Supplementary Information (SI) for Physical Chemistry Chemical Physics.

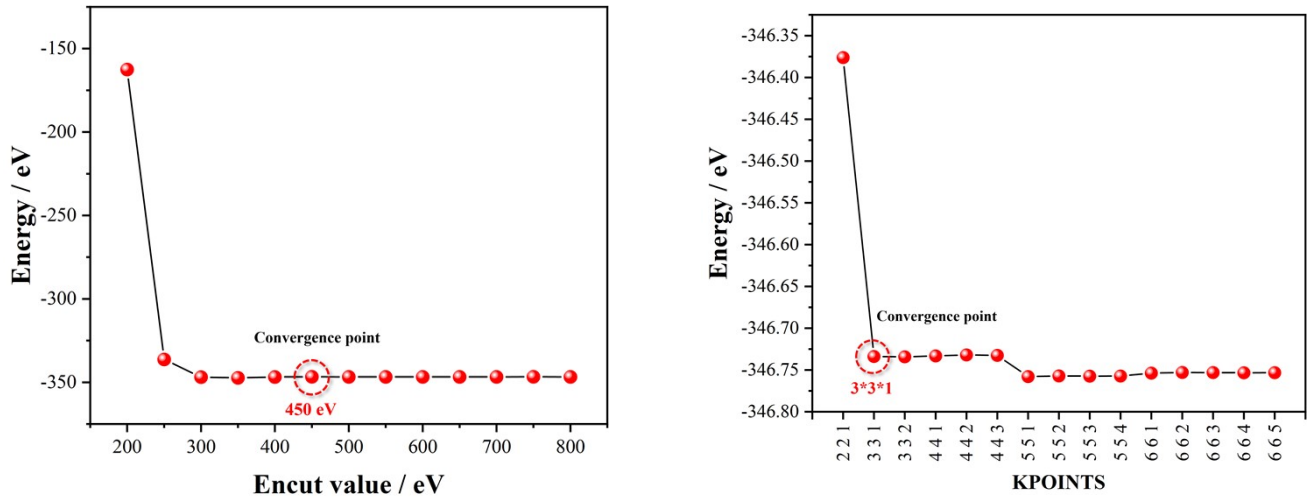
Mechanistic insights into CO_2 hydrogenation to methanol on Cu(110): Unveiling energy linear relationships and enhancing performance strategies

Huang Qin, Hai Zhang*, Xingzi Wang, Weidong Fan

School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai 200240, China

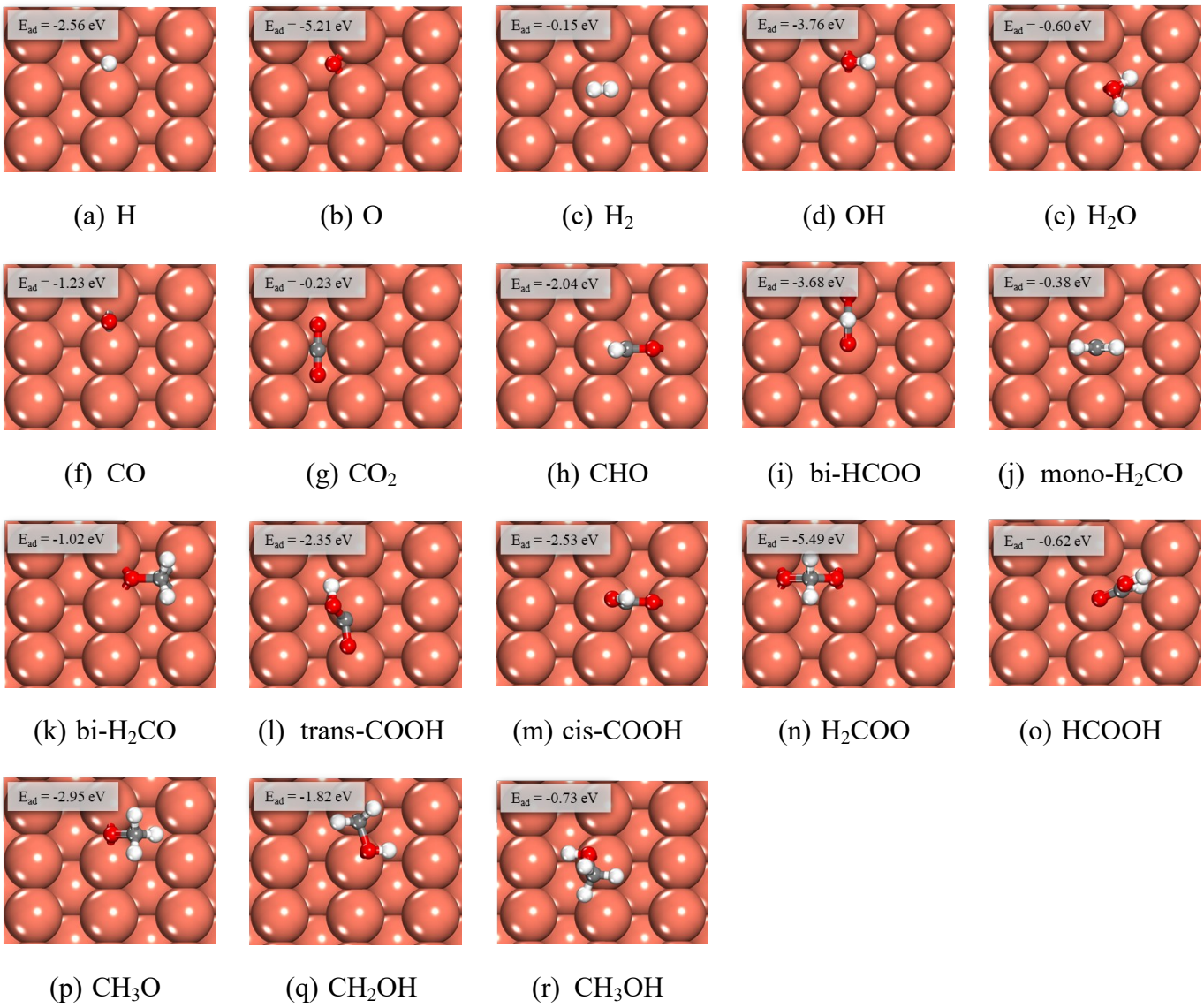
* Corresponding author.
Telephone: 021-34206052
E-mail: zhanghai@sjtu.edu.cn

1. Figure captions



(a) Convergence test on Encut value (b) Convergence test on Kpoints

Fig. S1. Convergence tests on calculation parameters, including (a) Encut value and (b) Kpoints.



