Supporting Information

CO_2 Reduction and Ethane Dehydrogenation on Transition Metal Catalysts: Mechanistic Insights, Reactivity Trends and Rational Design of Bimetallic Alloys

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SI-1 Reaction Scheme

The elementary reactions included in the MKM to understand the CO_2 assisted dehydrogenation of ethane on the terrace and stepped sites of transition metal catalysts are mentioned below. '*t' represents a free step site (111), '*s' represents a free step site (211), '*h' represents the hydrogen site and the subscript '(g)' represents the gas phase species. The superscript '**t**', '**s**' and '**h**' represents species adsorbed on terrace sites, step site and hydrogen site respectively. The following are the reaction steps studied for (111) sites:

$$CH_3CH_{3(g)} + *t + *t \rightarrow CH_3^t + CH_3^t$$
$$CH_3CH_{3(g)} + *t + *h \rightarrow CH_3CH_2^t + H^h$$
$$CH_3CH_{3(g)} + *t + OH^t \rightarrow H_2O^t + CH_3CH_2^t$$
$$CH_3CH_{3(g)} + *t + O^t \rightarrow CH_3CH_2{}^t + OH^t$$
$$CH_3CH_2^t + *t \rightarrow CH_3^t + CH_2^t$$
$$CH_2CH_2^t + *t \rightarrow CH_2^t + CH_2^t$$
$$CH_3CH_2^t + *h \rightarrow CH_2CH_2^t + H^h$$
$$CH_3CH_2^t + OH^t \rightarrow CH_2CH_2^t + H_2O^t$$
$$CH_3CH_2^t + O^t \rightarrow CH_2CH_2^t + OH^t$$
$$CH_2CH_2^t \rightarrow CH_2CH_{2(g)} + *t$$
$$CH^t + O^t \rightarrow CHO^t + *t$$
$$CHO^t + *h \rightarrow CO^t + H^h$$
$$COH^t + *h \rightarrow CO^t + H^h$$
$$CHO^t + O^t \rightarrow CO^t + OH^t$$
$$CHO^t + OH^t \rightarrow CO^t + H_2O^t$$
$$C^t + OH^t \rightarrow COH^t + *t$$
$$COH^t + OH^t \rightarrow CO^t + H_2O^t$$
$$COH^t + O^t \rightarrow CO^t + OH^t$$

$$C^t + O^t \rightarrow CO^t + *t$$
$$CH^t + *h \rightarrow C^t + H^h$$
$$C^t + H_2O^t \rightarrow CH^t + OH^t$$
$$C^t + OH^t \rightarrow CH^t + O^t$$
$$CH_2^t + *h \rightarrow CH^t + H^h$$
$$CH^t + H_2O^t \rightarrow CH_2^t + OH^t$$
$$CH^t + OH^t \rightarrow CH_2^t + O^t$$
$$CH_2^t + H^h \rightarrow CH_3^t + *h$$
$$CH_2^t + H_2O^t \rightarrow CH_3^t + OH^t$$
$$CH_2^t + OH^t \rightarrow CH_3^t + O^t$$
$$CH_3^t + H^h \rightarrow CH_{4(g)} + *t + *h$$
$$CH_3^t + H_2O^t \rightarrow CH_{4(g)} + OH^t + *t$$
$$CH_3^t + OH^t \rightarrow CH_{4(g)} + O^t + *t$$
$$H^h + H^h \rightarrow H_{2(g)} + *h + *h$$
$$O^t + H^h \rightarrow OH^t + *h$$
$$O^t + H_2O^t \rightarrow OH^t + OH^t$$
$$OH^t + Hh \rightarrow H_2O^t + *h$$
$$OH^t + OH^t \rightarrow H_2O^t + O^t$$
$$H_2O^t \rightarrow H_2O_{(g)} + *t$$
$$CO^t \rightarrow CO_{(g)} + *t$$
$$CO_{2(g)} + *t + *t \rightarrow CO^t + O^t$$
$$CO_{2(g)} + H^h + *t \rightarrow COOH^t + *h$$
$$COOH^t + *t \rightarrow CO^t + OH^t$$
$$CO_{2(g)} + H^h + *t \rightarrow HCOO^t + *h$$
$$HCOO^t + *t \rightarrow CHO^t + O^t$$

The following are the reaction steps studied for (211) sites:

$$CH_3CH_{3(g)} + *s + *s \rightarrow CH_3^s + CH_3^s$$
$$CH_3CH_{3(g)} + *s + *h \rightarrow CH_3CH_2^s + H^h$$
$$CH_3CH_{3(g)} + *s + OH^s \rightarrow H_2O^s + CH_3CH_2^s$$
$$CH_3CH_{3(g)} + *s + O^s \rightarrow CH_3CH_2^s + OH^s$$
$$CH_3CH_2^s + *s \rightarrow CH_3^s + CH_2^s$$
$$CH_2CH_2^s + *s \rightarrow CH_2^s + CH_2^s$$
$$CH_3CH_2^s + *h \rightarrow CH_2CH_2^s + H^h$$
$$CH_3CH_2^s + OH^s \rightarrow CH_2CH_2^s + H_2O^s$$
$$CH_3CH_2^s + O^s \rightarrow CH_2CH_2^s + OH^s$$
$$CH_2CH_2^s \rightarrow CH_2CH_{2(g)} + *s$$
$$CH^s + O^s \rightarrow CHO^s + *s$$
$$CHO^s + *h \rightarrow CO^s + H^h$$
$$COH^s + *h \rightarrow CO^s + H^h$$
$$CHO^s + O^s \rightarrow CO^s + OH^s$$
$$CHO^s + OH^s \rightarrow CO^s + H_2O^s$$
$$C^s + OH^s \rightarrow COH^s + *s$$
$$COH^s + OH^s \rightarrow CO^s + H_2O^s$$
$$COH^s + O^s \rightarrow CO^s + OH^s$$
$$C^s + O^s \rightarrow CO^s + *s$$
$$CH^s + *h \rightarrow C^s + H^h$$
$$C^s + H_2O^s \rightarrow CH^s + OH^s$$
$$C^s + OH^s \rightarrow CH^s + O^s$$

$$CH_2^s + *h \rightarrow CH^s + H^h$$
$$CH^s + H_2O^s \rightarrow CH_2^s + OH^s$$
$$CH^s + OH^s \rightarrow CH_2^s + O^s$$
$$CH_2^s + H^h \rightarrow CH_3^s + *h$$
$$CH_2^s + H_2O^s \rightarrow CH_3^s + OH^s$$
$$CH_2^s + OH^s \rightarrow CH_3^s + O^s$$
$$CH_3^s + H^h \rightarrow CH_{4(g)} + *s + *h$$
$$CH_3^s + H_2O^s \rightarrow CH_{4(g)} + OH^s + *s$$
$$CH_3^s + OH^s \rightarrow CH_{4(g)} + O^s + *s$$
$$H^h + H^h \rightarrow H_{2(g)} + *h + *h$$
$$O^s + H^h \rightarrow OH^s + *h$$
$$O^s + H_2O^s \rightarrow OH^s + OH^s$$
$$OH^s + Hh \rightarrow H_2O^s + *h$$
$$OH^s + OH^s \rightarrow H_2O^s + O^s$$
$$H_2O^s \rightarrow H_2O_{(g)} + *s$$
$$CO^s \rightarrow CO_{(g)} + *s$$
$$CO_{2(g)} + *s + *s \rightarrow CO^s + O^s$$
$$CO_{2(g)} + H^h + *s \rightarrow COOH^s + *h$$
$$COOH^s + *s \rightarrow CO^s + OH^s$$
$$CO_{2(g)} + H^h + *s \rightarrow HCOO^s + *h$$
$$HCOO^s + *s \rightarrow CHO^s + O^s$$
$$C^s + C^s \rightarrow C_2^s + *s$$
$$C_2^s \rightarrow C_{2(g)} + *s$$

