.42	-0.44	-0.38	-0.20
CH_3O	-2.68	-2.68	-2.61	-2.17	-2.56	-2.50	-2.72	-2.70	-2.64	-2.36	-2.11	-2.21	-2.04	-2.14	-2.27	-2.38	-1.76	-1.73	-2.02	-1.77	-1.81	-1.91	-2.09	-1.29
CH	-2.05	-1.86	-1.62	-1.65	-1.55	-1.68	-1.88	-2.14	-1.91	-1.61	-1.63	-2.31	-1.21	-1.85	-2.00	-2.22	-1.43	-1.55	-1.63	-1.98	-0.73	-1.09	-1.41	-0.22
CH_2OH	-1.41	-1.28	-1.26	-0.89	-1.21	-1.19	-1.38	-1.37	-1.62	-1.25	-1.05	-1.22	-1.01	-1.20	-1.22	-1.26	-0.87	-1.02	-1.25	-0.96	-1.10	-1.12	-1.18	-0.58
O	-4.96	-4.88	-5.06	-4.84	-4.91	-4.98	-5.06	-5.15	-4.82	-4.21	-4.32	-4.64	-4.39	-4.26	-4.47	-4.59	-3.97	-3.23	-3.60	-3.41	-3.27	-3.17	-3.20	-3.03
CH_2	-1.89	-1.84	-1.92	-1.44	-1.75	-1.76	-1.80	-1.87	-1.96	-1.59	-1.72	-1.82	-1.52	-1.55	-1.79	-2.04	-1.61	-1.23	-1.64	-1.43	-1.25	-1.15	-1.29	-0.88
OH	-4.29	-4.20	-4.11	-3.69	-4.09	-4.02	-4.18	-4.16	-4.14	-3.91	-3.68	-3.80	-3.49	-3.63	-3.73	-3.88	-3.34	-3.27	-3.52	-3.28	-3.29	-3.31	-3.32	-2.83
CH_3	-1.79	-1.61	-1.67	-1.27	-1.58	-1.53	-1.61	-1.61	-2.16	-1.83	-1.57	-1.59	-1.47	-1.57	-1.65	-1.71	-1.47	-1.50	-1.74	-1.48	-1.49	-1.51	-1.56	-1.14

Adsorb	Cr3	Cr4	Cr5	Cr6	Cr7	Cr8	Cr9	Cr10	Mn3	Mn4	Mn5	Mn6	Mn7	Mn8	Mn9	Mn10	Fe3	Fe4	Fe5	Fe6	Fe7	Fe8	Fe9	Fe10
CO_2	-1.03	-1.44	-1.26	-1.02	-1.33	-0.95	-1.27	-1.28	-1.44	-0.83	-1.45	-1.52	-1.72	-1.22	-1.45	-2.01	-1.11	-1.24	-0.89	-0.58	-0.60	-1.15	-0.78	-0.85
H	-0.15	-0.66	-0.27	-0.34	-0.31	-0.57	-0.36	-0.29	-0.16	-0.94	-0.30	-0.44	-1.08	-0.67	-0.40	-1.23	-0.49	-1.14	-0.59	-0.46	-0.34	-0.79	-0.01	-0.62
COOH	-0.70	-1.22	-0.93	-1.05	-0.82	-0.63	-0.81	-1.02	-1.05	-0.53	-0.74	-0.79	-1.44	-0.98	-1.11	-1.43	-1.02	-1.15	-0.74	-0.50	-0.44	-0.91	-0.50	-0.85
OOCH	-2.02	-2.56	-2.17	-2.18	-1.92	-1.98	-1.96	-1.75	-1.46	-1.61	-1.65	-1.84	-2.45	-1.74	-1.84	-2.62	-1.78	-1.96	-1.54	-1.35	-1.37	-1.71	-1.53	-1.67
CO	-0.15	-0.74	-0.71	-0.66	-0.64	-0.48	-0.85	-0.72	-0.77	-0.83	-0.82	-1.27	-1.69	-1.21	-1.07	-2.00	-1.06	-1.24	-1.17	-0.93	-0.69	-0.99	-0.64	-0.85
COHOH	0.67	0.14	0.44	0.57	0.48	0.82	0.37	0.30	0.19	0.18	0.18	0.01	-0.60	-0.02	-0.11	-0.42	0.02	-0.19	0.03	0.27	0.36	-0.09	0.36	0.39
CHO	-0.28	-0.77	-0.42	-0.47	-0.52	-0.52	-0.88	-1.01	-0.50	-0.64	-0.84	-0.75	-1.56	-0.71	-0.85	-1.51	-0.67	-0.83	-0.56	-0.16	-0.21	-0.53	-0.12	-0.46
COH	0.49	-0.22	-0.10	0.06	0.00	0.26	-0.21	-0.09	-0.06	-0.16	-0.13	-0.37	-0.73	-0.17	-0.15	-0.98	-0.26	-0.87	-0.62	-0.19	0.13	0.00	0.09	-0.26
CH_2O	-0.84	-1.40	-1.12	-1.15	-0.81	-0.97	-1.10	-1.13	-1.21	-1.12	-1.07	-1.30	-1.46	-1.07	-1.61	-2.24	-1.04	-1.17	-0.88	-0.63	-0.59	-1.10	-0.51	-0.88
C	0.68	-0.04	-0.15	0.15	0.24	0.56	-0.08	0.08	-0.35	-0.29	0.05	-0.32	-0.58	-0.15	-0.37	-1.48	0.03	-0.59	-0.22	0.18	0.50	0.06	0.46	0.04
CHOH	0.47	-0.12	-0.04	0.16	-0.08	-0.04	-0.07	-0.07	0.10	-0.13	-0.27	-0.20	-0.77	-0.22	-0.26	-1.11	-0.41	-0.67	-0.07	0.18	0.03	-0.16	0.17	0.11
CH_3O	-1.34	-1.91	-1.42	-1.28	-1.27	-1.24	-1.43	-1.30	-1.24	-1.64	-1.85	-1.71	-1.80	-1.37	-1.56	-2.29	-1.28	-1.49	-1.21	-0.84	-0.79	-1.25	-1.03	-1.26
CH	0.02	-0.40	-0.43	-0.21	-0.39	-0.40	-0.60	-0.62	-0.62	-0.52	-0.54	-0.87	-1.41	-0.91	-0.73	-1.51	-0.78	-1.19	-0.82	-0.33	-0.22	-0.41	-0.39	-0.68
CH_2OH	-0.73	-1.22	-0.80	-0.76	-0.66	-0.71	-0.76	-0.87	-0.57	-0.59	-0.88	-0.70	-1.31	-1.03	-0.85	-1.56	-0.80	-1.00	-0.58	-0.36	-0.30	-0.72	-0.44	-0.73
O	-2.57	-2.65	-2.59	-2.26	-2.48	-2.43	-2.93	-2.94	-2.35	-2.50	-2.62	-2.66	-3.32	-2.68	-2.59	-3.63	-2.43	-2.29	-2.01	-1.78	-1.85	-2.05	-1.93	-2.25
CH_2	-0.80	-0.71	-0.67	-0.50	-0.60	-0.27	-0.55	-0.76	-1.01	-0.81	-0.93	-0.75	-1.20	-0.84	-1.11	-1.52	-1.10	-1.21	-0.79	-0.42	-0.56	-0.67	-0.45	-0.56