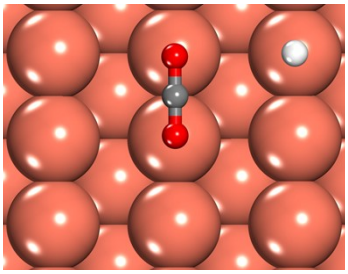
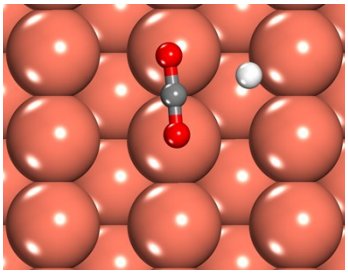
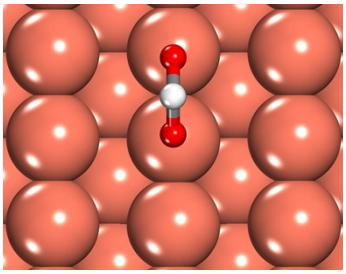
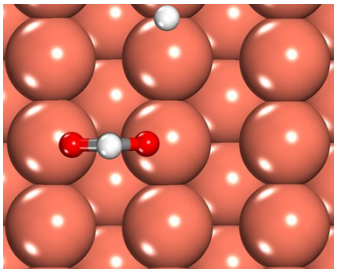
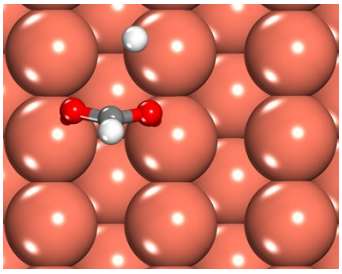
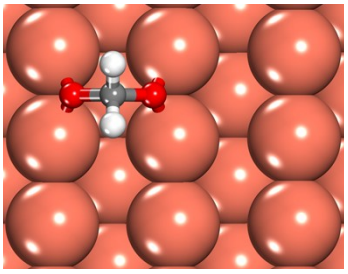
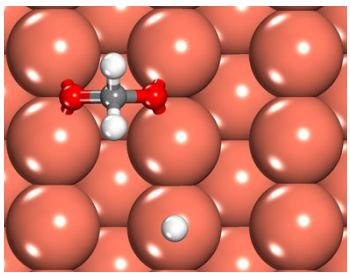
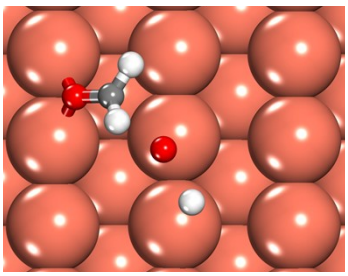
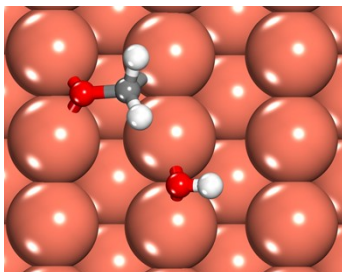
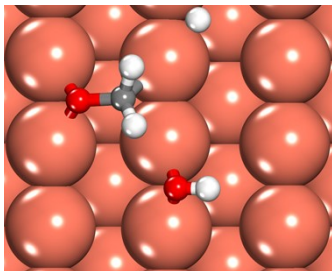
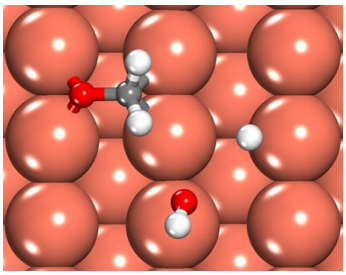
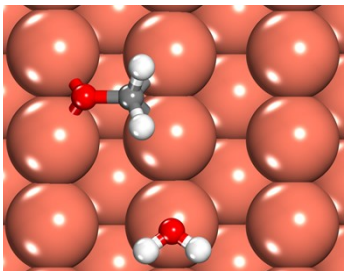
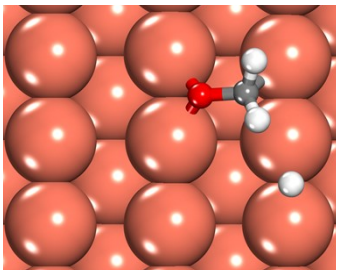
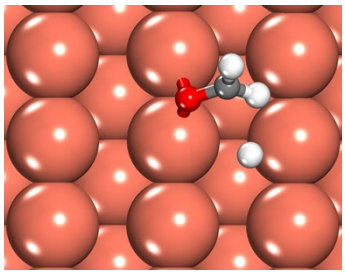
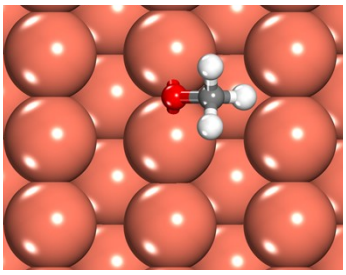
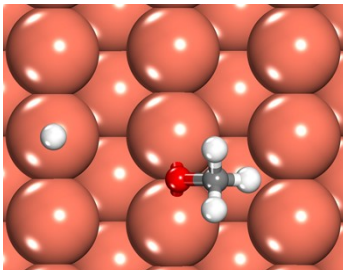
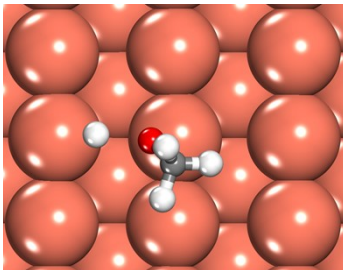
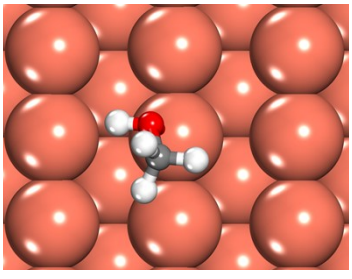
(a) H (b) O (c) H_2 (d) OH (e) H_2O

(f) CO (g) CO_2 (h) CHO (i) bi-HCOO (j) mono-H_2CO

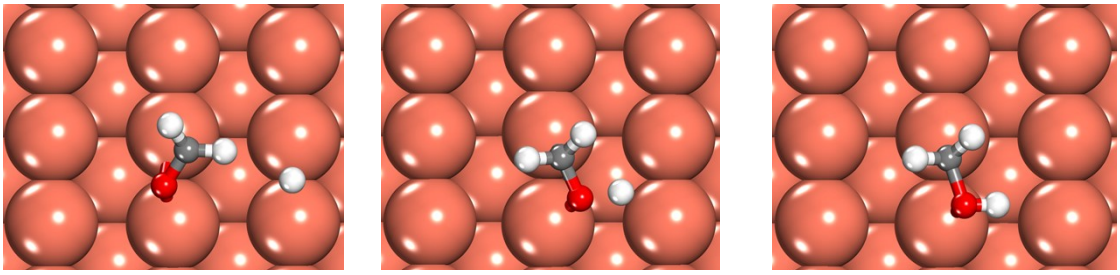
(k) bi-H_2CO (l) trans-COOH (m) cis-COOH (n) H_2COO (o) HCOOH

(p) CH_3O (q) CH_2OH (r) CH_3OH

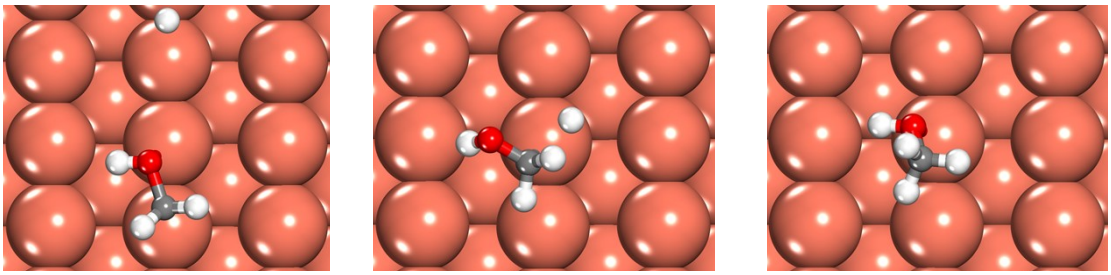
Fig. S2. The most thermodynamically stable configurations of reaction species on Cu(110) involved in CO_2 hydrogenation, labeled with the corresponding adsorption energies (Orange: Cu; Gray: C; Red: O; White: H).

