Supplementary Material

Homonuclear Multi-Atom Catalysts for CO_2 Electroreduction: A Comparison Density Functional Theory Study with Single-Atom Counterparts

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Table S1. Formation energies of homonuclear trimetallic atomic metals adsorbed on the surface oxygen sites of Mo_2CO_2 or embedded in the oxygen vacancies.

Structure	E_f (eV) embedment	F_f (eV) adsorption
Ti	-2.70	---
V	-1.89	---
Cr	-1.63	---
Mn	-2.38	-2.05
Fe	-2.04	-1.03
Co	-1.97	-0.72
Ni	-2.21	-0.76
Cu	-2.45	-1.28
Zn	-3.13	-2.46
Zr	-2.90	---
Nb	-1.96	-0.68
Mo	-1.50	-0.35
Ru	-1.71	0.50
Rh	-2.31	-0.16
Pd	-2.40	-0.48
Ag	-2.85	-2.03
Hf	-2.65	---
Ta	-1.69	-1.23
W	-0.90	0.48
Re	-1.13	0.71
Os	-1.22	1.16
Ir	-1.94	0.79
Pt	-2.65	-0.44
Au	-2.97	-1.67

Table S2. Formation energies of homonuclear bimetallic atomic metals adsorbed on the surface oxygen sites of Mo_2CO_2 or embedded in the oxygen vacancies.

Structure	E_f (eV) emdedment	E_f (eV) adsorption
Ti	-2.53	---
V	-1.84	---
Cr	-1.52	---
Mn	-0.62	---
Fe	-1.64	-1.43
Co	-1.88	-0.67
Ni	-2.08	-0.75
Cu	-2.46	-1.26
Zn	-3.13	-2.70
Zr	-2.66	---
Nb	-1.87	---
Mo	-1.41	-0.58
Ru	-1.60	0.58
Rh	-2.13	0.29
Pd	-2.30	-0.48
Ag	-2.91	-1.97
Hf	-2.35	---
Ta	-1.54	---
W	-0.85	0.73
Re	-1.03	1.67
Os	-1.09	1.81
Ir	-1.78	1.36
Pt	-2.56	0.27
Au	-3.02	-1.07

Table S3. Formation energies of homonuclear monometallic atomic metals adsorbed on the surface oxygen sites of Mo_2CO_2 or embedded in the oxygen vacancies.

Structure	E_f (eV) embedment	E_f (eV) adsorption
Ti	-1.87	---
V	-0.92	---
Cr	-1.49	---
Mn	-1.94	2.68
Fe	-0.59	0.06
Co	-1.32	-1.06
Ni	-1.87	-0.57
Cu	-2.30	-1.50
Zn	-2.62	-2.60
Zr	-3.80	1.48
Nb	-0.85	---
Mo	0.10	0.14
Ru	-0.53	1.16
Rh	-1.58	0.02
Pd	-2.29	-0.43
Ag	-2.83	-2.21
Hf	-1.53	---
Ta	-0.27	---
W	0.81	1.38
Re	0.71	1.62
Os	0.40	1.71
Ir	-0.86	2.66
Pt	-2.31	1.14
Au	-2.91	-0.83

Table S4. Reaction free energies for CO_2RR on the Ir TAC calculated by approximate solvation correction and explicit water bilayer solvation model, respectively.

Ir TAC	ΔG(approximate solvation)	ΔG (explicit solvation)
CO_2 →*HCOO	-0.46	-0.23
*HCOO → *HCOOH	0.21	0.36
*HCOOH → *CHO	0.22	0.42
*CHO → *CHOH	0.01	0.14
*CHOH → *CH	-0.51	-0.69
*CH → *CH_2	-0.23	-0.23
CH_2 →CH_3	-0.08	-0.07
*CH_3 → CH_4	-0.60	-0.76

Table S5. The fitted energy correction (ΔE) - electric potential (U) quadratic function for each reaction steps of CO_2RR on the Rh TAC at pH = 0.

Absorbate	Rh TAC
CO_2 →*HCOO	$\Delta E = 1.00 + 8.87\ U - 9.91\ U^2$
*HCOO → *HCOOH	$\Delta E = 0.87 + 5.45\ U - 5.17\ U^2$
*HCOOH → *CHO	$\Delta E = 0.76 + 9.61\ U - 10.00\ U^2$
*CHO → *CHOH	$\Delta E = 0.80 + 7.16\ U - 6.58\ U^2$
*CHOH → *CH	$\Delta E = 1.17 + 7.92\ U - 7.26\ U^2$
*CH → *CH_2	$\Delta E = 0.78 + 10.47\ U - 12.56\ U^2$
CH_2 →CH_3	$\Delta E = 0.77 + 9.79\ U - 12.01\ U^2$

