SUPPLEMENTARY INFORMATION

Dramatic change in the step edges of Cu(100) electrocatalyst upon exposure to CO: *Operando* observations by electrochemical STM and explanation using quantum mechanical calculations

Soonho Kwon[§a], Youn-Geun Kim[§b*], Jack H. Baricuatro[§b], and William A. Goddard III[a*]

[§]First authorship is equally shared

[a]*Liquid Sunlight Alliance (LiSA) and Materials and Process Simulation Center (MSC), California Institute of Technology, Pasadena, California 91125. USA*

[b]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA*

*To whom correspondence may be addressed: wag@caltech.edu, ORCID:0000-0003-0097-5716; ygkim@caltech.edu, ORCID: 0000-0002-5936-6520

Jack Baricuatro: jackhess@caltech.edu, ORCID: 0000-0002-9210-344X

Soonho Kwon: skwon@caltech.edu, ORCID: 0000-0002-9225-3018

Youn-Geun Kim: ygkim@caltech.edu, ORCID: 0000-0002-5936-6520

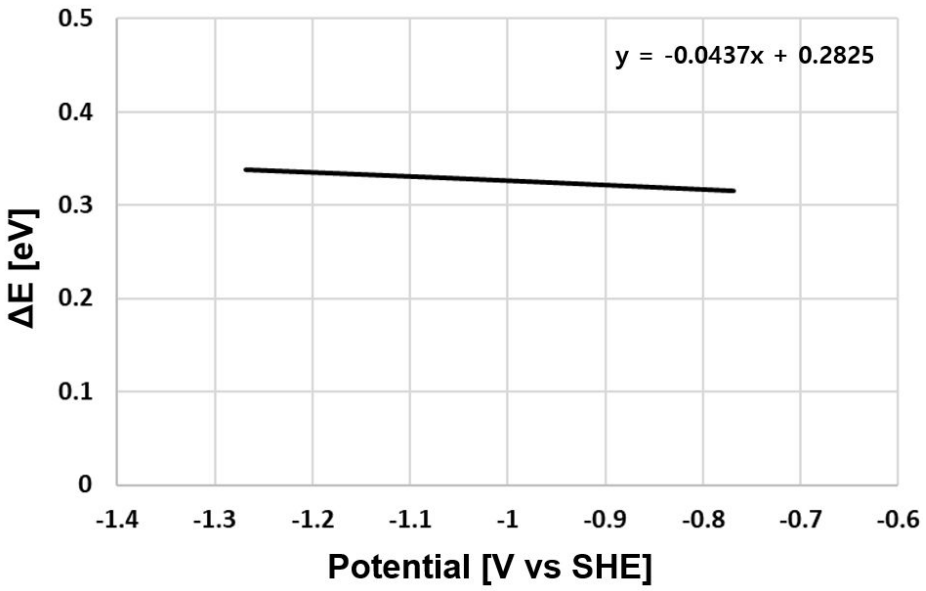

Figure S1. Grand canonical reaction energy of step edge formation along <001> direction from Cu(711) with CO 0.5 ML as function of potential. The reaction energy has a negligible potential dependence with a slope of 0.04 eV/V. The grand canonical calculations were performed using GCP-K method[1] to estimate the effect of applied potential on each step of the reactions. In this scheme, the electrochemical potential is the same for the starting point, reaction pathway, and ending point of each reaction, but the surface charge changes.