Reactions	*IS*	*TS*	*FS*
R1			
R2			
R3			
R4			
R5			
R6			

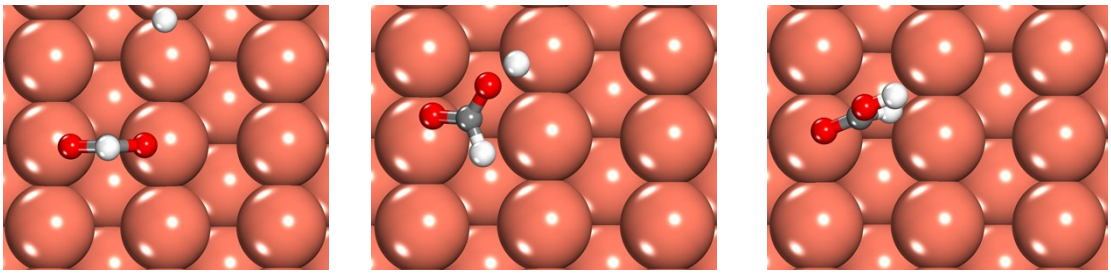
R7



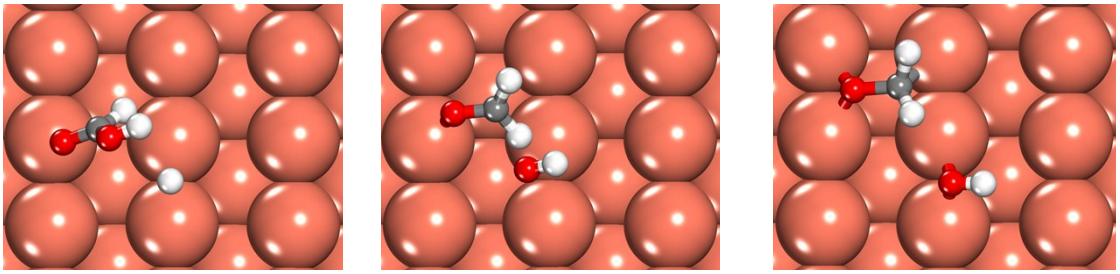
R8



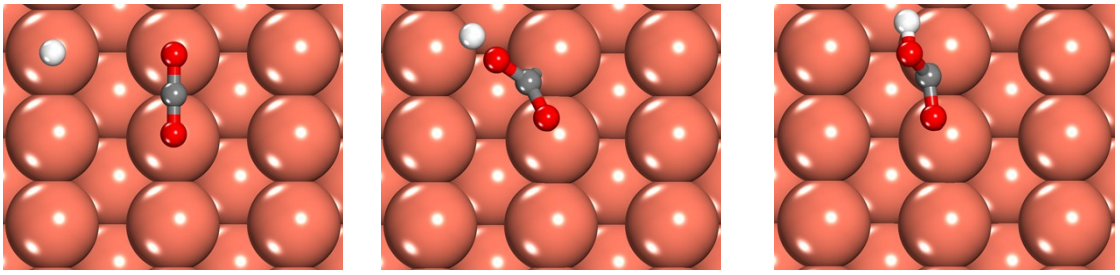
R9



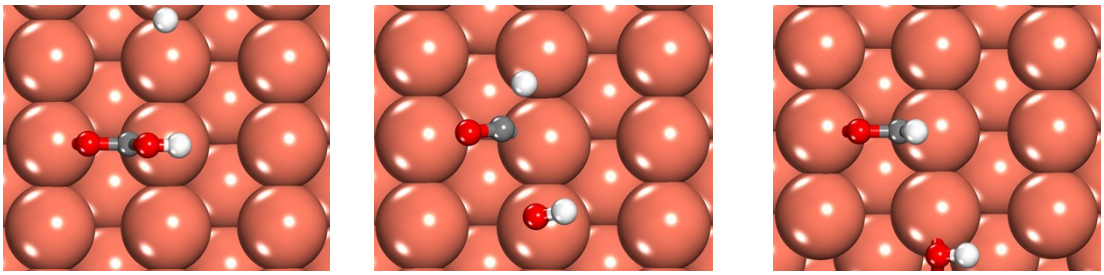
R10



R11



R12



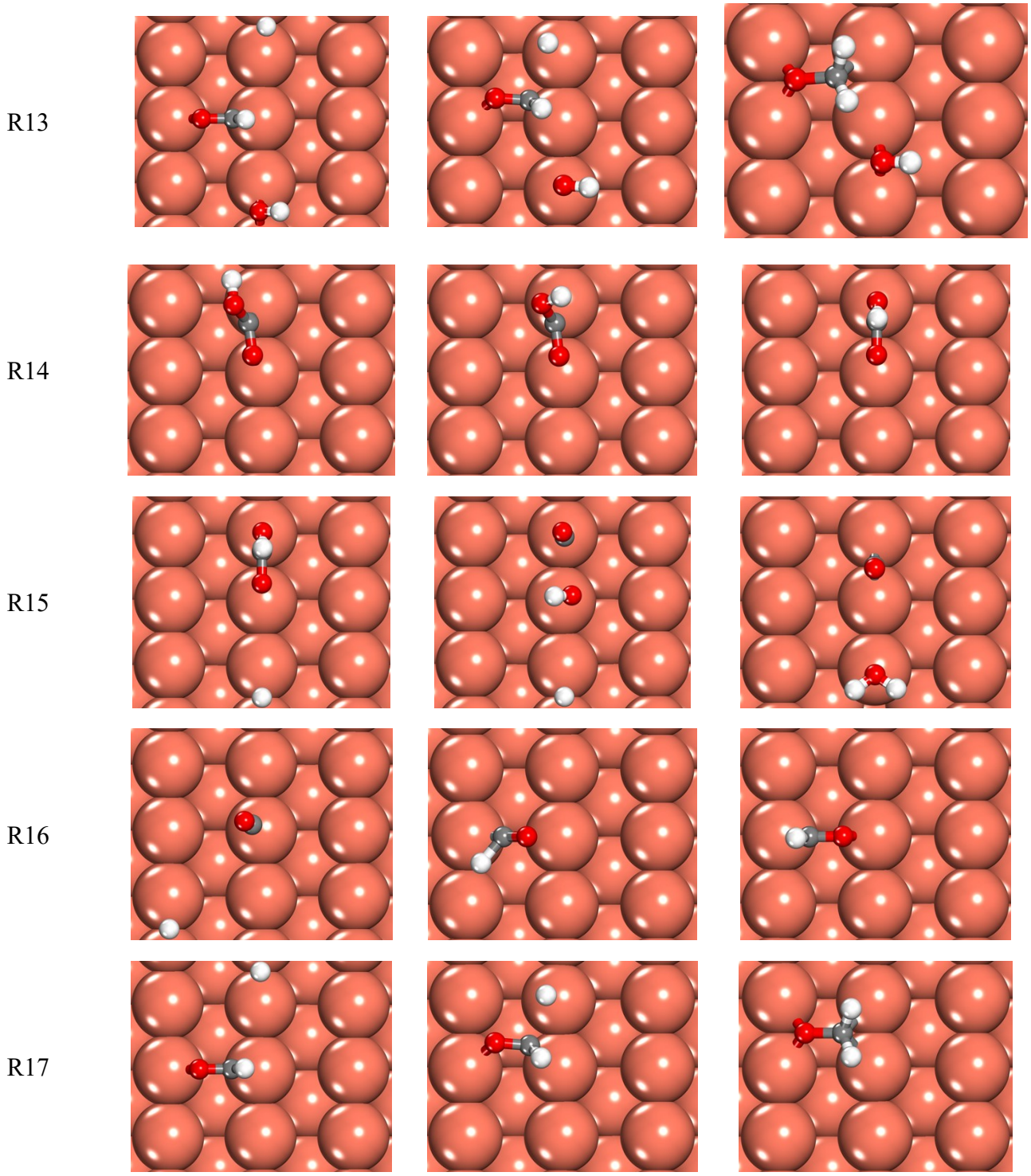
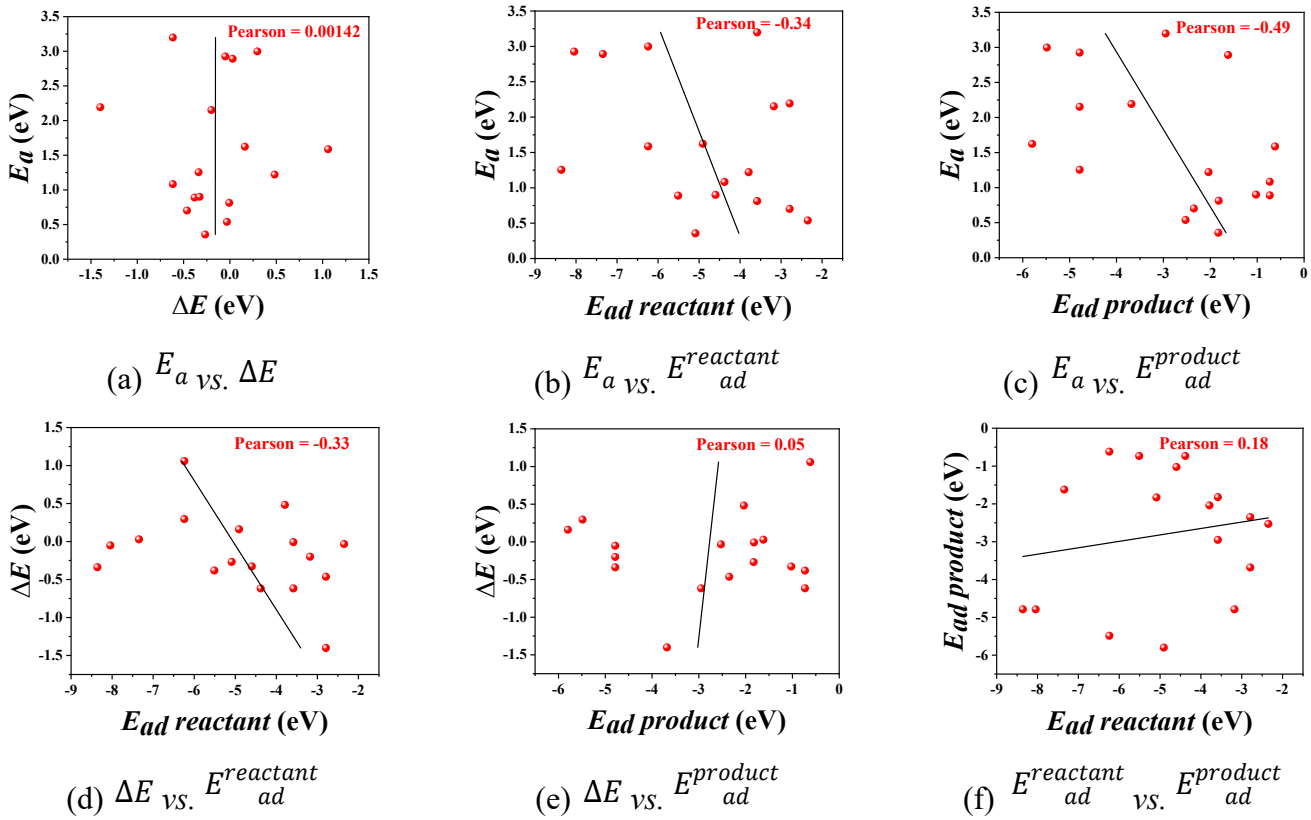


Fig. S3. Schematic diagrams of model structures for all elementary reactions (Orange: Cu; Gray: C; Red: O; White: H), where IS, TS and FS represent initial, transition and final states, respectively.



(a) $E_{a\ vs.}\ \Delta E$ (b) $E_{a\ vs.}\ E_{ad}^{reactant}$ (c) $E_{a\ vs.}\ E_{ad}^{product}$

(d) $\Delta E\ _{vs.}\ E_{ad}^{reactant}$ (e) $\Delta E\ _{vs.}\ E_{ad}^{product}$ (f) $E_{ad}^{reactant}\ _{vs.}\ E_{ad}^{product}$

Fig. S4. Correlation diagram of energy-related parameters of hydrogenation reactions on Cu(110) substrate, where energy parameters include activation energy (E_a), reaction energy (ΔE), adsorption energy of reactant ($E_{ad}^{reactant}$) and product ($E_{ad}^{product}$).

