Electronic Supplementary Information (ESI)

New aspects of C2 selectivity in electrochemical CO_2 reduction over oxide-derived copper

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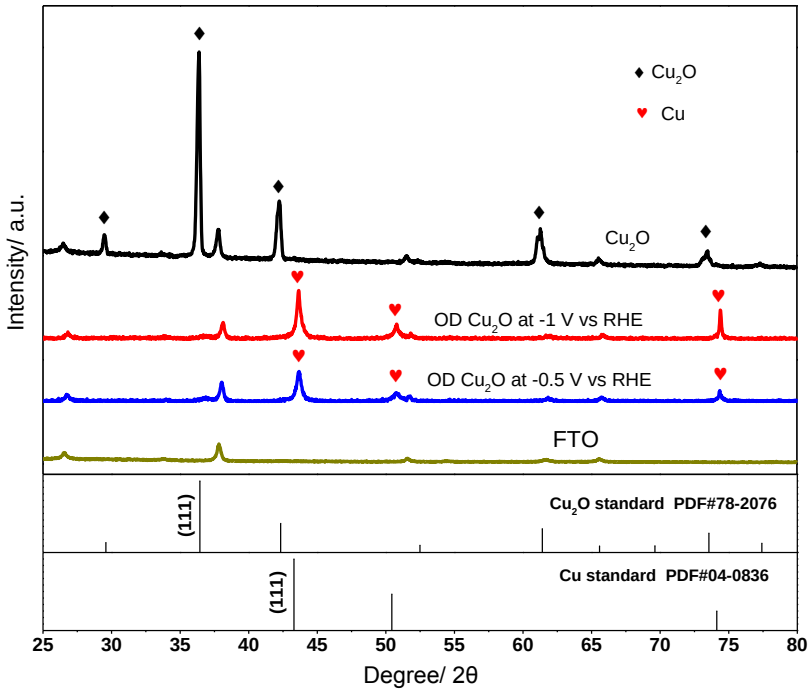

Figure S1. XRD patterns of the as-synthesized Cu_2O NWs and ODCu at –0.5 and –0.1 V vs RHE for 90 min in CO_2-saturated 0.1 M $KHCO_3$.

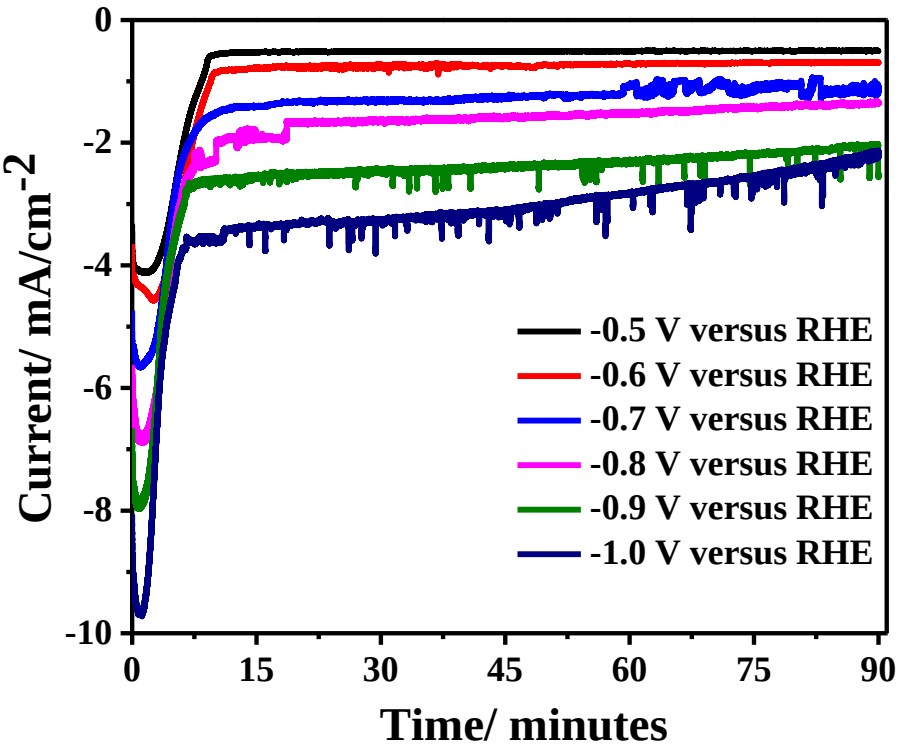

Figure S2. Total current density at different applied voltages in CO_2-saturated 0.1 M $KHCO_3$ electrolyte.