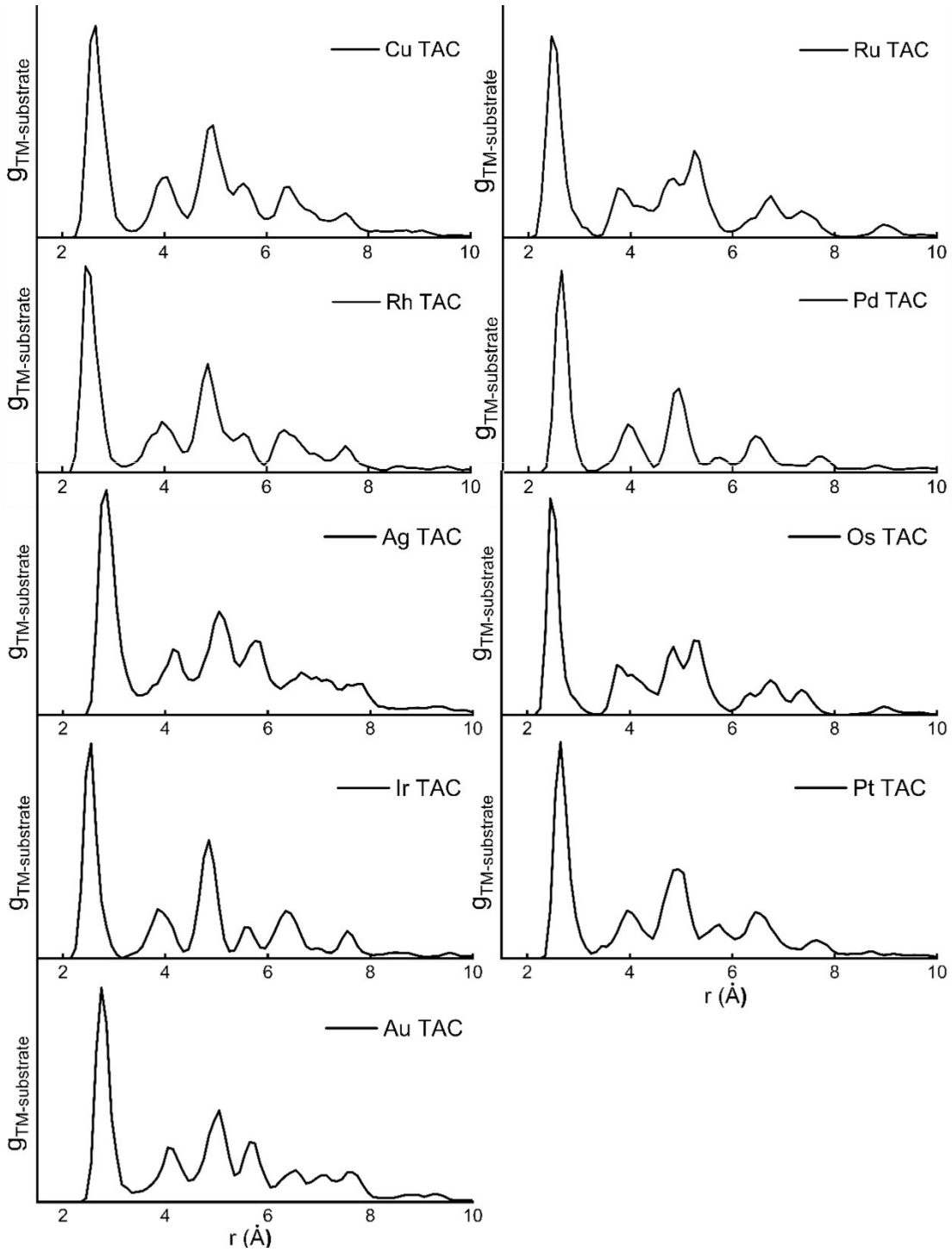

Fig. S1 Radial distribution function of selected TACs at 500 K after a 10 ps MD simulation.

