

Electronic Supplementary Information

Mechanistic Insights into Higher Alcohol Synthesis from Syngas on Rh/Cu Single-Atom Alloy

Catalysts

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This supplementary information is divided into two sections, briefly summarized below.

Section 1: Additional figures:

Figure S1. Initial state (left), transition state (middle), and final state (right) for some key elementary reactions on Rh/Cu(111) surface.

Figure S2. Initial state (left), transition state (middle), and final state (right) for some key elementary reactions on Rh/Cu(100) surface.

Section 2: Additional tables.

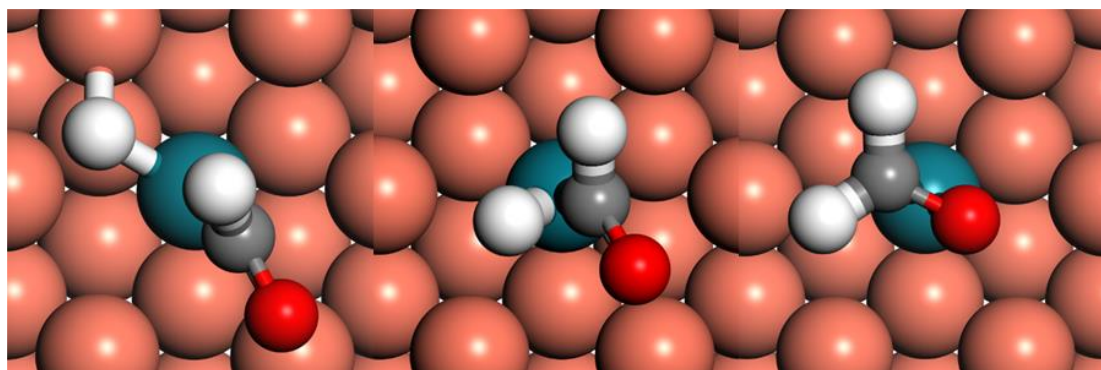
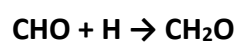
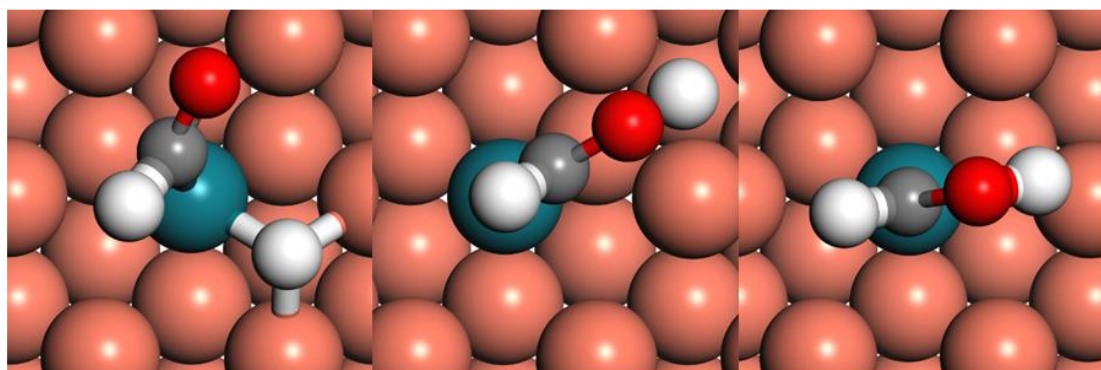
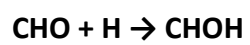
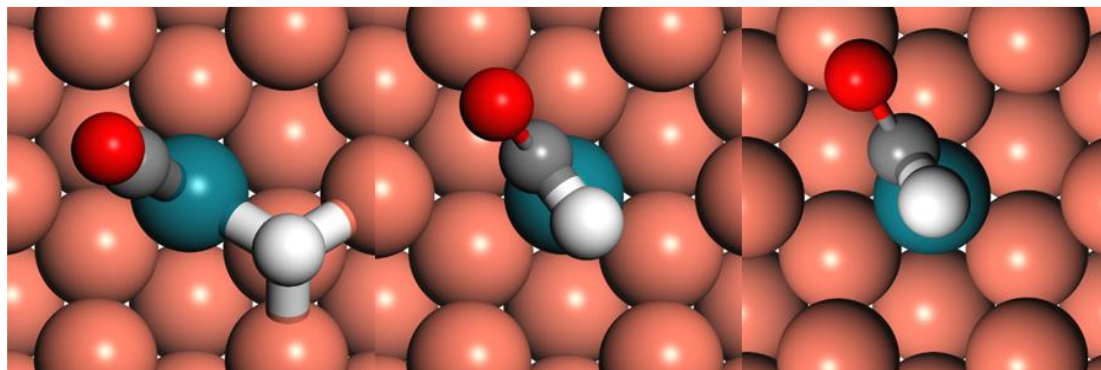
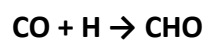
Table S1. Adsorption energies (eV) and key geometric parameters for the possible intermediates during ethanol formation from syngas on Rh/Cu SAA surfaces.

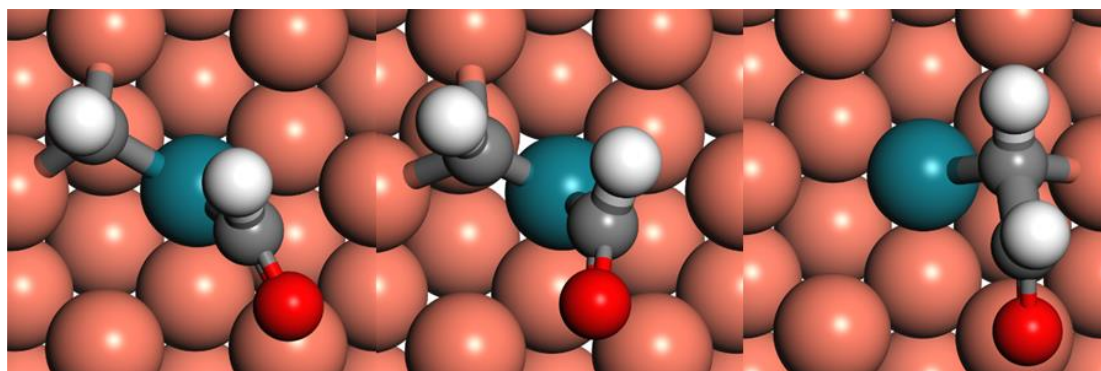
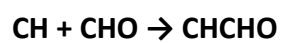
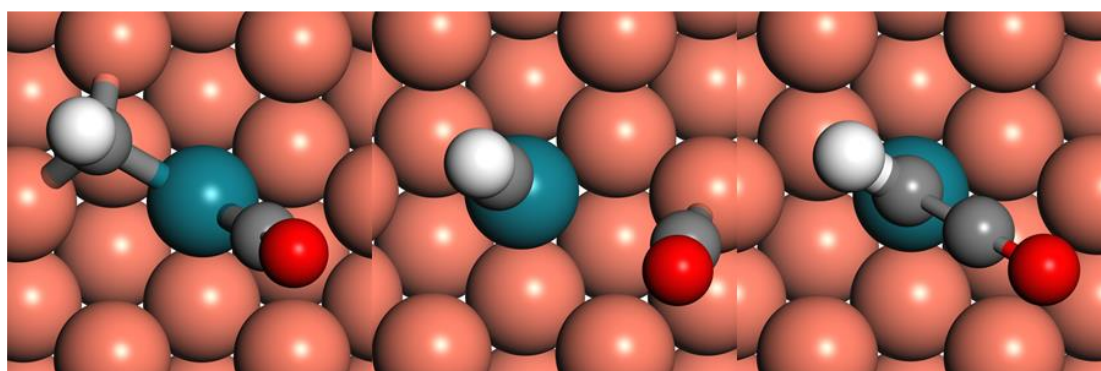
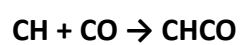
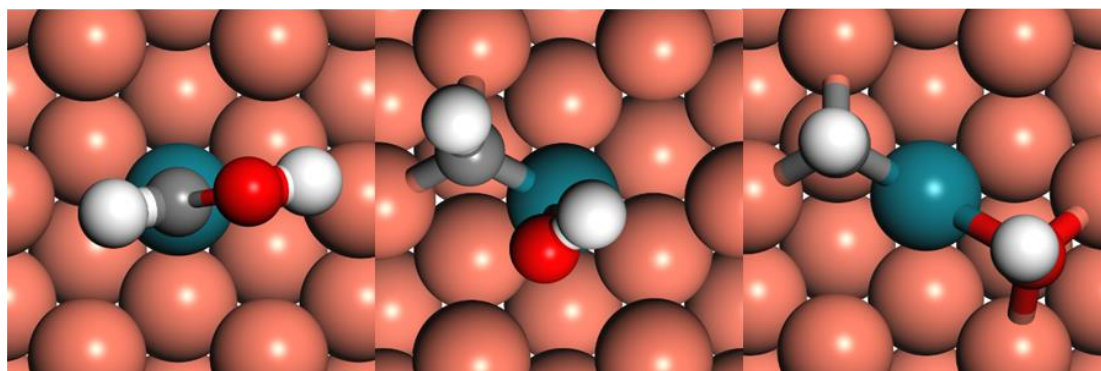
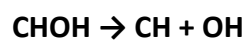
Table S2. Adsorption energies for several simple adsorbates on the Rh/Cu(111) and Rh/Cu(100) surfaces with a different number of atomic layers relaxed.