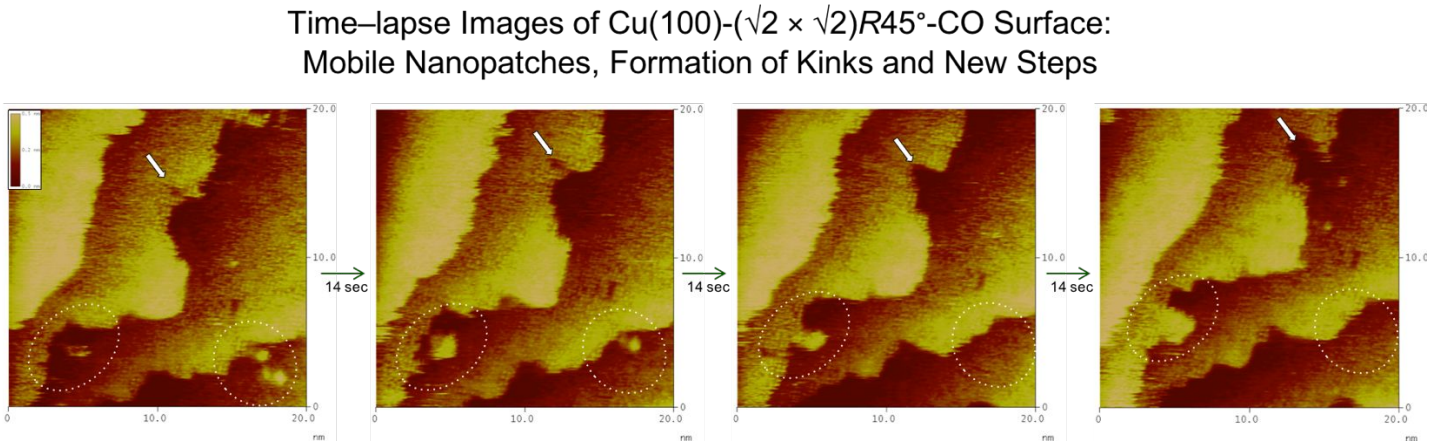

Figure S2. Time–lapse images of the Cu(100)-(√2 × √2)*R*45°-CO surface at -0.9 V in CO-saturated 0.1 M KOH solution. Bias voltage = 250 mV; tunneling current = 5 nA; scan rate = 18 Hz. White arrows indicate the same position on the surface. Circles highlight areas where there is cluster diffusion and formation of new steps. Other experimental details are indicated in the text.

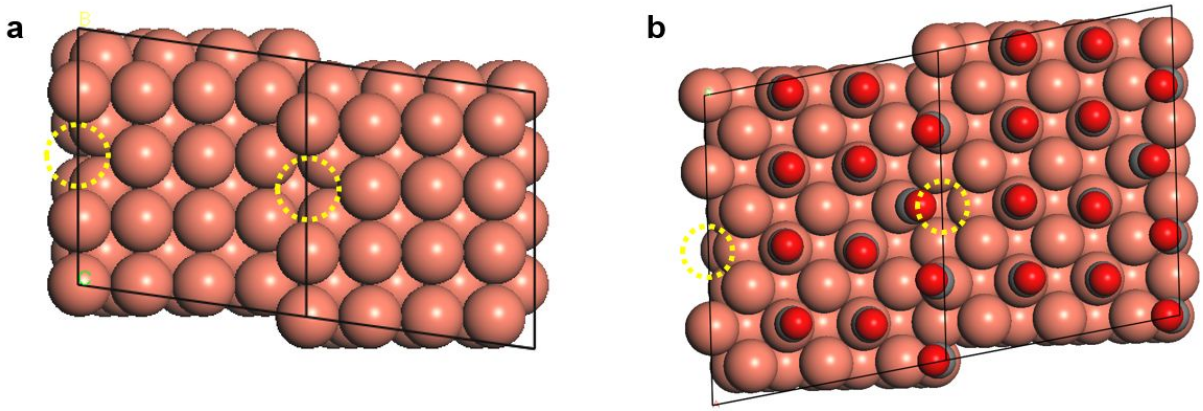

Figure S3. Kink formation on (a) Cu(711) without CO* and (b) Cu(610) with CO* at a surface coverage of 0.5 monolayer.

References

1. Huang, Y.; Nielsen, R. J.; Goddard, W. A., Reaction Mechanism for the Hydrogen Evolution Reaction on the Basal Plane Sulfur Vacancy Site of MoS2 Using Grand Canonical Potential Kinetics. *J. Am. Chem. Soc.* **2018,** *140*, 16773-16782.

Coordinates for all atomic structures

Cu610

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   Cu
    50
Selective dynamics
Direct
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  0.9729700090000009  0.8918899700000011  0.2268899990000008  F  F  F
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  0.6824299840000023  0.7297299709999976  0.2401899930000013  F  F  F
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  0.8918899589999967  0.5675699729999977  0.2535000049999994  F  F  F
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Cu711

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Cu

64

Selective dynamics

Direct

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Transition state forming step edge along the <001> direction on Cu711

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Cu

64

Selective dynamics

Direct

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Step edge formation along the <001> direction on Cu(711)

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0.0000000000000000	0.0000000000000000	22.4923992157000008

