

***Supplementary Material for “Adsorption, activation, and conversion of carbon dioxide on small copper-tin nanoclusters”***

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**1 Supplementary Tables**

**Table S1.** The energies ( $E$ ), zero-point energies ( $E_{\text{ZPE}}$ ), and entropies ( $S$ ) of  $\text{H}_2(\text{g})$ ,  $\text{CO}_2(\text{g})$  and  $\text{CO}(\text{g})$ , and  $\text{H}_2\text{O}$ . The entropies of  $\text{H}_2(\text{g})$ ,  $\text{CO}_2(\text{g})$  and  $\text{CO}(\text{g})$  were calculated at 1 atm. The entropy of  $\text{H}_2\text{O}(\text{g}=\text{l})$  was calculated at 0.035 atm, which corresponds to the vapor pressure of liquid water.

<b>Gas Phase</b>	<b><math>E</math></b>	<b><math>E_{\text{ZPE}}</math></b>	<b><math>TS</math></b>	<b><math>\Delta G</math></b>
<b><math>\text{H}_2</math></b>	-7.03	0.27	-0.40	-7.078
<b><math>\text{H}_2\text{O}</math></b>	-14.7	0.56	-0.67	-14.70
<b><math>\text{CO}(\text{g})</math></b>	-15.3	0.13	-0.59	-15.70
<b><math>\text{CO}_2</math></b>	-22.8	0.30	-0.66	-23.03

**Table S2.** Adsorption energy ( $\Delta E$ , in eV) of the cluster  $\text{Cu}_{4-n}\text{Sn}_n$  ( $n = 0-4$ ) on graphene and  $\gamma\text{-Al}_2\text{O}_3(100)$  ( $\Delta E = E(\text{Cu}_{4-n}\text{Sn}_n) + E(*) - E[(\text{Cu}_{4-n}\text{Sn}_n)\cdots*]$ , where  $*$  = graphene and  $\gamma\text{-Al}_2\text{O}_3(100)$ ). The average Bader charge ( $Q_B$ ) of Cu and Sn atoms in the isolated and supported clusters.

System	$\text{Cu}_{4-n}\text{Sn}_n$		$\text{Cu}_{4-n}\text{Sn}_n/\text{graphene}$			$\text{Cu}_{4-n}\text{Sn}_n/\gamma\text{-Al}_2\text{O}_3$		
	$Q_B(\text{Cu})$	$Q_B(\text{Sn})$	$\Delta E_{\text{ads}}$	$Q_B(\text{Cu})$	$Q_B(\text{Sn})$	$\Delta E_{\text{ads}}$	$Q_B(\text{Cu})$	$Q_B(\text{Sn})$
<b>Cu<sub>4</sub></b>	0.00	-	-0.99	0.04	-	-2.45	0.04	-
<b>Cu<sub>3</sub>Sn</b>	-0.67	2.01	-0.87	-0.58	2.12	-1.87	-0.71	2.15
<b>Cu<sub>2</sub>Sn<sub>2</sub></b>	-0.92	0.92	-0.81	-0.82	0.95	-1.78	-0.92	0.91
<b>CuSn<sub>3</sub></b>	-1.81	0.60	-0.77	-1.82	0.64	-2.17	-2.51	0.95

**Table S3.** Adsorption energy ( $\Delta E_{\text{CO}_2}$ , in eV), C–O bond length ( $d_{\text{C-O}}$ , in Å), bond angle ( $\theta_{\text{OCO}}$ , in degrees) of  $\text{CO}_2$ , and charge transfer from the catalyst to  $\text{CO}_2$  using Bader analysis ( $\Delta Q_{\text{B}}$ , in e) in  $\text{Cu}_{4-n}\text{-M}_n$  clusters of  $\text{M} = \text{Sn}$  [this work], Pd [1], Ni [1], Pt [1,2], and Zr [3] ( $n = 1\text{--}3$ ).

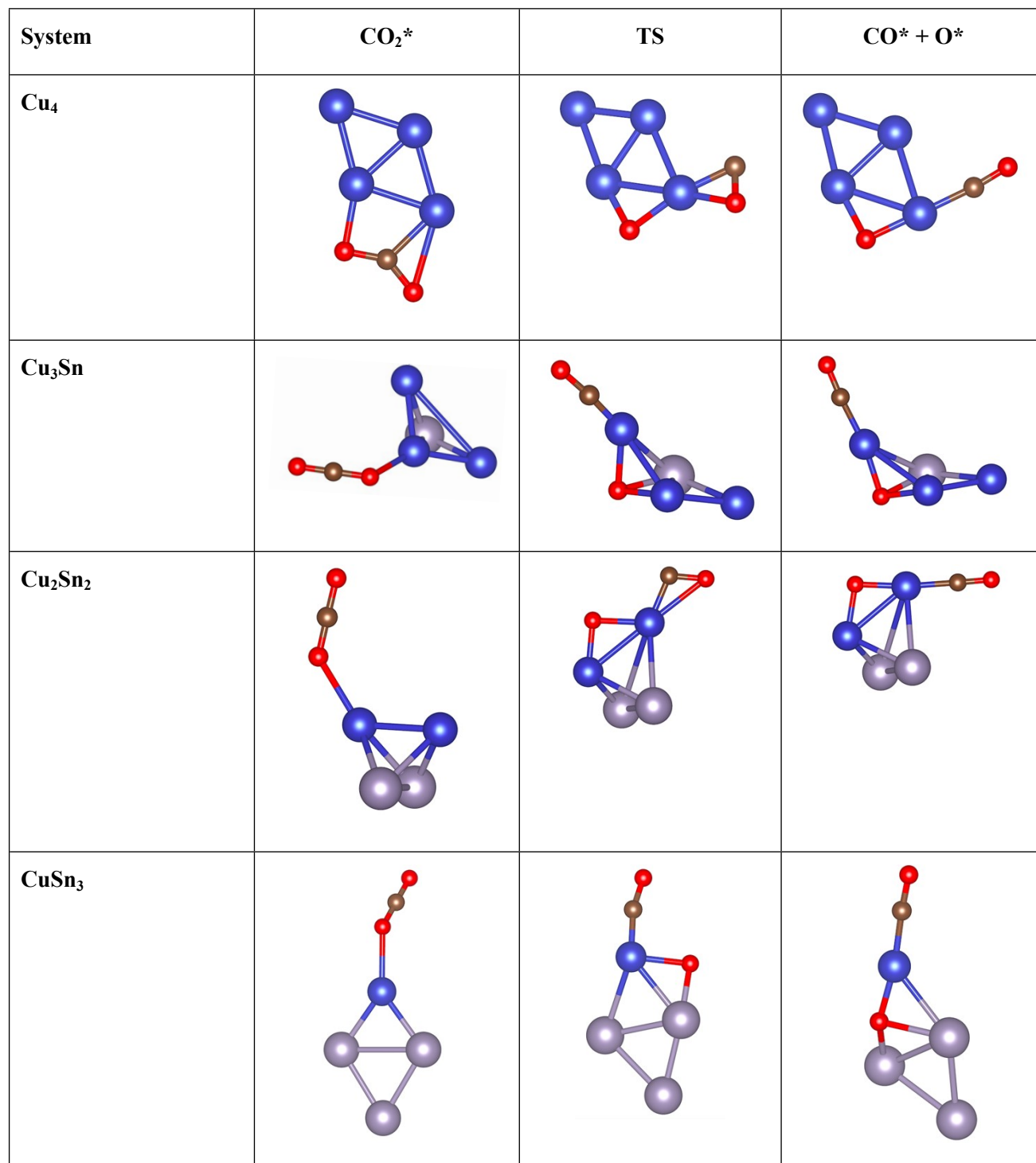
System	$\Delta E_{\text{CO}_2}$	$d_{\text{C-O}}$	$\theta_{\text{OCO}}$	$\Delta Q_{\text{B}}$
$\text{Cu}_3\text{Sn}$	-0.21	1.24	140.0	-0.51
$\text{Cu}_2\text{Sn}_2$	0.50	1.28	142.6	-0.52
$\text{CuSn}_3$	0.40	1.27	136.9	-0.70
$\text{Cu}_3\text{Pd}$	-1.25	1.28	137.5	-0.49
$\text{Cu}_2\text{Pd}_2$	-1.06	1.27	140.1	-0.45
$\text{CuPd}_3$	-0.84	1.27	140.5	-0.44
$\text{Cu}_3\text{Ni}$	-1.13	1.28	136.8	-0.55
$\text{Cu}_2\text{Ni}_2$	-1.17	1.29	126.0	-0.93
$\text{CuNi}_3$	-1.18	1.28	136.7	-0.65
$\text{Cu}_3\text{Pt}$	-1.01	1.29	132.5	-
$\text{Cu}_2\text{Pt}_2$	-1.64	1.29	136.6	-
$\text{CuPt}_3$	-1.44	1.28	137.2	-
$\text{Cu}_3\text{Zr}$	-1.73	1.36	130.3	-0.98
$\text{Cu}_2\text{Zr}_2$	-3.07	1.28	136.7	-1.29
$\text{CuZr}_3$	-1.27	1.27	132.3	-1.29