OH	-2.87	-3.34	-2.86	-2.93	-2.77	-2.55	-3.00	-3.07	-2.88	-2.90	-3.15	-2.96	-3.67	-2.84	-3.46	-3.83	-2.78	-2.92	-2.73	-2.42	-2.26	-2.79	-2.58	-2.90
CH_3	-0.95	-1.56	-1.27	-1.14	-1.06	-1.15	-1.11	-1.32	-1.19	-1.33	-1.57	-1.55	-1.96	-1.23	-1.41	-2.10	-1.31	-1.54	-1.37	-1.18	-1.00	-1.46	-1.01	-1.35

Adsorb	Co3	Co4	Co5	Co6	Co7	Co8	Co9	Co10	Ni3	Ni4	Ni5	Ni6	Ni7	Ni8	Ni9	Ni10	Cu3	Cu4	Cu5	Cu6	Cu7	Cu8	Cu9	Cu10
CO_2	-1.31	-0.78	-0.75	-0.32	-0.75	-0.67	-0.85	-0.68	-1.19	-1.28	-1.11	-0.72	-0.65	-0.72	-0.55	-0.57	-0.44	-0.30	-0.35	-0.05	0.14	-0.03	-0.18	-0.05
H	-0.57	-0.49	-0.43	-0.54	-0.27	-0.17	-0.20	-0.46	-0.36	-0.86	-0.53	-0.82	-0.34	-0.44	-0.26	-0.23	-0.38	-0.25	-0.87	-0.21	-0.36	0.31	-0.39	-0.07
COOH	-1.17	-0.71	-0.79	-0.40	-0.55	-0.61	-0.68	-0.64	-0.97	-1.13	-0.89	-0.82	-0.70	-0.79	-0.61	-0.57	-0.94	-0.30	-0.97	-0.24	-0.37	0.08	-0.72	-0.19
OOCH	-1.91	-1.58	-1.50	-1.29	-1.37	-1.52	-1.55	-1.45	-1.63	-1.84	-1.59	-1.38	-1.31	-1.43	-1.25	-1.21	-1.67	-0.98	-1.60	-0.94	-1.07	-0.59	-1.44	-0.96
CO	-1.33	-1.23	-1.27	-0.65	-1.12	-0.88	-0.98	-0.97	-1.45	-1.42	-1.50	-1.29	-1.01	-1.12	-1.10	-0.90	-0.84	-0.82	-0.66	-0.58	-0.32	-0.33	-0.40	-0.37
COHOH	-0.22	-0.17	-0.20	0.30	0.16	0.28	0.11	0.16	-0.26	-0.27	-0.40	-0.24	-0.29	-0.06	-0.01	0.18	-0.03	0.02	0.18	0.20	0.55	0.53	0.41	0.47
CHO	-0.89	-0.43	-0.52	0.02	-0.32	-0.29	-0.35	-0.29	-0.63	-0.75	-0.64	-0.38	-0.34	-0.47	-0.31	-0.23	-0.38	0.28	-0.31	0.42	0.18	0.65	-0.12	0.37
COH	-0.41	-0.06	-0.40	0.38	0.29	0.38	0.18	0.11	-0.57	-0.46	-0.61	-0.43	-0.25	-0.29	-0.27	-0.30	0.54	1.13	0.47	1.08	0.95	1.46	0.79	0.91
CH_2O	-1.18	-0.88	-0.83	-0.22	-0.60	-0.61	-0.72	-0.92	-0.89	-1.05	-1.05	-0.63	-0.53	-0.61	-0.48	-0.45	-0.51	-0.35	-0.30	0.19	0.20	0.19	-0.16	0.02
C	-0.02	-0.14	-0.43	0.64	0.47	0.50	0.34	0.17	-0.07	-0.48	-0.68	-0.60	-0.54	-0.49	-0.21	-0.06	1.33	0.79	0.85	1.19	1.83	2.04	1.42	1.35
CHOH	0.01	-0.09	-0.05	0.29	-0.19	0.32	0.13	-0.19	-0.55	-0.51	-0.20	-0.14	-0.07	-0.16	0.03	-0.03	0.11	0.26	-0.04	0.40	0.69	0.92	0.31	0.46
CH_3O	-1.06	-1.13	-1.13	-0.78	-0.85	-1.00	-1.13	-1.25	-0.84	-1.34	-0.94	-0.76	-0.66	-0.77	-0.74	-0.60	-1.04	-0.46	-1.20	-0.38	-0.32	-0.15	-0.97	-0.47
CH	-0.91	-0.62	-0.60	0.27	0.06	-0.02	-0.10	-0.07	-1.03	-1.20	-1.02	-0.58	-0.51	-0.43	-0.41	-0.61	-0.05	0.31	0.20	0.95	0.83	1.14	0.61	0.67
CH_2OH	-0.98	-0.68	-0.68	-0.33	-0.50	-0.45	-0.56	-0.55	-0.88	-1.06	-0.80	-0.65	-0.58	-0.63	-0.44	-0.43	-0.83	-0.20	-0.79	-0.12	-0.35	0.14	-0.65	-0.15
O	-1.95	-1.63	-1.56	-1.15	-1.48	-1.31	-1.73	-1.99	-1.36	-1.55	-1.45	-1.45	-1.21	-1.33	-1.31	-1.52	-0.70	-0.54	-0.75	-0.61	-0.47	-0.55	-1.11	-1.25
CH_2	-0.97	-0.78	-0.67	-0.21	-0.46	-0.36	-0.70	-0.66	-1.08	-1.05	-0.89	-0.50	-0.38	-0.50	-0.50	-0.49	-0.44	-0.36	-0.47	-0.31	0.15	0.19	-0.14	-0.25
OH	-2.79	-2.49	-2.42	-1.92	-2.36	-2.38	-2.47	-2.78	-2.47	-2.50	-2.57	-2.48	-2.17	-2.29	-2.27	-2.28	-2.47	-2.07	-2.82	-1.99	-1.88	-1.74	-2.56	-2.04
CH_3	-1.47	-1.29	-1.35	-1.17	-1.08	-1.05	-1.03	-1.49	-1.33	-1.41	-1.34	-1.24	-1.18	-1.26	-1.05	-1.00	-1.62	-1.01	-1.71	-0.99	-1.24	-0.60	-1.27	-0.83

Table S6: Potential-determining step (PDS) and the free energy change of PDS for different CHO* and COH* mediated reaction pathways on all nanoclusters. The PDS step in the red color indicates the lowest energy reaction pathway among all the reaction pathways. Although it seems like many reaction pathways have similar PDS values, there are intermediate steps that will decide the overall lowest energy reaction route.