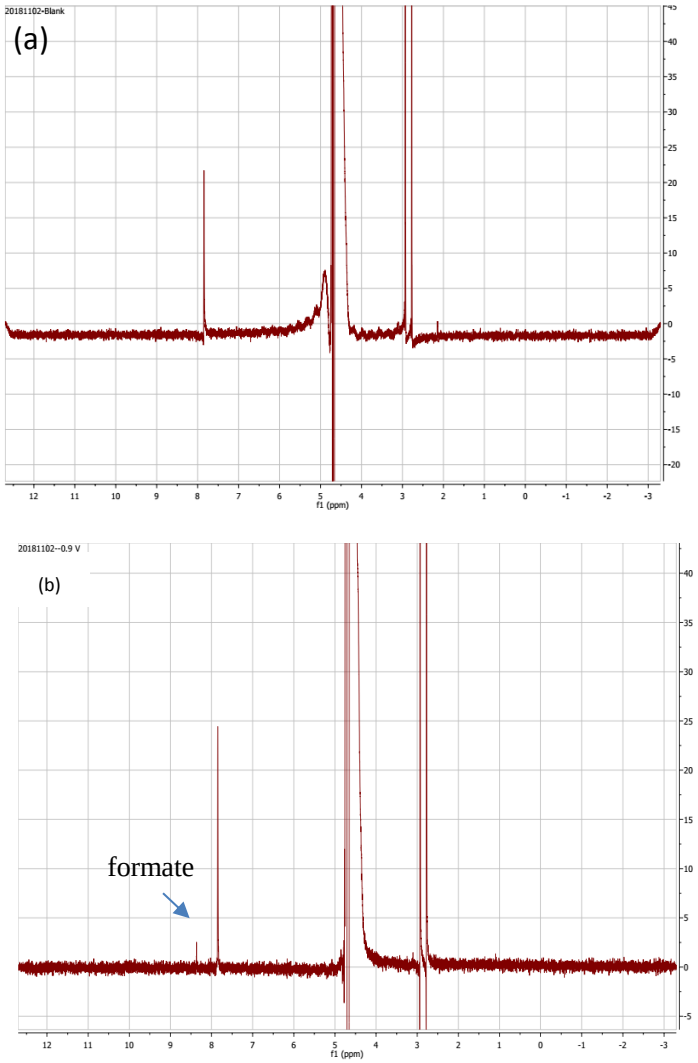

Figure S3. ^{1}HNMR of (a) blank and (b) the samples upon polarization at –0.9 V vs RHE for 90 min in CO_2-saturated 0.1 M $KHCO_3$ (pH 6.8).