SI-2 Methodology

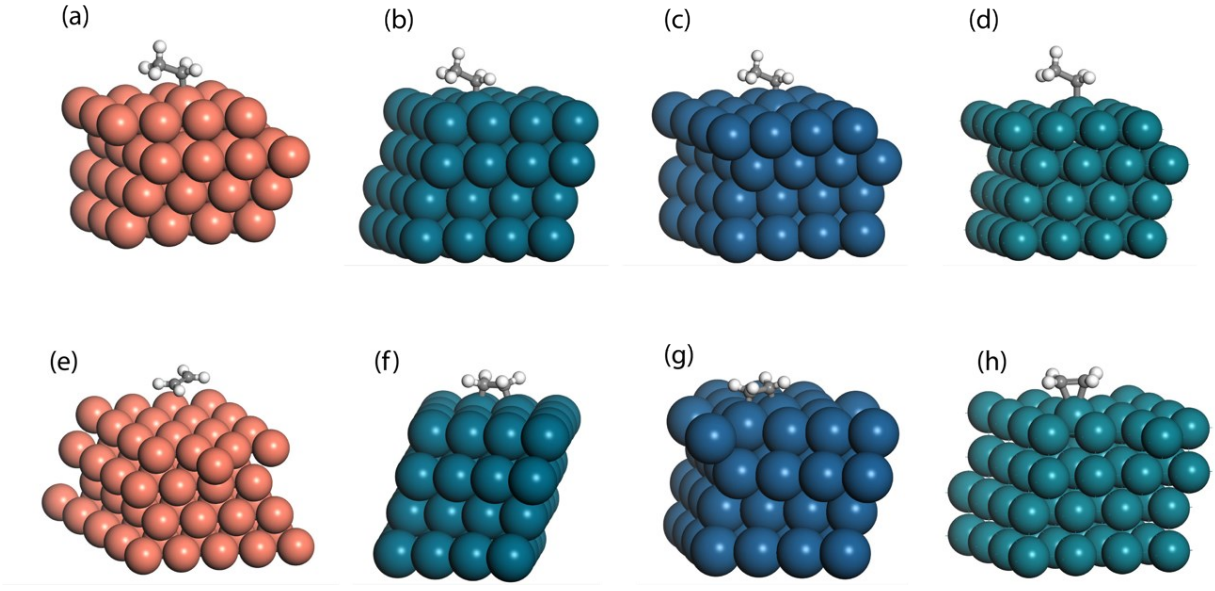

Figure SI-1 Adsorption of CH_3CH_2 on (a) Cu(111), (b) Pd(111), (c) Pt(111) and (d) Rh (111); adsorption of CH_2CH_2 on (e) Cu(111), (f) Pd(111), (g) Pt(111) and (h) Rh(111).

Table SI-1 Details of the reference used for CatMAP data, their source article and DFT set-up

Reference	Article	DFT Method	XC	Potential
1.	*Energy Environ. Sci.* **3**, 1311–1315 (2010)	DACAPO	RPBE	USPP
2.	*Top Catal.* **57**, 135–142 (2014)	DACAPO	RPBE	USPP
3.	*Phy. Rev. Lett.* **99**, 016105 (2007)	DACAPO	RPBE	USPP
4.	*Phys. Chem. Chem. Phys*. **13**, 20760–20765 (2011)	DACAPO	RPBE	USPP
5.	*J. Phys. Chem. C* **113**, 10548–10553 (2009)	DACAPO	RPBE	USPP
6.	*Angew. Chem. Int. Ed*. **47**, 4835 –4839 (2008)	DACAPO	RPBE	USPP
7.	*Catal. Lett*. **141**, 370–373 (2011)	DACAPO	RPBE	USPP
8.	*J. Catal,* **293**, 51–60 (2012)	DACAPO	RPBE	USPP
9.	*Angew. Chem. Int. Ed*. **51**, 272–274 (2012)	DACAPO	RPBE	USPP
10.	*J Catal*. **374**, 161–170 (2019).	Quantum Espresso	BEEF-vdW	GBRV
11.	*J. Am. Chem. Soc.* 133 (2011) 5009–5015 (only for Energy for C2(g))	VASP	PW91	USPP
12.	*New J. Phys.* **15**, 125021 (2013)	DACAPO	RPBE	USPP

Table SI-2 Carbon (E_C) and oxygen binding energies (E_O) over transition metal surfaces calculated using VASP plane-wave method.

Surface	E_C(VASP) (eV)	E_O(VASP) (eV)
Ag	6.05	2.50
Cu	4.59	1.42
Pd	2.44	1.59
Pt	2.45	1.80
Rh	2.15	0.75

Table SI-3 Carbon (E_C) and oxygen binding energies (E_O) over transition metal surfaces calculated using DACAPO plane-wave method.

Surface	E_C(DACAPO) (eV)	E_O(DACAPO) (eV)
Ag	5.57	2.05
Cu	4.36	1.07
Pd	2.52	1.55
Pt	2.16	1.62
Rh	1.95	0.55