	CHO Path I	RDS	CHO Path II	RDS	CHO Path III	RDS	CHO Path IV	RDS	COH Path V	RDS	COH Path VI	RDS	COH Path VII	RDS
Sc3	2.92	OH* → H_2O + *	1.45	CH_2O* → CH_2OH*	2.20	CHO* → CHOH*	2.20	CHO* → CHOH*	1.34	CO* → COH*	1.34	CO* → COH*	1.34	CO* → COH*
Sc4	2.84	OH* → H_2O + *	1.53	CH_2O* → CH_2OH*	2.37	CHO* → CHOH*	2.37	CHO* → CHOH*	1.62	CO* → COH*	1.62	CO* → COH*	1.62	CO* → COH*
Sc5	2.75	OH* → H_2O + *	1.53	CH_2O* → CH_2OH*	1.69	CHO* → CHOH*	1.69	CHO* → CHOH*	1.58	CO* → COH*	1.58	CO* → COH*	1.58	CO* → COH*
Sc6	2.33	OH* → H_2O + *	1.34	CH_2O* → CH_2OH*	1.67	CHO* → CHOH*	1.67	CHO* → CHOH*	1.70	CO* → COH*	1.70	CO* → COH*	1.70	CO* → COH*
Sc7	2.73	OH* → H_2O + *	1.41	CH_2O* → CH_2OH*	1.65	CHO* → CHOH*	1.65	CHO* → CHOH*	2.17	CO* → COH*	2.17	CO* → COH*	2.17	CO* → COH*
Sc8	2.66	OH* → H_2O + *	1.37	CH_2O* → CH_2OH*	1.72	CHO* → CHOH*	1.72	CHO* → CHOH*	1.88	CO* → COH*	1.88	CO* → COH*	1.88	CO* → COH*
Sc9	2.82	OH* → H_2O + *	1.38	CH_2O* → CH_2OH*	1.81	CHO* → CHOH*	1.81	CHO* → CHOH*	2.04	CO* → COH*	2.04	CO* → COH*	2.04	CO* → COH*
Sc10	2.80	OH* → H_2O + *	1.40	CH_2O* → CH_2OH*	1.60	CHO* → CHOH*	1.60	CHO* → CHOH*	1.90	CO* → COH*	1.90	CO* → COH*	1.90	CO* → COH*
Ti3	2.77	OH* → H_2O + *	0.82	CH_2O* → CH_2OH*	1.36	CHO* → CHOH*	1.36	CHO* → CHOH*	1.20	CO* → COH*	1.20	CO* → COH*	1.20	CO* → COH*
Ti4	2.55	OH* → H_2O + *	0.82	CH_2O* → CH_2OH*	1.72	CHO* → CHOH*	1.72	CHO* → CHOH*	1.19	CO* → COH*	1.19	CO* → COH*	1.19	CO* → COH*
Ti5	2.32	OH* → H_2O + *	0.81	CH_2O* → CH_2OH*	1.64	CHO* → CHOH*	1.64	CHO* → CHOH*	1.07	CO* → COH*	1.07	CO* → COH*	1.07	CO* → COH*
Ti6	2.44	OH* → H_2O + *	0.73	CH_2O* → CH_2OH*	1.27	CHO* → CHOH*	1.27	CHO* → CHOH*	0.61	CO* → COH*	0.61	CO* → COH*	0.61	CO* → COH*
Ti7	2.13	OH* → H_2O + *	1.03	CH_2O* → CH_2OH*	1.16	CHO* → CHOH*	1.16	CHO* → CHOH*	0.93	CO* → COH*	0.93	CO* → COH*	0.93	CO* → COH*
Ti8	2.27	OH* → H_2O + *	0.84	CH_2O* → CH_2OH*	1.13	CHO* → CHOH*	1.13	CHO* → CHOH*	1.08	CO* → COH*	1.08	CO* → COH*	1.08	CO* → COH*
Ti9	2.37	OH* → H_2O + *	0.94	CH_2O* → CH_2OH*	1.32	CHO* → CHOH*	1.32	CHO* → CHOH*	0.92	CO* → COH*	0.92	CO* → COH*	0.92	CO* → COH*
Ti10	2.52	OH* → H_2O + *	1.19	CH_2O* → CH_2OH*	1.88	CHO* → CHOH*	1.88	CHO* → CHOH*	0.95	CO* → COH*	0.95	CO* → COH*	0.95	CO* → COH*
V3	1.98	OH* → H_2O + *	0.85	CH_2O* → CH_2OH*	0.70	CHO* → CHOH*	0.70	CHO* → CHOH*	0.51	CO* → COH*	0.51	CO* → COH*	0.51	CO* → COH*
V4	1.91	OH* → H_2O + *	0.35	CH_2O* → CH_2OH*	1.01	CHO* → CHOH*	1.01	CHO* → CHOH*	0.36	COH* → C*	0.68	COH* → CHOH*	0.68	COH* → CHOH*
V5	2.16	OH* → H_2O + *	0.55	CH_2O* → CH_2OH*	1.78	CHO* → CHOH*	1.78	CHO* → CHOH*	0.44	CO* → COH*	0.75	COH* → CHOH*	0.75	COH* → CHOH*
V6	1.92	OH* → H_2O + *	0.74	CH_2O* → CH_2OH*	1.34	CHO* → CHOH*	1.34	CHO* → CHOH*	0.55	CH* → CH_2*	0.96	COH* → CHOH*	0.96	COH* → CHOH*
V7	1.93	OH* → H_2O + *	0.66	CH_2O* → CH_2OH*	1.31	CHO* → CHOH*	1.31	CHO* → CHOH*	0.64	CO* → COH*	0.64	CO* → COH*	0.64	CO* → COH*
V8	1.94	OH* → H_2O + *	0.53	CH_2O* → CH_2OH*	0.95	CHO* → CHOH*	0.95	CHO* → CHOH*	1.10	CO* → COH*	1.10	CO* → COH*	1.10	CO* → COH*
V9	1.96	OH* → H_2O + *	0.53	CH_2O* → CH_2OH*	1.05	CHO* → CHOH*	1.05	CHO* → CHOH*	0.61	CO* → COH*	0.61	CO* → COH*	0.61	CO* → COH*
V10	1.47	OH* → H_2O + *	0.66	CH_2O* → CH_2OH*	0.58	CHO* → CHOH*	0.58	CHO* → CHOH*	1.11	CO* → COH*	1.11	CO* → COH*	1.11	CO* → COH*
Cr3	1.51	OH* → H_2O + *	0.56	COOH* → CO*	0.75	CHO* → CHOH*	0.75	CHO* → CHOH*	0.64	CO* → COH*	0.64	CO* → COH*	0.64	CO* → COH*