Cu

64

Selective dynamics

Direct

0.1176500030000014	0.0147100000000009	0.2222999880000032	F	F	F
0.1176499999999976	0.2647100229999992	0.2222999880000032	F	F	F
0.1176499999999976	0.5147100280000032	0.2222999880000032	F	F	F
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0.2941200269999982	0.4117599859999999	0.2889199869999999	F	F	F
0.2941200169999973	0.6617599659999982	0.2889199869999999	F	F	F
0.2941200069999965	0.9117599459999965	0.2889199869999999	F	F	F
0.0196100000000001	0.1274500059999966	0.3111299810000006	F	F	F
0.0196099980000000	0.3774499860000020	0.3111299810000006	F	F	F
0.0196100020000003	0.6274500139999972	0.3111299810000006	F	F	F
0.0196099989999965	0.8774500419999995	0.3111299810000006	F	F	F
0.7451000040000011	0.0931399999999982	0.3333300119999976	F	F	F
0.7451000379999968	0.3431400099999991	0.3333300119999976	F	F	F
0.7451000189999988	0.5931400150000030	0.3333300119999976	F	F	F
0.7451000550000018	0.8431400429999982	0.3333300119999976	F	F	F
0.4705899639999984	0.0588200030000010	0.3555400070000019	F	F	F
0.4705899719999991	0.3088200130000018	0.3555400070000019	F	F	F
0.4705899819999999	0.5588200409999970	0.3555400070000019	F	F	F
0.4705899590000016	0.8088200219999990	0.3555400070000019	F	F	F
0.1960800069999991	0.0245099999999994	0.3777500010000026	F	F	F
0.1960799980000019	0.2745099899999985	0.3777500010000026	F	F	F
0.1960800120000030	0.5245100420000028	0.3777500010000026	F	F	F
0.1960800020000022	0.7745100220000012	0.3777500010000026	F	F	F
0.9226755971586411	0.2402662948768151	0.4007377856158256	T	T	T
0.9217391076266059	0.4899505575466633	0.4006641638595055	T	T	T
0.9219272002547614	0.7401651255227893	0.4008003862628433	T	T	T
0.9220842800821183	0.9903593221139469	0.4006479468413607	T	T	T
0.6494620864887387	0.2064737491493923	0.4235831609579274	T	T	T
0.6477972867542376	0.4561781951210968	0.4233871063792297	T	T	T
0.6491567492498613	0.7063572560054922	0.4229902856590022	T	T	T
0.6491813802415065	0.9561960980635504	0.4232870021685975	T	T	T
0.3736055050798742	0.1716814723292941	0.4451818941768574	T	T	T
0.3733994046208199	0.4221312805203601	0.4454138031948432	T	T	T
0.3755924472857032	0.6721465292966468	0.4448107577850481	T	T	T
0.3761993732750991	0.9212387910419032	0.4450311046399926	T	T	T
0.0974385849648777	0.1392292164199860	0.4687207922188759	T	T	T
0.0961100825756585	0.3842057768665801	0.4689688948769515	T	T	T
0.1006715625904148	0.6365162655580269	0.4667496907676331	T	T	T

0.1011653817945134	0.8882897407568324	0.4667170398605764	T	T	T
0.8246970705367834	0.1055325979174984	0.4914363487096455	T	T	T
0.8226916658401112	0.3510333083907978	0.4915450820164239	T	T	T
0.8222778390446763	0.5989463894169129	0.4908728448869694	T	T	T
0.8230116840009410	0.8572567892885027	0.4910569637898331	T	T	T
0.5516818480187728	0.0692927436226064	0.5117655725129655	T	T	T
0.5492363374591440	0.3186634155703975	0.5119005230023232	T	T	T
0.5485786358429222	0.5681082762666193	0.5134305636664447	T	T	T
0.5490897412804828	0.8197672064200131	0.5135766947634791	T	T	T
0.2790957159956757	0.0343605028097028	0.5328013820384612	T	T	T
0.2745807989926247	0.2839256015808506	0.5328972401059142	T	T	T
0.2764647529707026	0.5341352972530797	0.5330056457812870	T	T	T
0.2770840806032346	0.7840514641240106	0.5334772746596580	T	T	T
0.0062033923833769	0.9988273985850478	0.5532151681264397	T	T	T
0.7306954133597854	0.7163542563676336	0.5736974952240567	T	T	T
0.0042469446750192	0.5029200656813891	0.5533162004871277	T	T	T
0.0033279954260607	0.7504236330736437	0.5536972355560920	T	T	T