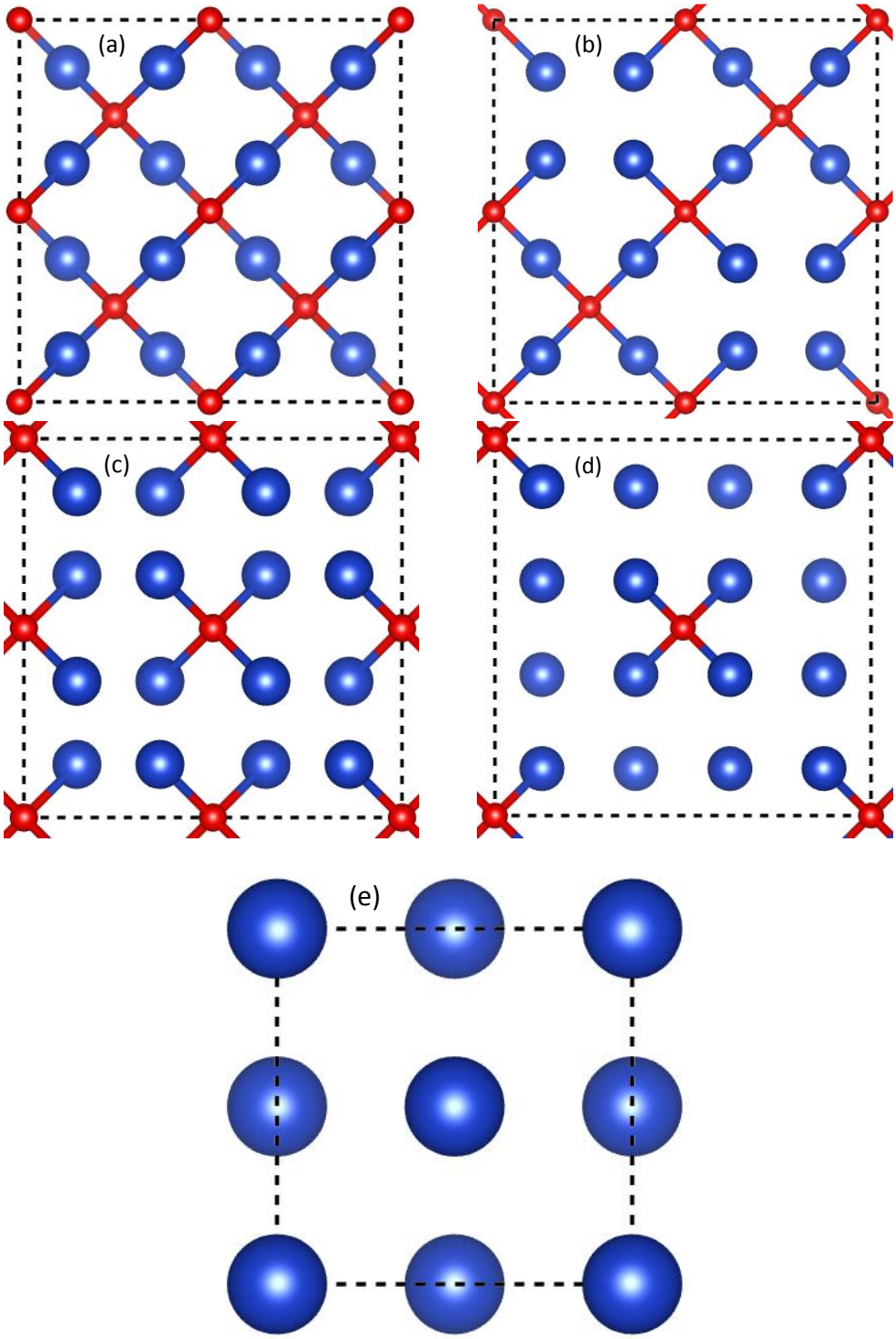

Figure S4. Optimized structure of (a) Cu_2O, (b) $Cu_2O_{0.75}$, (c) $Cu_2O_{0.50}$, (d) $Cu_2O_{0.25}$ and (e) Cu.