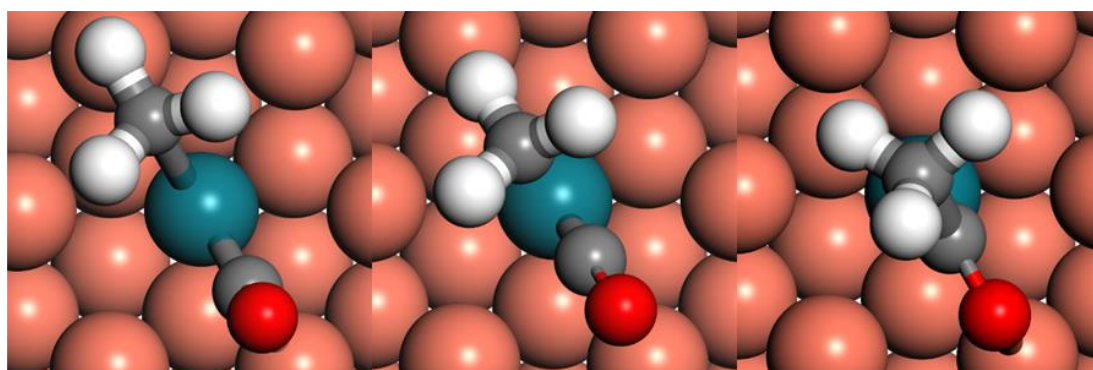
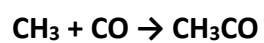
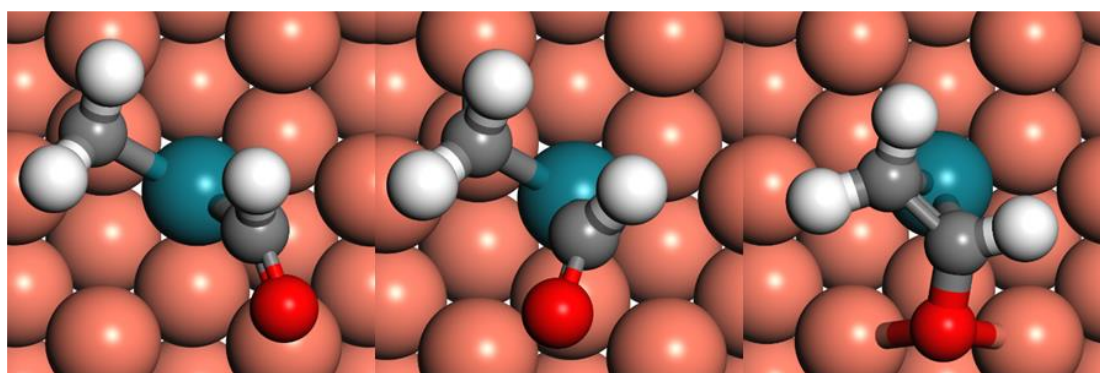
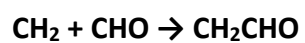
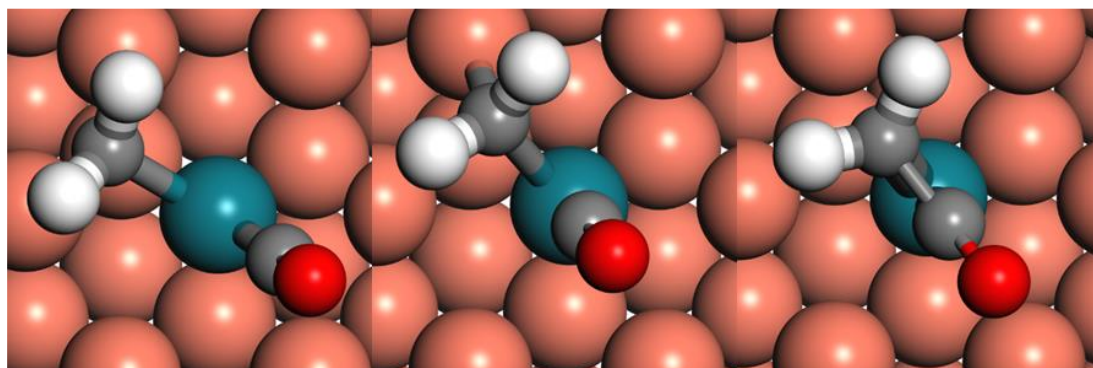
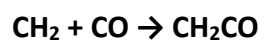
Table S3. Optimized fractional coordinates.

Table S4. Typical input files.

Fig. S1. Initial state (left), transition state (middle), and final state (right) for some key elementary reactions on Rh/Cu(111) surface.