2. Table captions

Table S1. Adsorption information of all reaction species on Cu(110) with different pre-sites, where *t*, *lb*, *sb* and *h* represent top site, long bridge site, short bridge site and hollow site, respectively.

Species	Site_*t*	Site_*lb*	Site_*sb*	Site_*h*
H	-2.02	-2.41	-2.56	-2.51
O	-5.21	-5.09	-4.90	-5.14
H_2	-0.15	-0.06	-0.06	-0.07
OH	-3.76	-3.44	-3.76	-3.76
H_2O	-0.55	-0.60	-0.48	-0.51
CO	-1.15	-0.82	-1.23	-1.23
CO_2	-0.19	-0.23	-0.20	-0.23
CHO	-1.75	-2.04	-1.81	-1.52
bi-HCOO	-2.81	-3.65	-3.68	-3.56
mono-H_2CO	-0.38	-0.17	-0.28	-1.02
bi-H_2CO	-0.78	-1.02	-0.78	-1.02
trans-COOH	-2.06	-2.35	-2.14	-2.35
cis-COOH	-2.15	-2.53	-2.22	-2.53
H_2COO	-4.32	-5.49	-4.18	-5.49
HCOOH	-0.50	-0.61	-0.26	-0.62
CH_3O	-2.95	-2.57	-2.95	-2.95
CH_2OH	-1.82	-1.72	-1.82	-1.76
CH_3OH	-0.59	-0.73	-0.71	-0.71

Table S2. Information summary of description eigenvalues for linear correlation analysis.