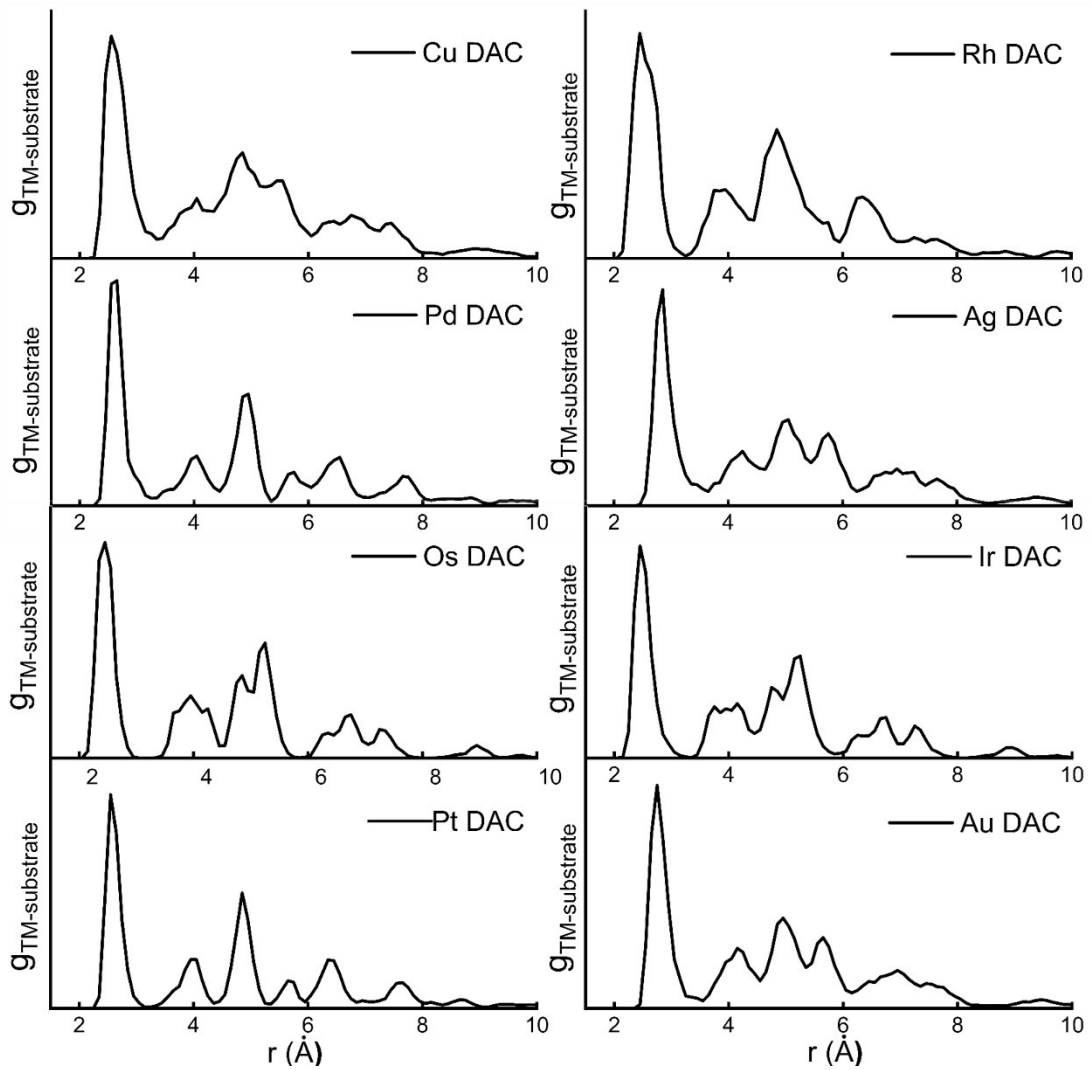

Fig. S2 Radial distribution function of selected DACs at 500 K after a 10 ps MD simulation.

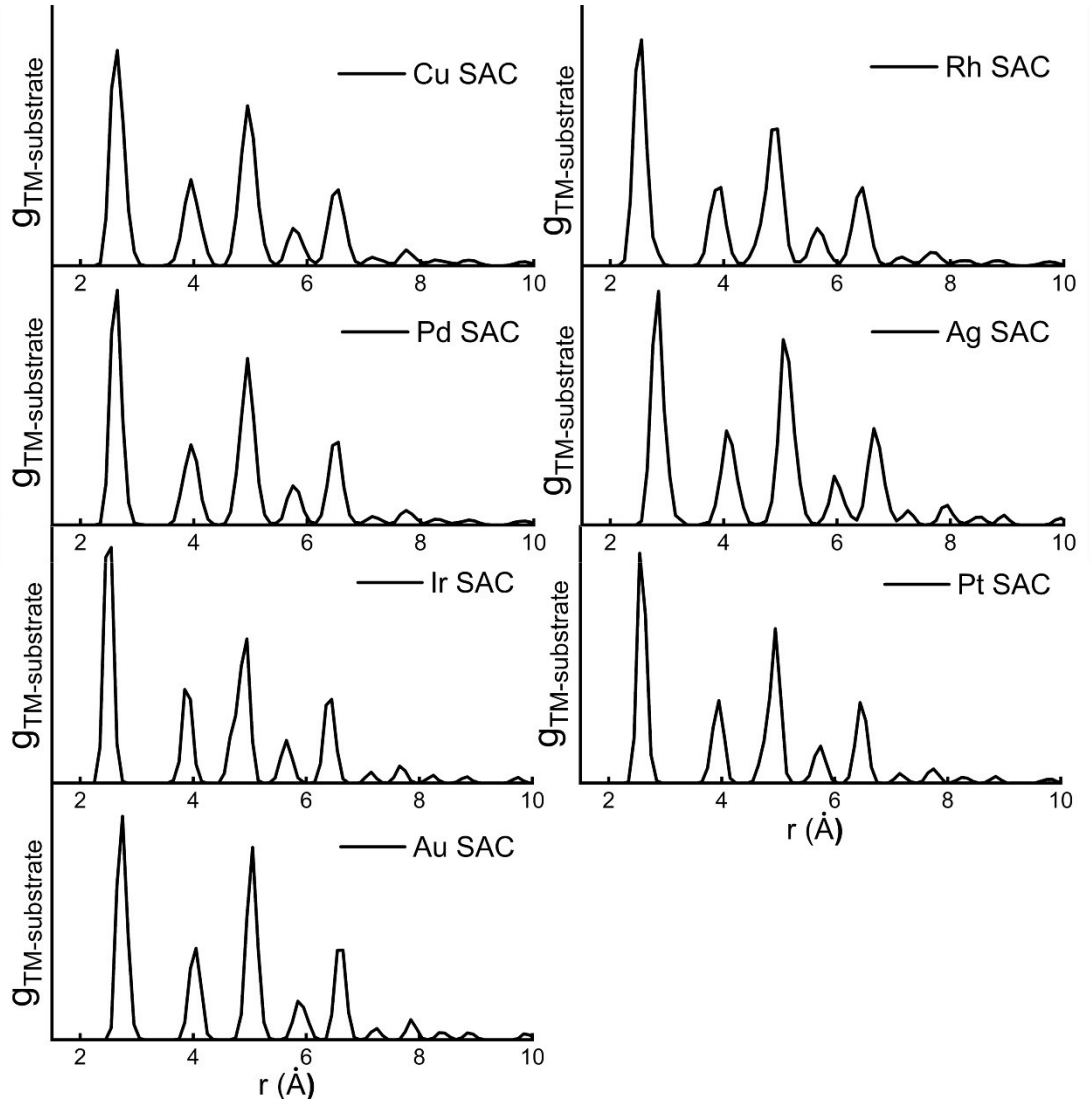

Fig. S3 Radial distribution function of selected SACs at 500 K after a 10 ps MD simulation.