[1] A. Alvarez-García, E. Flórez, A. Moreno and C. Jimenez-Orozco, *Mol. Catal.*, 2020, **484**, 110733. [2] L. E. Gálvez-González, J. O. Juárez-Sánchez, R. Pacheco-Contreras, I. L. Garzón, L. O. Paz-Borbón and A. Posada-Amarillas, *Phys. Chem. Chem. Phys.*, 2018, **20**, 17071–17080. [3] Megha, K. Mondal, T. K. Ghanty and A. Banerjee, *J. Phys. Chem. A*, 2021, **125**, 2558–2572.

**Table S4.** Adsorption energy ( $\Delta E_{\text{CO}_2}$ , in eV), C–O bond length ( $d_{\text{C-O}}$ , in Å), bond angle ( $\theta_{\text{OCO}}$ , in degrees) of  $\text{CO}_2$ , and the overall charge surface of  $\text{CO}_2$  ( $Q_{\text{B}}$  in e) using Bader analysis of the  $\text{CO}_2$  molecule physisorbed on graphene and  $\gamma\text{-Al}_2\text{O}_3$  supported  $\text{Cu}_{4-n}\text{Sn}_n$  ( $n = 0\text{--}4$ ) clusters.

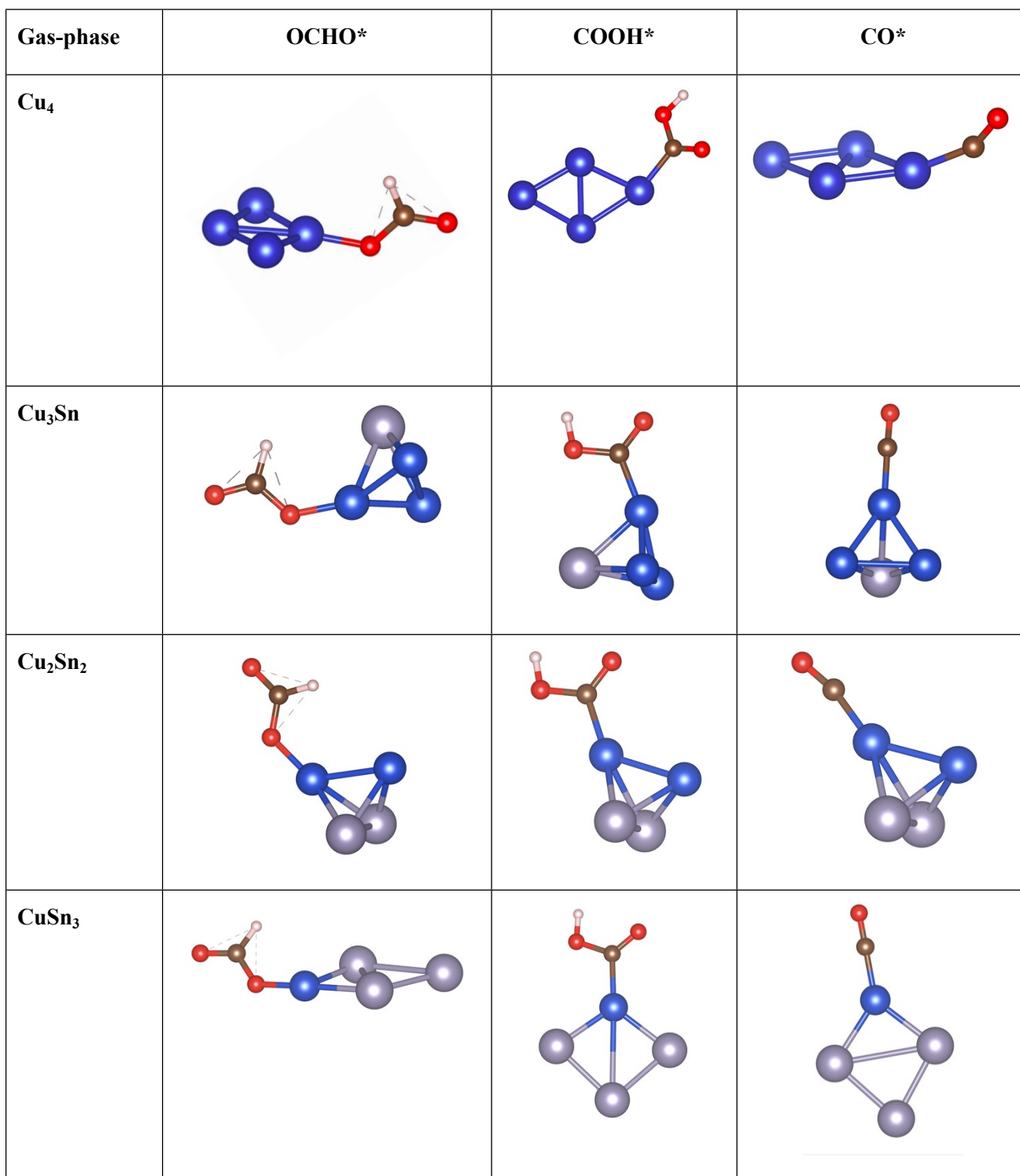
System	Graphene				$\gamma\text{-Al}_2\text{O}_3$			
	$\Delta E_{\text{CO}_2}$	$d_{\text{C-O}}$	$\theta_{\text{OCO}}$	$Q_{\text{B}}(\text{CO}_2)$	$\Delta E_{\text{CO}_2}$	$d_{\text{C-O}}$	$\theta_{\text{OCO}}$	$Q_{\text{B}}(\text{CO}_2)$
<b>Cu<sub>4</sub></b>	-0.18	1.19,1.17	177.4	-0.03	-0.21	1.18,1.17	179.5	-0.01
<b>Cu<sub>3</sub>Sn</b>	-0.14	1.18,1.17	179.1	-0.03	-0.50	1.25,1.29	129.5	-1.05
<b>Cu<sub>2</sub>Sn<sub>2</sub></b>	-0.12	1.18,1.17	179.0	-0.03	-0.04	1.19,1.17	179.9	0.00
<b>CuSn<sub>3</sub></b>	0.34	1.26,1.21	138.2	-1.57	-0.18	1.18,1.17	176.2	-0.03