Reaction	E_a	ΔE	$E_{ad}^{reactant}$	$E_{ad}^{product}$	*Atom number*	*Molar mass*	*valence electron count*	*Electronegativity*	*Electron affinity*
R1	2.19	-1.40	-2.79	-3.68	4	45.02	17	11.63	508.70
R2	3.00	0.30	-6.24	-5.49	5	46.03	18	13.83	581.50
R3	2.93	-0.05	-8.04	-4.79	6	47.03	19	16.03	654.30
R4	2.89	0.03	-7.35	-1.62	7	48.04	20	18.23	727.10
R5	3.20	-0.62	-3.58	-2.95	5	31.03	13	12.59	513.30
R6	0.89	-0.38	-5.51	-0.73	6	32.04	14	14.79	586.10
R7	0.81	-0.01	-3.58	-1.82	5	31.03	13	12.59	513.30
R8	1.08	-0.62	-4.38	-0.73	6	32.04	14	14.79	586.10
R9	1.59	1.06	-6.24	-0.62	5	46.03	18	13.83	581.50
R10	2.15	-0.20	-3.18	-4.79	6	47.03	19	16.03	654.30
R11	0.70	-0.46	-2.79	-2.35	4	45.02	17	11.63	508.70
R12	1.62	0.16	-4.91	-5.80	5	46.03	18	13.83	581.50
R13	1.26	-0.34	-8.36	-4.79	6	47.03	19	16.03	654.30
R14	0.54	-0.03	-2.35	-2.53	4	45.02	17	11.63	508.70
R15	0.36	-0.27	-5.09	-1.83	5	46.03	18	13.83	581.50
R16	1.22	0.48	-3.79	-2.04	3	29.02	11	8.19	367.70
R17	0.90	-0.33	-4.60	-1.02	4	30.03	12	10.39	440.50

Continue

First ionization energy	*Reactant charge*	*Product charge*	*Reactant – product charge*	*Reactant fermi level*	*Product fermi level*
5026.30	2.32	2.11	0.20	-0.34	-0.13
6338.30	2.66	2.53	0.13	-0.36	-0.11
7650.30	3.07	2.46	0.62	-0.34	-0.32
8962.30	3.00	2.50	0.50	-0.55	-0.26
6336.40	2.21	2.01	0.20	-0.35	-0.13
7648.40	2.56	2.02	0.53	-0.36	-0.02
6336.40	2.21	1.76	0.45	-0.35	-0.11
7648.40	2.31	2.02	0.28	-0.34	-0.02
6338.30	2.66	1.87	0.78	-0.36	0.02
7650.30	2.41	2.46	-0.04	-0.21	-0.32
5026.30	2.32	1.83	0.48	-0.34	-0.15
6338.30	2.38	2.27	0.10	-0.38	-0.33
7650.30	2.82	2.46	0.36	-0.56	-0.32
5026.30	1.83	1.95	-0.11	-0.15	-0.09
6338.30	2.49	1.91	0.58	-0.32	-0.31
3712.40	1.62	1.48	0.14	-0.40	-0.13
5024.40	2.03	1.67	0.36	-0.36	-0.12

Continue

$Reactant - product\ fermi\ level$	$Reactant\ IPDOS$	$Product\ IPDOS$	$Reactant - product\ IPDOS$	$Reaction\ deformation$
-0.25	-8.16	-7.87	-0.29	5.14
-0.02	-8.24	-8.60	0.36	7.47
-0.29	-8.96	-9.11	0.14	4.74
-0.23	-5.66	-5.50	-0.16	5.50
-0.33	-5.87	-6.20	0.33	6.76
-0.24	-5.66	-5.79	0.13	3.89
-0.32	-6.16	-6.20	0.04	6.85
-0.38	-8.16	-8.46	0.30	6.18
0.11	-8.83	-8.60	-0.24	7.58
-0.19	-8.51	-7.88	-0.63	3.50
-0.05	-8.25	-8.37	0.13	6.48
-0.24	-8.74	-8.60	-0.15	5.44
-0.07	-7.88	-7.89	0.02	2.54
0.00	-8.26	-8.73	0.47	6.53
-0.27	-5.29	-5.08	-0.21	5.52
-0.24	-5.44	-5.30	-0.15	3.95
-0.25	-8.16	-7.87	-0.29	5.14

Table S3. Chemical formulas of seven-dimensional SISSO variables and their correlation parameters, labelled with the activation energies of all elementary reactions involved in hydrogenation process.

$SISSO$	$Formula$	PCC
$SISSO_1^1$	2∗□□□□□□□□□□□□□+□□□	0.71
$SISSO_2^1$	$Chg_{Product} * (Chg_{Product}/IPDOS_{Product})$	-0.71
$SISSO_2^2$	$(AN/Fermi_{Product})/Derform$	0.20
$SISSO_3^1$	$Chg_{Product} * (Chg_{Product}/IPDOS_{Product})$	-0.71
$SISSO_3^2$	$(AN/Fermi_{Product})/Derform$	0.20
$SISSO_3^3$	$MM/(E_{ad}^{product} - IPDOS_{Product})$	0.15
$SISSO_4^1$	$Chg_{Product} * (Chg_{Product}/IPDOS_{Product})$	-0.71
$SISSO_4^2$	$(AN/Fermi_{Product})/Derform$	0.20
$SISSO_4^3$	$Fermi_{Reactant-Product}/(E_{ad}^{product} - IPDOS_{Product})$	0.15
$SISSO_4^4$	$(Fermi_{Product} * Fermi_{Reactant-Product})/FIE$	0.06
$SISSO_5^1$	$AN * Chg_{Product} - EN$	0.71
$SISSO_5^2$	$(MM * Chg_{Product})/IPDOS_{Product}$	-0.69
$SISSO_5^3$	$Fermi_{Reactant} * (E_{ad}^{product} + Derform)$	0.14
$SISSO_5^4$	$E_{ad}^{product} * (IPDOS_{Product} + Derform)$	0.09
$SISSO_5^5$	$Chg_{Product} + E_{ad}^{product} + Derform$	-0.10
$SISSO_6^1$	$AN * Chg_{Product} - EN$	0.71
$SISSO_6^2$	$(MM * Chg_{Product})/IPDOS_{Product}$	-0.69
$SISSO_6^3$	$Fermi_{Reactant} * (E_{ad}^{product} + Derform)$	0.14
$SISSO_6^4$	$E_{ad}^{product} * (IPDOS_{Product} + Derform)$	0.09
$SISSO_6^5$	$Chg_{Product} + E_{ad}^{product} + Derform$	-0.10
$SISSO_6^6$	$Chg_{Product}/(Derform - AN)$	0.41
$SISSO_7^1$	$AN * Chg_{Product} - EN$	0.71
$SISSO_7^2$	$(AN/Fermi_{Product})/Derform$	0.20
$SISSO_7^3$	$Fermi_{Reactant-Product}/(E_{ad}^{reactant} - IPDOS_{Product})$	0.15

$SISSO_7^4$	$(IPDOS_{Reactant-Product}/E_{ad}^{reactant})/Chg_{Reactant-Product}$	0.01
$SISSO_7^5$	$(E_{ad}^{product}+Derform)/EN$	-0.27
$SISSO_7^6$	$VEC/(AN+IPDOS_{Reactant})$	-0.11
$SISSO_7^7$	$IPDOS_{Product}/(AN+IPDOS_{Reactant})$	0.11

Table S4. Chemical formulas of seven-dimensional SISSO variables and their correlation parameters, labelled with the reaction energies of all elementary reactions involved in hydrogenation process.