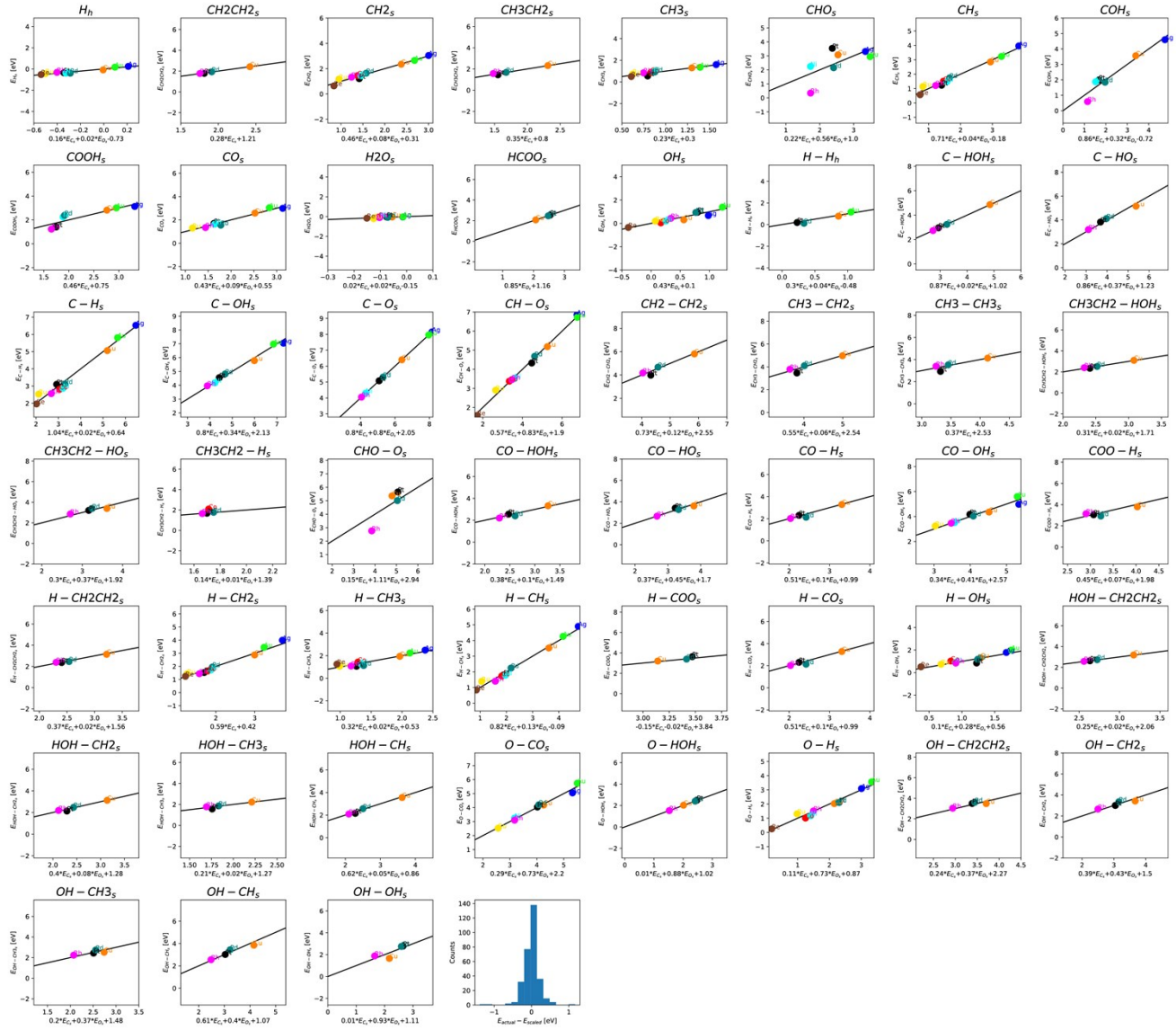

Figure SI-2 Scaling Relationship Plots

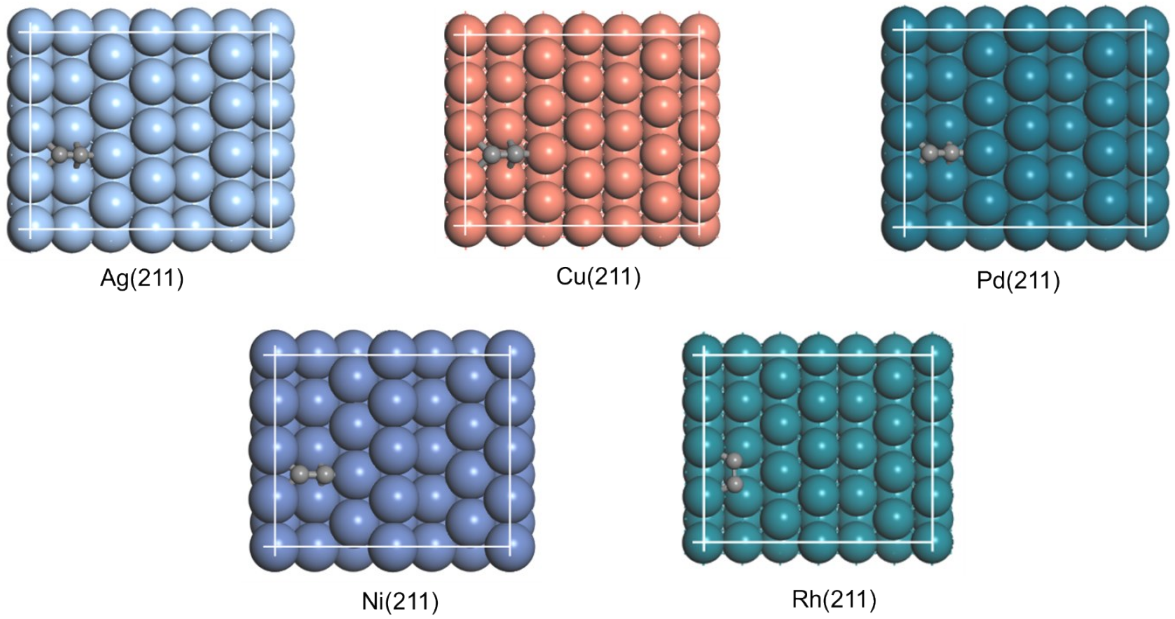

Figure SI-3 Geometry optimized adsorption configurations of C_2 species at the transition metals (211) surfaces.

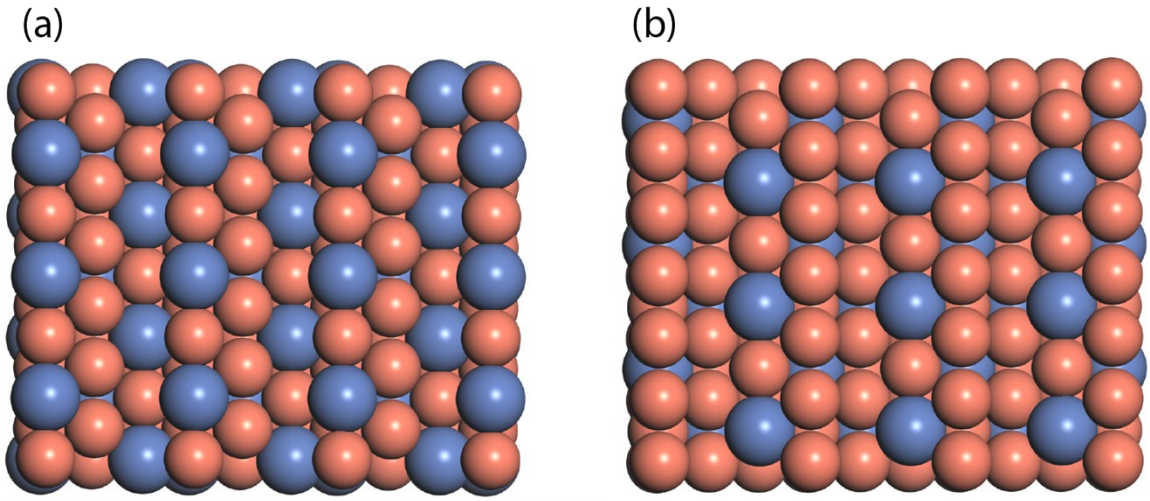

Figure SI-4 Top view of (a) AB and (b) AA termination of A_3B bimetallic alloys of Pt and Ni screened in the MKM.

SI-3 Reactivity of Terrace (111) Sites

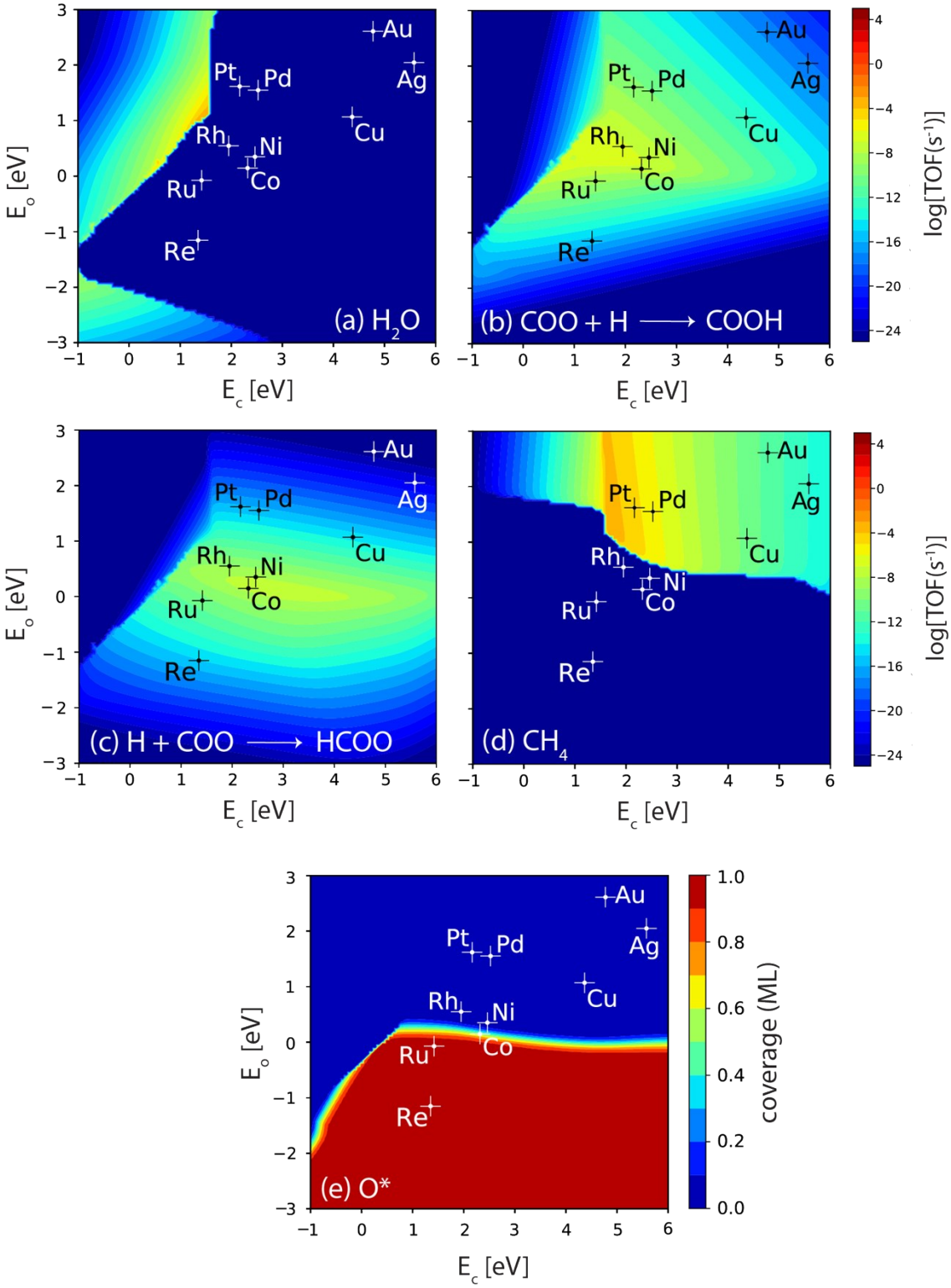

Figure SI-5 Volcano plots for the consumption rates of (a) H_2O; elementary reaction rates of CO_2 dissociation via (b) carboxyl (COOH) and (c) formate (HCOO) route; production rate plots of (d) CH_4 and (e) coverage of O* over (111) facets of transition metal catalysts. Error bar = 0.2 eV.