Cr4	1.98	OH* → H_2O + *	0.51	CH_2OH* → CH_2*	0.66	CHO* → CHOH*	0.66	CHO* → CHOH*	0.51	CO* → COH*	0.51	CO* → COH*	0.51	CO* → COH*
Cr5	1.50	OH* → H_2O + *	0.32	CH_2O* → CH_2OH*	0.38	CHO* → CHOH*	0.38	CHO* → CHOH*	0.61	CO* → COH*	0.61	CO* → COH*	0.61	CO* → COH*
Cr6	1.57	OH* → H_2O + *	0.40	CH_2O* → CH_2OH*	0.63	CHO* → CHOH*	0.63	CHO* → CHOH*	0.71	CO* → COH*	0.71	CO* → COH*	0.71	CO* → COH*
Cr7	1.41	OH* → H_2O + *	0.18	COOH* → CO*	0.44	CHO* → CHOH*	0.44	CHO* → CHOH*	0.64	CO* → COH*	0.64	CO* → COH*	0.64	CO* → COH*
Cr8	1.18	OH* → H_2O + *	0.44	CH_2OH* → CH_2*	0.48	CHO* → CHOH*	0.48	CHO* → CHOH*	0.74	CO* → COH*	0.74	CO* → COH*	0.74	CO* → COH*
Cr9	1.64	OH* → H_2O + *	0.35	CH_2O* → CH_2OH*	0.81	CHO* → CHOH*	0.81	CHO* → CHOH*	0.64	CO* → COH*	0.64	CO* → COH*	0.64	CO* → COH*
Cr10	1.71	OH* → H_2O + *	0.29	COOH* → CO*	0.94	CHO* → CHOH*	0.94	CHO* → CHOH*	0.63	CO* → COH*	0.63	CO* → COH*	0.63	CO* → COH*
Mn3	1.52	OH* → H_2O + *	0.64	CH_2O* → CH_2OH*	0.59	CHO* → CHOH*	0.59	CHO* → CHOH*	0.70	CO* → COH*	0.70	CO* → COH*	0.70	CO* → COH*
Mn4	1.54	OH* → H_2O + *	0.53	CH_2O* → CH_2OH*	0.50	CHO* → CHOH*	0.50	CHO* → CHOH*	0.67	CO* → COH*	0.67	CO* → COH*	0.67	CO* → COH*
Mn5	1.79	OH* → H_2O + *	0.21	CH_3* → CH_4+ *	0.57	CHO* → CHOH*	0.57	CHO* → CHOH*	0.69	CO* → COH*	0.69	CO* → COH*	0.69	CO* → COH*
Mn6	1.59	OH* → H_2O + *	0.60	CH_2O* → CH_2OH*	0.55	CHO* → CHOH*	0.55	CHO* → CHOH*	0.90	CO* → COH*	0.90	CO* → COH*	0.90	CO* → COH*
Mn7	2.31	OH* → H_2O + *	0.60	CH_3* → CH_4+ *	0.79	CHO* → CHOH*	0.79	CHO* → CHOH*	0.96	CO* → COH*	0.96	CO* → COH*	0.96	CO* → COH*
Mn8	1.47	OH* → H_2O + *	0.49	CO* → CHO*	0.49	CO* → CHO*	0.49	CO* → CHO*	1.04	CO* → COH*	1.04	CO* → COH*	1.04	CO* → COH*
Mn9	2.10	OH* → H_2O + *	0.75	CH_2O* → CH_2OH*	0.58	CHO* → CHOH*	0.58	CHO* → CHOH*	0.92	CO* → COH*	0.92	CO* → COH*	0.92	CO* → COH*
Mn10	2.46	OH* → H_2O + *	0.74	CH_3* → CH_4+ *	0.74	CH_3* → CH_4+ *	0.74	CH_3* → CH_4+ *	1.01	CO* → COH*	1.01	CO* → COH*	1.01	CO* → COH*
Fe3	1.42	OH* → H_2O + *	0.38	CO* → CHO*	0.38	CO* → CHO*	0.38	CO* → CHO*	0.79	CO* → COH*	0.79	CO* → COH*	0.79	CO* → COH*
Fe4	1.55	OH* → H_2O + *	0.40	CO* → CHO*	0.40	CO* → CHO*	0.40	CO* → CHO*	0.37	CO* → COH*	0.37	CO* → COH*	0.37	CO* → COH*
Fe5	1.37	OH* → H_2O + *	0.61	CO* → CHO*	0.61	CO* → CHO*	0.61	CO* → CHO*	0.55	CO* → COH*	0.55	COH* → CHOH*	0.55	COH* → CHOH*
Fe6	1.06	OH* → H_2O + *	0.77	CO* → CHO*	0.77	CO* → CHO*	0.77	CO* → CHO*	0.75	CO* → COH*	0.75	CO* → COH*	0.75	CO* → COH*
Fe7	0.89	OH* → H_2O + *	0.48	CO* → CHO*	0.48	CO* → CHO*	0.48	CO* → CHO*	0.81	CO* → COH*	0.81	CO* → COH*	0.81	CO* → COH*

Fe8	1.43	OH* → H_2O + *	0.46	CO* → CHO*	0.46	CO* → CHO*	0.46	CO* → CHO*	0.99	CO* → COH*	0.99	CO* → COH*	0.99	CO* → COH*
Fe9	1.22	OH* → H_2O + *	0.52	CO* → CHO*	0.52	CO* → CHO*	0.52	CO* → CHO*	0.73	CO* → COH*	0.73	CO* → COH*	0.73	CO* → COH*
Fe10	1.54	OH* → H_2O + *	0.39	CO* → CHO*	0.57	CHO* → CHOH*	0.57	CHO* → CHOH*	0.59	CO* → COH*	0.59	CO* → COH*	0.59	CO* → COH*
Co3	1.43	OH* → H_2O + *	0.44	CO* → CHO*	0.90	CHO* → CHOH*	0.90	CHO* → CHOH*	0.93	CO* → COH*	0.93	CO* → COH*	0.93	CO* → COH*
Co4	1.12	OH* → H_2O + *	0.80	CO* → CHO*	0.80	CO* → CHO*	0.80	CO* → CHO*	1.17	CO* → COH*	1.17	CO* → COH*	1.17	CO* → COH*
Co5	1.06	OH* → H_2O + *	0.75	CO* → CHO*	0.75	CO* → CHO*	0.75	CO* → CHO*	0.87	CO* → COH*	0.87	CO* → COH*	0.87	CO* → COH*
Co6	0.67	CO* → CHO*	0.67	CO* → CHO*	0.67	CO* → CHO*	0.67	CO* → CHO*	1.03	CO* → COH*	1.03	CO* → COH*	1.03	CO* → COH*
Co7	1.00	OH* → H_2O + *	0.80	CO* → CHO*	0.80	CO* → CHO*	0.80	CO* → CHO*	1.41	CO* → COH*	1.41	CO* → COH*	1.41	CO* → COH*