SISSO	*Formula*	*PCC*
$SISSO_1^1$	$IPDOS_{Reactant-Product} * (IPDOS_{Reactant-Product}/Fermi_{Product})$	0.72
$SISSO_2^1$	$(Chg_{Reactant-Product} - IPDOS_{Reactant-Product})/Fermi_{Product}$	0.71
$SISSO_2^2$	$IPDOS_{Reactant}/(E_{ad}^{product} + AN)$	0.57
$SISSO_3^1$	$(Chg_{Reactant-Product} - IPDOS_{Reactant-Product})/Fermi_{Product}$	0.71
$SISSO_3^2$	$IPDOS_{Reactant}/(E_{ad}^{product} + AN)$	0.57
$SISSO_3^3$	$IPDOS_{Reactant-Product}/(IPDOS_{Reactant} + Derform)$	-0.53
$SISSO_4^1$	$(Chg_{Reactant-Product} - IPDOS_{Reactant-Product})/Fermi_{Product}$	0.71
$SISSO_4^2$	$Fermi_{Reactant-Product}/(Chg_{Reactant-Product} + IPDOS_{Reactant-Product})$	0.33
$SISSO_4^3$	$Chg_{Product}/(E_{ad}^{product} + AN)$	-0.56
$SISSO_4^4$	$IPDOS_{Reactant}/(E_{ad}^{product} + AN)$	0.57
$SISSO_5^1$	$(Chg_{Reactant-Product} - IPDOS_{Reactant-Product})/Fermi_{Product}$	0.71
$SISSO_5^2$	$Chg_{Product}/(E_{ad}^{product} + AN)$	-0.56
$SISSO_5^3$	$IPDOS_{Reactant}/(E_{ad}^{product} + AN)$	0.57
$SISSO_5^4$	$Fermi_{Reactant}/(Chg_{Reactant-Product} + IPDOS_{Reactant-Product})$	0.30
$SISSO_5^5$	$Fermi_{Reactant-Product} + Fermi_{Reactant}/E_{ad}^{product}$	0.22
$SISSO_6^1$	$(Chg_{Reactant-Product} - IPDOS_{Reactant-Product})/Fermi_{Product}$	0.71
$SISSO_6^2$	$E_{ad}^{reactant}/(Chg_{Reactant-Product} + IPDOS_{Reactant-Product})$	0.32
$SISSO_6^3$	$Chg_{Product}/(E_{ad}^{product} + AN)$	-0.56
$SISSO_6^4$	$IPDOS_{Reactant}/(E_{ad}^{product} + AN)$	0.57
$SISSO_6^5$	$Fermi_{Reactant-Product} + Fermi_{Reactant}/E_{ad}^{product}$	0.22
$SISSO_6^6$	$FIE/(Fermi_{Product} - Fermi_{Reactant-Product})$	-0.06
$SISSO_7^1$	$Chg_{Reactant-Product} - IPDOS_{Reactant-Product})/Fermi_{Product}$	0.71
$SISSO_7^2$	$E_{ad}^{reactant}/(Chg_{Reactant-Product} + IPDOS_{Reactant-Product})$	0.32
$SISSO_7^3$	$Chg_{Product}/(E_{ad}^{product} + AN)$	-0.56

$SISSO_7^4$	$IPDOS_{Reactant}/(E_{ad}^{product} + AN)$	0.57
$SISSO_7^5$	$Fermi_{Reactant-Product} + Fermi_{Reactant}/E_{ad}^{product}$	0.22
$SISSO_7^6$	$E_{ad}^{reactant}/(Fermi_{Product} - Fermi_{Reactant-Product})$	0.02
$SISSO_7^7$	$IPDOS_{Reactant-Product} + EN/E_{ad}^{reactant}$	0.49

Table S5. Chemical formulas of seven-dimensional SISSO variables and their respective correlation parameters, labelled with the activation energies of elementary reactions with hydrogen attacking carbon atom.

$SISSO$	$Formula$	PCC	$RMSE$
$SISSO_1^1$	$IPDOS_{Product}/E_{ad}^{product} - EN$	-0.96	10.86
$SISSO_2^1$	$IPDOS_{Product}/E_{ad}^{product} - EN$	-0.96	10.86
$SISSO_2^2$	$Fermi_{Product}/(VEC - EN)$	-0.56	2.24
$SISSO_3^1$	$IPDOS_{Product}/E_{ad}^{product} - EN$	-0.96	10.86
$SISSO_3^2$	$Fermi_{Product}/(VEC - EN)$	-0.56	2.24
$SISSO_3^3$	$(Chg_{Product} + Derform)/EA$	-0.27	2.13
$SISSO_4^1$	$(E_{ad}^{product} - AN)/Chg_{Product}$	-0.95	5.66
$SISSO_4^2$	$Fermi_{Reactant-Product} + Derform/MM$	0.18	2.22
$SISSO_4^3$	$Chg_{Reactant-Product} + AN/Derform$	-0.06	1.30
$SISSO_4^4$	$IPDOS_{Reactant-Product}/(E_{ad}^{product} + Fermi_{Product})$	0.04	2.07
$SISSO_5^1$	$IPDOS_{Reactant}/(E_{ad}^{product} - EN)$	-0.96	10.79
$SISSO_5^2$	$(E_{ad}^{product} * FIE)/MM$	-0.96	455.04
$SISSO_5^3$	$VEC/(IPDOS_{Product} + Derform)$	-0.62	3205.35
$SISSO_5^4$	$EN/(Chg_{Reactant-Product} - Derform)$	-0.21	4.40
$SISSO_5^5$	$Chg_{Product}/(IPDOS_{Reactant-Product} - Chg_{Reactant})$	-0.13	2.90
$SISSO_6^1$	$IPDOS_{Product}/E_{ad}^{product} - EN$	-0.96	10.86
$SISSO_6^2$	$Fermi_{Reactant} * (E_{ad}^{product} + VEC)$	0.01	6.14
$SISSO_6^3$	$Derform * (Fermi_{Reactant} + Fermi_{Product})$	-0.25	4.57
$SISSO_6^4$	$(MM * IPDOS_{Reactant-Product})/ E_{ad}^{product}$	0.11	3.38
$SISSO_6^5$	$MM/(Fermi_{Reactant} - IPDOS_{Reactant})$	0.12	3.94
$SISSO_6^6$	$(FIE * IPDOS_{Reactant})/E_{ad}^{reactant}$	0.35	9841.01
$SISSO_7^1$	$IPDOS_{Product}/E_{ad}^{product} - EN$	-0.96	10.86
$SISSO_7^2$	$(E_{ad}^{product} * FIE)/MM$	-0.96	455.04
$SISSO_7^3$	$Fermi_{Reactant-Product} + Derform/MM$	0.18	2.22

$SISSO_7^4$	$Derform/EN - Chg_{Reactant-Product}$	0.10	1.92
$SISSO_7^5$	$(MM * IPDOS_{Reactant-Product})/E_{ad}^{product}$	0.11	3.38
$SISSO_7^6$	$(FIE * IPDOS_{Product})/E_{ad}^{reactant}$	0.34	9403.61
$SISSO_7^7$	$E_{ad}^{product}$	-0.82	5.20

Table S6. Chemical formulas of seven-dimensional SISSO variables and their respective correlation parameters, labelled with the reaction energies of elementary reactions with hydrogen attacking carbon atom.