Cu711 with CO 0.5 ML

1.00000000000000

9.0944004059000001	0.0000000000000000	0.0000000000000000
-1.3991367633000000	9.9918163488000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.4923992157000008

Cu	C	O
64	6	6

Selective dynamics

Direct

0.1176500030000014	0.0147100000000009	0.2222999880000032	F	F	F
0.1176499999999976	0.2647100229999992	0.2222999880000032	F	F	F
0.1176499999999976	0.5147100280000032	0.2222999880000032	F	F	F
0.1176499970000009	0.7647100080000016	0.2222999880000032	F	F	F
0.8431400090000025	0.2303900020000000	0.2444999980000020	F	F	F
0.8431399890000009	0.4803900060000004	0.2444999980000020	F	F	F
0.8431400260000004	0.7303900349999992	0.2444999980000020	F	F	F
0.8431400099999991	0.9803900630000015	0.2444999980000020	F	F	F
0.5686299859999977	0.1960800029999987	0.2667100130000009	F	F	F
0.5686299660000032	0.4460800069999991	0.2667100130000009	F	F	F
0.5686299509999984	0.6960800350000014	0.2667100130000009	F	F	F
0.5686299609999992	0.9460800629999966	0.2667100130000009	F	F	F
0.2941200240000015	0.1617600049999979	0.2889199869999999	F	F	F
0.2941200269999982	0.4117599859999999	0.2889199869999999	F	F	F
0.2941200169999973	0.6617599659999982	0.2889199869999999	F	F	F
0.2941200069999965	0.9117599459999965	0.2889199869999999	F	F	F
0.0196100000000001	0.1274500059999966	0.3111299810000006	F	F	F
0.0196099980000000	0.3774499860000020	0.3111299810000006	F	F	F
0.0196100020000003	0.6274500139999972	0.3111299810000006	F	F	F
0.0196099989999965	0.8774500419999995	0.3111299810000006	F	F	F
0.7451000040000011	0.0931399999999982	0.3333300119999976	F	F	F
0.7451000379999968	0.3431400099999991	0.3333300119999976	F	F	F
0.7451000189999988	0.5931400150000030	0.3333300119999976	F	F	F
0.7451000550000018	0.8431400429999982	0.3333300119999976	F	F	F
0.4705899639999984	0.0588200030000010	0.3555400070000019	F	F	F
0.4705899719999991	0.3088200130000018	0.3555400070000019	F	F	F
0.4705899819999999	0.5588200409999970	0.3555400070000019	F	F	F
0.4705899590000016	0.8088200219999990	0.3555400070000019	F	F	F
0.1960800069999991	0.0245099999999994	0.3777500010000026	F	F	F
0.1960799980000019	0.2745099899999985	0.3777500010000026	F	F	F
0.1960800120000030	0.5245100420000028	0.3777500010000026	F	F	F
0.1960800020000022	0.7745100220000012	0.3777500010000026	F	F	F