## 2 Supplementary Figures

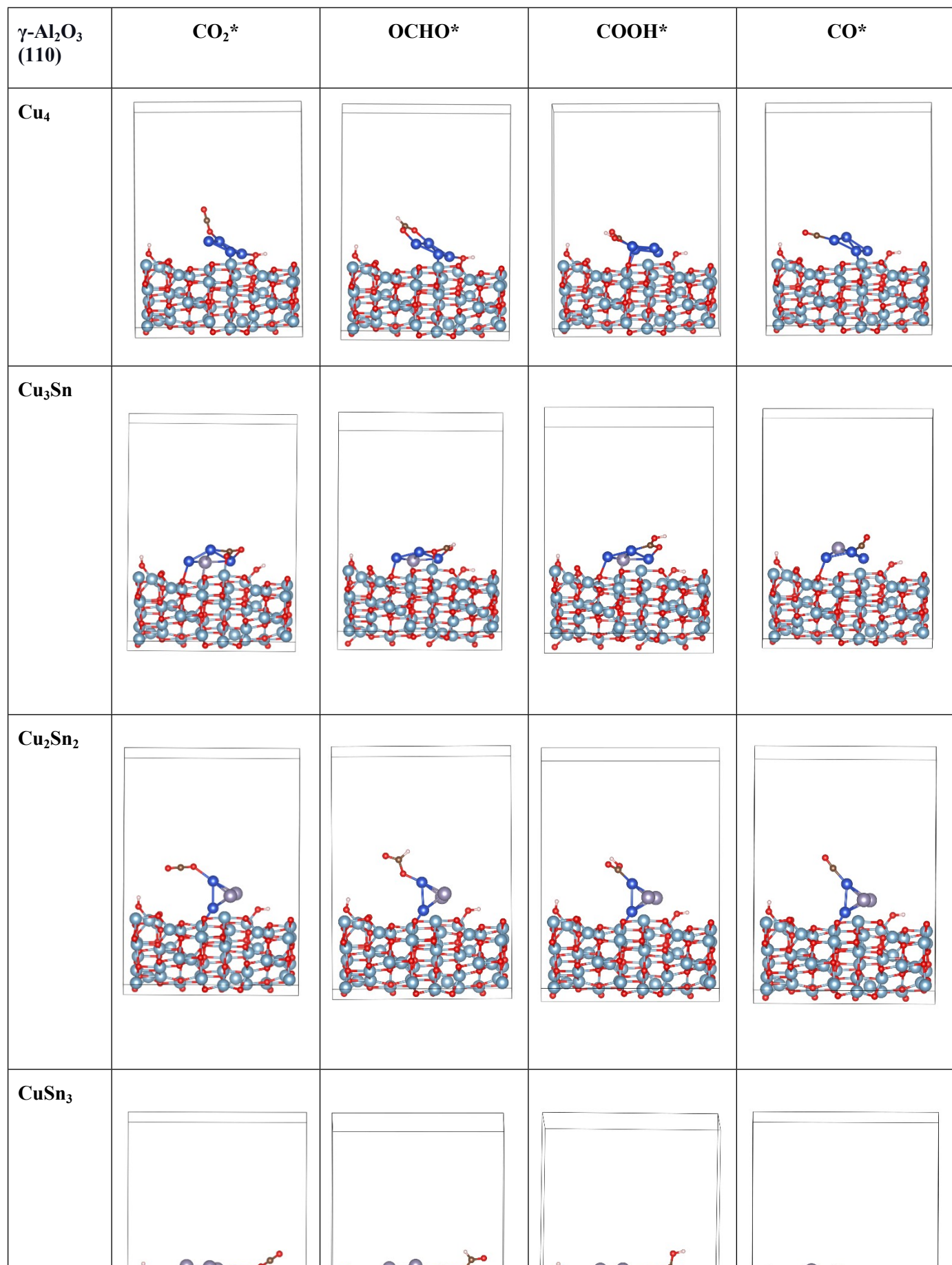
**Figure S1.** Structures of initial state, transition state, and final state involved in the gas phase  $\text{CO}_2$  direct dissociation to CO ( $\text{CO}_2^* \rightarrow \text{CO}^* + \text{O}^*$ ) over  $\text{Cu}_4$ ,  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_2\text{Sn}_2$ , and  $\text{CuSn}_3$ .