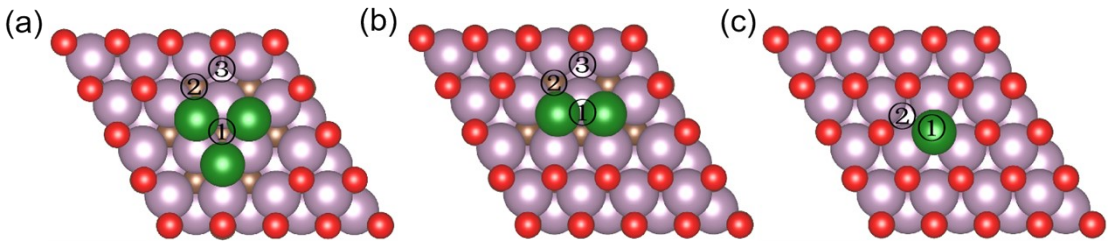

Fig. S4 The considered adsorption sites on TACs, DACs, and SACs. Green, red, purple, and brown spheres represent TM, O, Mo, and C atoms, respectively.

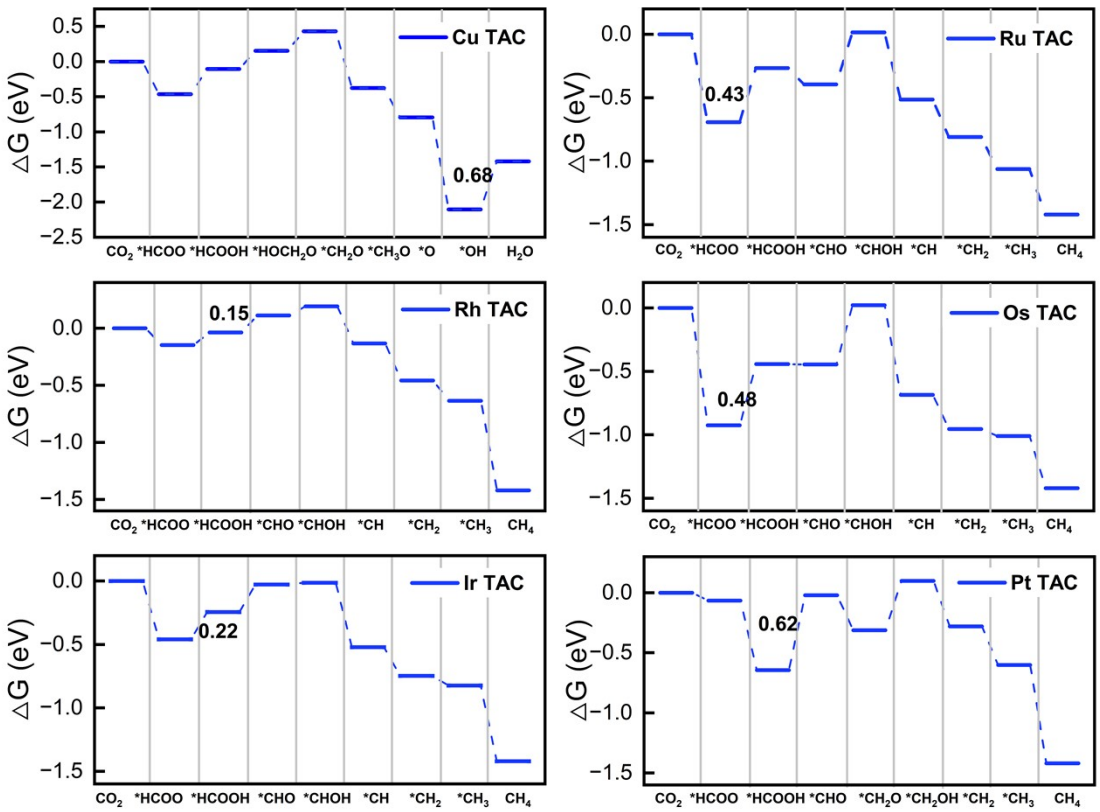

Fig. S5 Free energy diagram for CO_2RR on the six TACs (Cu, Ru, Rh, Os, Ir, and Pt).