SI-4 Reactivity of Step (211) Sites

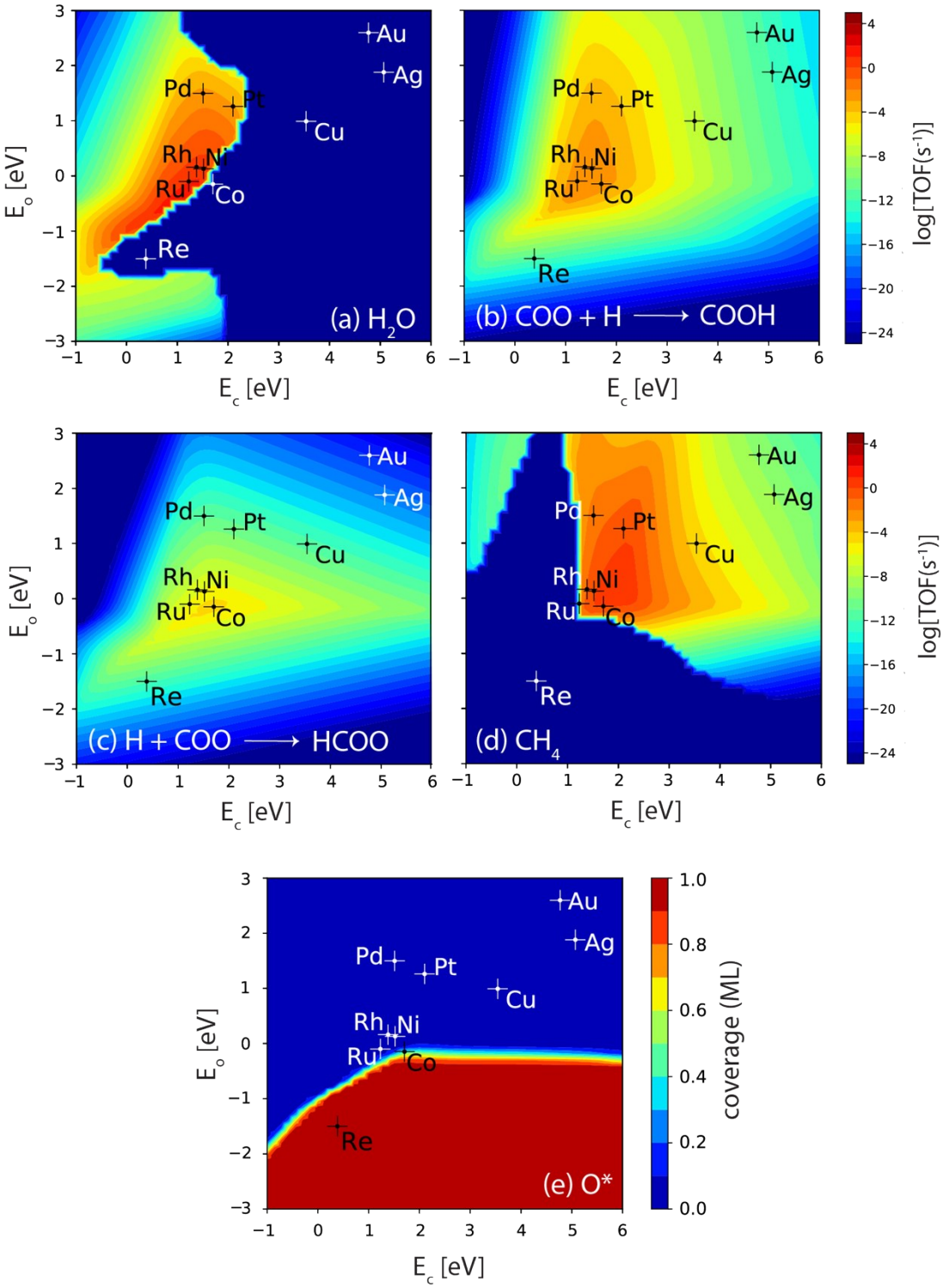

Figure SI-6 Volcano plots for the consumption rates of (a) H_2O; elementary reaction rates of CO_2 dissociation via (b) carboxyl (COOH) and (c) formate (HCOO) route; production rate plots of (d) CH_4 and (e) coverage of O* over (211) facets of transition metal catalysts. Error bar = 0.2 eV.

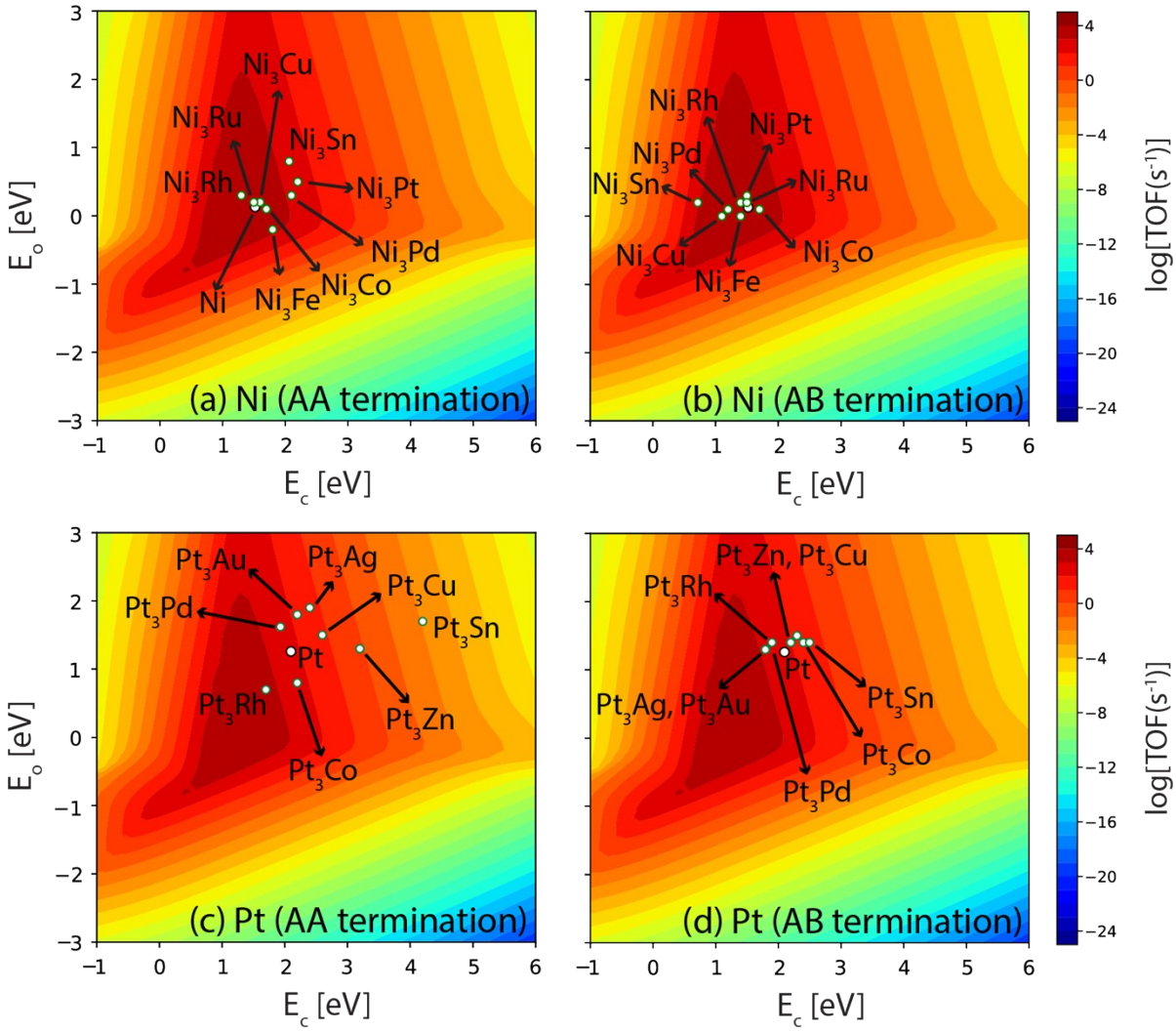

Figure SI-7 Volcano plots for H_2 production rates over (a) AA surface termination and (b) AB surface termination of Ni based A_3B alloys; and (c) AA surface termination and (d) AB surface termination of Pt based A_3B alloys

SI-5 Reaction Energetics

The formation energies of the species used in the model are listed in Table SI-1. The formation energies of all the species are referenced with respect to methane, hydrogen, and water; for C, H and O atom respectively. The energies have been obtained from previous literature[1-12] and calculated in this work. The literature source for the formation energies and respective DFT

setup employed is given in Table SI-2. The descriptor energies for Ni and Pt based A_3B alloys have been taken from the study on methane steam reforming conducted by Xu et al[13].