**Figure S2.** Structures of the intermediates OCHO\*, COOH\*, and \*CO involved in the electrocatalytic CO<sub>2</sub> reduction reactions over Cu<sub>4</sub>, Cu<sub>3</sub>Sn, Cu<sub>2</sub>Sn<sub>2</sub>, and CuSn<sub>3</sub>.

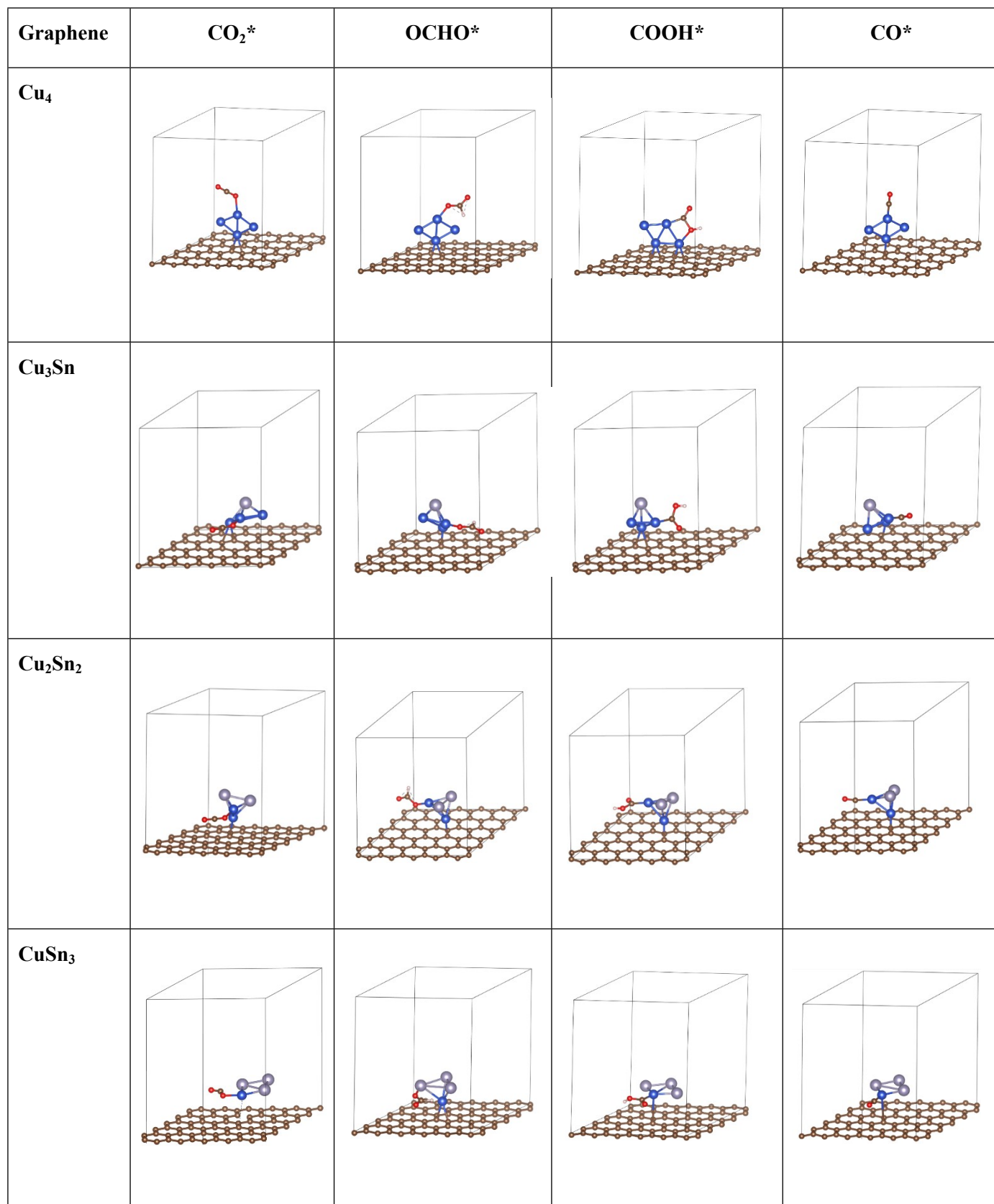


**Figure S3.** Structures of the intermediates  $\text{OCHO}^*$ ,  $\text{COOH}^*$ , and  $^*\text{CO}$  involved in the electrocatalytic  $\text{CO}_2$  reduction reactions on  $\text{Cu}_4$ ,  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_2\text{Sn}_2$ , and  $\text{CuSn}_3$  supported by the  $\gamma\text{-Al}_2\text{O}_3$  (110) surface.



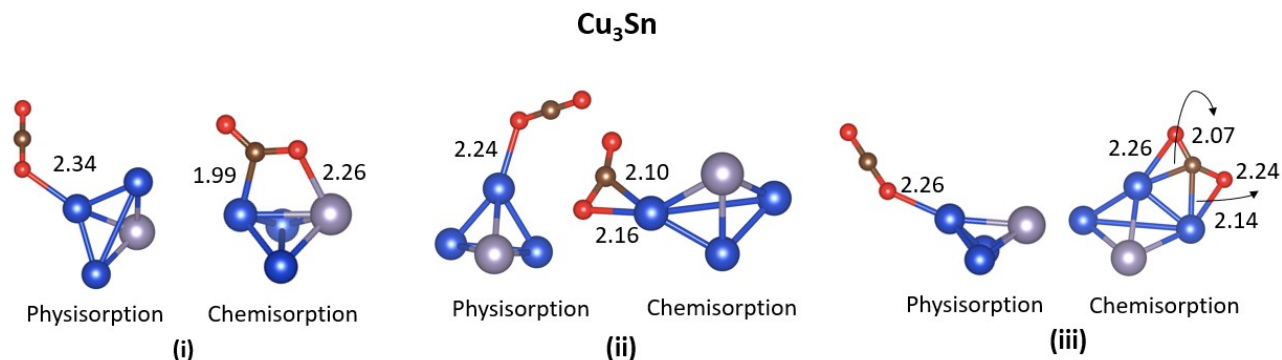


**Figure S4.** Configurations of the intermediates  $\text{OCHO}^*$ ,  $\text{COOH}^*$ , and  $\text{CO}^*$  involved in the  $\text{CO}_2$  reduction reactions over  $\text{Cu}_4$ ,  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_2\text{Sn}_2$ , and  $\text{CuSn}_3$  supported by graphene.