$SISSO$	$Formula$	PCC	$RMSE$
$SISSO_1^1$	$Chg_{Product}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.99	0.59
$SISSO_2^1$	$Chg_{Product}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.99	0.59
$SISSO_2^2$	$Derform/IPDOS_{Product} - Chg_{Reactant}$	0.25	2.78
$SISSO_3^1$	$Chg_{Product}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.99	0.59
$SISSO_3^2$	$Derform/IPDOS_{Product} - Chg_{Reactant}$	0.25	2.78
$SISSO_3^3$	$E_{ad}^{product}/(VEC - EN)$	0.08	2.90
$SISSO_4^1$	$Chg_{Reactant}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.98	0.61
$SISSO_4^2$	$E_{ad}^{reactant}/IPDOS_{Product} - Chg_{Reactant-Product}$	0.96	0.96
$SISSO_4^3$	$Chg_{Reactant-Product} + EN * Fermi_{Reactant}$	0.08	3.76
$SISSO_4^4$	$Fermi_{Reactant}/(VEC - EN)$	-0.01	0.76
$SISSO_5^1$	$Chg_{Reactant}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.98	0.61
$SISSO_5^2$	$Chg_{Product}/(VEC - EN)$	-0.01	2.56
$SISSO_5^3$	$MM/(IPDOS_{Product} + Derform)$	0.18	7648.54
$SISSO_5^4$	$Chg_{Reactant}/(IPDOS_{Product} - Derform)$	0.02	0.65
$SISSO_5^5$	$(Fermi_{Reactant} * IPDOS_{Reactant})/Derform$	0.05	1.02
$SISSO_6^1$	$Chg_{Product}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.99	0.59
$SISSO_6^2$	$E_{ad}^{reactant}/(Chg_{Reactant} + Fermi_{Reactant})$	-0.94	2.32
$SISSO_6^3$	$E_{ad}^{product}/AN - AN$	0.22	4.85
$SISSO_6^4$	$VEC/(IPDOS_{Product} + Derform)$	-0.18	1396.36
$SISSO_6^5$	$FIE/Derform - EA$	0.04	584.00
$SISSO_6^6$	$AN - Derform - Chg_{Reactant}$	0.06	2.92
$SISSO_7^1$	$Chg_{Product}/E_{ad}^{reactant} - Chg_{Reactant-Product}$	0.99	0.59
$SISSO_7^2$	$(EA/E_{ad}^{reactant})/Fermi_{Reactant}$	-0.94	364.99
$SISSO_7^3$	$Chg_{Product} * AN * EN$	-0.16	125.95

$SISSO_7^4$	$Fermi_{Product}/(VEC - EN)$	0.09	0.69
$SISSO_7^5$	$MM/Derform - Chg_{Product}$	0.00	5.31
$SISSO_7^6$	$E_{ad}^{product}$	-0.10	2.91
$SISSO_7^7$	$E_{ad}^{product}$	-0.10	2.91

Table S7. Chemical formulas of seven-dimensional SISSO variables and their respective correlation parameters, labelled with the activation energies of elementary reactions with hydrogen attacking oxygen atom.

$SISSO$	$Formula$	PCC	$RMSE$
$SISSO_1^1$	$(Derform/E_{ad}^{reactant})/Chg_{Reactant-Product}$	1.00	3.14
$SISSO_2^1$	$VEC/EA-Fermi_{Reactant}$	1.00	0.70
$SISSO_2^2$	$(VEC-EN)/Fermi_{Product}$	1.00	136.28
$SISSO_3^1$	$(Derform/E_{ad}^{reactant})/Chg_{Reactant-Product}$	1.00	3.14
$SISSO_3^2$	$IPDOS_{Reactant}+Chg_{Product}*IPDOS_{Reactant-Product}$	-0.02	8.19
$SISSO_3^3$	$AN/E_{ad}^{reactant}-IPDOS_{Reactant-Product}$	0.06	2.25
$SISSO_4^1$	$(Derform/E_{ad}^{reactant})/Chg_{Reactant-Product}$	1.00	3.14
$SISSO_4^2$	$Chg_{Reactant-Product}/E_{ad}^{product}-IPDOS_{Reactant}$	0.03	5.60
$SISSO_4^3$	$Fermi_{Reactant-Product}*IPDOS_{Reactant-Product}-Fermi_{Reactant-Product}$	-0.01	0.82
$SISSO_4^4$	$Chg_{Product}*Chg_{Reactant-Product}-IPDOS_{Reactant-Product}$	0.07	0.47
$SISSO_5^1$	$(Derform/E_{ad}^{reactant})/Chg_{Reactant-Product}$	1.00	3.14
$SISSO_5^2$	$IPDOS_{Reactant}+Chg_{Product}*IPDOS_{Reactant-Product}$	-0.02	8.19
$SISSO_5^3$	$Chg_{Product}*IPDOS_{Product}-E_{ad}^{reactant}$	-0.08	9.94
$SISSO_5^4$	$N/E_{ad}^{reactant}-IPDOS_{Reactant-Product}$	0.06	2.25
$SISSO_5^5$	$E_{ad}^{reactant}$	-0.82	5.78
$SISSO_6^1$	$(Derform/E_{ad}^{reactant})/Chg_{Reactant-Product}$	1.00	3.14
$SISSO_6^2$	$(IPDOS_{Reactant}-VEC)/IPDOS_{Product}$	-1.00	2.23
$SISSO_6^3$	$IPDOS_{Reactant-Product}/Fermi_{Reactant}-IPDOS_{Product}$	0.02	6.29
$SISSO_6^4$	$IPDOS_{Reactant-Product}+E_{ad}^{reactant}/AN$	0.02	1.92
$SISSO_6^5$	$Chg_{Product}*(E_{ad}^{reactant}+VEC)$	0.06	19.82
$SISSO_6^6$	$E_{ad}^{reactant}$	-0.82	5.78
$SISSO_7^1$	$(Derform/E_{ad}^{reactant})/Chg_{Reactant-Product}$	1.00	3.14
$SISSO_7^2$	$(Chg_{Product}/Fermi_{Reactant})/Chg_{Reactant}$	1.00	3.19

$SISSO_7^3$	$VEC * Fermi_{Product} - AN$	1.00	7.02
$SISSO_7^4$	$(Chg_{Product} * IPDOS_{Reactant})/FIE$	-0.05	1.06
$SISSO_7^5$	$IPDOS_{Reactant} * (EA - Chg_{Reactant})$	0.04	17.14
$SISSO_7^6$	$E_{ad}^{reactant}$	-0.82	5.78
$SISSO_7^7$	$E_{ad}^{product}$	0.74	2.44

Table S8. Chemical formulas of seven-dimensional SISSO variables and their respective correlation parameters, labelled with the reaction energies of elementary reactions with hydrogen attacking oxygen atom.