0.9226346113977573	0.2402803677471844	0.3997963151929734	T	T	T
0.9232184540354957	0.4902894615143608	0.4007010724484648	T	T	T
0.9226988835262470	0.7401517626765282	0.3997855414420186	T	T	T
0.9232236915235804	0.9902861596629750	0.4006809345206000	T	T	T
0.6485986890270869	0.2049480432660952	0.4238709285977268	T	T	T
0.6487352314979662	0.4568983579175771	0.4239106415410990	T	T	T
0.6487284897866963	0.7048955272946510	0.4238154387965594	T	T	T
0.6485557956236332	0.9568576396056859	0.4238818871161017	T	T	T
0.3753539891929957	0.1722191274003821	0.4461124665391491	T	T	T
0.3749309316247584	0.4216273691725597	0.4458478106406217	T	T	T
0.3753788505055040	0.6723391971284925	0.4461599850977063	T	T	T
0.3749640254202099	0.9215983634603403	0.4458597692869056	T	T	T
0.1006605768921604	0.1375596522817146	0.4682443228347019	T	T	T
0.0999074614389547	0.3879393078023429	0.4682908941828289	T	T	T
0.1008949067927847	0.6375194323827794	0.4683378941365858	T	T	T
0.0998925433930936	0.8877944729706611	0.4681786012906666	T	T	T
0.8258755070979317	0.1029579805273463	0.4906412755096040	T	T	T
0.8238630344314946	0.3529255491045938	0.4909382245904679	T	T	T
0.8261258183745873	0.6029027809850486	0.4907009293643267	T	T	T
0.8239524104257738	0.8527536506716835	0.4908057925460917	T	T	T
0.5538704878387075	0.0686500502286792	0.5162902114631787	T	T	T
0.5534159089528745	0.3185805912376775	0.5117136815424713	T	T	T
0.5540538532606877	0.5686122942880886	0.5162046482644175	T	T	T
0.5535310745918777	0.8186024340027784	0.5117662732267236	T	T	T
0.2781466725532953	0.0352098503733624	0.5333596550801836	T	T	T
0.2794728803408876	0.2852685996221883	0.5376234073792403	T	T	T
0.2783795877044153	0.5351831507514527	0.5333549559181343	T	T	T
0.2797042646644445	0.7852376456772197	0.5376835425154923	T	T	T
0.0040405930695683	0.0002527968927848	0.5570855621276269	T	T	T
0.0018387697040514	0.2502859275757173	0.5545146118074166	T	T	T
0.0044482328205451	0.5002903701826924	0.5574164512312144	T	T	T
0.0020377634783826	0.7504146114909127	0.5545544275508461	T	T	T
0.5908962714035461	0.0707220027310689	0.5968479437896140	T	T	T
0.5929977835361689	0.5748522554393145	0.5966121386481376	T	T	T
0.3130969842666637	0.2944738911737281	0.6181468799515498	T	T	T
0.3109435725421702	0.7967266086660227	0.6183548791611987	T	T	T
-0.0082524024265869	0.0032393219786176	0.6384941598790799	T	T	T
-0.0089095001055718	0.5059358924756197	0.6388241760867331	T	T	T
0.6109986900597112	0.0729178773511931	0.6477601784240878	T	T	T
0.6147220449937141	0.5800026203608959	0.6474001479592699	T	T	T
0.3368023856568078	0.2993238303091996	0.6688129549763837	T	T	T
0.3329867099870004	0.8029462149327419	0.6691324254261126	T	T	T
-0.0034822269586237	0.0077190472668578	0.6898900240597502	T	T	T
-0.0057316795820551	0.5120697427331850	0.6902014095445980	T	T	T

Transition state forming step edge along the <001> direction on Cu711 with CO 0.5 ML

1.00000000000000

9.0944004059000001	0.0000000000000000	0.0000000000000000
-1.3991367633000000	9.9918163488000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.4923992157000008

Cu	C	O
64	6	6

Selective dynamics

Direct

0.1176500030000014	0.0147100000000009	0.2222999880000032	F	F	F
0.1176499999999976	0.2647100229999992	0.2222999880000032	F	F	F
0.1176499999999976	0.5147100280000032	0.2222999880000032	F	F	F
0.1176499970000009	0.7647100080000016	0.2222999880000032	F	F	F
0.8431400090000025	0.2303900020000000	0.2444999980000020	F	F	F