### 3 Isomers of Cu<sub>3</sub>Sn

#### 3.1 CO<sub>2</sub> adsorption and activation on the isomers of Cu<sub>3</sub>Sn

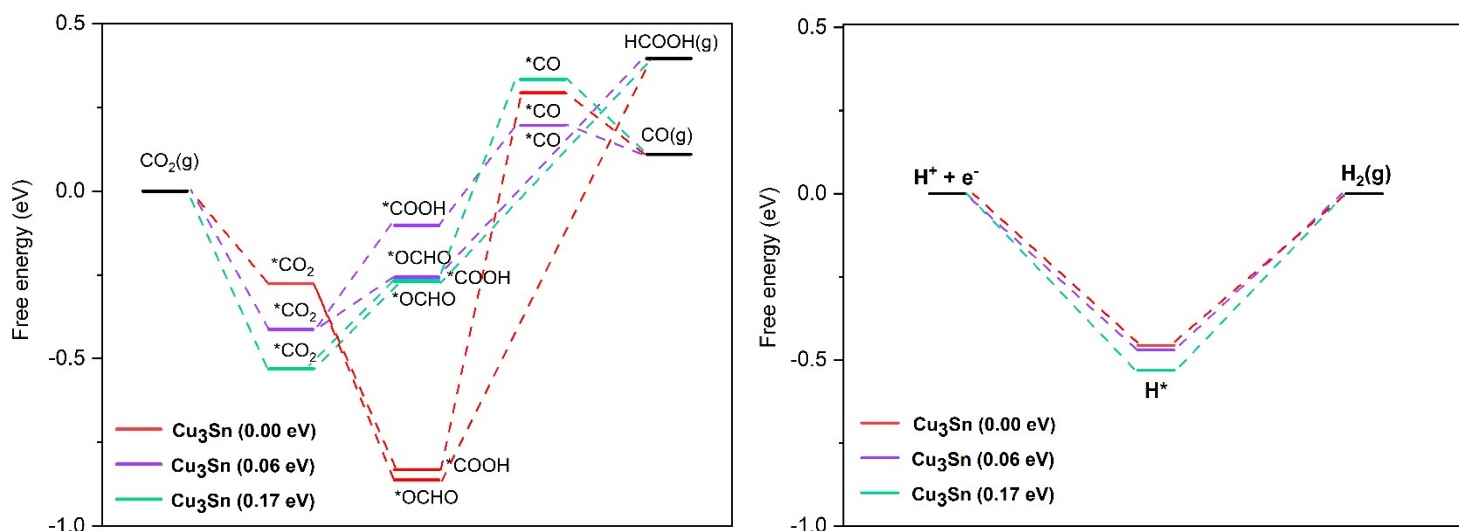


**Figure S5.** Lowest energy structures of CO<sub>2</sub> physisorbed and chemisorbed starting from the three most stable isomers of Cu<sub>3</sub>Sn. The C<sub>2v</sub> isomer (ii) rearranged to the C<sub>s</sub> (i) isomer upon CO<sub>2</sub> chemisorption. The C<sub>3v</sub> isomer (iii) rearranged to the C<sub>s</sub> (i) isomer upon CO<sub>2</sub> physisorption and chemisorption,

**Table S5:** Adsorption energy ( $\Delta E_{\text{CO}_2}$ , in eV), C–O bond length ( $d_{\text{C-O}}$ , in Å), bond angle ( $\theta_{\text{OCO}}$ , in degrees) of CO<sub>2</sub>, and charge transfer from the catalyst to CO<sub>2</sub> using Bader analysis ( $Q_{\text{B}}(\text{CO}_2)$ , in e) when physisorbed and chemisorbed on the three most stable isomers of Cu<sub>3</sub>Sn. For comparison, the bond length and bond angle of the CO<sub>2</sub> molecule in the gas phase are 1.18 Å and 180 degrees, respectively.

System	Physisorption				Chemisorption			
	$\Delta E_{\text{CO}_2}$	$d_{\text{C-O}}$	$\theta_{\text{OCO}}$	$Q_{\text{B}}(\text{CO}_2)$	$\Delta E_{\text{CO}_2}$	$d_{\text{C-O}}$	$\theta_{\text{OCO}}$	$Q_{\text{B}}(\text{CO}_2)$
<b>Cu<sub>3</sub>Sn (i)</b>	-0.15	1.18, 1.17	179.2	-0.02	0.29	1.29, 1.22	133.1	-0.64
<b>Cu<sub>3</sub>Sn (ii)</b>	-0.21	1.19, 1.17	179.1	-0.02	-0.17	1.23, 1.19	155.2	-0.29
<b>Cu<sub>3</sub>Sn (iii)</b>	-0.32	1.18, 1.17	179.5	-0.03	-0.21	1.23, 1.24	142.6	-0.52

### 3.2 Electrochemical CO<sub>2</sub> reduction to CO and HCOOH on the isomers of Cu<sub>3</sub>Sn



**Figure S6.** (a) Gibbs free energy diagram for CO<sub>2</sub> reduction pathways to HCOOH and CO on the three lowest energy isomers of Cu<sub>3</sub>Sn. (b) Gibbs free energy diagram for hydrogen evolution reaction on the three lowest energy isomers of Cu<sub>3</sub>Sn.

The energetic pathway for the electrochemical CO<sub>2</sub> reduction to HCOOH and CO is also explored on the three lowest energy isomers of Cu<sub>3</sub>Sn as their energy difference is within 0.20 eV. However, upon optimization, the C<sub>2v</sub> and C<sub>3v</sub> isomers of Cu<sub>3</sub>Sn rearrange to the most stable C<sub>s</sub> isomer. Therefore, the energetic pathways reported in Figure S6 correspond to three active sites of the same isomer (C<sub>s</sub>). The formation of the intermediates \*COOH ( $\Delta G_{\text{COOH}^*} = -0.56$  eV) and \*OCHO ( $\Delta G_{\text{OCHO}^*} = -0.59$  eV) is favorable on the lowest energy isomer of Cu<sub>3</sub>Sn relative to the other isomers as indicated by its large negative Gibbs free energy change (red lines on **Figure S6(a)**). Although the lowest energy isomer leads to the favorable \*COOH and \*OCHO intermediate formation, the next proton/electron step to form \*CO and HCOOH would require a large amount of energy for the lowest energy isomer compared with the other two isomers. For HCOOH formation, the most stable isomer has a Gibbs free energy of 1.26 eV, whereas the second and third isomers have 0.65 eV and 0.66 eV, respectively. Therefore, HCOOH formation is unfavorable on the most stable isomer of Cu<sub>3</sub>Sn relative to the other two isomers. In addition, CO formation is not favorable on the most stable isomer of Cu<sub>3</sub>Sn ( $\Delta G_{\text{CO}^*} = 1.12$  eV). For the second and third most stable isomer of Cu<sub>3</sub>Sn,  $\Delta G_{\text{CO}^*}$  is 0.25 eV and 0.61 eV, respectively. The CO formation is also favorable on the second most stable isomer ( $\Delta G_{\text{CO(g)}} = 0.26$  eV). Overall, CO formation is favorable on the second most stable isomer compared to HCOOH. The third most stable isomer has a similar energetic pathway for both CO and HCOOH formation. The energetics of the hydrogen evolution reaction (**Figure S6(b)**) is not significantly affected by the isomer on which the reaction occurs and is only slightly more favorable on the stable C<sub>s</sub> isomer compared to the C<sub>2v</sub> and C<sub>3v</sub> isomers of Cu<sub>3</sub>Sn ( $\Delta G_{\text{H}} = -0.46$  eV >  $-0.47$  eV >  $-0.53$  eV, respectively) as the Gibbs free energy change becomes more negative.