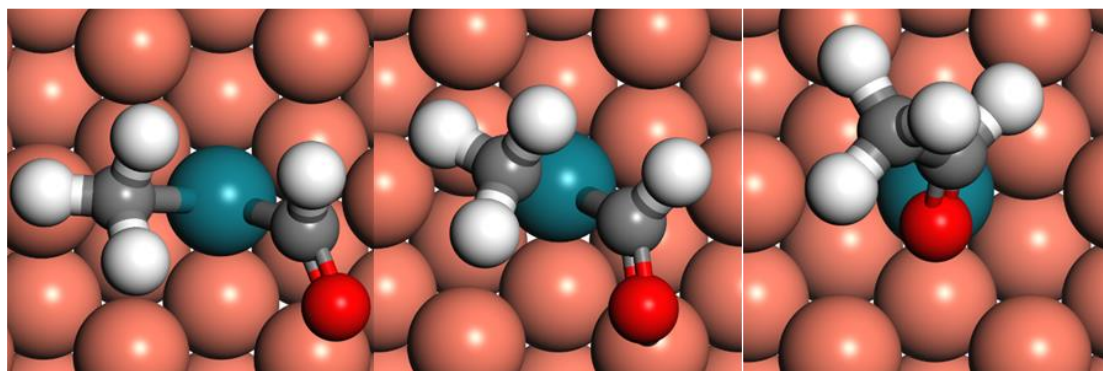
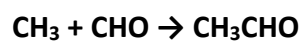
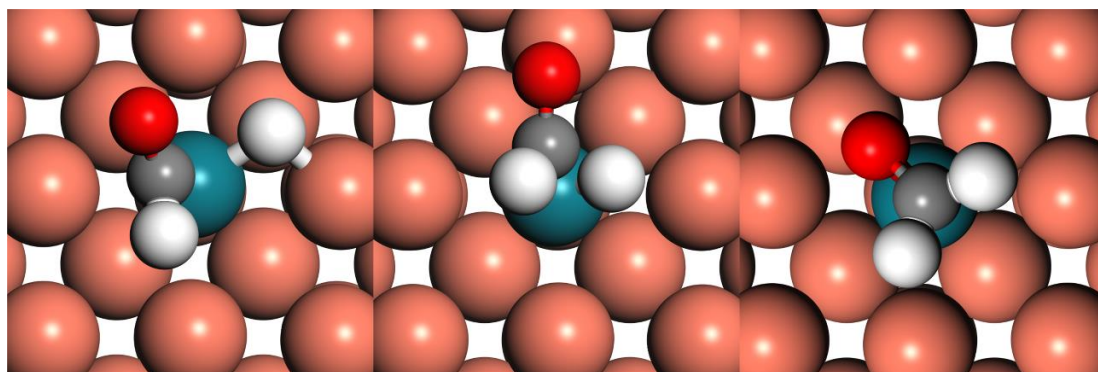
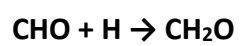
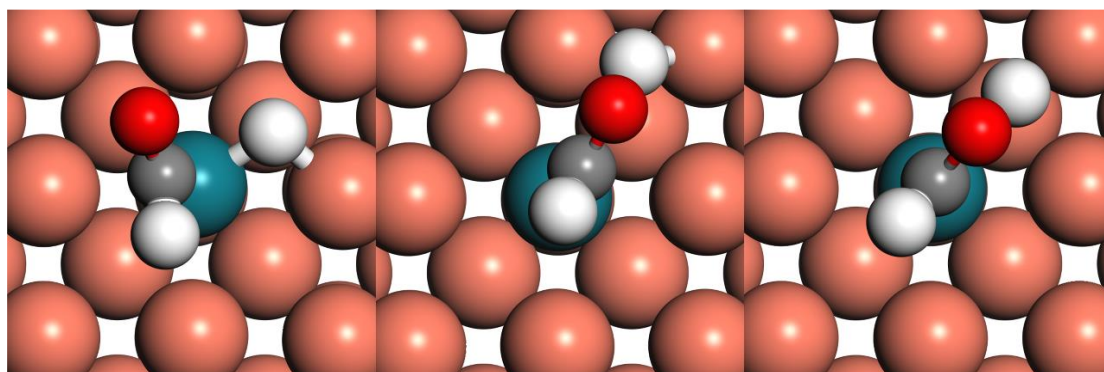
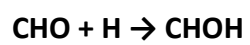
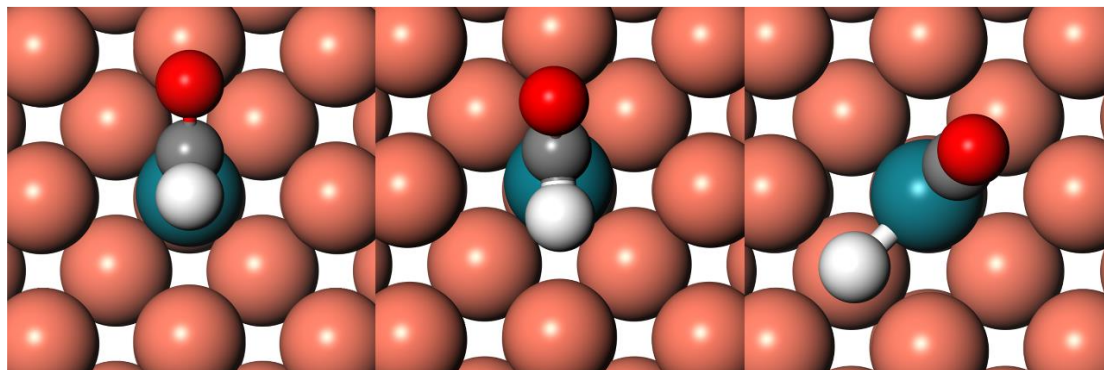
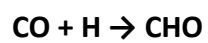
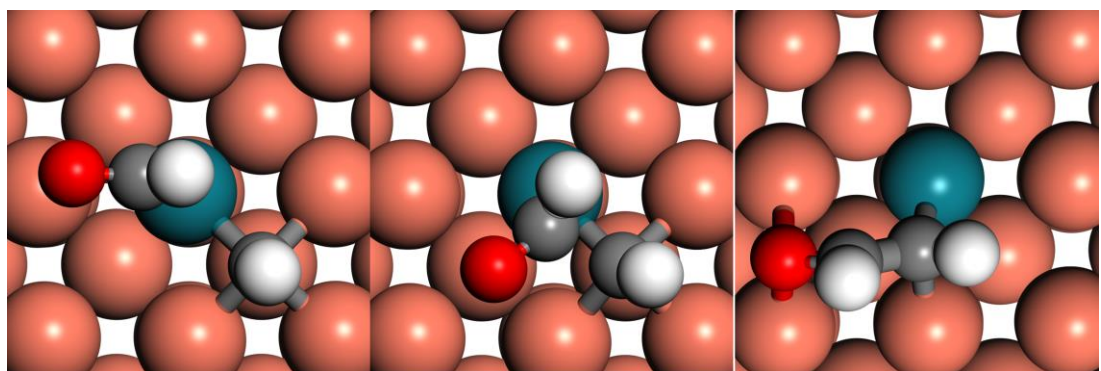
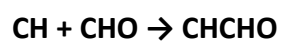
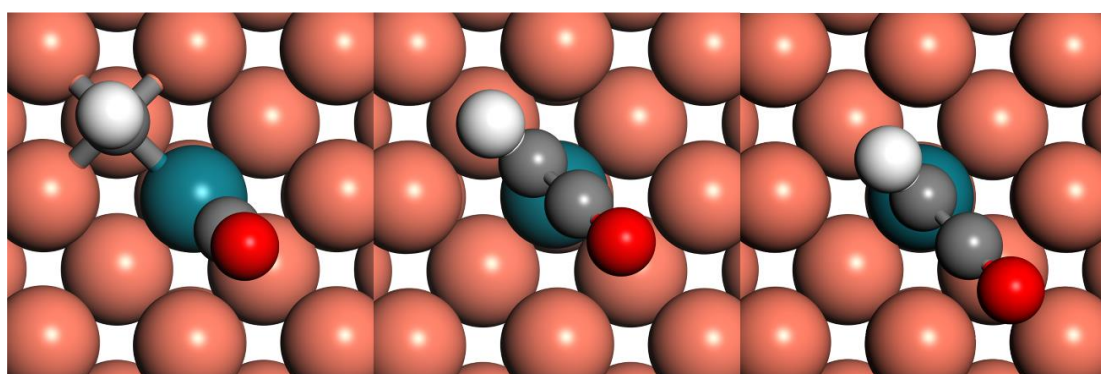
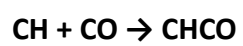
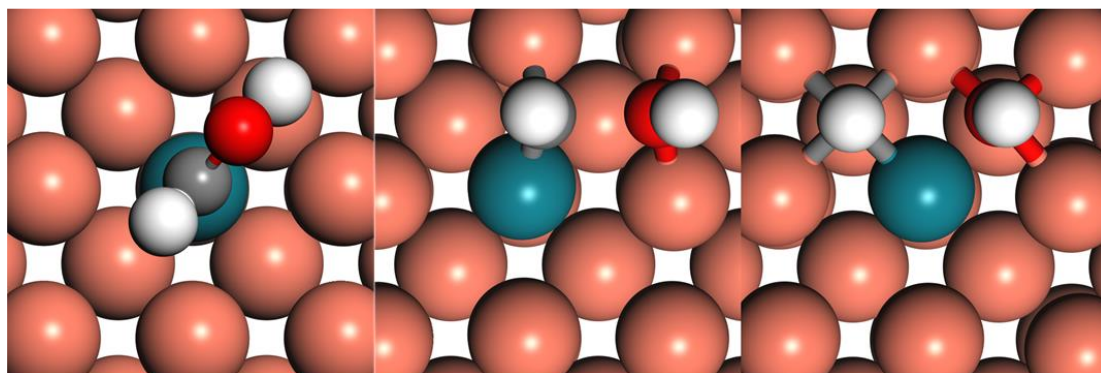
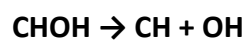
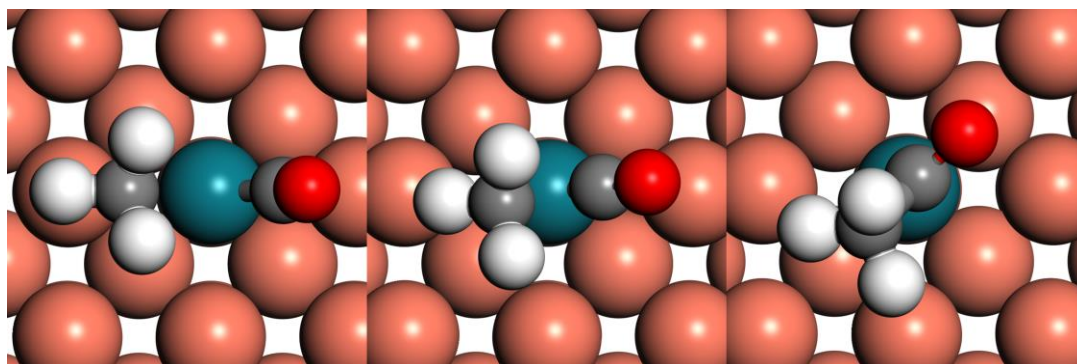
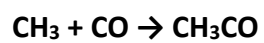
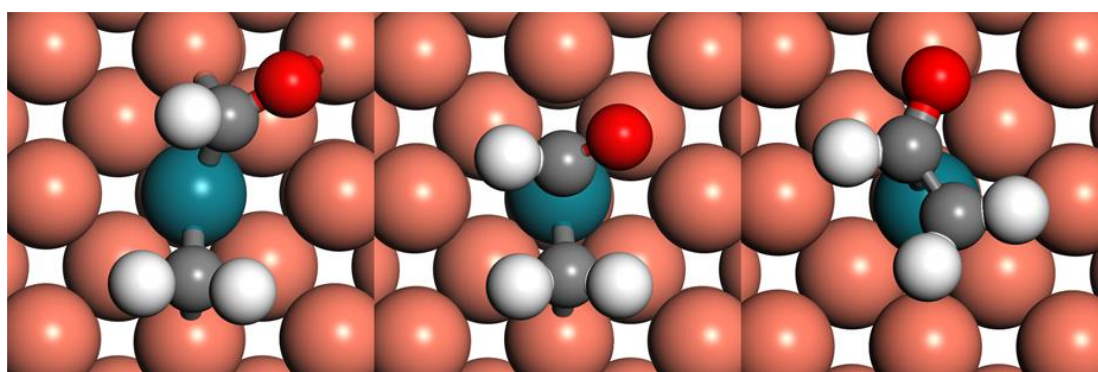
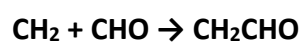
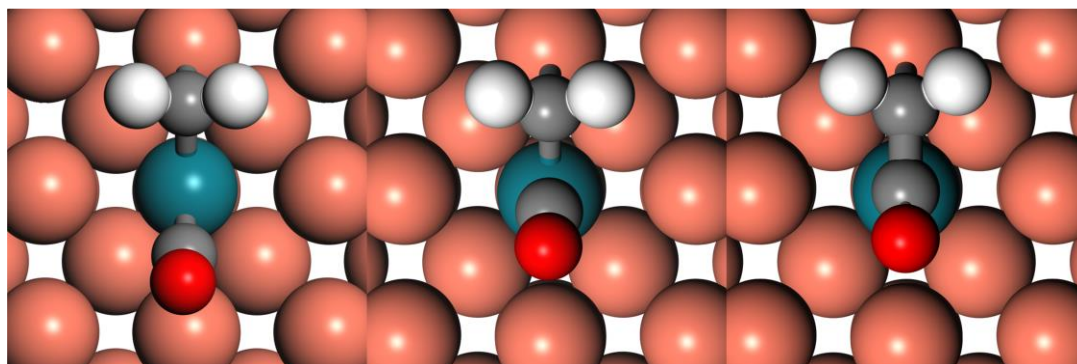
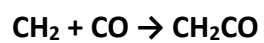


Fig. S2. Initial state (left), transition state (middle), and final state (right) for some key elementary reactions on Rh/Cu(100) surface.







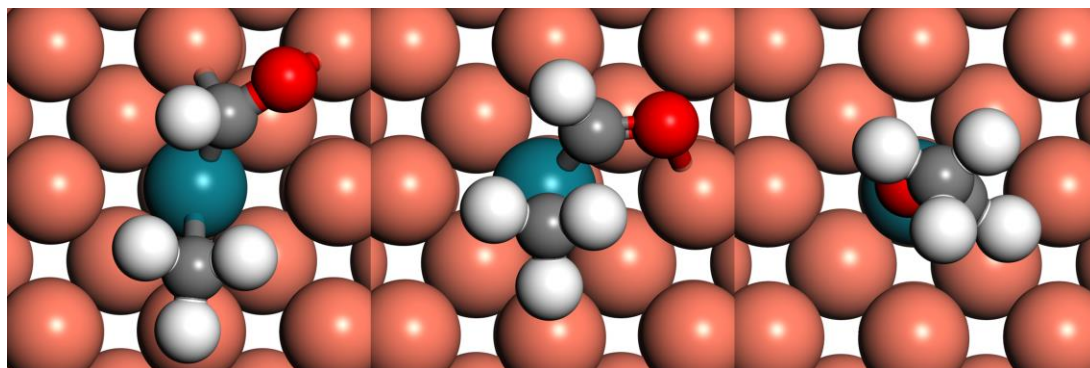
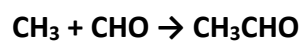


Table S1. Adsorption energies (eV) and key geometric parameters for the possible intermediates during ethanol formation from syngas on Rh/Cu SAA surfaces.