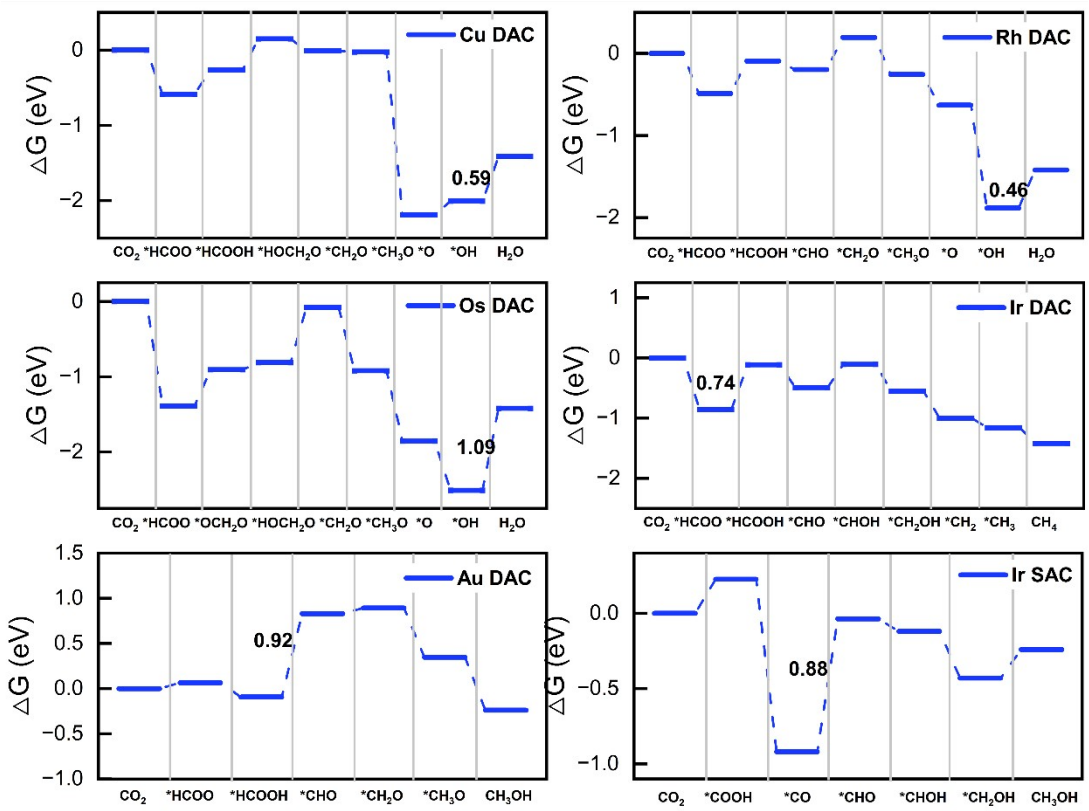

Fig. S6 Free energy diagram for CO_2RR on the five DACs (Cu, Rh, Os, Ir, and Au) and one SAC (Ir).

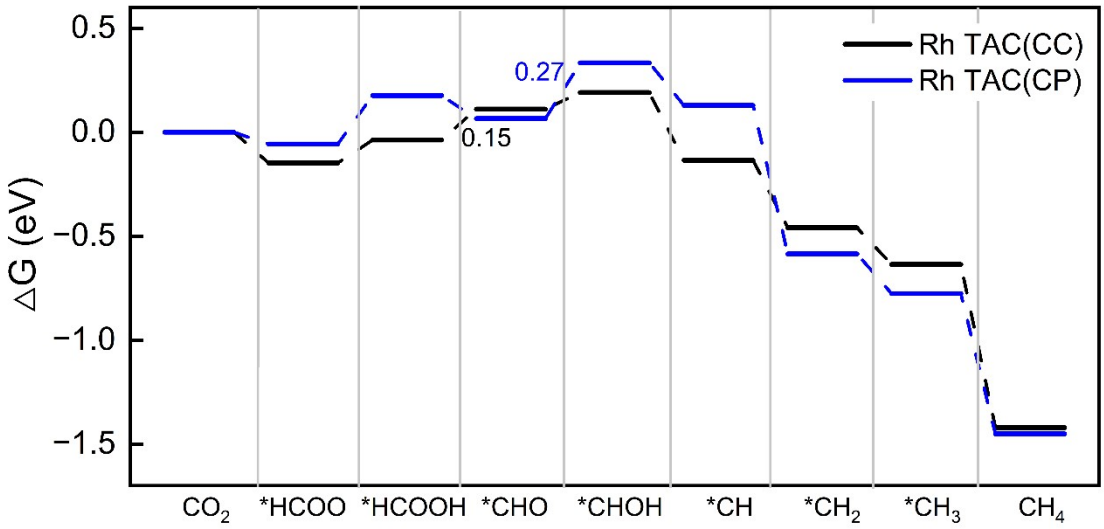

Fig. S7 Free energy diagrams for CH_4 production on Rh TAC calculated by constant charge (CC) method at 0 V *vs*. RHE and constant potential (CP) method at 0 V *vs*. RHE (pH = 0).