## 4 Optimized structures from VASP calculations

### 4.1 Output file of the structure CO<sub>2</sub>\* on Cu<sub>4</sub>

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu C O
4 1 2
Direct
0.3322031404215622 0.4335422547892733 0.3754624124267636
0.4001778917169503 0.3427562798763475 0.3769006900910341
0.3617810664899679 0.3897077098547399 0.4803440413080935
0.3658039227234937 0.3894873682556010 0.2718609395575484
0.4444816329907226 0.1979858050475443 0.3714149520257379
0.4330840213486624 0.1408903508992054 0.3652808611217466
0.4562603333086415 0.2556867432772805 0.3770481094690901
```

### 4.2 Output file of the structure OCHO\* on Cu<sub>4</sub>

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu C O H
4 1 2 1
Direct
0.3157343606633489 0.4061142096935271 0.3787849996288486
0.4117433652381521 0.3350116003615042 0.3848563291748377
0.3502973514431957 0.3668505398534521 0.4814610785964675
0.3667391297595159 0.3715054854295801 0.2809002507772291
0.4927935433851829 0.2213546719035406 0.3655117384761724
0.5448417169096942 0.1891572915703819 0.3672751231992351
0.4891549910378572 0.2870013241292639 0.3778809107668195
0.4436670425630709 0.1969378500587524 0.3520480243804052
```

### 4.3 Output file of the structure COOH\* on Cu<sub>4</sub>

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu C O H
4 1 2 1
Direct
0.3176582357644264 0.3797042688750523 0.3766785138875832
0.4353672901269192 0.3768386216942616 0.3784748952287060
0.3708738788814401 0.3667425026842963 0.4794587610625314
0.3707222120592704 0.3787271633195886 0.2750464546224052
0.2958604667324281 0.3577003414096041 0.5374062326514135
0.2485850807753991 0.4083956993463147 0.5308840059947144
0.2889202671147260 0.3121707586380680 0.5775845568217406
0.2132585655453880 0.3988016200328275 0.5632715097309209
```

### 4.4 Output file of the structure CO\* on Cu<sub>4</sub>

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu C O
4 1 1
Direct
0.3195240733417180 0.3772806707077123 0.3661074812459262
0.4307762390136034 0.3869476572822066 0.3738244385216944
0.3793451552354767 0.3504789783806075 0.4733158449410695
0.3722426880290186 0.4127815124608674 0.2681417687061725
```

0.3563354400340373 0.2952784551542962 0.5444478433693263  
 0.3553388633461481 0.2430472510143105 0.5685925992158225

#### 4.5 Output file of the structure CO<sub>2</sub>\* on Cu<sub>3</sub>Sn

```

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu Sn C O
3 1 1 2
Direct
0.5858364640896905 0.6768506712555261 0.5943665727840358
0.7049626852861390 0.6719102193488843 0.6005956995581360
0.5670089845773324 0.6574743629704216 0.7102442565454560
0.6409081660135113 0.5755525949303979 0.6499922018914543
0.5501258519192382 0.7056399628527908 0.4448700612470222
0.5667062278969706 0.6891181202455080 0.3911460884889656
0.5338346282171130 0.7217690933964834 0.4994736574849286

```

#### 4.6 Output file of the structure OCHO\* on Cu<sub>3</sub>Sn

```

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu Sn C O H
3 1 1 2 1
Direct
0.6220267189845075 0.7155396983952258 0.5808590867267327
0.6901984221660697 0.6329886537837126 0.6313055295632211
0.5664258004196725 0.6669385932763134 0.6736368249260067
0.5856567093300029 0.5926838393354856 0.5735183580737484
0.6151221177973127 0.7505991366141700 0.4440256680590480
0.6112161563481848 0.7903425531444697 0.3976951722195139
0.6105954069000958 0.7687110965387944 0.5080021570202078
0.6226496760541451 0.6954273709118368 0.4343146574115373

```

#### 4.7 Output file of the structure COOH\* on Cu<sub>3</sub>Sn

```

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu Sn C O H
3 1 1 2 1
Direct
0.6379991389292942 0.6382310268518449 0.5711118254717048
0.6657784766921291 0.5818806914441078 0.6729610970449765
0.6447961816896619 0.7101080235887132 0.6678887846864773
0.5488059354305995 0.6288284378609427 0.6601016363140326
0.6002520853451260 0.6342497240185909 0.4843592858639700
0.5310644149956326 0.6328394580655073 0.4813513516090067
0.6348004541224743 0.6334138394614780 0.4339278427164784
0.5191418637950780 0.6311222437088246 0.4334811922933541

```

#### 4.8 Output file of the structure CO\* on Cu<sub>3</sub>Sn

```

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
Cu Sn C O
3 1 1 1
Direct
0.6227696590439393 0.6454794864623281 0.5663391584548805
0.6941857576630852 0.6700273972453346 0.6596487504172543

```



0.5655531687255220 0.6840413005356112 0.6642647959322758  
0.6187324783596608 0.5706074212512817 0.6739665416671841  
0.6220601654024591 0.6378632370610049 0.4761799872069545  
0.6218543438053175 0.6218405914444389 0.4198697453214528

#### 4.9 Output file of the structure CO<sub>2</sub>\* on Cu<sub>2</sub>Sn<sub>2</sub>

1.000000000000000  
20.000000000000000 0.000000000000000 0.000000000000000  
0.000000000000000 20.000000000000000 0.000000000000000  
0.000000000000000 0.000000000000000 20.000000000000000  
Cu Sn C O  
2 2 1 2

Direct

0.6966153945473721 0.6663150467838221 0.6219174618596028  
0.5724061410167423 0.6845924901977725 0.6221407533495267  
0.6218105728063108 0.5842198705275052 0.5551153855246369  
0.6233983559491421 0.5911976213056747 0.6979179121438861  
0.5379212394467956 0.8456886970393285 0.6168593072670632  
0.5198658663209059 0.7896462996806548 0.6226529970997703  
0.5564374129127287 0.9009714024652453 0.6102771607555262