Intermediates	Rh/Cu(111)		Rh/Cu(100)	
	E_{ad}	Adsorption Site	E_{ad}	Adsorption Site
CO	-1.64	C _{d-t}	-1.80	C _{d-t}
C	-5.71	C _{d-h}	-5.27	C _{d-h}
O	-6.34	O _{d-h}	-5.63	O _{d-h}
CHO	-2.02	C _{d-t}	-2.24	C _{d-t}
COH	-3.34	C _{d-t}	-3.58	C _{d-t}
CHOH	-3.62	C _{d-t}	-3.59	C _{d-t}
CH ₂ O	-0.46	C _{d-t}	-0.65	C _{d-t}
CH ₂ OH	-1.48	C _{d-t}	-1.70	C _{d-t}
CH ₃ O	-2.14	O _{d-h}	-2.34	O _{d-h}
CH ₃ OH	-0.42	O _{d-t}	-0.50	O _{d-t}
CH	-4.39	C _{d-h}	-5.07	C _{d-h}
CH ₂	-3.19	C _{d-b}	-3.17	C _{d-b}
CH ₃	-1.52	C _{d-h}	-1.70	C _{d-h}
CH ₄	-0.13	-	-0.14	-
CHCO	-1.42	C(H) _{d-t}	-1.52	C(H) _{d-t}
CHCHO	-1.01	C(H) _{d-t}	-1.13	C(H) _{d-t}
CH ₂ CO	-0.88	C(H) _{d-t}	-1.20	C(H) _{d-t}
CH ₂ CHO	-1.32	C(H) _{d-t}	-1.07	C(H) _{d-t}
CH ₃ CO	-1.96	C(O) _{d-t}	-2.11	C(O) _{d-t}
CH ₃ COH	-2.34	C(O) _{d-t}	-2.57	C(O) _{d-t}
CH ₃ CHO	-0.35	-	-0.51	-
CH ₃ CHOH	-1.42	C _{d-t}	-1.68	C _{d-t}
CH ₃ CH ₂ O	-1.87	O _{d-h}	-2.07	O _{d-h}
CH ₃ CH ₂ OH	-0.41	-	-0.54	-
H	-3.55	H _{d-t}	-3.55	H _{d-t}
H ₂	-0.22	-	-0.33	-
OH	-3.88	O _{d-h}	-3.12	O _{d-h}
H ₂ O	-0.27	-	-0.33	-

Table S2. Adsorption energies for several simple adsorbates on the Rh/Cu(111) and Rh/Cu(100) surfaces with a different number of atomic layers relaxed.

		$E_{ad}(eV)$			
Layers relaxed		CO	C	O	H
Rh/Cu(111)	1	-1.64	-5.71	-6.34	-3.55
	2	-1.66	-5.71	-6.36	-3.56
	3	-1.66	-5.71	-6.35	-3.55
Rh/Cu(100)	1	-1.81	-6.58	-6.57	-3.54
	2	-1.81	-6.58	-6.59	-3.55
	3	-1.80	-6.57	-6.59	-3.55

Table S3. Optimized fractional coordinates.

H-CO Rh/Cu(100)	Cu Rh C O H			
	1.0000000000000000			
	7.6679000000000004	0.0000000000000000	0.0000000000000000	
	0.0000000000000000	7.6679000000000004	0.0000000000000000	
	0.0000000000000000	0.0000000000000000	13.6146999999999991	
	Cu Rh C O H			
	26	1	1	1
	Selective dynamics			
	Direct			
	0.0000000000000000	0.1666688402300522	0.1327241878263905	F F F
	0.1666688402300522	0.0000000000000000	0.0000000000000000	F F F
	0.1662712390306511	-0.0022424856069391	0.2673436382762973	T T T
	0.3333376804600975	0.1666688402300522	0.1327241878263905	F F F
	0.5000065206901496	0.0000000000000000	0.0000000000000000	F F F
	0.4997536945084138	0.0065149312655810	0.2667619271818923	T T T
	0.6666753609202019	0.1666688402300522	0.1327241878263905	F F F
	0.8333442011502470	0.0000000000000000	0.0000000000000000	F F F
	0.8333436647393340	0.9978178198878033	0.2673198709147468	T T T
	0.0000000000000000	0.5000065206901496	0.1327241878263905	F F F
	0.1666688402300522	0.3333376804600975	0.0000000000000000	F F F
	0.1637276108962195	0.3310937394049639	0.2678107260870029	T T T
	0.3333376804600975	0.5000065206901496	0.1327241878263905	F F F
	0.5000065206901496	0.3333376804600975	0.0000000000000000	F F F
	0.6666753609202019	0.5000065206901496	0.1327241878263905	F F F
	0.8333442011502470	0.3333376804600975	0.0000000000000000	F F F
	0.8384966024583448	0.3310103690021852	0.2679101634372273	T T T
	0.0000000000000000	0.8333442011502470	0.1327241878263905	F F F
	0.1666688402300522	0.6666753609202019	0.0000000000000000	F F F
	0.1662827340127671	0.6651578345473055	0.2673934826371221	T T T
	0.3333376804600975	0.8333442011502470	0.1327241878263905	F F F
	0.5000065206901496	0.6666753609202019	0.0000000000000000	F F F
	0.4995036563388847	0.6829746121281811	0.2679634581527156	T T T
	0.6666753609202019	0.8333442011502470	0.1327241878263905	F F F
	0.8333442011502470	0.6666753609202019	0.0000000000000000	F F F
	0.8332680478458524	0.6652035127021068	0.2673091644180289	T T T
	0.5013565487293019	0.3507589574212912	0.2859046199609856	T T T
	0.5059941198358999	0.4216195739193817	0.4185771234695195	T T T
	0.5121130733391148	0.5310806850838508	0.4815446644704494	T T T
	0.4983988694192233	0.2724117583130475	0.4332200443974589	T T T

H-CO Rh/Cu(111)	Cu Rh C O H
	1.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 -3.8339499999999997 6.6405961900000001 0.0000000000000000 0.0000000000000000 0.0000000000000000 19.1738999999999997
	Cu Rh C O H 26 1 1 1 1
	Selective dynamics
	Direct
	0.2929540879960022 0.1427755333075625 0.2193522795853962 T T T 0.0740787133764584 0.0370448665995440 0.0000000000000000 F F F 0.1852133131750904 0.2593140661968150 0.1088458790334812 F F F 0.6305821380552858 0.1411698561397930 0.2184406147709744 T T T 0.4074163938365558 0.0370448665995440 0.0000000000000000 F F F 0.5185509936351949 0.2593140661968150 0.1088458790334812 F F F 0.9641832757403002 0.1459536734763266 0.2190893490377451 T T T 0.7407540742966533 0.0370448665995440 0.0000000000000000 F F F 0.8518886740952922 0.2593140661968150 0.1088458790334812 F F F 0.2931150198985357 0.4793301658637448 0.2186759856012864 T T T 0.0740364784000534 0.3702980771068383 0.0000000000000000 F F F 0.1851710781986975 0.5925672767041092 0.1088458790334812 F F F 0.4073741588601507 0.3702980771068383 0.0000000000000000 F F F 0.5185087586587898 0.5925672767041092 0.1088458790334812 F F F 0.9687823363500591 0.4802714602288265 0.2192612473997663 T T T 0.7407118393202556 0.3702980771068383 0.0000000000000000 F F F 0.8518464391188871 0.5925672767041092 0.1088458790334812 F F F 0.2969205893385314 0.8126217367929037 0.2192508774208815 T T T 0.0740695378679563 0.7037018765027483 0.0000000000000000 F F F 0.1852041376666058 0.9259710761000194 0.1088458790334812 F F F 0.6305358715767553 0.8164078691431078 0.2179133676027657 T T T 0.4074072183280708 0.7037018765027483 0.0000000000000000 F F F 0.5185418181267129 0.9259710761000194 0.1088458790334812 F F F 0.9675829905593895 0.8167045618758437 0.2190284851415585 T T T 0.7407448987881580 0.7037018765027483 0.0000000000000000 F F F 0.8518794985868173 0.9259710761000194 0.1088458790334812 F F F 0.6312752009424348 0.4772095998094154 0.2309607801144714 T T T 0.6418551442478578 0.4004514880956925 0.3249558874189482 T T T 0.6577794955810762 0.2944676393188240 0.3676656497992180 T T T 0.6196339025223473 0.5345435380583251 0.3390933827576074 T T T

CHO-H Rh/Cu(100)	Cu Rh C O H
	1.000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 13.6146999999999991 Cu Rh C O H 26 1 1 1 2 Selective dynamics Direct 0.0000000000000000 0.1666688402300522 0.1327241878263905 F F F 0.1666688402300522 0.0000000000000000 0.0000000000000000 F F F 0.1657612935243426 0.9984450576870839 0.2678863527198245 T T T 0.3333376804600974 0.1666688402300522 0.1327241878263905 F F F 0.5000065206901496 0.0000000000000000 0.0000000000000000 F F F 0.4983909152068889 0.0029767492508711 0.2686379345944701 T T T 0.6666753609202019 0.1666688402300522 0.1327241878263905 F F F 0.8333442011502470 0.0000000000000000 0.0000000000000000 F F F 0.8314146592418283 1.0022797710369917 0.2685737036957067 T T T 0.0000000000000000 0.5000065206901496 0.1327241878263905 F F F 0.1666688402300522 0.3333376804600974 0.0000000000000000 F F F 0.1643849343009574 0.3318428006113556 0.2685120835726303 T T T 0.3333376804600974 0.5000065206901496 0.1327241878263905 F F F 0.5000065206901496 0.3333376804600974 0.0000000000000000 F F F 0.6666753609202019 0.5000065206901496 0.1327241878263905 F F F 0.8333442011502470 0.3333376804600974 0.0000000000000000 F F F 0.8370666508760820 0.3325200237164087 0.2675156691237709 T T T 0.0000000000000000 0.8333442011502470 0.1327241878263905 F F F 0.1666688402300522 0.6666753609202019 0.0000000000000000 F F F 0.1682384953660707 0.6657422531856289 0.2668693001446428 T T T 0.3333376804600974 0.8333442011502470 0.1327241878263905 F F F 0.5000065206901496 0.6666753609202019 0.0000000000000000 F F F 0.5052701093050971 0.6787877062168362 0.2699831912187181 T T T 0.6666753609202019 0.8333442011502470 0.1327241878263905 F F F 0.8333442011502470 0.6666753609202019 0.0000000000000000 F F F 0.8316422634674623 0.6722791830677824 0.2718531665458864 T T T 0.5004362378249378 0.3370938205282430 0.2814299722078536 T T T 0.5541611275761397 0.4011228993214211 0.4148938352945832 T T T 0.6250873348672088 0.5361187029168978 0.4504383845656817 T T T 0.5113434879308497 0.3055159142455994 0.4709332760408088 T T T 0.6718237093054458 0.6408132326612567 0.3671943773933193 T T T