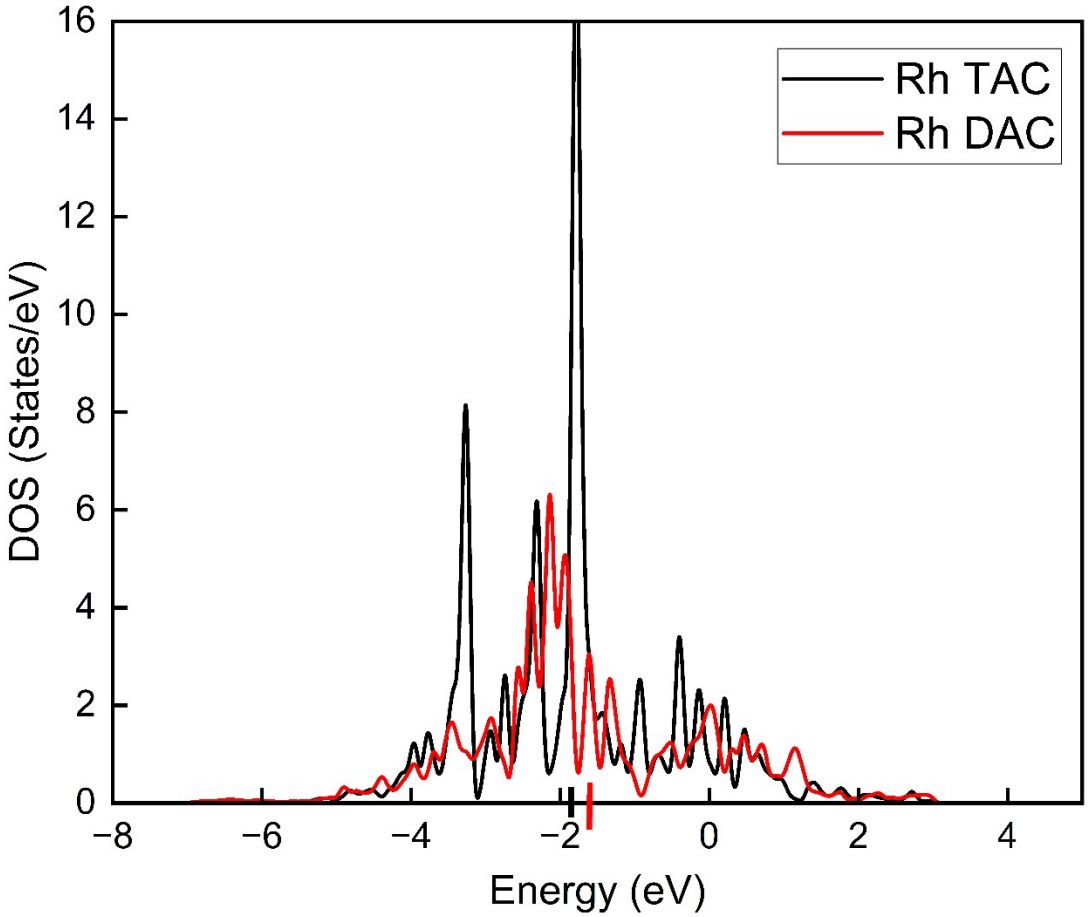

Fig. S8 Projected density of states (DOS) of the *d*-band for Rh atoms in Rh TAC and DAC. The vertical black and red lines indicate the *d*-band center.

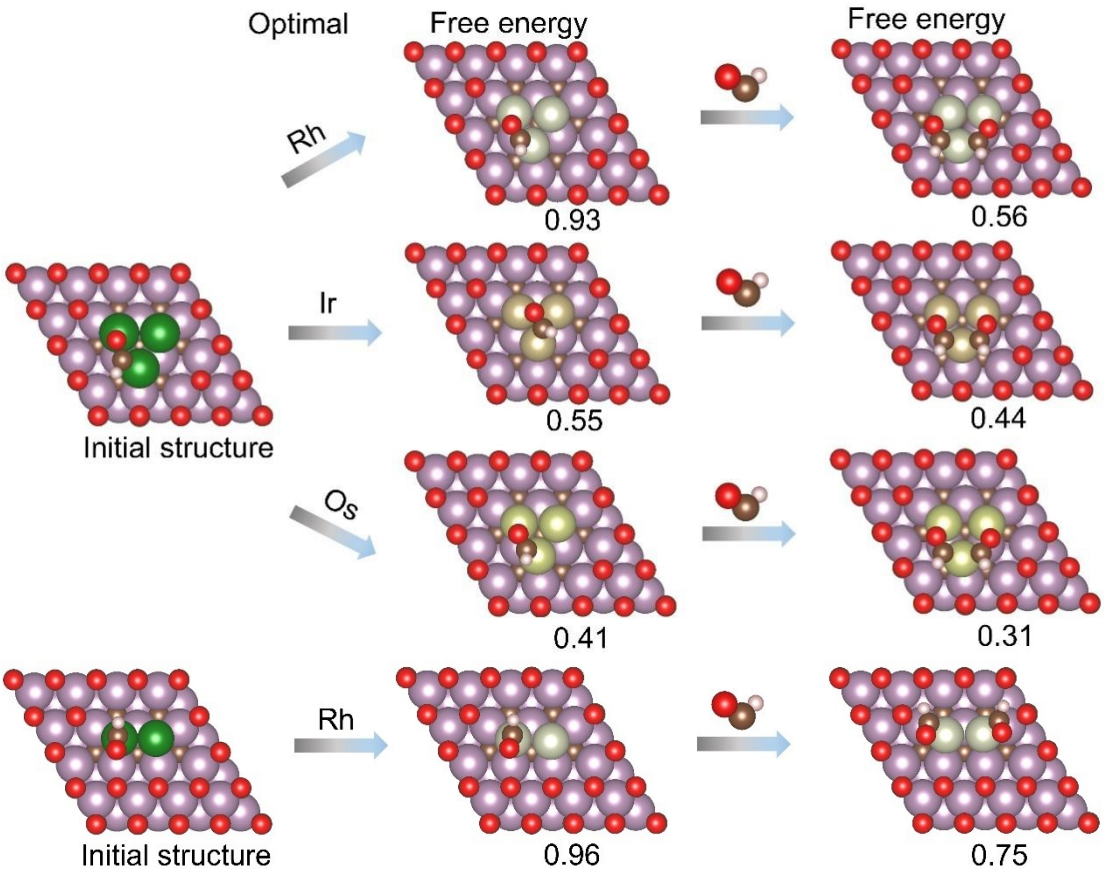

Fig. S9 Adsorption structure and free energy of single *CHO and double *CHO intermediates on Rh, Ir, Os TACs, and Rh DAC.