#### 4.10 Output file of the structure OCHO\* on Cu<sub>2</sub>Sn<sub>2</sub>

1.000000000000000  
20.000000000000000 0.000000000000000 0.000000000000000  
0.000000000000000 20.000000000000000 0.000000000000000  
0.000000000000000 0.000000000000000 20.000000000000000  
Cu Sn C O H  
2 2 1 2 1

Direct

0.6723077135282978 0.6885985857165124 0.6207639416039115  
0.5450078730341161 0.6681560426030160 0.6178981038211546  
0.6259660652698642 0.5880760905712563 0.5544562794025083  
0.6217016300530247 0.5969565779632262 0.6960661354838535  
0.4881333700632453 0.7955993225860141 0.5964603070809460  
0.4780734322604800 0.7312557170270466 0.6100927505847906  
0.4433367021204475 0.8367691009718285 0.5890468325906113  
0.5424171816705368 0.8106865725610959 0.5910536964322226

#### 4.11 Output file of the structure COOH\* on Cu<sub>2</sub>Sn<sub>2</sub>

1.000000000000000  
20.000000000000000 0.000000000000000 0.000000000000000  
0.000000000000000 20.000000000000000 0.000000000000000  
0.000000000000000 0.000000000000000 20.000000000000000  
Cu Sn C O H  
2 2 1 2 1

Direct

0.6718790576992717 0.6818015542751255 0.6237207773357554  
0.5483431533061704 0.6491000989422488 0.6156892109988803  
0.6335066373569447 0.5760318805336055 0.5519182085703918  
0.6232808897188278 0.5780271254768081 0.6928501647981662  
0.7083497193169350 0.7719386630654412 0.6271414643991449  
0.7776212860310423 0.7753396902046674 0.6216926911324947  
0.6748296667562528 0.8228606829148575 0.6337800624235186  
0.7892745718145520 0.8232732835872412 0.6232269253416511

#### 4.12 Output file of the structure CO\* on Cu<sub>2</sub>Sn<sub>2</sub>

1.000000000000000  
20.000000000000000 0.000000000000000 0.000000000000000  
0.000000000000000 20.000000000000000 0.000000000000000  
0.000000000000000 0.000000000000000 20.000000000000000  
Cu Sn C O  
2 2 1 1

Direct

0.6657631360671203 0.6895795368573943 0.6207215369566370  
0.5492747649230623 0.6419409326043493 0.6222315295257417

0.6386678620437110 0.5801147345100972 0.5539524549724888  
 0.6320175448678853 0.5722212150954604 0.6945302235012392  
 0.7126287401282312 0.7680984446579942 0.6337140771356360  
 0.7513369229699904 0.8108766572747044 0.6321996139082664

#### 4.13 Output file of the structure CO<sub>2</sub>\* on CuSn<sub>3</sub>

1.0000000000000000  
 20.0000000000000000 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 20.0000000000000000 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 20.0000000000000000  
 Cu Sn C O  
 1 3 1 2

Direct

0.3824674805773327 0.4726233322265898 0.3568601618148293  
 0.4630873366983508 0.3752526263928857 0.3709706638878743  
 0.3120538372768848 0.3677353788781446 0.3717861095221195  
 0.3932433921637468 0.2525289604029624 0.3884080383322299  
 0.3888943381670273 0.6204448958145647 0.2891539591946994  
 0.3776282982418451 0.5843841736446009 0.3347378054174541  
 0.4000982868747940 0.6558921656402603 0.2431772988308048

#### 4.14 Output file of the structure OCHO\* on CuSn<sub>3</sub>

1.0000000000000000  
 20.0000000000000000 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 20.0000000000000000 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 20.0000000000000000  
 Cu Sn C O H  
 1 3 1 2 1

Direct

0.4228488488804558 0.4765797604966053 0.3904583812142235  
 0.4428680841370110 0.3546037078503730 0.4062300258107996  
 0.3260992467242971 0.4053574379309879 0.3368921008951489  
 0.3665547939819547 0.2517447110492554 0.3644471140947516  
 0.3882653470530713 0.5991552124237316 0.3237792478982016  
 0.3993948303851198 0.5637996814183950 0.3794428898320987  
 0.3886023248205248 0.6602706787096437 0.3219518618938224  
 0.3777429770175544 0.5679768011209987 0.2773373723609645

#### 4.15 Output file of the structure COOH\* on CuSn<sub>3</sub>

1.0000000000000000  
 20.0000000000000000 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 20.0000000000000000 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 20.0000000000000000  
 Cu Sn C O H  
 1 3 1 2 1

Direct

0.3905057179305729 0.4086206558724044 0.3501368005787810  
 0.4903997461396656 0.3339942273452721 0.3648279739427878  
 0.2896216891825887 0.3483403641799825 0.3921331953092491  
 0.3895719565483162 0.2573276484674807 0.4184112156033848  
 0.3868490565339258 0.4959017853220189 0.3088160024025797  
 0.3222862575973764 0.5120113258139511 0.2885122876011721  
 0.4337231933995156 0.5340340467607163 0.3003798437867005  
 0.3252403576680294 0.5568739542381564 0.2673302137753418

#### 4.16 Output file of the structure CO\* on CuSn<sub>3</sub>

1.0000000000000000  
 20.0000000000000000 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 20.0000000000000000 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 20.0000000000000000  
 Cu Sn C O  
 1 3 1 1

Direct

0.3885867162347054 0.4393073513240751 0.3511729888513244  
0.4729762739874559 0.3488531176560699 0.3776510638020412  
0.3015484805683926 0.3515054590101911 0.3785232356635717  
0.3857658119403240 0.2464456915263966 0.4120577041184177  
0.3888916134782150 0.5251150210125033 0.3204899770559706  
0.3888575837909016 0.5787339114707564 0.2984585635086781