Co8	1.02	OH* → H_2O + *	0.59	CO* → CHO*	0.61	CHO* → CHOH*	0.61	CHO* → CHOH*	1.26	CO* → COH*	1.26	CO* → COH*	1.26	CO* → COH*
Co9	1.10	OH* → H_2O + *	0.62	CO* → CHO*	0.62	CO* → CHO*	0.62	CO* → CHO*	1.16	CO* → COH*	1.16	CO* → COH*	1.16	CO* → COH*
Co10	1.41	OH* → H_2O + *	0.68	CO* → CHO*	0.68	CO* → CHO*	0.68	CO* → CHO*	1.08	CO* → COH*	1.08	CO* → COH*	1.08	CO* → COH*
Ni3	1.11	OH* → H_2O + *	0.82	CO* → CHO*	0.82	CO* → CHO*	0.82	CO* → CHO*	0.88	CO* → COH*	0.88	CO* → COH*	0.88	CO* → COH*
Ni4	1.14	OH* → H_2O + *	0.66	CO* → CHO*	0.66	CO* → CHO*	0.66	CO* → CHO*	0.95	CO* → COH*	0.95	CO* → COH*	0.95	CO* → COH*
Ni5	1.21	OH* → H_2O + *	0.86	CO* → CHO*	0.86	CO* → CHO*	0.86	CO* → CHO*	0.89	CO* → COH*	0.89	CO* → COH*	0.89	CO* → COH*
Ni6	1.11	OH* → H_2O + *	0.91	CO* → CHO*	0.91	CO* → CHO*	0.91	CO* → CHO*	0.86	CO* → COH*	0.86	CO* → COH*	0.86	CO* → COH*
Ni7	0.81	OH* → H_2O + *	0.67	CO* → CHO*	0.67	CO* → CHO*	0.67	CO* → CHO*	0.76	CO* → COH*	0.76	CO* → COH*	0.76	CO* → COH*
Ni8	0.93	OH* → H_2O + *	0.65	CO* → CHO*	0.65	CO* → CHO*	0.65	CO* → CHO*	0.83	CO* → COH*	0.83	CO* → COH*	0.83	CO* → COH*
Ni9	0.91	OH* → H_2O + *	0.79	CO* → CHO*	0.79	CO* → CHO*	0.79	CO* → CHO*	0.83	CO* → COH*	0.83	CO* → COH*	0.83	CO* → COH*
Ni10	0.92	OH* → H_2O + *	0.67	CO* → CHO*	0.67	CO* → CHO*	0.67	CO* → CHO*	0.60	CO* → COH*	0.60	CO* → COH*	0.60	CO* → COH*
Cu3	1.11	OH* → H_2O + *	0.46	CO* → CHO*	0.49	CHO* → CHOH*	0.49	CHO* → CHOH*	1.38	CO* → COH*	1.38	CO* → COH*	1.38	CO* → COH*
Cu4	1.10	CO* → CHO*	1.10	CO* → CHO*	1.10	CO* → CHO*	1.10	CO* → CHO*	1.95	CO* → COH*	1.95	CO* → COH*	1.95	CO* → COH*
Cu5	1.45	OH* → H_2O + *	0.36	CO* → CHO*	0.36	CO* → CHO*	0.36	CO* → CHO*	1.14	CO* → COH*	1.14	CO* → COH*	1.14	CO* → COH*
Cu6	1.00	CO* → CHO*	1.00	CO* → CHO*	1.00	CO* → CHO*	1.00	CO* → CHO*	1.66	CO* → COH*	1.66	CO* → COH*	1.66	CO* → COH*
Cu7	0.52	OH* → H_2O + *	0.50	CO* → CHO*	0.50	CHO* → CHOH*	0.50	CHO* → CHOH*	1.27	CO* → COH*	1.27	CO* → COH*	1.27	CO* → COH*
Cu8	0.98	CO* → CHO*	0.98	CO* → CHO*	0.98	CO* → CHO*	0.98	CO* → CHO*	1.79	CO* → COH*	1.79	CO* → COH*	1.79	CO* → COH*
Cu9	1.20	OH* → H_2O + *	0.51	CH_2OH* → CH_2*	0.51	CH_2OH* → CH_2*	0.43	CHO* → CHOH*	1.19	CO* → COH*	1.19	CO* → COH*	1.19	CO* → COH*
Cu10	0.75	CO* → CHO*	0.75	CO* → CHO*	0.75	CO* → CHO*	0.7472	CO* → CHO*	1.28	CO* → COH*	1.28	CO* → COH*	1.28	CO* → COH*

	CHO Path VIII	RDS	CHO Path IX	RDS	CHO Path X	RDS	COH Path XI	RDS
Sc3	2.56	$CH_3O^* \rightarrow CH_3OH + *$	1.45	$CH_2O^* \rightarrow CH_2OH^*$	2.20	$CHO^* \rightarrow CHOH^*$	1.34	$CO^* \rightarrow COH^*$
Sc4	2.56	$CH_3O^* \rightarrow CH_3OH + *$	1.53	$CH_2O^* \rightarrow CH_2OH^*$	2.37	$CHO^* \rightarrow CHOH^*$	1.62	$CO^* \rightarrow COH^*$
Sc5	2.50	$CH_3O^* \rightarrow CH_3OH + *$	1.53	$CH_2O^* \rightarrow CH_2OH^*$	1.69	$CHO^* \rightarrow CHOH^*$	1.58	$CO^* \rightarrow COH^*$
Sc6	2.05	$CH_3O^* \rightarrow CH_3OH + *$	1.34	$CH_2O^* \rightarrow CH_2OH^*$	1.67	$CHO^* \rightarrow CHOH^*$	1.70	$CO^* \rightarrow COH^*$
Sc7	2.44	$CH_3O^* \rightarrow CH_3OH + *$	1.41	$CH_2O^* \rightarrow CH_2OH^*$	1.65	$CHO^* \rightarrow CHOH^*$	2.17	$CO^* \rightarrow COH^*$
Sc8	2.39	$CH_3O^* \rightarrow CH_3OH + *$	1.37	$CH_2O^* \rightarrow CH_2OH^*$	1.72	$CHO^* \rightarrow CHOH^*$	1.88	$CO^* \rightarrow COH^*$
Sc9	2.60	$CH_3O^* \rightarrow CH_3OH + *$	1.38	$CH_2O^* \rightarrow CH_2OH^*$	1.81	$CHO^* \rightarrow CHOH^*$	2.04	$CO^* \rightarrow COH^*$