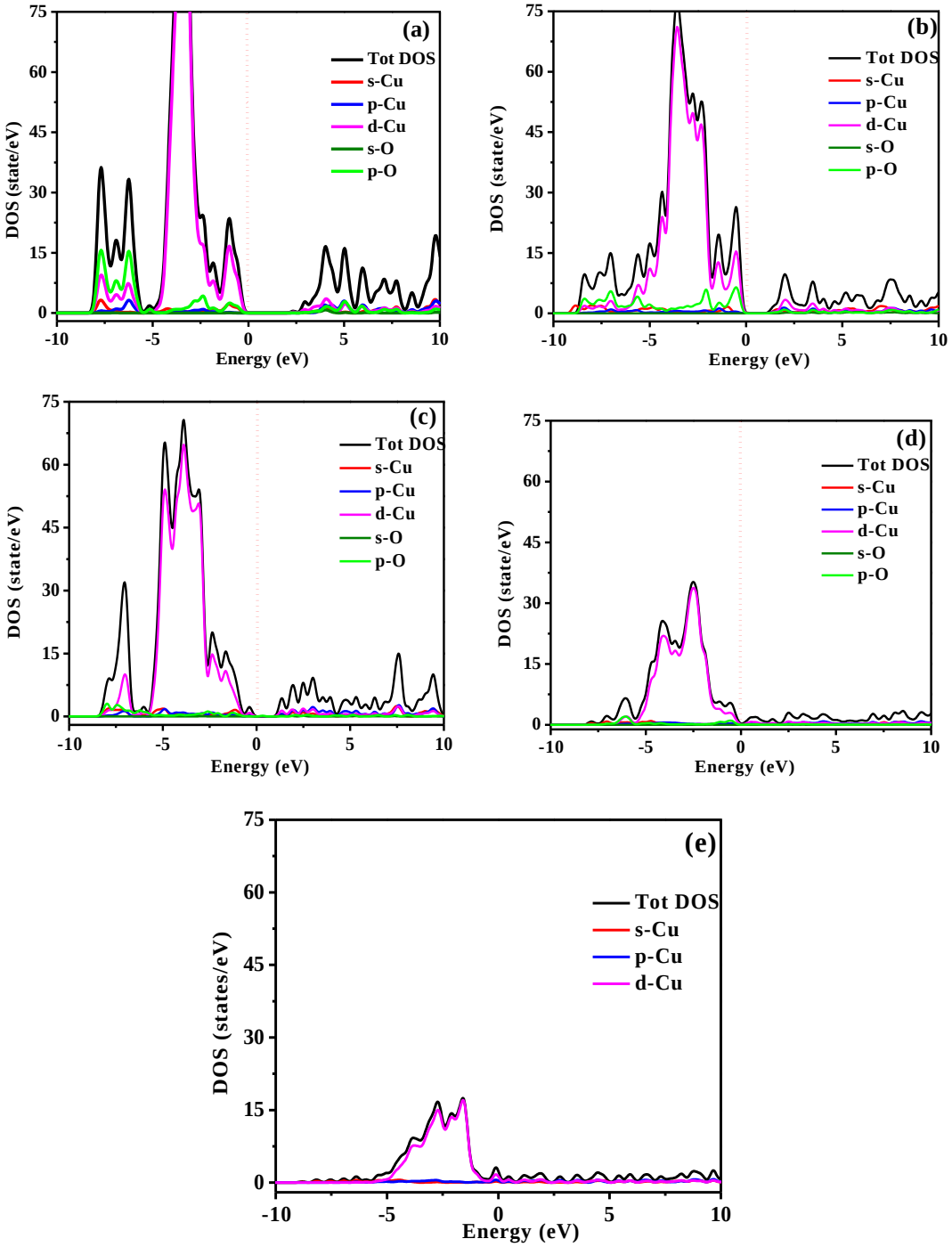

Figure S5. Total density of states of (a) Cu_2O, (b) $Cu_2O_{0.75}$, (c) $Cu_2O_{0.50}$, (d) $Cu_2O_{0.25}$ and (e) Cu.

Table S1. Calculated total energies of different systems

Systems	Total Energy (eV)
clean Cu(111)	–279.63
clean Cu_2O(111)	–237.02
isolated OCCO	–30.05
OCCO adsorbed on Cu(111)	–312.88
OCCO adsorbed on Cu_2O(111)	–272.56

The data of calculations

1. TOTEN

1) TOTEN Cu

free energy TOTEN = 544.01209894 eV

free energy TOTEN = -310.94863142 eV

free energy TOTEN = -349.09110945 eV

free energy TOTEN = -349.92710880 eV

free energy TOTEN = -311.42242599 eV

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free energy TOTEN = -279.63550811 eV

2) TOTEN Cu_2O

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2. Structure geometry

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Cu
4
Direct
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Cu O
16 8
Direct
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0.3750000000000000 0.3750000000000000 0.7500000000000000
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(3) POSCAR_$Cu_2O_{0.25}$

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     0.0000000000000000     0.0000000000000000     2.7949763029051491
   Cu     O
     8      1
Direct
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  0.0000000000000000  0.2945288037124518  0.2419244773225013
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(4) POSCAR_$Cu_2O_{0.50}$

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   Cu     O
    16     4
Direct
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  0.1402238284721939  0.3597761715278062  0.2802484112772020
  0.3597761715278062  0.3597761715278062  0.7197515887227981
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0.00000000E+00   0.00000000E+00   0.00000000E+00
0.00000000E+00   0.00000000E+00   0.00000000E+00
0.00000000E+00   0.00000000E+00   0.00000000E+00