0.8431399890000009	0.4803900060000004	0.2444999980000020	F	F	F
0.8431400260000004	0.7303900349999992	0.2444999980000020	F	F	F
0.8431400099999991	0.9803900630000015	0.2444999980000020	F	F	F
0.5686299859999977	0.1960800029999987	0.2667100130000009	F	F	F
0.5686299660000032	0.4460800069999991	0.2667100130000009	F	F	F
0.5686299509999984	0.6960800350000014	0.2667100130000009	F	F	F
0.5686299609999992	0.9460800629999966	0.2667100130000009	F	F	F
0.2941200240000015	0.1617600049999979	0.2889199869999999	F	F	F
0.2941200269999982	0.4117599859999999	0.2889199869999999	F	F	F
0.2941200169999973	0.6617599659999982	0.2889199869999999	F	F	F
0.2941200069999965	0.9117599459999965	0.2889199869999999	F	F	F
0.0196100000000001	0.1274500059999966	0.3111299810000006	F	F	F
0.0196099980000000	0.3774499860000020	0.3111299810000006	F	F	F
0.0196100020000003	0.6274500139999972	0.3111299810000006	F	F	F
0.0196099989999965	0.8774500419999995	0.3111299810000006	F	F	F
0.7451000040000011	0.0931399999999982	0.3333300119999976	F	F	F
0.7451000379999968	0.3431400099999991	0.3333300119999976	F	F	F
0.7451000189999988	0.5931400150000030	0.3333300119999976	F	F	F
0.7451000550000018	0.8431400429999982	0.3333300119999976	F	F	F
0.4705899639999984	0.0588200030000010	0.3555400070000019	F	F	F
0.4705899719999991	0.3088200130000018	0.3555400070000019	F	F	F
0.4705899819999999	0.5588200409999970	0.3555400070000019	F	F	F
0.4705899590000016	0.8088200219999990	0.3555400070000019	F	F	F
0.1960800069999991	0.0245099999999994	0.3777500010000026	F	F	F
0.1960799980000019	0.2745099899999985	0.3777500010000026	F	F	F
0.1960800120000030	0.5245100420000028	0.3777500010000026	F	F	F
0.1960800020000022	0.7745100220000012	0.3777500010000026	F	F	F
0.9245416618154433	0.2383514528679215	0.3989125024827828	T	T	T
0.9240935584785452	0.4921346015571689	0.3993842746713662	T	T	T
0.9227033392747931	0.7409649590087121	0.4001693506364575	T	T	T
0.9230342082743771	0.9901031875265311	0.4011154902575701	T	T	T
0.6461767034420960	0.2022454201898197	0.4228934760232645	T	T	T
0.6456426970129190	0.4590121262305196	0.4230347190280599	T	T	T
0.6483123600131186	0.7059683709244415	0.4241745211586019	T	T	T
0.6498560133747329	0.9572344230135921	0.4246223051787884	T	T	T
0.3758543373689852	0.1725109536085063	0.4463611581095466	T	T	T
0.3745190952999521	0.4217250980155794	0.4464647860602901	T	T	T
0.3747455424766924	0.6720159666177495	0.4466099710109998	T	T	T
0.3764579355305280	0.9216750336931402	0.4460071964575001	T	T	T
0.1002077728878469	0.1389155940913000	0.4690177917807000	T	T	T
0.0990183367377874	0.3838015688917453	0.4679437216724987	T	T	T
0.0995627691916737	0.6350636240548095	0.4683235930765353	T	T	T
0.1009741943153153	0.8879549298624587	0.4684821871838780	T	T	T
0.8300874940725717	0.1073243720146519	0.4915701741973774	T	T	T
0.8259119177653432	0.3516172395085577	0.4820198487831599	T	T	T
0.8232625154404156	0.6028021719629465	0.4902791567481518	T	T	T
0.8250579765314831	0.8543576190486531	0.4916723483548041	T	T	T
0.5595499001864730	0.0711451416583677	0.5182277126983350	T	T	T
0.5565108755162719	0.3188098459101782	0.5121552748458583	T	T	T
0.5515251763002961	0.5678716125327155	0.5179029759376855	T	T	T
0.5536134333426699	0.8189741479402783	0.5123186158035232	T	T	T
0.2815754470351212	0.0362271579523322	0.5331170886113160	T	T	T
0.2765924178145138	0.2841725602791686	0.5365534245397690	T	T	T
0.2715584983390724	0.5328002592690632	0.5340680884941800	T	T	T
0.2790468630900950	0.7852321477121825	0.5375328356159259	T	T	T
0.0089979795143386	0.9988417944108636	0.5565274216242463	T	T	T
0.7641471674506568	0.3488463139236769	0.5824861451641113	T	T	T
0.9987813748958192	0.4940554956592106	0.5558230194668587	T	T	T
0.0010760576131850	0.7451469900706911	0.5542499314290231	T	T	T

0.5780517402111697	0.0514114676956811	0.5994111072941232	T	T	T
0.5782041498801315	0.5899508165800557	0.5989283023982706	T	T	T
0.2957164329519869	0.2952991543518060	0.6176975262723325	T	T	T
0.2968840372822162	0.7902957314824879	0.6190059146227193	T	T	T
0.9846107168996083	0.0247871000298291	0.6364391031207226	T	T	T
0.9205610093577666	0.4450386420058606	0.6334955202612333	T	T	T
0.5866055926464560	0.0376211365040264	0.6505031688344709	T	T	T
0.5885015493779244	0.6087850870479737	0.6497892307904279	T	T	T
0.3151698068353074	0.3024307883250389	0.6685684827311085	T	T	T
0.3140110416322389	0.7935376341262150	0.6700799694607790	T	T	T
0.9754321935399837	0.0336843357367719	0.6874472987748935	T	T	T
0.9374621033152177	0.4607579293271631	0.6850098945468948	T	T	T