Sc10	2.58	$CH_3O^* \rightarrow CH_3OH + *$	1.40	$CH_2O^* \rightarrow CH_2OH^*$	1.60	$CHO^* \rightarrow CHOH^*$	1.90	$CO^* \rightarrow COH^*$
Ti3	2.53	$CH_3O^* \rightarrow CH_3OH + *$	1.51	$CH_2OH^* \rightarrow CH_3OH + *$	1.51	$CH_2OH^* \rightarrow CH_3OH + *$	1.51	$CH_2OH^* \rightarrow CH_3OH + *$
Ti4	2.24	$CH_3O^* \rightarrow CH_3OH + *$	1.14	$CH_2OH^* \rightarrow CH_3OH + *$	1.72	$CHO^* \rightarrow CHOH^*$	1.19	$CO^* \rightarrow COH^*$
Ti5	1.99	$CH_3O^* \rightarrow CH_3OH + *$	0.94	$CH_2OH^* \rightarrow CH_3OH + *$	1.64	$CHO^* \rightarrow CHOH^*$	1.07	$CO^* \rightarrow COH^*$
Ti6	2.09	$CH_3O^* \rightarrow CH_3OH + *$	1.10	$CH_2OH^* \rightarrow CH_3OH + *$	1.27	$CHO^* \rightarrow CHOH^*$	1.10	$CH_2OH^* \rightarrow CH_3OH + *$
Ti7	1.92	$CH_3O^* \rightarrow CH_3OH + *$	1.03	$CH_2O^* \rightarrow CH_2OH^*$	1.16	$CHO^* \rightarrow CHOH^*$	0.93	$CO^* \rightarrow COH^*$
Ti8	2.02	$CH_3O^* \rightarrow CH_3OH + *$	1.09	$CH_2OH^* \rightarrow CH_3OH + *$	1.13	$CHO^* \rightarrow CHOH^*$	1.09	$CH_2OH^* \rightarrow CH_3OH + *$
Ti9	2.15	$CH_3O^* \rightarrow CH_3OH + *$	1.11	$CH_2OH^* \rightarrow CH_3OH + *$	1.32	$CHO^* \rightarrow CHOH^*$	1.11	$CH_2OH^* \rightarrow CH_3OH + *$
Ti10	2.26	$CH_3O^* \rightarrow CH_3OH + *$	1.19	$CH_2O^* \rightarrow CH_2OH^*$	1.88	$CHO^* \rightarrow CHOH^*$	1.14	$CH_2OH^* \rightarrow CH_3OH + *$
V3	1.64	$CH_3O^* \rightarrow CH_3OH + *$	0.85	$CH_2O^* \rightarrow CH_2OH^*$	0.75	$CH_2OH^* \rightarrow CH_3OH + *$	0.75	$CH_2OH^* \rightarrow CH_3OH + *$
V4	1.61	$CH_3O^* \rightarrow CH_3OH + *$	0.90	$CH_2OH^* \rightarrow CH_3OH + *$	1.01	$CHO^* \rightarrow CHOH^*$	0.90	$CH_2OH^* \rightarrow CH_3OH + *$
V5	1.90	$CH_3O^* \rightarrow CH_3OH + *$	1.13	$CH_2OH^* \rightarrow CH_3OH + *$	1.78	$CHO^* \rightarrow CHOH^*$	1.13	$CH_2OH^* \rightarrow CH_3OH + *$
V6	1.65	$CH_3O^* \rightarrow CH_3OH + *$	0.84	$CH_2OH^* \rightarrow CH_3OH + *$	1.34	$CHO^* \rightarrow CHOH^*$	0.96	$COH^* \rightarrow CHOH^*$
V7	1.69	$CH_3O^* \rightarrow CH_3OH + *$	0.98	$CH_2OH^* \rightarrow CH_3OH + *$	1.31	$CHO^* \rightarrow CHOH^*$	0.98	$CH_2OH^* \rightarrow CH_3OH + *$
V8	1.79	$CH_3O^* \rightarrow CH_3OH + *$	1.00	$CH_2OH^* \rightarrow CH_3OH + *$	1.00	$CH_2OH^* \rightarrow CH_3OH + *$	1.10	$CO^* \rightarrow COH^*$
V9	1.98	$CH_3O^* \rightarrow CH_3OH + *$	1.06	$CH_2OH^* \rightarrow CH_3OH + *$	1.06	$CH_2OH^* \rightarrow CH_3OH + *$	1.06	$CH_2OH^* \rightarrow CH_3OH + *$
V10	1.17	$CH_3O^* \rightarrow CH_3OH + *$	0.66	$CH_2O^* \rightarrow CH_2OH^*$	0.58	$CHO^* \rightarrow CHOH^*$	1.11	$CO^* \rightarrow COH^*$
Cr3	1.22	$CH_3O^* \rightarrow CH_3OH + *$	0.61	$CH_2OH^* \rightarrow CH_3OH + *$	0.75	$CHO^* \rightarrow CHOH^*$	0.64	$CO^* \rightarrow COH^*$
Cr4	1.79	$CH_3O^* \rightarrow CH_3OH + *$	1.10	$CH_2OH^* \rightarrow CH_3OH + *$	1.10	$CH_2OH^* \rightarrow CH_3OH + *$	1.10	$CH_2OH^* \rightarrow CH_3OH + *$
Cr5	1.30	$CH_3O^* \rightarrow CH_3OH + *$	0.69	$CH_2OH^* \rightarrow CH_3OH + *$	0.69	$CH_2OH^* \rightarrow CH_3OH + *$	0.69	$CH_2OH^* \rightarrow CH_3OH + *$
Cr6	1.16	$CH_3O^* \rightarrow CH_3OH + *$	0.64	$CH_2OH^* \rightarrow CH_3OH + *$	0.64	$CH_2OH^* \rightarrow CH_3OH + *$	0.71	$CO^* \rightarrow COH^*$
Cr7	1.16	$CH_3O^* \rightarrow CH_3OH + *$	0.54	$CH_2OH^* \rightarrow CH_3OH + *$	0.54	$CH_2OH^* \rightarrow CH_3OH + *$	0.64	$CO^* \rightarrow COH^*$
Cr8	1.12	$CH_3O^* \rightarrow CH_3OH + *$	0.59	$CH_2OH^* \rightarrow CH_3OH + *$	0.59	$CH_2OH^* \rightarrow CH_3OH + *$	0.74	$CO^* \rightarrow COH^*$