(5) POSCAR_$Cu_2O_{0.75}$

mp-361_Cu2O
1.00000000000000

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   9.8355183351850872   0.0000000000000000   0.0000000000000000
   0.0000000000000000   9.8355183351850872   0.0000000000000000
   0.0000000000000000   0.0000000000000000   2.5147972244102266
  Cu     O
  16     6
Direct
  0.1231655693077686  0.1231655693077686  0.7473390677829055
  0.1231655693077686  0.3768344306922313  0.2526609322170942
  0.3768344306922313  0.3768344306922313  0.7473390677829055
  0.3768344306922313  0.1231655693077686  0.2526609322170942
  0.6355622064166839  0.1355622064166837  0.7837252386832986
  0.6355622064166840  0.3644377935833162  0.2162747613167014
  0.8644377935833160  0.3644377935833162  0.7837252386832987
  0.8644377935833160  0.1355622064166837  0.2162747613167013
  0.1355622064166838  0.6355622064166840  0.7837252386832986
  0.1355622064166838  0.8644377935833160  0.2162747613167014
  0.3644377935833162  0.8644377935833160  0.7837252386832986
  0.3644377935833162  0.6355622064166840  0.2162747613167014
  0.6231655693077685  0.6231655693077685  0.7473390677829055
  0.6231655693077685  0.8768344306922315  0.2526609322170942
  0.8768344306922315  0.8768344306922315  0.7473390677829055
  0.8768344306922315  0.6231655693077685  0.2526609322170942
  0.0000000000000000  0.0000000000000000  0.0177015176506743
  0.2500000000000000  0.2500000000000000  0.5000000000000000
  0.5000000000000000  0.0000000000000000 -0.0177015176506743
  0.0000000000000000  0.5000000000000000 -0.0177015176506743
  0.5000000000000000  0.5000000000000000  0.0177015176506744
  0.7500000000000000  0.7500000000000000  0.5000000000000000