Table SI-4 Formation energies of the species used in the MKM. Formation energies are references to CH_4, H_2O and H_2.

Species	Facet	Surface	Formation Energy
C_2	gas	None	2.30
CH_2CH_2	gas	None	2.25
CH_3CH3	gas	None	0.80
CH_4	gas	None	0.00
CO	gas	None	2.77
CO_2	gas	None	2.47
H_2	gas	None	0.00
H_2O	gas	None	0.00
C	111	Ag	5.57
C	111	Au	4.77
C	111	Co	2.32
C	111	Co	2.32
C	111	Cu	4.36
C	111	Ni	2.46
C	111	Pd	2.52
C	111	Pt	2.16
C	111	Re	1.35
C	111	Ru	1.42
C-C	111	Ag	10.97
C-C	111	Au	9.69
C-C	111	Cu	9.03
C-C	111	Ni	5.99
C-C	111	Pd	6.09
C-C	111	Pt	5.51
C-C	111	Rh	5.18
C-H	111	Ag	6.53
C-H	111	Au	5.81
C-H	111	Co	2.81
C-H	111	Cu	5.06
C-H	111	Ni	2.87
C-H	111	Pd	3.12

C-H	111	Pt	3.10
C-H	111	Re	1.96
C-H	111	Rh	2.56
C-H	111	Rh	2.56
C-H	111	Ru	2.53
C-HO	111	Cu	5.15
C-HO	111	Pd	4.12
C-HO	111	Pt	3.82
C-HO	111	Rh	3.19
C-HOH	111	Cu	4.86
C-HOH	111	Pd	3.24
C-HOH	111	Pt	2.96
C-HOH	111	Rh	2.73
C-O	111	Ag	8.15
C-O	111	Au	7.96
C-O	111	Cu	6.40
C-O	111	Ni	4.30
C-O	111	Pd	5.31
C-O	111	Pt	5.08
C-O	111	Rh	4.05
C-OH	111	Ag	7.05
C-OH	111	Au	6.98
C-OH	111	Cu	5.78
C-OH	111	Ni	4.18
C-OH	111	Pd	4.82
C-OH	111	Pt	4.55
C-OH	111	Rh	3.96
CH	111	Ag	3.96
CH	111	Au	3.23
CH	111	Co	1.51
CH	111	Cu	2.85
CH	111	Ni	1.48
CH	111	Pd	1.74
CH	111	Pt	1.23
CH	111	Re	0.57
CH	111	Rh	1.21
CH	111	Ru	1.14
CH-O	111	Ag	6.86
CH-O	111	Au	6.72
CH-O	111	Co	3.38
CH-O	111	Cu	5.19
CH-O	111	Ni	3.51

CH-O	111	Pd	4.68
CH-O	111	Pt	4.33
CH-O	111	Re	1.59
CH-O	111	Rh	3.46
CH-O	111	Ru	2.91
CH_2	111	Ag	3.04
CH_2	111	Au	2.65
CH_2	111	Co	1.45
CH_2	111	Cu	2.35
CH_2	111	Ni	1.44
CH_2	111	Pd	1.64
CH_2	111	Pt	1.21
CH_2	111	Re	0.64
CH_2	111	Rh	1.33
CH_2	111	Ru	1.17
CH_2-CH_2	111	Cu	5.81
CH_2-CH_2	111	Pd	4.67
CH_2-CH_2	111	Pt	3.99
CH_2-CH_2	111	Rh	4.18
CH_2CH_2	111	Cu	2.42
CH_2CH_2	111	Pd	1.93
CH_2CH_2	111	Pt	1.78
CH_2CH_2	111	Rh	1.77
CH_3	111	Ag	1.60
CH_3	111	Au	1.35
CH_3	111	Co	0.89
CH_3	111	Cu	1.30
CH_3	111	Ni	0.93
CH_3	111	Pd	0.92
CH_3	111	Pt	0.55
CH_3	111	Re	0.50
CH_3	111	Rh	0.84
CH_3	111	Ru	0.73
CH_3-CH_2	111	Cu	4.97
CH_3-CH_2	111	Pd	4.10
CH_3-CH_2	111	Pt	3.46
CH_3-CH_2	111	Rh	3.79
CH_3-CH_3	111	Cu	4.13
CH_3-CH_3	111	Pd	3.52
CH_3-CH_3	111	Pt	2.93
CH_3-CH_3	111	Rh	3.39
CH_3CH_2	111	Cu	2.32

CH_3CH_2	111	Pd	1.68
CH_3CH_2	111	Pt	1.45
CH_3CH_2	111	Rh	1.57
CH_3CH_2-H	111	Co	2.09
CH_3CH_2-H	111	Pd	1.77
CH_3CH_2-H	111	Pt	1.68
CH_3CH_2-H	111	Rh	1.65
CH_3CH_2-HO	111	Cu	3.40
CH_3CH_2-HO	111	Pd	3.39
CH_3CH_2-HO	111	Pt	3.21
CH_3CH_2-HO	111	Rh	2.86
CH_3CH_2-HOH	111	Cu	3.10
CH_3CH_2-HOH	111	Pd	2.52
CH_3CH_2-HOH	111	Pt	2.34
CH_3CH_2-HOH	111	Rh	2.40
CHO	111	Ag	3.31
CHO	111	Au	2.94
CHO	111	Cu	3.07
CHO	111	Ni	2.24
CHO	111	Pd	2.15
CHO	111	Pt	3.54
CHO	111	Rh	0.34
CHO-O	111	Cu	5.36
CHO-O	111	Pd	5.01
CHO-O	111	Pt	5.65
CHO-O	111	Rh	2.76
CO	111	Ag	2.99
CO	111	Au	3.04
CO	111	Cu	2.58
CO	111	Cu	2.58
CO	111	Ni	1.63
CO	111	Pd	1.55
CO	111	Pd	1.55
CO	111	Pt	1.70
CO	111	Pt	1.70
CO	111	Rh	1.34
CO	111	Rh	1.34
CO	111	Ru	1.30
CO-H	111	Cu	3.28
CO-H	111	Pd	2.13
CO-H	111	Pt	2.30
CO-H	111	Rh	2.02

CO-HO	111	Cu	3.62
CO-HO	111	Pd	3.28
CO-HO	111	Pt	3.43
CO-HO	111	Rh	2.66
CO-HOH	111	Cu	3.32
CO-HOH	111	Pd	2.40
CO-HOH	111	Pt	2.56
CO-HOH	111	Rh	2.20
CO-OH	111	Ag	4.98
CO-OH	111	Ag	4.98
CO-OH	111	Au	5.59
CO-OH	111	Au	5.59
CO-OH	111	Cu	4.36
CO-OH	111	Cu	4.36
CO-OH	111	Ni	3.51
CO-OH	111	Ni	3.51
CO-OH	111	Pd	4.04
CO-OH	111	Pd	4.04
CO-OH	111	Pt	4.18
CO-OH	111	Pt	4.18
CO-OH	111	Rh	3.47
CO-OH	111	Rh	3.47
CO-OH	111	Ru	3.24
CO-OH	111	Ru	3.24
COH	111	Ag	4.60
COH	111	Cu	3.56
COH	111	Ni	1.87
COH	111	Pd	1.84
COH	111	Pt	1.99
COH	111	Rh	0.59
COO-H	111	Cu	3.79
COO-H	111	Pd	2.92
COO-H	111	Pt	3.05
COO-H	111	Rh	3.14
COOH	111	Ag	3.13
COOH	111	Au	3.01
COOH	111	Cu	2.82
COOH	111	Ni	2.25
COOH	111	Pd	2.39
COOH	111	Pt	1.41
COOH	111	Rh	1.23
H	111	Ag	0.24