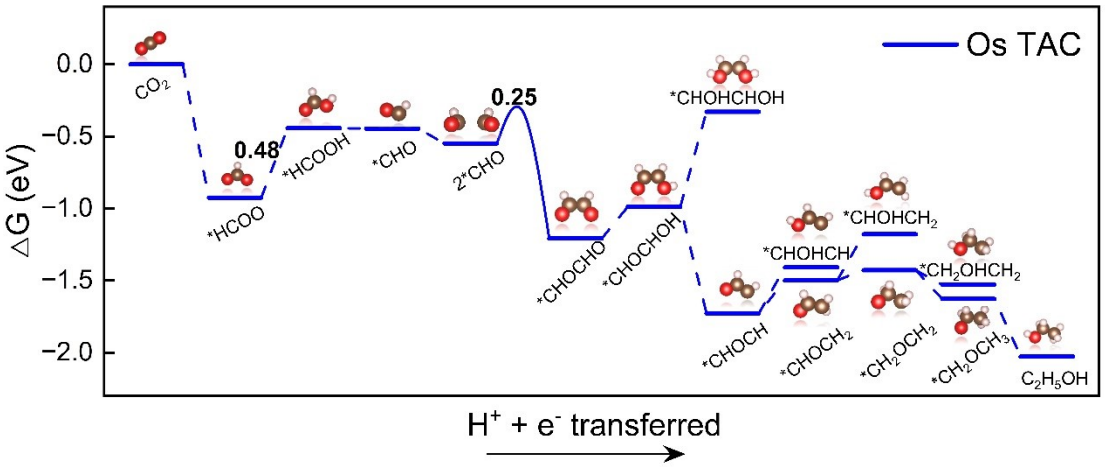

Fig. S10 Free energy diagram for C_2H_5OH production on Os TAC. Atomic structures of the intermediates are shown as insets. Gray, red, and white spheres represent C, O, and H atoms, respectively.

Optimized geometries

The optimized atomic geometries for Rh TAC, Os TAC, Ir TAC, and Rh DAC

*Rh TAC (fractional coordinates)

1.00000000000000

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-5.9939999579999999 10.3819124678999994 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.2723007202000005

Rh Mo C O

3 32 16 25

Direct

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*Os TAC (fractional coordinates)

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Os Mo C O

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Direct

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*Ir TAC (fractional coordinates)

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Ir	Mo	C	O
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Direct

0.4254993862586925	0.3508539892508558	0.3183615116557165
0.4255527684072511	0.5744222957010098	0.3184603150781672
0.6490792725293484	0.5744538348431777	0.3183770444347571
0.0782460617928061	0.1654956246096484	0.2371956970447710
0.3289520537839363	0.1579431401076307	0.2372496437166808
0.5872220653345877	0.1654833764276723	0.2371961791003974
0.8333275161381165	0.1666883621060348	0.2383785916362298
0.0782540605040404	0.4127645236575239	0.2371921010815056
0.3244328924779122	0.4123048112867553	0.2308141487535698
0.5877830197575986	0.4122603300315731	0.2307411666487689
0.8345267365126268	0.4127872283942265	0.2371912408675696
0.0825380125986669	0.6650574644424093	0.2374364164684622
0.3290169908954155	0.6709953252106745	0.2371920963873279
0.5876891858217718	0.6755227296690388	0.2307793834624262
0.8420492940948661	0.6710497600950739	0.2372371312667838
0.0825153920953096	0.9174874208143009	0.2374436012440935
0.3349559893083524	0.9174705334062710	0.2374446255270778
0.5872400978094515	0.9217526913476279	0.2371925412707343
0.8345070828467527	0.9217564267755021	0.2371931961535812
0.1654631113998808	0.0823068078381582	0.1102721065509070
0.4168327266245090	0.0823054515559325	0.1102648906877122
0.6672233959008660	0.0836200202890358	0.1099068859733149
0.9163850122223179	0.0836191207467671	0.1099081541024613
0.1659358924166044	0.3329605992513289	0.1114100669990966
0.4152040240194865	0.3304216307340478	0.1121290977290340
0.6670290451646549	0.3329706067506096	0.1114049508762402
0.9163867839889474	0.3327835557598226	0.1099059871074556
0.1654753675075236	0.5831547840880383	0.1102481169123059
0.4152150085218264	0.5847857389551880	0.1121100072853649
0.6695730709531292	0.5847945745006915	0.1121210072041023