  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
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  0.00000000E+00  0.00000000E+00  0.00000000E+00
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  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
```

0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00

2) OCCO adsorbed geometry

(1) POSCAR_Cu

CONTCARCu
1.00000000000000
10.1048002242999999 0.0000000000000000 0.0000000000000000
-5.0524001122000000 8.7510136943999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 23.2504997252999992
Cu O C
80 2 2
Direct
0.0000415259777622 0.0001805602436433 0.3588397140668504
-0.0003658043822531 0.2489412303964707 0.3587977329688091
0.2465183287921035 0.2471625606524975 0.3573188597128536
0.2504062736285568 0.0000887184177177 0.3584667399899272
0.5000093717832975 0.0002075707185263 0.3586578712946409
0.4998573554009333 0.2471774103100109 0.3579850781518562
0.7515054016144963 0.2487746660671452 0.3587307045125647
0.7506556353955075 0.0001207132691428 0.3588346652605435
0.0017497586155874 0.4999611448211182 0.3580277880850666
0.0032909631661225 0.7520587652741000 0.3588659794939568
0.2508042232092555 0.7511115217653622 0.3582461166524032
0.2458103474221105 0.4998619392813312 0.3572477175155790
0.4894792250666513 0.4996511741555102 0.3597626813363516
0.4998297632367660 0.7529820745930040 0.3575135029155007
0.7536112484016646 0.7526835445034225 0.3588517181551589
0.7545265270821045 0.5002709414516385 0.3643247146903869
0.1679048966775530 0.3334577228155374 0.2673702538933481
0.1673441524338632 0.0826851345958898 0.2673790425456808
0.4183930000949480 0.0839695821448100 0.2677555443319402
0.4186520687848106 0.3348268094862938 0.2688181852763944
0.6688028577886880 0.3355798725022452 0.2692230547156159
0.6680479244884275 0.0835512001382445 0.2681003011019410
0.9180913957058732 0.0835534192655679 0.2679140269239999

0.9175373313011846 0.3337554400355257 0.2680933958091471
0.1672103123446956 0.8329564160223555 0.2678417387463415
0.1676476530153622 0.5841406012918171 0.2671295196977970
0.4183857815878370 0.5828520328728481 0.2679854115012947
0.4178732963148089 0.8337065230102481 0.2673479935128359
0.6683162208893113 0.8324575642590611 0.2683629205829282
0.6666588157280943 0.5818447130403336 0.2699435487121130
0.9156576191843248 0.5826034079696241 0.2692548717969677
0.9175378595073748 0.8329446926014642 0.2681234085633705
0.3354842210267470 0.1674077327363832 0.1775832036707524
0.3350978944163183 0.4165768180086079 0.1770955040313086
0.0846750932390991 0.4168917261717220 0.1774001432584550
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0.8352714874769860 0.1670539860034451 0.1775895017767203
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0.5857231383043645 0.1677265215727509 0.1779185525449340
0.3347186362223165 0.6665529648417582 0.1770906351245830
0.3345669633583306 0.9168600891915104 0.1774737242585121
0.0844740374920725 0.9164043149506891 0.1773004232152349
0.0838719426848332 0.6664053979880962 0.1775931472457564
0.8339960666620362 0.6662396763119308 0.1780309031887896
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0.5849860071524493 0.6664381843300664 0.1774863216745176
0.0006837098416001 -0.0001601688013264 0.0869652467438818
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0.7509161763152792 0.2499289796592716 0.0871721510304078
0.7509189162165579 -0.0000527472914126 0.0871014640676660
0.0010011833855575 0.5000631093808708 0.0868796750535769
0.0004833944557306 0.7498896649502417 0.0870764347926844
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0.2506725386590922 0.5000331289075108 0.0867226268241888
0.5008769730035905 0.5002201571780969 0.0867586212042552
0.5009340200053690 0.7502662678685144 0.0869881419207725
0.7508568730833127 0.7499372495846334 0.0870540596264597
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0.1667705176872601 0.3331801101640036 -0.0040184331864573
0.1668665567840121 0.0832464178166392 -0.0039072100368525
0.4169988562036059 0.0831941605127683 -0.0036969580191562

0.4169268349216468	0.3332893713414750	-0.0037719209201346
0.6672208608781867	0.3332615185972027	-0.0035499637765462
0.6670603491319640	0.0833420531090657	-0.0036436173089435
0.9170723993886710	0.0834736306698727	-0.0038134054215967
0.9169362290087267	0.3331289296153778	-0.0037780198200556
0.1669285997242528	0.8332399317565721	-0.0038417999797542
0.1669890414571187	0.5835600876315852	-0.0039868102876174
0.4170682066757699	0.5834851684804436	-0.0038100500900311
0.4169224925266600	0.8334140949968786	-0.0037511637069791
0.6669862819833861	0.8335182613831333	-0.0036536851710172
0.6671038897976297	0.5833674853900731	-0.0037536903033734
0.9170493966196727	0.5834606911086718	-0.0038789535458754
0.9171650694032041	0.8334409756489995	-0.0037288761878076
0.5391575744916943	0.5079948667287052	0.4425515774373283
0.8431392489767674	0.5163296576760310	0.5189953970593383
0.6709119438787345	0.5120465482794587	0.4396937706506049
0.7576436076096960	0.5143657646423883	0.4841950521884581