Step edge formation along the <001> direction on Cu(711) with CO 0.5 ML

1.00000000000000

9.0944004059000001	0.0000000000000000	0.0000000000000000
-1.3991367633000000	9.9918163488000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.4923992157000008

Cu	C	O
64	6	6

Selective dynamics

Direct

0.1176500030000014	0.0147100000000009	0.2222999880000032	F	F	F
0.1176499999999976	0.2647100229999992	0.2222999880000032	F	F	F
0.1176499999999976	0.5147100280000032	0.2222999880000032	F	F	F
0.1176499970000009	0.7647100080000016	0.2222999880000032	F	F	F
0.8431400090000025	0.2303900020000000	0.2444999980000020	F	F	F
0.8431399890000009	0.4803900060000004	0.2444999980000020	F	F	F
0.8431400260000004	0.7303900349999992	0.2444999980000020	F	F	F
0.8431400099999991	0.9803900630000015	0.2444999980000020	F	F	F
0.5686299859999977	0.1960800029999987	0.2667100130000009	F	F	F
0.5686299660000032	0.4460800069999991	0.2667100130000009	F	F	F
0.5686299509999984	0.6960800350000014	0.2667100130000009	F	F	F
0.5686299609999992	0.9460800629999966	0.2667100130000009	F	F	F
0.2941200240000015	0.1617600049999979	0.2889199869999999	F	F	F
0.2941200269999982	0.4117599859999999	0.2889199869999999	F	F	F
0.2941200169999973	0.6617599659999982	0.2889199869999999	F	F	F
0.2941200069999965	0.9117599459999965	0.2889199869999999	F	F	F
0.0196100000000001	0.1274500059999966	0.3111299810000006	F	F	F
0.0196099980000000	0.3774499860000020	0.3111299810000006	F	F	F
0.0196100020000003	0.6274500139999972	0.3111299810000006	F	F	F
0.0196099989999965	0.8774500419999995	0.3111299810000006	F	F	F
0.7451000040000011	0.0931399999999982	0.3333300119999976	F	F	F
0.7451000379999968	0.3431400099999991	0.3333300119999976	F	F	F
0.7451000189999988	0.5931400150000030	0.3333300119999976	F	F	F
0.7451000550000018	0.8431400429999982	0.3333300119999976	F	F	F
0.4705899639999984	0.0588200030000010	0.3555400070000019	F	F	F
0.4705899719999991	0.3088200130000018	0.3555400070000019	F	F	F
0.4705899819999999	0.5588200409999970	0.3555400070000019	F	F	F
0.4705899590000016	0.8088200219999990	0.3555400070000019	F	F	F
0.1960800069999991	0.0245099999999994	0.3777500010000026	F	F	F
0.1960799980000019	0.2745099899999985	0.3777500010000026	F	F	F
0.1960800120000030	0.5245100420000028	0.3777500010000026	F	F	F
0.1960800020000022	0.7745100220000012	0.3777500010000026	F	F	F
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0.9236331249037246	0.4909360180258286	0.4006187298830810	T	T	T
0.9238885181611939	0.7402846887231678	0.3998909832856979	T	T	T
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0.6490986624755972	0.4559028703669696	0.4227736109277227	T	T	T
0.6501177662793927	0.7067306370231230	0.4226317617334200	T	T	T
0.6487927217611699	0.9573364808414235	0.4239752979460482	T	T	T
0.3752918374861381	0.1722002270188531	0.4460830909311778	T	T	T
0.3729376863800895	0.4210742160715812	0.4452317810069195	T	T	T
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0.0989066093132145	0.1395920889403520	0.4688966740099127	T	T	T
0.0971294389895167	0.3853515657351536	0.4690524387931712	T	T	T
0.1016551860323582	0.6360384914777203	0.4685787381700566	T	T	T
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0.5512667426614777	0.5685824839793895	0.5116532521454413	T	T	T
0.5535690462771308	0.8170131662862292	0.5124093777536977	T	T	T
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0.3328864205653513	0.8050293235910980	0.6695046258053113	T	T	T
-0.0070514029731616	0.0669414432699642	0.6857615020627807	T	T	T
-0.0080478696269571	0.4533342950485202	0.6883288272902005	T	T	T
0.6892447039775368	0.7241186589615491	0.7071826141112912	T	T	T