H	111	Au	0.17
H	111	Cu	-0.09
H	111	Cu	-0.09
H	111	Ni	-0.39
H	111	Pd	-0.40
H	111	Pd	-0.40
H	111	Pt	-0.35
H	111	Pt	-0.35
H	111	Re	-0.53
H	111	Rh	-0.32
H	111	Rh	-0.32
H	111	Ru	-0.44
H-CH	111	Ag	4.90
H-CH	111	Au	4.26
H-CH	111	Co	1.73
H-CH	111	Cu	3.52
H-CH	111	Ni	1.78
H-CH	111	Pd	2.24
H-CH	111	Pt	1.80
H-CH	111	Re	0.84
H-CH	111	Rh	1.40
H-CH	111	Ru	1.39
$H-CH_2$	111	Ag	3.99
$H-CH_2$	111	Au	3.45
$H-CH_2$	111	Co	1.65
$H-CH_2$	111	Cu	2.87
$H-CH_2$	111	Ni	1.73
$H-CH_2$	111	Pd	1.95
$H-CH_2$	111	Pt	1.53
$H-CH_2$	111	Re	1.24
$H-CH_2$	111	Rh	1.44
$H-CH_2$	111	Ru	1.43
$H-CH_2CH_2$	111	Cu	3.15
$H-CH_2CH_2$	111	Pd	2.46
$H-CH_2CH_2$	111	Pt	2.37
$H-CH_2CH_2$	111	Rh	2.39
$H-CH_3$	111	Ag	2.49
$H-CH_3$	111	Au	2.23
$H-CH_3$	111	Co	1.43
$H-CH_3$	111	Cu	1.94
$H-CH_3$	111	Ni	1.27
$H-CH_3$	111	Pd	1.13

$H\text{-}CH_3$	111	Pt	1.06
H-CH3	111	Re	1.25
$H\text{-}CH_3$	111	Rh	1.08
$H\text{-}CH_3$	111	Ru	1.06
H-CO	111	Cu	3.28
H-CO	111	Pd	2.13
H-CO	111	Pt	2.30
H-CO	111	Rh	2.02
H-COO	111	Cu	3.20
H-COO	111	Pd	3.39
H-COO	111	Pt	3.63
H-H	111	Au	1.15
H-H	111	Cu	0.78
H-H	111	Pd	0.12
H-H	111	Pt	0.19
H-OH	111	Ag	1.78
H-OH	111	Au	2.00
H-OH	111	Co	1.03
H-OH	111	Cu	1.30
H-OH	111	Cu	1.30
H-OH	111	Ni	0.91
H-OH	111	Pd	1.18
H-OH	111	Pd	1.18
H-OH	111	Pt	0.85
H-OH	111	Re	0.52
H-OH	111	Rh	0.85
H-OH	111	Ru	0.74
H_2O	111	Ag	-0.04
H_2O	111	Au	-0.03
H_2O	111	Co	-0.05
H_2O	111	Cu	-0.04
H_2O	111	Ni	-0.05
H_2O	111	Pd	-0.08
H_2O	111	Pt	-0.05
H_2O	111	Re	-0.17
H_2O	111	Rh	-0.11
H_2O	111	Ru	-0.21
HCO	111	Ag	3.31
HCO	111	Au	2.94
HCO	111	Cu	3.07
HCO	111	Ni	2.24
HCO	111	Pd	2.15

HCO	111	Pt	3.54
HCO	111	Rh	0.34
HCOO	111	Cu	2.07
HCOO	111	Pd	2.47
HCOO	111	Pt	2.54
HOH-CH	111	Cu	3.56
HOH-CH	111	Pd	2.57
HOH-CH	111	Pt	2.15
HOH-CH	111	Rh	2.09
$HOH-CH_2$	111	Cu	3.13
$HOH-CH_2$	111	Pd	2.48
$HOH-CH_2$	111	Pt	2.14
$HOH-CH_2$	111	Rh	2.19
$HOH-CH_2CH_2$	111	Cu	3.19
$HOH-CH_2CH_2$	111	Pd	2.73
$HOH-CH_2CH_2$	111	Pt	2.63
$HOH-CH_2CH_2$	111	Rh	2.57
$HOH-CH_3$	111	Cu	2.22
$HOH-CH_3$	111	Pd	1.86
$HOH-CH_3$	111	Pt	1.57
$HOH-CH_3$	111	Rh	1.77
O	111	Ag	2.05
O	111	Au	2.61
O	111	Co	0.15
O	111	Cu	1.07
O	111	Ni	0.35
O	111	Pd	1.55
O	111	Pt	1.62
O	111	Re	-1.15
O	111	Rh	0.55
O	111	Ru	-0.07
O-CO	111	Ag	5.05
O-CO	111	Au	5.74
O-CO	111	Cu	4.18
O-CO	111	Ni	3.25
O-CO	111	Pd	4.20
O-CO	111	Pt	4.04
O-CO	111	Rh	3.10
O-CO	111	Ru	2.53
O-H	111	Ag	3.09
O-H	111	Au	3.56
O-H	111	Co	1.02

O-H	111	Cu	2.03
O-H	111	Cu	2.03
O-H	111	Ni	1.18
O-H	111	Pd	2.12
O-H	111	Pt	2.12
O-H	111	Re	0.25
O-H	111	Rh	1.52
O-H	111	Ru	1.31
O-HOH	111	Cu	2.02
O-HOH	111	Pd	2.40
O-HOH	111	Pt	2.49
O-HOH	111	Rh	1.52
OH	111	Ag	0.67
OH	111	Au	1.39
OH	111	Co	0.05
OH	111	Cu	0.30
OH	111	Cu	0.30
OH	111	Ni	0.20
OH	111	Pd	0.94
OH	111	Pd	0.94
OH	111	Pt	0.96
OH	111	Pt	0.96
OH	111	Re	-0.35
OH	111	Rh	0.43
OH	111	Rh	0.43
OH	111	Ru	0.19
OH-CH	111	Cu	3.85
OH-CH	111	Pd	3.44
OH-CH	111	Pt	3.02
OH-CH	111	Rh	2.55
$OH-CH_2$	111	Cu	3.42
$OH-CH_2$	111	Pd	3.36
$OH-CH_2$	111	Pt	3.00
$OH-CH_2$	111	Rh	2.65
$OH-CH_2CH_2$	111	Cu	3.48
$OH-CH_2CH_2$	111	Pd	3.61
$OH-CH_2CH_2$	111	Pt	3.49
$OH-CH_2CH_2$	111	Rh	3.03
$OH-CH_3$	111	Cu	2.52
$OH-CH_3$	111	Pd	2.74
$OH-CH_3$	111	Pt	2.44
$OH-CH_3$	111	Rh	2.23

OH-OH	111	Cu	1.66
OH-OH	111	Pd	2.75
OH-OH	111	Pt	2.79
OH-OH	111	Rh	1.88
C	211	Ag	5.07
C	211	Au	4.77
C	211	Co	1.70
C	211	Cu	3.54
C	211	Ni	1.52
C	211	Pd	1.51
C	211	Pt	2.10
C	211	Re	0.38
C	211	Rh	1.38
C	211	Ru	1.23
C-C	211	Ag	11.02
C-C	211	Au	10.36
C-C	211	Co	5.07
C-C	211	Cu	8.22
C-C	211	Pt	6.03
C-C	211	Rh	4.51
C-C	211	Ru	4.37
C-H	211	Cu	4.31
C-H	211	Ni	2.02
C-H	211	Pd	2.25
C-H	211	Pt	3.06
C-H	211	Rh	1.97
C-H	211	Ru	1.74
C-HO	211	Ag	5.92
C-HO	211	Cu	4.15
C-HO	211	Pd	2.73
C-HO	211	Pt	3.26
C-HO	211	Rh	2.01
C-HOH	211	Ag	5.40
C-HOH	211	Cu	4.03
C-HOH	211	Pd	2.29
C-HOH	211	Pt	2.83
C-HOH	211	Rh	2.08
C-O	211	Ag	8.07
C-O	211	Au	8.18
C-O	211	Co	3.19
C-O	211	Ni	3.43
C-O	211	Pd	4.63