Cr9	1.31	$CH_3O^* \rightarrow CH_3OH + *$	0.64	$CH_2OH^* \rightarrow CH_3OH + *$	0.81	$CHO^* \rightarrow CHOH^*$	0.64	$CH_2OH^* \rightarrow CH_3OH + *$
Cr10	1.18	$CH_3O^* \rightarrow CH_3OH + *$	0.75	$CH_2OH^* \rightarrow CH_3OH + *$	0.94	$CHO^* \rightarrow CHOH^*$	0.75	$CH_2OH^* \rightarrow CH_3OH + *$
Mn3	1.12	$CH_3O^* \rightarrow CH_3OH + *$	0.64	$CH_2O^* \rightarrow CH_2OH^*$	0.59	$CHO^* \rightarrow CHOH^*$	0.70	$CO^* \rightarrow COH^*$
Mn4	1.52	$CH_3O^* \rightarrow CH_3OH + *$	0.53	$CH_2O^* \rightarrow CH_2OH^*$	0.50	$CHO^* \rightarrow CHOH^*$	0.67	$CO^* \rightarrow COH^*$
Mn5	1.73	$CH_3O^* \rightarrow CH_3OH + *$	0.77	$CH_2OH^* \rightarrow CH_3OH + *$	0.77	$CH_2OH^* \rightarrow CH_3OH + *$	0.77	$CH_2OH^* \rightarrow CH_3OH + *$
Mn6	1.59	$CH_3O^* \rightarrow CH_3OH + *$	0.60	$CH_2O^* \rightarrow CH_2OH^*$	0.59	$CH_2OH^* \rightarrow CH_3OH + *$	0.90	$CO^* \rightarrow COH^*$
Mn7	1.68	$CH_3O^* \rightarrow CH_3OH + *$	1.19	$CH_2OH^* \rightarrow CH_3OH + *$	1.19	$CH_2OH^* \rightarrow CH_3OH + *$	1.19	$CH_2OH^* \rightarrow CH_3OH + *$
Mn8	1.25	$CH_3O^* \rightarrow CH_3OH + *$	0.91	$CH_2OH^* \rightarrow CH_3OH + *$	0.91	$CH_2OH^* \rightarrow CH_3OH + *$	1.04	$CO^* \rightarrow COH^*$
Mn9	1.45	$CH_3O^* \rightarrow CH_3OH + *$	0.75	$CH_2O^* \rightarrow CH_2OH^*$	0.74	$CH_2OH^* \rightarrow CH_3OH + *$	0.92	$CO^* \rightarrow COH^*$
Mn10	2.17	$CH_3O^* \rightarrow CH_3OH + *$	1.44	$CH_2OH^* \rightarrow CH_3OH + *$	1.44	$CH_2OH^* \rightarrow CH_3OH + *$	1.44	$CH_2OH^* \rightarrow CH_3OH + *$
Fe3	1.16	$CH_3O^* \rightarrow CH_3OH + *$	0.69	$CH_2OH^* \rightarrow CH_3OH + *$	0.69	$CH_2OH^* \rightarrow CH_3OH + *$	0.79	$CO^* \rightarrow COH^*$
Fe4	1.37	$CH_3O^* \rightarrow CH_3OH + *$	0.88	$CH_2OH^* \rightarrow CH_3OH + *$	0.88	$CH_2OH^* \rightarrow CH_3OH + *$	0.88	$CH_2OH^* \rightarrow CH_3OH + *$
Fe5	1.10	$CH_3O^* \rightarrow CH_3OH + *$	0.61	$CO^* \rightarrow CHO^*$	0.61	$CO^* \rightarrow CHO^*$	0.55	$COH^* \rightarrow CHOH^*$
Fe6	0.77	$CO^* \rightarrow CHO^*$	0.77	$CO^* \rightarrow CHO^*$	0.77	$CO^* \rightarrow CHO^*$	0.75	$CO^* \rightarrow COH^*$
Fe7	0.67	$CH_3O^* \rightarrow CH_3OH + *$	0.48	$CO^* \rightarrow CHO^*$	0.48	$CO^* \rightarrow CHO^*$	0.81	$CO^* \rightarrow COH^*$

Fe8	**1.13**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.60**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.60**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.99**	**$CO^* \rightarrow COH^*$**
Fe9	**0.91**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.52**	**$CO^* \rightarrow CHO^*$**	**0.52**	**$CO^* \rightarrow CHO^*$**	**0.73**	**$CO^* \rightarrow COH^*$**
Fe10	**1.15**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.61**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.61**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.61**	**$CH_2OH^* \rightarrow CH_3OH + *$**
Co3	**0.94**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.87**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.90**	**$CHO^* \rightarrow CHOH^*$**	**0.93**	**$CO^* \rightarrow COH^*$**
Co4	**1.01**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.80**	**$CO^* \rightarrow CHO^*$**	**0.80**	**$CO^* \rightarrow CHO^*$**	**1.17**	**$CO^* \rightarrow COH^*$**
Co5	**1.01**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.75**	**$CO^* \rightarrow CHO^*$**	**0.75**	**$CO^* \rightarrow CHO^*$**	**0.87**	**$CO^* \rightarrow COH^*$**
Co6	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.67**	**$CO^* \rightarrow CHO^*$**	**1.03**	**$CO^* \rightarrow COH^*$**