CHO-H Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.173899999999997
	Cu Rh C O H		
	26	1	1 1 2
	Selective dynamics		
	Direct		
	0.2978193635255131	0.1484209445161431	0.2194004896105813 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6301818625318580	0.1445537483333986	0.2194983324547248 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9656443402095788	0.1495116957595177	0.2189673928392105 T T T
	0.7407540742966533	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2978533273329774	0.4828323885942373	0.2193896433428265 T T T
	0.0740364784000534	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781987053	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9713684640272652	0.4804592921539768	0.2183234220324685 T T T
	0.7407118393202556	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2923203124198593	0.8128705761812917	0.2249462146875023 T T T
	0.0740695378679563	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376666221	0.9259710761000194	0.1088458790334812 F F F
	0.6301521373731900	0.8189654608043373	0.2195005112210197 T T T
	0.4074072183280864	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181267442	0.9259710761000194	0.1088458790334812 F F F
	0.9713420834385375	0.8243152385567666	0.2182761858547327 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985868486	0.9259710761000194	0.1088458790334812 F F F
	0.6357183806447966	0.4845403076450009	0.2295717190031097 T T T
	0.7523753730175722	0.5428918773091527	0.3219957554899999 T T T
	0.9301950461989815	0.6318523592787176	0.3464488076632715 T T T
	0.6342302186334117	0.4837780325242459	0.3628559475597394 T T T
	1.0627061022933793	0.6980753845083117	0.2886713676211280 T T T

H-CHO Rh/Cu(100)	Cu Rh C O H
	1.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 13.6146999999999991
	Cu Rh C O H 26 1 1 1 2
	Selective dynamics
	Direct
	0.0000000000000000 0.1666688402300522 0.1327241878263905 F F F 0.1666688402300522 0.0000000000000000 0.0000000000000000 F F F 0.1684152832953667 0.0008061716059304 0.2675741243213036 T T T 0.3333376804600974 0.1666688402300522 0.1327241878263905 F F F 0.5000065206901496 0.0000000000000000 0.0000000000000000 F F F 0.5028659243067670 0.0043724056950970 0.2677546749303834 T T T 0.6666753609202019 0.1666688402300522 0.1327241878263905 F F F 0.8333442011502470 0.0000000000000000 0.0000000000000000 F F F 0.8344202575132761 0.9982798745065422 0.2673405168683110 T T T 0.0000000000000000 0.5000065206901496 0.1327241878263905 F F F 0.1666688402300522 0.3333376804600974 0.0000000000000000 F F F 0.1552402565050496 0.3329386098781406 0.2671418041747037 T T T 0.3333376804600974 0.5000065206901496 0.1327241878263905 F F F 0.5000065206901496 0.3333376804600974 0.0000000000000000 F F F 0.6666753609202019 0.5000065206901496 0.1327241878263905 F F F 0.8333442011502470 0.3333376804600974 0.0000000000000000 F F F 0.8308314534667792 0.3321627073595759 0.2684576543429972 T T T 0.0000000000000000 0.8333442011502470 0.1327241878263905 F F F 0.1666688402300522 0.6666753609202019 0.0000000000000000 F F F 0.1655595791619185 0.6672150363387704 0.2661127075774832 T T T 0.3333376804600974 0.8333442011502470 0.1327241878263905 F F F 0.5000065206901496 0.6666753609202019 0.0000000000000000 F F F 0.5038671212919299 0.6835678589511985 0.2738662955161723 T T T 0.6666753609202019 0.8333442011502470 0.1327241878263905 F F F 0.8333442011502470 0.6666753609202019 0.0000000000000000 F F F 0.8376113221846809 0.6679909063742212 0.2668062794542590 T T T 0.4906754026805807 0.3362026094091212 0.2814133727062482 T T T 0.4737908465853100 0.4422947169753852 0.4163249528891280 T T T 0.4749884464504189 0.6061554465330242 0.4249316500334164 T T T 0.4217427937812114 0.3635587222380645 0.4773831136022190 T T T 0.6237223387914148 0.3703532874765808 0.3830058471764241 T T T

H-CHO Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.173899999999997
	Cu Rh C O H		
	26	1	1 1 2
	Selective dynamics		
	Direct		
	0.2916477014684471	0.1431512032330332	0.2192069640865622 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6295490834826130	0.1418580240838938	0.2196734457763097 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9624809199342845	0.1465594845187169	0.2191916030259570 T T T
	0.7407540742966533	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2923362237630735	0.4802504180184773	0.2201857514651941 T T T
	0.0740364784000534	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781987035	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9677047075845268	0.4813165896753091	0.2186065055915736 T T T
	0.7407118393202556	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2964299521690107	0.8140402489180127	0.2194500621277913 T T T
	0.0740695378679563	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376666183	0.9259710761000194	0.1088458790334812 F F F
	0.6296575048667835	0.8168260047525623	0.2194839351366393 T T T
	0.4074072183280827	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181267368	0.9259710761000194	0.1088458790334812 F F F
	0.9670216047786643	0.8176983044206311	0.2186744205994062 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985868413	0.9259710761000194	0.1088458790334812 F F F
	0.6286990243119116	0.4794847140010932	0.2297194565559612 T T T
	0.6817553454179254	0.4655927812359932	0.3371991925404834 T T T
	0.6836845548766028	0.3227230809347076	0.3650205876283737 T T T
	0.7513007553625276	0.6148178574344223	0.3626029495441579 T T T
	0.5040312052706331	0.4255293542788682	0.3067636990885446 T T T

CH-CO Rh/Cu(100)	Cu Rh C O H			
	1.000000000000000			
	7.6679000000000004	0.000000000000000	0.000000000000000	
	0.000000000000000	7.6679000000000004	0.000000000000000	
	0.000000000000000	0.000000000000000	13.614699999999991	
	Cu Rh C O H			
	26	1	2	1 1
	Selective dynamics			
	Direct			
	0.000000000000000	0.1666688402300522	0.1327241878263905	F F F
	0.1666688402300522	0.000000000000000	0.000000000000000	F F F
	0.1671952635063078	0.9979778119573324	0.2679446262089631	T T T
	0.3333376804600974	0.1666688402300522	0.1327241878263905	F F F
	0.5000065206901496	0.000000000000000	0.000000000000000	F F F
	0.5014675515829128	1.0014528970732341	0.2669427340857604	T T T
	0.6666753609202019	0.1666688402300522	0.1327241878263905	F F F
	0.8333442011502470	0.000000000000000	0.000000000000000	F F F
	0.8336804874871456	-0.0006652582511616	0.2678619088468677	T T T
	0.000000000000000	0.5000065206901496	0.1327241878263905	F F F
	0.1666688402300522	0.3333376804600974	0.000000000000000	F F F
	0.1583507299610480	0.3324003259480166	0.2683208397956156	T T T
	0.3333376804600974	0.5000065206901496	0.1327241878263905	F F F
	0.5000065206901496	0.3333376804600974	0.000000000000000	F F F
	0.6666753609202019	0.5000065206901496	0.1327241878263905	F F F
	0.8333442011502470	0.3333376804600974	0.000000000000000	F F F
	0.8329084928983423	0.3317190947667890	0.2668745654225324	T T T
	0.000000000000000	0.8333442011502470	0.1327241878263905	F F F
	0.1666688402300522	0.6666753609202019	0.000000000000000	F F F
	0.1665274917730213	0.6669012927512878	0.2662362758824260	T T T
	0.3333376804600974	0.8333442011502470	0.1327241878263905	F F F
	0.5000065206901496	0.6666753609202019	0.000000000000000	F F F
	0.5008969765105685	0.6755955086026560	0.2692616572744537	T T T
	0.6666753609202019	0.8333442011502470	0.1327241878263905	F F F
	0.8333442011502470	0.6666753609202019	0.000000000000000	F F F
	0.8352013872333144	0.6665568019559042	0.2678304823857542	T T T
	0.4948051803432921	0.3390082734384156	0.2800098672541489	T T T
	0.4459005792557819	0.4094700931738891	0.4199593383750927	T T T
	0.5496441006568425	0.3171083299106701	0.4773203036914564	T T T
	0.6450646553514275	0.2320995702411645	0.5259243998360168	T T T
	0.3503307393425514	0.4978325124036923	0.4507539348628994	T T T