C-O	211	Pt	4.11
C-O	211	Re	1.21
C-O	211	Rh	3.03
C-O	211	Ru	2.80
C-OH	211	Ag	6.57
C-OH	211	Cu	4.83
C-OH	211	Ni	2.36
C-OH	211	Pd	3.34
C-OH	211	Pt	3.30
C-OH	211	Rh	2.64
C_2	211	Ag	5.80
C_2	211	Cu	4.44
C_2	211	Ni	3.57
C_2	211	Pd	4.03
C_2	211	Rh	4.23
CH	211	Ag	3.96
CH	211	Au	3.43
CH	211	Co	1.16
CH	211	Cu	2.70
CH	211	Ni	1.22
CH	211	Pd	1.57
CH	211	Pt	1.19
CH	211	Re	0.06
CH	211	Rh	1.01
CH	211	Ru	0.71
CH-O	211	Ag	6.96
CH-O	211	Au	7.28
CH-O	211	Cu	5.08
CH-O	211	Pd	4.87
CH-O	211	Pt	4.76
CH-O	211	Rh	3.28
CH-O	211	Ru	2.58
CH_2	211	Ag	2.87
CH_2	211	Au	2.23
CH_2	211	Co	0.79
CH_2	211	Cu	2.22
CH_2	211	Ni	1.14
CH_2	211	Pd	1.28
CH_2	211	Pt	0.76
CH_2	211	Re	0.21
CH_2	211	Rh	0.76
CH_2	211	Ru	0.69

CH_2-CH_2	211	Ag	5.75
CH_2-CH_2	211	Au	4.94
CH_2-CH_2	211	Cu	4.43
CH_2-CH_2	211	Pd	3.34
CH_2-CH_2	211	Pt	3.16
CH_2-CH_2	211	Rh	2.55
CH_2-CH_2	211	Ru	2.25
CH_2CH_2	211	Ag	2.39
CH_2CH_2	211	Cu	2.26
CH_2CH_2	211	Pd	1.72
CH_2CH_2	211	Pt	1.58
CH_2CH_2	211	Pt	1.58
CH_2CH_2	211	Rh	1.48
CH_3	211	Ag	1.39
CH_3	211	Au	1.10
CH_3	211	Co	0.04
CH_3	211	Cu	0.97
CH_3	211	Ni	0.39
CH_3	211	Pd	0.79
CH_3	211	Pt	0.46
CH_3	211	Re	-0.13
CH_3	211	Rh	0.36
CH_3	211	Ru	0.06
CH_3-CH_2	211	Ag	4.63
CH_3-CH_2	211	Au	4.05
CH_3-CH_2	211	Cu	3.89
CH_3-CH_2	211	Pd	3.07
CH_3-CH_2	211	Pt	2.64
CH_3-CH_2	211	Rh	2.39
CH_3-CH_2	211	Ru	2.33
CH_3-CH_3	211	Ag	4.53
CH_3-CH_3	211	Au	4.41
CH_3-CH_3	211	Cu	3.75
CH_3-CH_3	211	Pt	3.39
CH_3-CH_3	211	Rh	2.72
CH_3-CH_3	211	Ru	2.42
CH_3CH_2	211	Ag	2.30
CH_3CH_2	211	Au	1.94
CH_3CH_2	211	Cu	1.91
CH_3CH_2	211	Pd	1.68
CH_3CH_2	211	Pt	1.22
CH_3CH_2	211	Rh	1.26

CH_3CH_2	211	Ru	1.06
CH_3CH_2-H	211	Ag	3.04
CH_3CH_2-H	211	Au	2.59
CH_3CH_2-H	211	Cu	2.52
CH_3CH_2-H	211	Pd	2.24
CH_3CH_2-H	211	Pt	1.48
CH_3CH_2-H	211	Rh	1.45
CH_3CH_2-HO	211	Ag	3.54
CH_3CH_2-HO	211	Cu	2.75
CH_3CH_2-HO	211	Pd	2.88
CH_3CH_2-HO	211	Pt	2.50
CH_3CH_2-HO	211	Rh	1.90
CH_3CH_2-HOH	211	Ag	3.01
CH_3CH_2-HOH	211	Cu	2.62
CH_3CH_2-HOH	211	Pd	2.43
CH_3CH_2-HOH	211	Pt	2.07
CH_3CH_2-HOH	211	Rh	1.98
CH_3CH_2-OH	211	Cu	3.12
CH_3CH_2-OH	211	Pd	3.10
CH_3CH_2-OH	211	Pt	2.90
CH_3CH_2-OH	211	Rh	2.36
CHO	211	Ag	3.21
CHO	211	Au	2.88
CHO	211	Cu	2.75
CHO	211	Pd	1.84
CHO	211	Pt	1.79
CHO	211	Rh	1.83
CHO-O	211	Ag	5.36
CHO-O	211	Cu	4.13
CHO-O	211	Pd	4.79
CHO-O	211	Pt	4.15
CHO-O	211	Rh	3.20
CO	211	Ag	2.87
CO	211	Au	2.57
CO	211	Co	1.40
CO	211	Cu	2.28
CO	211	Ni	1.25
CO	211	Pd	1.22
CO	211	Pt	1.11
CO	211	Re	0.75
CO	211	Rh	1.07
CO	211	Ru	0.98

CO-H	211	Ag	5.35
CO-H	211	Cu	4.30
CO-H	211	Pd	2.59
CO-H	211	Pt	2.50
CO-H	211	Rh	2.93
CO-HO	211	Ag	4.03
CO-HO	211	Cu	3.07
CO-HO	211	Pd	2.48
CO-HO	211	Pt	2.41
CO-HO	211	Rh	1.74
CO-HOH	211	Ag	3.51
CO-HOH	211	Cu	2.95
CO-HOH	211	Pd	3.37
CO-HOH	211	Pt	2.07
CO-HOH	211	Rh	1.85
CO-OH	211	Ag	3.75
CO-OH	211	Au	4.14
CO-OH	211	Cu	2.97
CO-OH	211	Pd	3.10
CO-OH	211	Pt	2.80
CO-OH	211	Rh	2.40
CO-OH	211	Ru	2.27
COH	211	Ag	4.59
COH	211	Cu	3.57
COH	211	Cu	3.55
COH	211	Pd	1.90
COH	211	Pt	1.92
COH	211	Rh	1.94
COO-H	211	Ag	4.36
COO-H	211	Cu	3.88
COO-H	211	Pd	2.85
COO-H	211	Pt	2.62
COO-H	211	Rh	2.60
COOH	211	Cu	2.70
COOH	211	Cu	2.39
COOH	211	Pd	2.17
COOH	211	Pd	2.03
COOH	211	Pt	1.94
COOH	211	Pt	1.55
COOH	211	Rh	1.59
H	211	Ag	0.24
H	211	Au	0.17

H	211	Cu	-0.09
H	211	Ni	-0.39
H	211	Pd	-0.40
H	211	Pt	-0.35
H	211	Re	-0.69
H	211	Rh	-0.32
H	211	Ru	-0.44
H-CH	211	Ag	4.74
H-CH	211	Au	4.58
H-CH	211	Co	1.78
H-CH	211	Cu	3.27
H-CH	211	Ni	1.93
H-CH	211	Pd	2.05
H-CH	211	Pt	2.35
H-CH	211	Re	0.60
H-CH	211	Rh	1.54
H-CH	211	Ru	1.07
$H-CH_2$	211	Ag	3.52
$H-CH_2$	211	Au	2.81
$H-CH_2$	211	Co	0.99
$H-CH_2$	211	Cu	2.50
$H-CH_2$	211	Ni	1.41
$H-CH_2$	211	Pd	1.53
$H-CH_2$	211	Pt	0.94
$H-CH_2$	211	Re	0.28
$H-CH_2$	211	Rh	0.79
$H-CH_2$	211	Ru	0.68
$H-CH_2CH_2$	211	Ag	3.40
$H-CH_2CH_2$	211	Au	3.37
$H-CH_2CH_2$	211	Cu	2.80
$H-CH_2CH_2$	211	Pd	2.28
$H-CH_2CH_2$	211	Pt	1.99
$H-CH_2CH_2$	211	Pt	1.99
$H-CH_2CH_2$	211	Rh	1.61
$H-CH_2CH_2$	211	Rh	1.61
$H-CH_3$	211	Ag	2.23
$H-CH_3$	211	Au	1.83
$H-CH_3$	211	Co	0.86
$H-CH_3$	211	Cu	1.70
$H-CH_3$	211	Ni	1.13
$H-CH_3$	211	Pd	0.83
$H-CH_3$	211	Pt	0.73