Co7	**0.80**	**$CO^* \rightarrow CHO^*$**	**0.80**	**$CO^* \rightarrow CHO^*$**	**0.80**	**$CO^* \rightarrow CHO^*$**	**1.41**	**$CO^* \rightarrow COH^*$**
Co8	**0.88**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.59**	**$CO^* \rightarrow CHO^*$**	**0.61**	**$CHO^* \rightarrow CHOH^*$**	**1.26**	**$CO^* \rightarrow COH^*$**
Co9	**1.01**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.62**	**$CO^* \rightarrow CHO^*$**	**0.62**	**$CO^* \rightarrow CHO^*$**	**1.16**	**$CO^* \rightarrow COH^*$**
Co10	**1.13**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.68**	**$CO^* \rightarrow CHO^*$**	**0.68**	**$CO^* \rightarrow CHO^*$**	**1.08**	**$CO^* \rightarrow COH^*$**
Ni3	**0.82**	**$CO^* \rightarrow CHO^*$**	**0.82**	**$CO^* \rightarrow CHO^*$**	**0.82**	**$CO^* \rightarrow CHO^*$**	**0.88**	**$CO^* \rightarrow COH^*$**
Ni4	**1.22**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.94**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.94**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.95**	**$CO^* \rightarrow COH^*$**
Ni5	**0.86**	**$CO^* \rightarrow CHO^*$**	**0.86**	**$CO^* \rightarrow CHO^*$**	**0.86**	**$CO^* \rightarrow CHO^*$**	**0.89**	**$CO^* \rightarrow COH^*$**
Ni6	**0.91**	**$CO^* \rightarrow CHO^*$**	**0.91**	**$CO^* \rightarrow CHO^*$**	**0.91**	**$CO^* \rightarrow CHO^*$**	**0.86**	**$CO^* \rightarrow COH^*$**
Ni7	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.76**	**$CO^* \rightarrow COH^*$**
Ni8	**0.65**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.65**	**$CO^* \rightarrow CHO^*$**	**0.65**	**$CO^* \rightarrow CHO^*$**	**0.83**	**$CO^* \rightarrow COH^*$**
Ni9	**0.79**	**$CO^* \rightarrow CHO^*$**	**0.79**	**$CO^* \rightarrow CHO^*$**	**0.79**	**$CO^* \rightarrow CHO^*$**	**0.83**	**$CO^* \rightarrow COH^*$**
Ni10	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.67**	**$CO^* \rightarrow CHO^*$**	**0.60**	**$CO^* \rightarrow COH^*$**
Cu3	**0.92**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.72**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.72**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**1.38**	**$CO^* \rightarrow COH^*$**
Cu4	**1.10**	**$CO^* \rightarrow CHO^*$**	**1.10**	**$CO^* \rightarrow CHO^*$**	**1.10**	**$CO^* \rightarrow CHO^*$**	**1.95**	**$CO^* \rightarrow COH^*$**
Cu5	**1.08**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.67**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.67**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**1.14**	**$CO^* \rightarrow COH^*$**
Cu6	**1.00**	**$CO^* \rightarrow CHO^*$**	**1.00**	**$CO^* \rightarrow CHO^*$**	**1.00**	**$CO^* \rightarrow CHO^*$**	**1.66**	**$CO^* \rightarrow COH^*$**
Cu7	**0.50**	**$CO^* \rightarrow CHO^*$**	**0.50**	**$CO^* \rightarrow CHO^*$**	**0.50**	**$CHO^* \rightarrow CHOH^*$**	**1.27**	**$CO^* \rightarrow COH^*$**
Cu8	**0.98**	**$CO^* \rightarrow CHO^*$**	**0.98**	**$CO^* \rightarrow CHO^*$**	**0.98**	**$CO^* \rightarrow CHO^*$**	**1.79**	**$CO^* \rightarrow COH^*$**
Cu9	**0.85**	**$CH_3O^* \rightarrow CH_3OH + *$**	**0.53**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**0.53**	**$CH_2OH^* \rightarrow CH_3OH + *$**	**1.19**	**$CO^* \rightarrow COH^*$**
Cu10	**0.7472**	**$CO^* \rightarrow CHO^*$**	**0.75**	**$CO^* \rightarrow CHO^*$**	**0.75**	**$CO^* \rightarrow CHO^*$**	**1.28**	**$CO^* \rightarrow COH^*$**

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