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(2) POSCAR_Cu_2O

CONTCAR1
1.00000000000000
8.5391998290999993 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.0762996674000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.0571994780999994
Cu O C
56 26 2
Direct
0.2014615371815277 0.1830082828201165 0.0252670699708381
0.2374925673620507 0.0022243596019939 0.1509956535085485
0.2687172546253633 0.2428398221379319 0.2516949626986544
0.2580423463554037 0.0491821257726902 0.3645246959397446
0.1104767245191337 -0.0049728922784812 0.0038941211090119
0.2657439557074107 0.2356118242171555 0.1310620611463856
0.2184423068936015 -0.0197433711512800 0.2655956028669961
0.2197135584734305 0.2455398170801448 0.3689496267452156
0.0185058133794275 0.3721999734743204 0.0572759724541412
-0.0219844304092196 0.1158124613605159 0.1921977898709458
0.0175356707942018 0.3638498330661962 0.3134554542228788
-0.0243670867479266 0.1304249683498724 0.0782853322291125
0.0301238505567067 0.3605592842887724 0.1882175559640973
0.0559994159868246 0.1440615815543783 0.3063010148219781
0.7335827964295540 0.3659303953587603 0.0206193647262628
0.7228471841972924 -0.0040597230433847 0.1213010684805584
0.7619724778315533 0.2484698886126560 0.2417674582262897
0.8789093590308764 -0.0016339808468341 0.3402819367517503

0.8335972210635529 -0.0072560151909018 0.0138595823602354
0.7491329922302344 0.2523208887431544 0.1217498265215753
0.7198292313064100 0.0071266847658081 0.2552140856300794
0.6951918902839378 0.2850501342660566 0.3473568930628845
0.4896500526076447 0.3720518941324992 0.0730591118391011
0.4972638066184794 0.1220698089026946 0.1952786212892440
0.4965992534145925 0.3760091713743559 0.2918941646020887
0.5053601535674237 0.1151634274197604 0.0619219816838199
0.4898716022297194 0.3739534037717064 0.1833686655701615
0.5195209279703373 0.1267117362960963 0.3230638331810666
0.1878057123957626 0.8034081471964236 0.0248571185734939
0.2494184868524507 0.4969719205777517 0.1169609181201496
0.2694361707589341 0.7645470911507024 0.2526853719777963
0.2930807216595666 0.5302492974304207 0.3740575354041120
0.3386614723862205 0.5028985308694611 0.0081638249809698
0.2533917795494238 0.7634532769817143 0.1350356355607094
0.2562540114561897 0.4925984636662345 0.2494835478481998
0.2306945853641761 0.7233285609054355 0.3588627270573101
-0.0163923216076293 0.8744146867010674 0.0837431622795601
0.0248908942006199 0.6324494587095855 0.1904454680059674
-0.0024268858684298 0.8184008127186609 0.3237928581357949
0.0174937600189538 0.6194186916227798 0.0597735425509346
-0.0300943983384737 0.8807793617625552 0.1944059539247219
0.0165052861249323 0.5969698409778440 0.3197227198705940
0.6956705541769348 0.7083810274912870 0.0233816508378774
0.7760475704225687 0.4972491630925384 0.1297838964256752
0.7603865186860345 0.7293207464886443 0.2517863695184679
0.6375259724534383 0.4833359965404997 0.3614618944815916
0.6066307864637106 0.5318742531614331 -0.0141737320743092
0.7644995511936850 0.7441856614360411 0.1292182858368025
0.7790416559741272 0.4963221198412847 0.2358156042943360
0.7141851215702920 0.6662335894701797 0.3777385845779246
0.5062525922613398 0.8676937837716723 0.0611657381219914
0.4930864933225206 0.6283586521779150 0.1865036798947678
0.5303616279337874 0.8910461558355162 0.3217948872939259
0.4874325907449751 0.6247817245377197 0.0772101102024253
0.5040543132115521 0.8748254285036396 0.1972728104514501
0.5045062388004597 0.6365011100523973 0.2959041711567763
0.0996717894756106 0.0055834064717167 0.0933670175509737
0.1318014296860683 0.2267021676581744 0.1921560641667600
0.0930365334516455 -0.0463996869280280 0.3308947194209415
0.3794274396014095 0.2401124216171861 0.0647227943823765
0.3751440385996645 -0.0025199681835839 0.2098841721948188
0.3947476816804225 0.2512783248461332 0.3152280883849594

0.6300633291524288	-0.0088380182309781	0.0506238148441173
0.6192665558643815	0.2478883132248662	0.1833937353418406
0.6597651224297475	0.0110658067015406	0.3311739032360831
0.8710810987913467	0.2597315661010161	0.0577419672302712
0.8306529403149995	0.0001847189445349	0.1888304383660004
0.8795161128775119	0.2467122415889215	0.3068443020293506
0.1435916488661285	0.4960990993447879	0.0490176060610510
0.1206282380751298	0.7680459521690161	0.1965222240743545
0.1579790058974249	0.4810386589705515	0.3190302539434838
0.3646067175096298	0.7535782478878962	0.0685773299258019
0.3644192134785690	0.5022199996659140	0.1824123800760117
0.4058425117628233	0.7687288151351219	0.3132484256195126
0.6201434855055886	0.4975181391504669	0.0777824121647416
0.6310799272217580	0.7495123935377235	0.1897811762443672
0.6080590408812150	0.5030731310007530	0.2818946724975319
0.8849775866235668	0.7404608344535522	0.0644409678188085
0.9328849741935652	0.4956601961865310	0.1829161863934313
0.8602345458816811	0.7028293993381386	0.3202626152607200
0.4150219416714263	0.5880244311386504	0.4295360255751002
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0.5745421147486323	0.5748245967379448	0.4251599851188901
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