H-CH_3	211	Re	0.49
H-CH_3	211	Rh	0.66
H-CH_3	211	Ru	0.52
H-CO	211	Ag	3.70
H-CO	211	Au	3.30
H-CO	211	Cu	3.11
H-CO	211	Pd	1.97
H-CO	211	Pt	1.85
H-CO	211	Rh	1.82
H-COH	211	Cu	4.12
H-COH	211	Pd	2.43
H-COH	211	Pt	2.49
H-COH	211	Rh	2.54
H-COO	211	Ag	3.47
H-COO	211	Cu	2.89
H-COO	211	Pd	2.99
H-COO	211	Pt	2.87
H-COO	211	Rh	2.63
H-H	211	Ag	1.40
H-H	211	Au	1.15
H-H	211	Cu	0.78
H-H	211	Pd	0.12
H-H	211	Rh	0.00
H-OH	211	Au	1.82
H-OH	211	Cu	0.80
H-OH	211	Ni	0.35
H-OH	211	Pd	0.82
H-OH	211	Pt	0.72
H-OH	211	Rh	0.49
H-OH	211	Ru	-0.01
H_2O	211	Ag	-0.12
H_2O	211	Co	-0.37
H_2O	211	Cu	-0.18
H_2O	211	Ni	-0.32
H_2O	211	Pd	-0.18
H_2O	211	Pt	-0.14
H_2O	211	Re	-0.58
H_2O	211	Rh	-0.29
H_2O	211	Ru	-0.57
HCO	211	Ag	3.08
HCO	211	Au	2.88
HCO	211	Au	2.66

HCO	211	Cu	2.75
HCO	211	Cu	2.78
HCO	211	Pd	1.84
HCO	211	Pt	1.79
HCO	211	Pt	1.65
HCO	211	Rh	1.83
HCO	211	Rh	1.75
HCO	211	Ru	1.49
HCOO	211	Ag	2.02
HCOO	211	Cu	1.57
HCOO	211	Pd	1.99
HCOO	211	Pt	1.85
HCOO	211	Rh	1.18
HOH-CH	211	Ag	4.44
HOH-CH	211	Cu	3.30
HOH-CH	211	Pd	2.34
HOH-CH	211	Pt	2.04
HOH-CH	211	Rh	1.76
$HOH-CH_2$	211	Ag	3.51
$HOH-CH_2$	211	Cu	2.89
$HOH-CH_2$	211	Pd	2.09
$HOH-CH_2$	211	Pt	1.67
$HOH-CH_2$	211	Rh	1.55
$HOH-CH_2CH_2$	211	Ag	2.97
$HOH-CH_2CH_2$	211	Cu	3.85
$HOH-CH_2CH_2$	211	Pd	2.95
$HOH-CH_2CH_2$	211	Pt	2.50
$HOH-CH_2CH_2$	211	Rh	0.79
$HOH-CH_3$	211	Ag	2.23
$HOH-CH_3$	211	Cu	1.82
$HOH-CH_3$	211	Pd	1.67
$HOH-CH_3$	211	Pt	1.42
$HOH-CH_3$	211	Rh	1.20
O	211	Ag	1.88
O	211	Au	2.60
O	211	Co	-0.15
O	211	Cu	0.99
O	211	Ni	0.13
O	211	Pd	1.50
O	211	Pt	1.26
O	211	Re	-1.50
O	211	Rh	0.16

O	211	Ru	-0.10
O-CO	211	Ag	5.10
O-CO	211	Au	5.45
O-CO	211	Co	2.73
O-CO	211	Cu	3.92
O-CO	211	Ni	2.77
O-CO	211	Pd	3.99
O-CO	211	Pt	3.53
O-CO	211	Rh	2.56
O-CO	211	Ru	2.35
O-H	211	Ag	2.80
O-H	211	Au	3.18
O-H	211	Cu	1.63
O-H	211	Ni	0.68
O-H	211	Pd	1.75
O-H	211	Pt	1.60
O-H	211	Rh	0.73
O-H	211	Ru	0.27
O-HOH	211	Ag	2.65
O-HOH	211	Cu	1.83
O-HOH	211	Pd	2.28
O-HOH	211	Pt	2.10
O-HOH	211	Rh	1.03
OH	211	Ag	0.49
OH	211	Au	0.94
OH	211	Cu	-0.04
OH	211	Ni	-0.50
OH	211	Pd	0.34
OH	211	Pt	0.36
OH	211	Rh	-0.37
OH	211	Ru	-0.69
OH-CH	211	Ag	4.97
OH-CH	211	Cu	3.43
OH-CH	211	Pd	2.78
OH-CH	211	Pt	2.47
OH-CH	211	Rh	1.69
$OH-CH_2$	211	Ag	4.03
$OH-CH_2$	211	Cu	3.01
$OH-CH_2$	211	Pd	2.53
$OH-CH_2$	211	Pt	2.10
$OH-CH_2$	211	Rh	1.48
$OH-CH_2CH_2$	211	Ag	3.49

$OH\text{-}CH_2CH_2$	211	Cu	3.04
$OH\text{-}CH_2CH_2$	211	Pd	3.36
$OH\text{-}CH_2CH_2$	211	Pt	3.38
$OH\text{-}CH_2CH_2$	211	Rh	2.75
$OH\text{-}CH_3$	211	Ag	2.76
$OH\text{-}CH_3$	211	Cu	1.94
$OH\text{-}CH_3$	211	Pd	2.11
$OH\text{-}CH_3$	211	Pt	1.85
$OH\text{-}CH_3$	211	Rh	1.13
OH-OH	211	Ag	1.98
OH-OH	211	Cu	1.07
OH-OH	211	Pd	1.72
OH-OH	211	Pt	1.76
OH-OH	211	Rh	0.50
C	211	Ni_3Fe (AA)	1.8
O	211	Ni_3Fe (AA)	-0.2
C	211	Ni_3Fe (AB)	1.4
O	211	Ni_3Fe (AB)	0
C	211	Ni_3Co	1.7
O	211	Ni_3Co	0.1
C	211	Ni_3Cu (AA)	1.6
O	211	Ni_3Cu (AA)	0.2
C	211	Ni_3Cu (AB)	1.1
O	211	Ni_3Cu (AB)	0
C	211	Ni_3Sn (AA)	2.7
O	211	Ni_3Sn (AA)	0.8
C	211	Ni_3Sn (AB)	1.8
O	211	Ni_3Sn (AB)	0.2
C	211	Ni_3Pd (AA)	2.1
O	211	Ni_3Pd (AA)	0.3
C	211	Ni_3Pd (AB)	1.3

O	211	Ni_3Pd (AB)	-0.7
C	211	Ni_3Pt (AA)	2.2
O	211	Ni_3Pt (AA)	0.5
C	211	Ni_3Pt (AB)	1.5
O	211	Ni_3Pt (AB)	0.3
C	211	Ni_3Rh (AA)	1.3
O	211	Ni_3Rh (AA)	0.3
C	211	Ni_3Rh (AB)	1.4
O	211	Ni_3Rh (AB)	0.2
C	211	Ni_3Ru (AA)	1.5
O	211	Ni_3Ru (AA)	0.2
C	211	Pt_3Co (AA)	2.2
O	211	Pt_3Co (AA)	0.8
C	211	Pt_3Co (AB)	2.4
O	211	Pt_3Co (AB)	1.4
C	211	Pt_3Cu (AA)	2.6
O	211	Pt_3Cu (AA)	1.5
C	211	Pt_3Cu (AB)	2.2
O	211	Pt_3Cu (AB)	1.4
C	211	Pt_3Zn (AA)	3.2
O	211	Pt_3Zn (AA)	1.3
C	211	Pt_3Zn (AB)	2.2
O	211	Pt_3Zn (AB)	1.4
C	211	Pt_3Rh (AA)	1.7
O	211	Pt_3Rh	0.7

		(AA)	
C	211	Pt_3Rh (AB)	1.9
O	211	Pt_3Rh (AB)	1.4
C	211	Pt_3Pd (AA)	2
O	211	Pt_3Pd (AA)	1.6
C	211	Pt_3Pd (AB)	1.9
O	211	Pt_3Pd (AB)	1.3
C	211	Pt_3Ag (AA)	2.4
O	211	Pt_3Ag (AA)	1.9
C	211	Pt_3Ag (AB)	1.8
O	211	Pt_3Ag (AB)	1.3
C	211	Pt_3Au (AA)	2.2
O	211	Pt_3Au (AA)	1.8
C	211	Pt_3Au (AB)	1.8
O	211	Pt_3Au (AB)	1.3
C	211	Pt_3Sn (AA)	4.2
O	211	Pt_3Sn (AA)	1.7
C	211	Pt_3Sn (AB)	2.5
O	211	Pt_3Sn (AB)	1.4

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