0.9177007138842042	0.5831709876630802	0.1102576932222331
0.1666752596270868	0.8333349655206390	0.1081530724830215
0.4168493389819238	0.8345298332017889	0.1102510170816327
0.6670379987287743	0.8340624794222824	0.1114044037448540
0.9176885687583257	0.8345314782733615	0.1102691847792964
0.9990702166611068	0.0009281947963295	0.1734406153115041
0.2472273517448488	0.9944504283259213	0.1728706140604287
0.5018422520317314	0.0009189621070166	0.1734396270426503
0.7511503339996785	0.0023181421321912	0.1734044944077606
0.9976800766812191	0.2488499625240677	0.1734058773033106
0.2449259005724988	0.2411082470716288	0.1746357990025530
0.4961520411280365	0.2410676968262903	0.1746230806058142
0.7511603746296220	0.2488474017532067	0.1734035738388345
0.9990864322678041	0.4981661493359179	0.1734349846209865
0.2448909923843338	0.5038265809178708	0.1746003783261938
0.4999649432939105	0.4999915305183428	0.1738565447280283
0.7589473668097517	0.5038563171161955	0.1746136861181234
0.0055497039179017	0.7527775097651774	0.1728697629364475
0.2472438298954077	0.7527698664834915	0.1728679777192400
0.4961809635264290	0.7551034633839672	0.1746021674265932
0.7588882252668051	0.7550710627824779	0.1746305332407751
0.9981081654267375	0.0018996699544281	0.2932972240027769
0.2499881941027310	0.0000180899277279	0.2936022966098676
0.5037555568544794	0.0018698908077050	0.2932974619441222
0.7485285820457058	0.9970139507768694	0.2936891192342795
0.0030005003221560	0.2514812624483887	0.2936906837328451
0.7484625189394204	0.2515496835107088	0.2936846168347645
0.9981452688134143	0.4962595327477854	0.2932935022779878
-0.0000295101566702	0.7500119917505814	0.2935955626654640
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0.2506462856798752 0.4989760396125641 0.0552653045131872

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0.7483533282528860 0.4989985148095561 0.0552739550190597

0.9977811104546782 0.7489015493127066 0.0537243468194084

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0.5010154102751396 0.7493488366719038 0.0552648267423618

0.7483597122424267 0.7493667813797023 0.0552781290942128

*Rh DAC (fractional coordinates)

1.00000000000000

11.9879999160999997 0.0000000000000000 0.0000000000000000

-5.9939999579999999 10.3819124678999994 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.2723007202000005

Rh Mo C O

2 32 16 27

Direct

0.4165845340057088 0.5593346549584253 0.3187830149104584

0.6428451332952754 0.5593144169288071 0.3187549114588285

0.0832644993114467 0.1684317035072615 0.2364924016655435

0.3323409167660204 0.1647040377369287 0.2364385965224195

0.5851691789983409 0.1684457898194487 0.2364877327844458

0.8345864274763849	0.1691818116313705	0.2369838110580100
0.0784617517394016	0.4141390167109060	0.2374153435927828
0.3261404464367731	0.4068546644675609	0.2360079776968562
0.5807035073212645	0.4068549380617656	0.2359974635900094
0.8356833092710814	0.4141605426468878	0.2374200168187661
0.0830234353684663	0.6660299803429955	0.2376244130389391
0.3321576253954129	0.6736547914501522	0.2354611346001682
0.5872128934677642	0.6744824437114949	0.2310613228990656
0.8416016956743078	0.6737307949463529	0.2354567080413089
0.0836864783511095	0.9182369221140514	0.2364338148142206
0.3345840210277486	0.9182336338619399	0.2364574176771366
0.5881181897721128	0.9254465858354793	0.2353691494731847
0.8373720096039724	0.9254451118966610	0.2353704213537825
0.1660745684512012	0.0826864797685005	0.1081493723686128
0.4165781399464767	0.0826628921893466	0.1081525002640812
0.6675004984905588	0.0849000851061209	0.1087536548773609
0.9173847729340420	0.0849002477141240	0.1087586866921794
0.1665028639256781	0.3337419490074789	0.1105802868937610
0.4158151420416935	0.3316397809718105	0.1104426744808363
0.6671974526483349	0.3337182295660426	0.1105831528777500
0.9170186543104513	0.3340540423682428	0.1091471193902114
0.1662680076386610	0.5832975841327979	0.1113378879542859
0.4159981729963706	0.5842992507418002	0.1137297925919534
0.6682783991026444	0.5843141523323938	0.1137257471877931
0.9170218972532027	0.5832917580931914	0.1113379005294023
0.1667419403136501	0.8334889825045831	0.1085343811150883
0.4170939717877865	0.8347389207847917	0.1097180627936540
0.6672607794504678	0.8345232596944135	0.1110401330614664
0.9176494522753974	0.8347556050809483	0.1097165170057619
0.0014715335237777	0.0027818992764880	0.1722564594589512

0.2496481389050712	-0.0007356227190702	0.1727570365187637
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0.9993825689444890	0.2509343576073579	0.1726890354478037
0.2461226218142102	0.2429433818118668	0.1711341211197359
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0.7515344144519981	0.2509292546625631	0.1726853072154756
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0.4984301770318569	0.4968743193485753	0.1768241521631561
0.7523273657611039	0.5001725483289874	0.1772738660380560
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0.9992809510148897	0.4984767348465836	0.2935616366961843
0.9981378994048965	0.7508129230863104	0.2929174161048678
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0.9984056161035070	-0.0002338997899258	0.0527947093700764
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0.5013307906377469	-0.0002559183625155	0.0527927349978053
0.7497632401005775	-0.0004517968733044	0.0534543230514901

0.0013961571504312	0.2521047423851900	0.0533147772849911
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0.7506863184438496	0.2521072937056299	0.0533140332625019
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0.2520139895184649	0.5013568262747711	0.0561733626005871
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