CH-CO Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.173899999999997
	Cu Rh C O H		
	26	1	2 1 1
	Selective dynamics		
	Direct		
	0.2917644298212557	0.1428036056058299	0.2186979675595609 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6289463711875561	0.1470035267200740	0.2182093773073126 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9617691963254605	0.1493718222782142	0.2171157399076920 T T T
	0.7407540742966533	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2830550607374983	0.4773204513391217	0.2225222114931461 T T T
	0.0740364784000534	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781987087	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9641097836141421	0.4821588311065779	0.2181978758885603 T T T
	0.7407118393202556	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2954852124018955	0.8156039264098018	0.2204117929367941 T T T
	0.0740695378679563	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376666293	0.9259710761000194	0.1088458790334812 F F F
	0.6337569099322941	0.8280289781852372	0.2225460129660767 T T T
	0.4074072183280932	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181267578	0.9259710761000194	0.1088458790334812 F F F
	0.9682900414275631	0.8193182959843446	0.2187003243338154 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985868623	0.9259710761000194	0.1088458790334812 F F F
	0.6303387823509053	0.4807771077936908	0.2305571121878063 T T T
	0.7230466701247933	0.3885918921048661	0.3680730688425499 T T T
	0.5104132895253209	0.6006114191492643	0.2855009551665325 T T T
	0.8020143841831298	0.3164065301747129	0.3969553530648990 T T T
	0.5029447579642303	0.6077776211292120	0.3423632940247844 T T T

CH-CHO Rh/Cu(100)	Cu Rh C O H
	1.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 13.6146999999999991
	Cu Rh C O H
	26 1 2 1 2
	Selective dynamics
	Direct
	0.0000000000000000 0.1666688402300522 0.1327241878263905 F F F 0.1666688402300522 0.0000000000000000 0.0000000000000000 F F F 0.1678507044590584 0.9989037540191672 0.2666330582869185 T T T 0.3333376804600974 0.1666688402300522 0.1327241878263905 F F F 0.5000065206901496 0.0000000000000000 0.0000000000000000 F F F 0.5064105384843700 0.9892740019079242 0.2739306227589128 T T T 0.6666753609202019 0.1666688402300522 0.1327241878263905 F F F 0.8333442011502470 0.0000000000000000 0.0000000000000000 F F F 0.8326609585979043 1.0001668313290188 0.2733342417799238 T T T 0.0000000000000000 0.5000065206901496 0.1327241878263905 F F F 0.1666688402300522 0.3333376804600974 0.0000000000000000 F F F 0.1565855948894100 0.3335359267297258 0.2667599476078317 T T T 0.3333376804600974 0.5000065206901496 0.1327241878263905 F F F 0.5000065206901496 0.3333376804600974 0.0000000000000000 F F F 0.6666753609202019 0.5000065206901496 0.1327241878263905 F F F 0.8333442011502470 0.3333376804600974 0.0000000000000000 F F F 0.8319888016435236 0.3329825995373215 0.2744535259282869 T T T 0.0000000000000000 0.8333442011502470 0.1327241878263905 F F F 0.1666688402300522 0.6666753609202019 0.0000000000000000 F F F 0.1678700345856424 0.6656161241201158 0.2674842085079404 T T T 0.3333376804600974 0.8333442011502470 0.1327241878263905 F F F 0.5000065206901496 0.6666753609202019 0.0000000000000000 F F F 0.5009748594541300 0.6670089064788806 0.2666737396625992 T T T 0.6666753609202019 0.8333442011502470 0.1327241878263905 F F F 0.8333442011502470 0.6666753609202019 0.0000000000000000 F F F 0.8332385782384847 0.6662566001351720 0.2671060161279429 T T T 0.4920328037864525 0.3343972164748001 0.2788386965559269 T T T 0.4819076397751986 0.2550004733691750 0.4260242186238092 T T T 0.6597131510136700 0.1686430889798982 0.3516517987418622 T T T 0.3612594538614525 0.1598019141286745 0.4526537856628455 T T T 0.5355417471670706 0.3570642317342111 0.4748551222599093 T T T 0.7239028683836815 0.1468750472592944 0.4231165131976112 T T T

CH-CHO Rh/Cu(111)	Cu Rh C O H
	1.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 -3.8339499999999997 6.6405961900000001 0.0000000000000000 0.0000000000000000 0.0000000000000000 19.1738999999999997 Cu Rh C O H 26 1 2 1 2 Selective dynamics Direct 0.2933552108166868 0.1360833417425265 0.2247640804508569 T T T 0.0740787133764584 0.0370448665995440 0.0000000000000000 F F F 0.1852133131750904 0.2593140661968150 0.1088458790334812 F F F 0.6357716527058053 0.1470698999987495 0.2173047561601521 T T T 0.4074163938365558 0.0370448665995440 0.0000000000000000 F F F 0.5185509936351949 0.2593140661968150 0.1088458790334812 F F F 0.9613568015581880 0.1468946268338404 0.2164443640829087 T T T 0.7407540742966532 0.0370448665995440 0.0000000000000000 F F F 0.8518886740952922 0.2593140661968150 0.1088458790334812 F F F 0.2832661695477431 0.4764324871246303 0.2223813846638039 T T T 0.0740364784000533 0.3702980771068383 0.0000000000000000 F F F 0.1851710781986924 0.5925672767041092 0.1088458790334812 F F F 0.4073741588601507 0.3702980771068383 0.0000000000000000 F F F 0.5185087586587898 0.5925672767041092 0.1088458790334812 F F F 0.9629316262645713 0.4793975314027488 0.2193414083589994 T T T 0.7407118393202552 0.3702980771068383 0.0000000000000000 F F F 0.8518464391188871 0.5925672767041092 0.1088458790334812 F F F 0.2890219030074151 0.8139048874312393 0.2260902645424659 T T T 0.0740695378679561 0.7037018765027483 0.0000000000000000 F F F 0.1852041376665952 0.9259710761000193 0.1088458790334812 F F F 0.6302557875572505 0.8216095055554501 0.2241801039984270 T T T 0.4074072183280606 0.7037018765027483 0.0000000000000000 F F F 0.5185418181266925 0.9259710761000193 0.1088458790334812 F F F 0.9633887978507187 0.8148124970641005 0.2168576477641587 T T T 0.7407448987881580 0.7037018765027483 0.0000000000000000 F F F 0.8518794985867970 0.9259710761000193 0.1088458790334812 F F F 0.6310714842781709 0.4783595906583590 0.2245062847451505 T T T 0.2968498685103555 -0.0068038064060595 0.3198479231722525 T T T 0.5125893488578087 0.5834188746745684 0.2852232905400172 T T T 0.4420477137767739 0.0135408011838681 0.3530490809107003 T T T 0.1634754442478549 -0.0243570856544696 0.3491619224382760 T T T 0.5041946334556034 0.5836989428682091 0.3423265180178124 T T T

CH ₂ -CO Rh/Cu(100)	Cu Rh C O H		
	1.0000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	0.0000000000000000	7.6679000000000004	0.0000000000000000
	0.0000000000000000	0.0000000000000000	13.6146999999999991
	Cu Rh C O H		
	26 1 2 1 2		
	Selective dynamics		
	Direct		
	0.0000000000000000	0.1666688402300522	0.1327241878263905 F F F
	0.1666688402300522	0.0000000000000000	0.0000000000000000 F F F
	0.1641216286739189	0.9990569126257651	0.2667230268181398 T T T
	0.3333376804600975	0.1666688402300522	0.1327241878263905 F F F
	0.5000065206901496	0.0000000000000000	0.0000000000000000 F F F
	0.4997597481114557	0.9975619455779711	0.2745815368502597 T T T
	0.6666753609202019	0.1666688402300522	0.1327241878263905 F F F
	0.8333442011502470	0.0000000000000000	0.0000000000000000 F F F
	0.8355350600623496	0.9990139135983067	0.2667003863863386 T T T
	0.0000000000000000	0.5000065206901496	0.1327241878263905 F F F
	0.1666688402300522	0.3333376804600975	0.0000000000000000 F F F
	0.1620197700182390	0.3327316033974332	0.2673769782707808 T T T
	0.3333376804600975	0.5000065206901496	0.1327241878263905 F F F
	0.5000065206901496	0.3333376804600975	0.0000000000000000 F F F
	0.6666753609202019	0.5000065206901496	0.1327241878263905 F F F
	0.8333442011502470	0.3333376804600975	0.0000000000000000 F F F
	0.8385447995408311	0.3326893910537809	0.2673902031051026 T T T
	0.0000000000000000	0.8333442011502470	0.1327241878263905 F F F
	0.1666688402300522	0.6666753609202019	0.0000000000000000 F F F
	0.1665777674557072	0.6664885628588759	0.2670525224446734 T T T
	0.3333376804600975	0.8333442011502470	0.1327241878263905 F F F
	0.5000065206901496	0.6666753609202019	0.0000000000000000 F F F
	0.4999572168211384	0.6759596316459610	0.2676776272843401 T T T
	0.6666753609202019	0.8333442011502470	0.1327241878263905 F F F
	0.8333442011502470	0.6666753609202019	0.0000000000000000 F F F
	0.8333736889278769	0.6664577463909825	0.2670416069700274 T T T
	0.5003434573316358	0.3440946213338587	0.2887756463713047 T T T
	0.5014013087929517	0.3899416278200612	0.4222851497215980 T T T
	0.5001857855908085	0.1350306987980232	0.3989900169083057 T T T
	0.5023434460729592	0.4528435525934253	0.5010367747434831 T T T
	0.6173255911257577	0.1123919840124175	0.4425934729365420 T T T
	0.3830307475630007	0.1130631164410922	0.4426882460434521 T T T

CH ₂ -CO Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.1738999999999997
	Cu Rh C O H		
	26	1	2 1 2
	Selective dynamics		
	Direct		
	0.2929398009604902	0.1416506689898734	0.2196069328532163 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6319899019543641	0.1396195082526158	0.2181967247789551 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9651196869421728	0.1454937397534956	0.2190129771509130 T T T
	0.7407540742966532	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2917785229901511	0.4778676871978562	0.2177012003600884 T T T
	0.0740364784000533	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781986924	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9697031715791302	0.4777450428212976	0.2196047630661945 T T T
	0.7407118393202552	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2952927218199579	0.8127728050366346	0.2193926558625919 T T T
	0.0740695378679561	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376665952	0.9259710761000193	0.1088458790334812 F F F
	0.6258677174047890	0.8135559008724911	0.2234484326695111 T T T
	0.4074072183280606	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181266925	0.9259710761000193	0.1088458790334812 F F F
	0.9706662707301489	0.8172693323531852	0.2178907001760759 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985867970	0.9259710761000193	0.1088458790334812 F F F
	0.6339322200124125	0.4746916567997623	0.2310709928836053 T T T
	0.6445055228724674	0.4307573388818906	0.3261268092170815 T T T
	0.5878762770382601	0.6498961416151139	0.3113961393544273 T T T
	0.6591096491483677	0.3721342615364397	0.3812551722031434 T T T
	0.4456680459676520	0.5810756095825345	0.3399017771426433 T T T
	0.7108148334996569	0.7542927848311111	0.3450461744426866 T T T