$SISSO$	$Formula$	PCC	$RMSE$
$SISSO_1^1$	$(MM * FIE)/Chg_{Reactant-Product}$	-1.00	435550.30
$SISSO_2^1$	$(MM * FIE)/Chg_{Reactant-Product}$	-1.00	435550.30
$SISSO_2^2$	$Fermi_{Product} + AN/Chg_{Reactant}$	-0.05	2.05
$SISSO_3^1$	$(E_{ad}^{reactant}/Chg_{Product})/Fermi_{Reactant-Product}$	1.00	8.31
$SISSO_3^2$	$(IPDOS_{Reactant}/Chg_{Product})/AN$	-0.05	1.08
$SISSO_3^3$	$(VEC/Chg_{Product})/IPDOS_{Product}$	0.14	1.37
$SISSO_4^1$	$(MM * FIE)/Chg_{Reactant-Product}$	-1.00	435550.30
$SISSO_4^2$	$Fermi_{Product} + AN/Chg_{Reactant}$	-0.05	2.05
$SISSO_4^3$	$Chg_{Product} + Chg_{Product}/IPDOS_{Product}$	0.08	1.66
$SISSO_4^4$	$(VEC/Chg_{Product})/IPDOS_{Product}$	0.14	1.37
$SISSO_5^1$	$(MM * FIE)/Chg_{Reactant-Product}$	-1.00	435550.30
$SISSO_5^2$	$(Chg_{Reactant} + IPDOS_{Reactant})/VEC$	-0.02	0.70
$SISSO_5^3$	$(Chg_{Reactant-Product}/IPDOS_{Reactant})/Derform$	-0.04	0.61
$SISSO_5^4$	$AN/MM - Chg_{Product}$	0.06	1.89
$SISSO_5^5$	$Chg_{Reactant} * IPDOS_{Reactant-Product} - Derform$	-0.05	5.14
$SISSO_6^1$	$(MM * FIE)/Chg_{Reactant-Product}$	-1.00	435550.30
$SISSO_6^2$	$EA/AN - VEC$	0.03	95.92
$SISSO_6^3$	$(Chg_{Reactant} + IPDOS_{Reactant-Product})/Derform$	0.08	0.75
$SISSO_6^4$	$Chg_{Product} + Chg_{Product}/IPDOS_{Reactant}$	0.04	1.66
$SISSO_6^5$	$(VEC/Chg_{Product})/IPDOS_{Product}$	0.14	1.37
$SISSO_6^6$	$EN + VEC/Derform$	0.15	16.47
$SISSO_7^1$	$(MM * FIE)/Chg_{Reactant-Product}$	-1.00	435550.30
$SISSO_7^2$	$EA/AN - VEC$	0.03	95.92
$SISSO_7^3$	$Chg_{Product} + Chg_{Reactant}/IPDOS_{Product}$	-0.01	1.59

$SISSO_7^4$	$Chg_{Product} + Chg_{Product}/IPDOS_{Reactant}$	0.04	1.66
$SISSO_7^5$	$Derform/(Chg_{Reactant} + IPDOS_{Reactant-Product})$	-0.13	2.11
$SISSO_7^6$	$E_{ad}^{reactant}$	-0.66	4.95
$SISSO_7^7$	AN	0.05	5.03

Table S9. Reaction energy summary for hydrogenation reactions where H adatom attacks carbon on the surface of Cu-based bimetallic alloys.

Model	Elementary reaction	Reaction energy
Cu-Au	$(CO_2 + H)^* \rightarrow$ bi-HCOO*	-0.62
	(bi-HCOO + H)* $\rightarrow$ bi-H_2COO*	-0.10
	(bi-H_2CO + H)* $\rightarrow$ CH_3O^*	-0.57
	$(CH_2OH + H)^* \rightarrow CH_3OH^*$	-0.96
	$(CO + H)^* \rightarrow CHO^*$	0.47
	(CHO + H)* $\rightarrow$ bi-H_2CO*	-0.38
Cu-Ni	$(CO_2 + H)^* \rightarrow$ bi-HCOO*	-0.32
	(bi-HCOO + H)* $\rightarrow$ bi-H_2COO*	-0.53
	(bi-H_2CO + H)* $\rightarrow$ CH_3O^*	0.10
	$(CH_2OH + H)^* \rightarrow CH_3OH^*$	-0.04
	$(CO + H)^* \rightarrow CHO^*$	0.92
	(CHO + H)* $\rightarrow$ bi-H_2CO*	0.83
Cu-Pd	$(CO_2 + H)^* \rightarrow$ bi-HCOO*	-0.52
	(bi-HCOO + H)* $\rightarrow$ bi-H_2COO*	-0.38
	(bi-H_2CO + H)* $\rightarrow$ CH_3O^*	-0.09
	$(CH_2OH + H)^* \rightarrow CH_3OH^*$	-0.27
	$(CO + H)^* \rightarrow CHO^*$	0.91
	(CHO + H)* $\rightarrow$ bi-H_2CO*	-0.16
Cu-Pt	$(CO_2 + H)^* \rightarrow$ bi-HCOO*	-0.11
	(bi-HCOO + H)* $\rightarrow$ bi-H_2COO*	-0.62
	(bi-H_2CO + H)* $\rightarrow$ CH_3O^*	-0.41
	$(CH_2OH + H)^* \rightarrow CH_3OH^*$	0.35

	$(CO + H)^* \rightarrow CHO^*$	1.22
	$(CHO + H)^* \rightarrow bi\text{-}H_2CO^*$	0.27
Cu-Zn	$(CO_2 + H)^* \rightarrow bi\text{-}HCOO^*$	-0.97
	$(bi\text{-}HCOO + H)^* \rightarrow bi\text{-}H_2COO^*$	-0.14
	$(bi\text{-}H_2CO + H)^* \rightarrow CH_3O^*$	-1.04
	$(CH_2OH + H)^* \rightarrow CH_3OH^*$	-0.82
	$(CO + H)^* \rightarrow CHO^*$	0.32
	$(CHO + H)^* \rightarrow bi\text{-}H_2CO^*$	-0.34

3. Computational details of SISSO

Input file of SISSO

```
!>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>!
ptype=1
ntask=1
task_weighting=1
scmt=.false.
desc_dim=7
nsample=17
!nsample=(n1,n2,...)
restart=0
!>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
nsf= 18
ops='(+)(-)(*)(/)'
fcomplexity=2
!funit=(1:2)
fmax_min=1e-6
fmax_max=1e6
nf_sis=20
!>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
method_so='L0'
nl1l0= 1
fit_intercept=.true.
metric='RMSE'
nmodels=300
isconvex=(1,1)
bwidth=0.001
```