CH ₂ -CHO Rh/Cu(100)	Cu Rh C O H
	1.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 13.6146999999999991
	Cu Rh C O H
	26 1 2 1 3
	Selective dynamics
	Direct
	0.0000000000000000 0.1666688402300522 0.1327241878263905 F F F 0.1666688402300522 0.0000000000000000 0.0000000000000000 F F F 0.1645705905348370 -0.0027805474124885 0.2672985110023742 T T T 0.3333376804600974 0.1666688402300522 0.1327241878263905 F F F 0.5000065206901496 0.0000000000000000 0.0000000000000000 F F F 0.4995059787363609 1.0033874235293341 0.2756246852008122 T T T 0.6666753609202019 0.1666688402300522 0.1327241878263905 F F F 0.8333442011502470 0.0000000000000000 0.0000000000000000 F F F 0.8354344230613302 0.9966878144292638 0.2667500188394225 T T T 0.0000000000000000 0.5000065206901496 0.1327241878263905 F F F 0.1666688402300522 0.3333376804600974 0.0000000000000000 F F F 0.1627615417589348 0.3312979120566903 0.2666948472108369 T T T 0.3333376804600974 0.5000065206901496 0.1327241878263905 F F F 0.5000065206901496 0.3333376804600974 0.0000000000000000 F F F 0.6666753609202019 0.5000065206901496 0.1327241878263905 F F F 0.8333442011502470 0.3333376804600974 0.0000000000000000 F F F 0.8384890250172715 0.3316789879166104 0.2667386007876009 T T T 0.0000000000000000 0.8333442011502470 0.1327241878263905 F F F 0.1666688402300522 0.6666753609202019 0.0000000000000000 F F F 0.1671357967416200 0.6652357047556708 0.2672282307504221 T T T 0.3333376804600974 0.8333442011502470 0.1327241878263905 F F F 0.5000065206901496 0.6666753609202019 0.0000000000000000 F F F 0.4992444704072967 0.6799939813137845 0.2676099994991176 T T T 0.6666753609202019 0.8333442011502470 0.1327241878263905 F F F 0.8333442011502470 0.6666753609202019 0.0000000000000000 F F F 0.8333204743753995 0.6660304926692149 0.2675363704053900 T T T 0.4995140763480409 0.3458526532480085 0.2865987881302020 T T T 0.5172879778059125 0.1533390908532798 0.3968178109015613 T T T 0.5090852367397649 0.4131787622930244 0.4318819896833035 T T T 0.6400703205774281 0.4745865764857979 0.4698181794535380 T T T 0.3797700159325150 0.4259661297136392 0.4673318149824417 T T T 0.6403215306671872 0.1286996632911142 0.4346382071667128 T T T 0.4070596419926401 0.1260262276052628 0.4454234359844547 T T T

CH ₂ -CHO Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.1738999999999997
	Cu Rh C O H		
	26	1	2 1 3
	Selective dynamics		
	Direct		
	0.2916499458379622	0.1403215869627138	0.2197578791524218 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6342073322201575	0.1404493100358201	0.2178988372831628 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9642297818488951	0.1450261603875212	0.2186018481143985 T T T
	0.7407540742966532	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2959452433175532	0.4839911945171803	0.2197672320640932 T T T
	0.0740364784000533	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781986924	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9691084600916988	0.4773110241571921	0.2184858877573271 T T T
	0.7407118393202552	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2949086498858489	0.8141163667618212	0.2193112471904136 T T T
	0.0740695378679561	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376665952	0.9259710761000193	0.1088458790334812 F F F
	0.6246815335668489	0.8128761931535756	0.2230417493113563 T T T
	0.4074072183280606	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181266925	0.9259710761000193	0.1088458790334812 F F F
	0.9672385615337401	0.8151209342465934	0.2188141253424636 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985867970	0.9259710761000193	0.1088458790334812 F F F
	0.6352862843180740	0.4751126520557985	0.2300132991157517 T T T
	0.5153859314703970	0.5930023252846173	0.3036853138975633 T T T
	0.6127642297537195	0.3974788198287869	0.3329432764398866 T T T
	0.4816142520688305	0.2315822815830968	0.3538873520550282 T T T
	0.7471256090912576	0.4928014503217042	0.3651438791171189 T T T
	0.6150619738325076	0.7153360151046978	0.3389042887078897 T T T
	0.3716216214854718	0.5025048093139943	0.3310227235939538 T T T

CH ₃ -CO Rh/Cu(100)	Cu Rh C O H			
	1.000000000000000			
	7.6679000000000004	0.0000000000000000	0.0000000000000000	
	0.0000000000000000	7.6679000000000004	0.0000000000000000	
	0.0000000000000000	0.0000000000000000	13.614699999999991	
	Cu Rh C O H			
	26	1	2	1 3
	Selective dynamics			
	Direct			
	0.0000000000000000	0.1666688402300522	0.1327241878263905	F F F
	0.1666688402300522	0.0000000000000000	0.0000000000000000	F F F
	0.1656890817800558	0.9988250339121163	0.2667583374353464	T T T
	0.3333376804600974	0.1666688402300522	0.1327241878263905	F F F
	0.5000065206901496	0.0000000000000000	0.0000000000000000	F F F
	0.4992878094265483	0.9952775610597624	0.2677197890039595	T T T
	0.6666753609202019	0.1666688402300522	0.1327241878263905	F F F
	0.8333442011502470	0.0000000000000000	0.0000000000000000	F F F
	0.8327281681074119	0.9981667941051632	0.2671406258227206	T T T
	0.0000000000000000	0.5000065206901496	0.1327241878263905	F F F
	0.1666688402300522	0.3333376804600974	0.0000000000000000	F F F
	0.1646299943371883	0.3332317114660285	0.2634849864083600	T T T
	0.3333376804600974	0.5000065206901496	0.1327241878263905	F F F
	0.5000065206901496	0.3333376804600974	0.0000000000000000	F F F
	0.6666753609202019	0.5000065206901496	0.1327241878263905	F F F
	0.8333442011502470	0.3333376804600974	0.0000000000000000	F F F
	0.8405922845478023	0.3323984752405571	0.2658859990465423	T T T
	0.0000000000000000	0.8333442011502470	0.1327241878263905	F F F
	0.1666688402300522	0.6666753609202019	0.0000000000000000	F F F
	0.1657078538585877	0.6671458765274383	0.2670985961870702	T T T
	0.3333376804600974	0.8333442011502470	0.1327241878263905	F F F
	0.5000065206901496	0.6666753609202019	0.0000000000000000	F F F
	0.4983995620852750	0.6704439200581014	0.2682385126782127	T T T
	0.6666753609202019	0.8333442011502470	0.1327241878263905	F F F
	0.8333442011502470	0.6666753609202019	0.0000000000000000	F F F
	0.8326258201155283	0.6681106745881799	0.2668858156293683	T T T
	0.5059140569391583	0.3336290930357855	0.2956398305831931	T T T
	0.6289988484271793	0.3446363375138709	0.4117626826040534	T T T
	0.3933007713617906	0.3086011604003130	0.4597224678889323	T T T
	0.7340840112846791	0.3560768246775630	0.4753380394465144	T T T
	0.4163769301367274	0.1824084005211550	0.4937289874929841	T T T
	0.2640076829420028	0.3117937080776001	0.4263979675016893	T T T
	0.4052767731441043	0.4160561400989378	0.5113825698072140	T T T

CH ₃ -CO Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.173899999999997
	Cu Rh C O H		
	26 1 2 1 3		
	Selective dynamics		
	Direct		
	0.2936138210323846	0.1453970012812923	0.2190728228449227 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6307427159872550	0.1446897359378304	0.2173303811470113 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9646017136199716	0.1483501327061424	0.2192443683673307 T T T
	0.7407540742966533	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2926269611469469	0.4810091813221464	0.2183496556838626 T T T
	0.0740364784000534	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781987040	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9675067674446804	0.4819032912412225	0.2190000011895216 T T T
	0.7407118393202556	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2964602851073976	0.8141234571385347	0.2191214315784319 T T T
	0.0740695378679563	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376666194	0.9259710761000194	0.1088458790334812 F F F
	0.6311211482198269	0.8195354630977124	0.2155095514433380 T T T
	0.4074072183280837	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181267388	0.9259710761000194	0.1088458790334812 F F F
	0.9682772100016931	0.8195127458924435	0.2185836292443174 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985868433	0.9259710761000194	0.1088458790334812 F F F
	0.6311336801369650	0.4813922095352154	0.2395252566492124 T T T
	0.6347349767460125	0.3591590050259944	0.3225460536335066 T T T
	0.6248481377787501	0.5921362674631278	0.3572024356954979 T T T
	0.6381916538084745	0.2560674192126562	0.3679443378206115 T T T
	0.4887327301591800	0.5016025152434255	0.3873898008553007 T T T
	0.6202168299066443	0.7195020891624335	0.3340466429585208 T T T
	0.7614587598179197	0.6458158897131647	0.3878809939857432 T T T

CH ₃ -CHO Rh/Cu(100)	Cu Rh C O H
	1.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 7.6679000000000004 0.0000000000000000 0.0000000000000000 0.0000000000000000 13.6146999999999991
	Cu Rh C O H
	26 1 2 1 4
	Selective dynamics
	Direct
	0.0000000000000000 0.1666688402300522 0.1327241878263905 F F F 0.1666688402300522 0.0000000000000000 0.0000000000000000 F F F 0.1695727240793698 0.0010188962164650 0.2673504587704495 T T T 0.3333376804600974 0.1666688402300522 0.1327241878263905 F F F 0.5000065206901496 0.0000000000000000 0.0000000000000000 F F F 0.5044196238436529 0.9954456735194726 0.2652023321220886 T T T 0.6666753609202019 0.1666688402300522 0.1327241878263905 F F F 0.8333442011502470 0.0000000000000000 0.0000000000000000 F F F 0.8365949860168710 -0.0028072886096135 0.2668875494334424 T T T 0.0000000000000000 0.5000065206901496 0.1327241878263905 F F F 0.1666688402300522 0.3333376804600974 0.0000000000000000 F F F 0.1608623912621368 0.3336425537034523 0.2668646229614051 T T T 0.3333376804600974 0.5000065206901496 0.1327241878263905 F F F 0.5000065206901496 0.3333376804600974 0.0000000000000000 F F F 0.6666753609202019 0.5000065206901496 0.1327241878263905 F F F 0.8333442011502470 0.3333376804600974 0.0000000000000000 F F F 0.8382048218516609 0.3242027889767929 0.2709405284045351 T T T 0.0000000000000000 0.8333442011502470 0.1327241878263905 F F F 0.1666688402300522 0.6666753609202019 0.0000000000000000 F F F 0.1679821960788913 0.6670888144974469 0.2670406452788016 T T T 0.3333376804600974 0.8333442011502470 0.1327241878263905 F F F 0.5000065206901496 0.6666753609202019 0.0000000000000000 F F F 0.4963671429502185 0.6716480965843390 0.2656847644453155 T T T 0.6666753609202019 0.8333442011502470 0.1327241878263905 F F F 0.8333442011502470 0.6666753609202019 0.0000000000000000 F F F 0.8358343208873518 0.6712446773533302 0.2708357521806479 T T T 0.4881134794634016 0.3333662791611461 0.2898736605345573 T T T 0.5997866691465270 0.4710506919991047 0.3943379339413383 T T T 0.4989030923252219 0.2502348318375691 0.4524485940695547 T T T 0.7684957553887265 0.4843334053309995 0.3938350710021737 T T T 0.5315161046330589 0.5582396231762370 0.4461033650595488 T T T 0.5011855798910076 0.1112240740612400 0.4350200956793580 T T T 0.3733600445347836 0.2884873548660034 0.4829220027970416 T T T 0.6032369952913462 0.2722506666382327 0.5055410909304973 T T T

CH ₃ -CHO Rh/Cu(111)	Cu Rh C O H		
	1.000000000000000		
	7.6679000000000004	0.0000000000000000	0.0000000000000000
	-3.8339499999999997	6.6405961900000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.173899999999997
	Cu Rh C O H		
	26	1	2 1 4
	Selective dynamics		
	Direct		
	0.2939552023154427	0.1487383000727728	0.2183972687848248 T T T
	0.0740787133764584	0.0370448665995440	0.0000000000000000 F F F
	0.1852133131750904	0.2593140661968150	0.1088458790334812 F F F
	0.6289103459856112	0.1418849910139780	0.2224143558230962 T T T
	0.4074163938365558	0.0370448665995440	0.0000000000000000 F F F
	0.5185509936351949	0.2593140661968150	0.1088458790334812 F F F
	0.9658864823578812	0.1490096536607134	0.2186425814593523 T T T
	0.7407540742966532	0.0370448665995440	0.0000000000000000 F F F
	0.8518886740952922	0.2593140661968150	0.1088458790334812 F F F
	0.2920477961266116	0.4811608079286342	0.2173757704142054 T T T
	0.0740364784000533	0.3702980771068383	0.0000000000000000 F F F
	0.1851710781986924	0.5925672767041092	0.1088458790334812 F F F
	0.4073741588601507	0.3702980771068383	0.0000000000000000 F F F
	0.5185087586587898	0.5925672767041092	0.1088458790334812 F F F
	0.9699248406081076	0.4854944165269227	0.2169327153645828 T T T
	0.7407118393202552	0.3702980771068383	0.0000000000000000 F F F
	0.8518464391188871	0.5925672767041092	0.1088458790334812 F F F
	0.2968175758971113	0.8153948827860257	0.2186193288600174 T T T
	0.0740695378679561	0.7037018765027483	0.0000000000000000 F F F
	0.1852041376665952	0.9259710761000193	0.1088458790334812 F F F
	0.6320223556454030	0.8198917740758732	0.2172621403250557 T T T
	0.4074072183280606	0.7037018765027483	0.0000000000000000 F F F
	0.5185418181266925	0.9259710761000193	0.1088458790334812 F F F
	0.9703157742040316	0.8220625231911697	0.2192374637330859 T T T
	0.7407448987881580	0.7037018765027483	0.0000000000000000 F F F
	0.8518794985867970	0.9259710761000193	0.1088458790334812 F F F
	0.6354687064598279	0.4894878206484854	0.2360233405529087 T T T
	0.5558536043871691	0.5239555631926882	0.3505220145732417 T T T
	0.7297507526531354	0.4126378765608378	0.3221839747276927 T T T
	0.6589440845768763	0.2258503936949641	0.3321264347456300 T T T
	0.8663534158185571	0.5177137506381336	0.3513101739361379 T T T
	0.6741708818461408	0.6304981169030892	0.3851304480589454 T T T
	0.4773924604154410	0.6002689480784310	0.3306651536077150 T T T
	0.4475637513198782	0.3880245056830331	0.3777728152532024 T T T

Table S4. Typical input files.

Note 1: VASP requires at least 4 input files: POSCAR (from Table S3), POTCAR (generated from the official PAW plane wave basis set library), INCAR, and KPOINTS. The following shows contents of the typical INCAR and KPOINTS files. The INCAR file differs slightly for different jobs: structural relaxation (local minimum optimization), transition state optimization, and harmonic frequency calculations. The KPOINTS file may differ if the kpoint grid differs.

Note 2: To use the BEEF-vdW exchange-correlation functional, the libbeef package (<https://github.com/vossjo/libbeef>) has to be compiled and linked with the VASP binary. In addition, to use the CI-NEB or dimer method for transition state optimization, the VASP Transition State Tools (VTST, <http://theory.cm.utexas.edu/vtsttools/index.html>) also has to be incorporated into the VASP source tree prior to compilation.

Note 3: Our INCAR files are usually generated using MedeA (a GUI for VASP, <http://archive.materialsdesign.com/medea/medea-vasp>), so some of the options may not be absolutely necessary.

INCAR

Local minimum optimization:

SYSTEM = CO

LUSE_VDW=.TRUE.

AGGAC=0.0000

GGA=BF

ENCUT = 400

PREC = Normal

EDIFF = 1.0e-07

ALGO = Fast

ISPIN = 1
ISMEAR = 1
SIGMA = 0.2
LREAL = .FALSE.
IBRION = 2
NSW = 100
ISIF = 0
EDIFFG = -0.01
NELMIN = 2
VOSKOWN = 1
NBLOCK = 1
NWRITE = 1
NELM=60
INIWAV = 1
ISTART = 0
ICHARG = 2
LWAVE = .FALSE.
LCHARG = .FALSE.
ADDGRID = .FALSE.
LASPH=.TRUE.
Zab_VDW=-1.8867

CI-NEB method for transition states

LUSE_VDW=.TRUE.
AGGAC=0.0000
GGA=BF

ENCUT = 400
PREC = Normal
EDIFF = 1.0e-07
ALGO = Fast
ISPIN = 1
ISMEAR = 1
SIGMA = 0.2
LREAL = .FALSE.
RWIGS = 1.17 1.25 0.77 0.73 0.32
IBRION = 3
NSW = 400
ISIF = 0
EDIFFG = -0.05
NELMIN = 2
VOSKOWN = 1
NBLOCK = 1
NWRITE = 1
NELM=60
INIWAV = 1
ISTART = 0
ICHARG = 2
LWAVE = .FALSE.
LCHARG = .FALSE.
ADDGRID = .FALSE.
LASPH=.TRUE.

Zab_VDW=-1.8867

ICHAIN = 0

POTIM = 0.05

IMAGES = 5

SPRING = -5

LCLIMB = .FALSE.

Dimer method for transition states

LUSE_VDW=.TRUE.

AGGAC=0.0000

GGA=BF

ENCUT = 400

PREC = Normal

EDIFF = 1.0e-07

ALGO = Fast

ISPIN = 1

ISMEAR = 1

SIGMA = 0.2

LREAL = .FALSE.

NSW = 900

ISIF = 0

EDIFFG = -0.001

NELMIN = 2

VOSKOWN = 1

NBLOCK = 1

NWRITE = 1

NELM=60
INIWAV = 1
ISTART = 0
ICHARG = 2
LWAVE = .FALSE.
LCHARG = .FALSE.
ADDGRID = .FALSE.
LASPH=.TRUE.
Zab_VDW=-1.8867
ICHAIN = 2
IBRION = 3
POTIM = 0.0
DdR = 0.005
DRotMax = 4
DFNMin = 0.01
DFNMax = 1.0
IOPT = 2

Calculation for frequency

LUSE_VDW=.TRUE.
AGGAC=0.0000
GGA=BF
ENCUT = 400
PREC = Normal
EDIFF = 1.0e-07
ALGO = Fast

ISPIN = 1
ISMEAR = 1
SIGMA = 0.2
LREAL = .FALSE.
IBRION = 5
NFREE = 2
POTIM = 0.015
NELMIN = 2
VOSKOWN = 1
NBLOCK = 1
NWRITE = 1
NELM=60
INIWAV = 1
ISTART = 0
ICHARG = 2
LWAVE = .FALSE.
LCHARG = .FALSE.
ADDGRID = .FALSE.
LASPH = .TRUE.
Zab_VDW = -1.8867

KPOINTS

Automatic mesh

0

Gamma

4 4 1

0. 0. 0.