#### 4.17 Output file of the structure CO<sub>2</sub>\* on Cu<sub>4</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

```

1.000000000000000
16.0489997863999996 0.0000000000000000 0.0000000000000000
-0.0582879140000000 10.0169307487000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.7133998870999996
O Al H Cu C
76 48 4 4 1
Direct
0.4313463175415247 0.3956297330575590 0.0602052788721155
0.4293245012436175 0.6808655064816542 0.2690696993604087
0.0283535986100489 0.8317047016090512 0.9894763174882680
0.0425450429146584 0.1243302178578051 0.2106823883054688
0.0388461578966041 0.3436281828691073 0.1449879942303570
0.4334556938719458 0.9179575378119794 0.2001488899234788
0.1815517925325473 0.7723115033423769 0.0818933449158654
0.2783275541998049 0.1857176220634302 0.3556641315016283
0.2980744737674511 0.2099701543248931 0.0334700843633702
0.2885221382148568 0.4977653025937985 0.2418238535772607
0.2967902069305842 0.9467287406089679 0.0905626081584187
0.1752334597932105 0.5443618446679708 0.1575807461143270
0.0624071414964201 0.2146496229432160 0.0458053710838970
0.0635096768112826 0.4987763439493121 0.2601963640383037
0.4214887491334011 0.7505748655884397 0.0860661802660481
0.4175483328578943 0.0565721717867338 0.3001857896813674
0.4146888847611334 0.5386798500155121 0.1649188759332281
0.0632392324947177 0.9760762270443313 0.1116737390912618
0.3332952770634278 0.7722648464356082 0.9862910985124217
0.3036644126326254 0.1321620667047774 0.2247105932003985
0.1818194057186657 0.3774639922715928 0.0401622067731128
0.1684933193066225 0.6806925017401924 0.2678132379394532
0.1748178392161432 0.9158531126696274 0.1921007896701914
0.3026521885425899 0.3543200041488497 0.1421821313429858
0.4221744005646956 0.1552275897624251 0.1302800011773705
0.0414042913943388 0.5602469004982765 0.0680380915005599
0.0482981577853383 0.8660472632369147 0.2812671770033244
0.1625895196112444 0.0236773653759032 0.0220350310657821
0.1634342396422832 0.3185478010483407 0.2364352281426527
0.3070011474741778 0.7269591357345984 0.1778367621019917
0.0439330169976084 0.7311376488983267 0.1745931176274321
0.4404482859057302 0.0102020656997516 0.0212386030107346
0.4339891322654889 0.3174487929252272 0.2289871020455271
0.3104685318778195 0.5705791962867768 0.0732363280189468
0.3034770786336514 0.8837015035582988 0.2915885073954975
0.1772561731453997 0.1553469242909958 0.1272116871275206
0.9092630662187469 0.3951948000688483 0.0614487581695325
0.9348763678928227 0.7032188853390927 0.2642497870452105
0.5353604757538782 0.8272837472978241 0.9861666018500987
0.5370682122680884 0.1213377338981088 0.2125259263815826
0.5402378686578367 0.3343608662493339 0.1435222057524757
0.9379979414235871 0.9215731732666694 0.1967685036230498
0.6800242054782645 0.7745202838878247 0.0909265269080464
0.7949802757908253 0.2349965285101069 0.3295767007600535
0.7921133475928782 0.2084628604323480 0.0391721874479478
0.7872990721532169 0.4806888073076011 0.2531540202369488
0.7962313223996693 0.9495319386579341 0.0984409726977438
0.6796465483165373 0.5453147467419879 0.1665082980369348
0.5609213835564014 0.2032742756409811 0.0448331531587271
0.5571838372668257 0.4933297516012874 0.2591186389438067
0.9140608284192973 0.7483904151038713 0.0868496417022814
0.9237600312430833 0.0568245934061177 0.2980198643226254
0.9131452805460383 0.5405208265583741 0.1620496728215500
0.5613203351330859 0.9703336997404881 0.1145858796593411
0.8224382398604233 0.7869416138806832 0.9967885074834328

```

0.8068187184459245 0.1201627542749457 0.2178942907879559  
0.6760872874611545 0.3734462511888386 0.0434670723652618  
0.6687298654896078 0.6776260964622844 0.2731573516415945  
0.6709846932236244 0.9157299015239505 0.1986783121568573  
0.7982528351528356 0.3537608459977346 0.1469104698160385  
0.9250621629213781 0.1636827028745807 0.1308483252080871  
0.5473660720150625 0.5634432064707017 0.0724455402052238  
0.5384384757654012 0.8610342777044991 0.2848505856910483  
0.6643922588042009 0.0158132109225180 0.0250714143857277  
0.6604054573960094 0.3125867972741787 0.2377099521912947  
0.8053977247925459 0.7291476188711933 0.1799809197946036  
0.5414145670384197 0.7294898555487871 0.1808737796516268  
0.9356954137162418 0.0177062193617644 0.0239581708434368  
0.9317724075776352 0.3072245172824012 0.2339419845292025  
0.8015730763904524 0.5719898359496184 0.0774512074737813  
0.8030633292007078 0.8951486029470758 0.2942525150783759  
0.6732782647952266 0.1504645616475102 0.1296939492367621  
0.3231460580441171 0.4494062880320688 0.9569215502776367  
0.9169908826262558 0.4462312971258147 0.3523647198808632  
0.5860180863273964 0.2101039584292136 0.5583402447702087  
0.5509644360152424 0.2708808201231265 0.4569115987224348  
0.2917474579198438 0.7632420643301574 0.0614065050529488  
0.3071506423544758 0.0641618580375792 0.3007432783526179  
0.1849019471835471 0.1933342782177729 0.0419967719172687  
0.1754455218954105 0.5065145494982359 0.2421984259109303  
0.1850368512153744 0.9539512391013760 0.1067641848116355  
0.2888553718490880 0.5424268574209807 0.1564952728044001  
0.4169204229915159 0.3411675910973899 0.1408459284921293  
0.0610880188443150 0.9287511056096267 0.2012295376597221  
0.0767876317225814 0.3908783943302357 0.0661774172960735  
0.0509423779213313 0.6833174489374154 0.2619069722653743  
0.4304891946737271 0.8337588320838973 0.0031743299182749  
0.4194553450616770 0.1117133304953245 0.2168691828282802  
0.0538799708551260 0.9860454193497956 0.0245499399027075  
0.0493291026159021 0.3297045515008595 0.2307058091089275  
0.4212575956762361 0.7463032799117230 0.1708996737508401  
0.2359467289078876 0.2419906282523576 0.1852327465544934  
0.2983518174168125 0.3983806493165319 0.0309406686334011  
0.2374883981094919 0.8012358061697764 0.2345681823009269  
0.0513218992101466 0.1567736460223315 0.12694125017111053  
0.4320955149812656 0.5717983321933932 0.0767867436731662  
0.4245054822495025 0.8764456837112388 0.2839722255318455  
0.1112866976426160 0.6594310287801205 0.1165889767236386  
0.3610902858528707 0.0814780453878619 0.0652604170054288  
0.3977242185979583 0.4909120674125688 0.2534509635456642  
0.7915417988985084 0.7615621144274450 0.0842110132532269  
0.8131558439581730 0.0781935807553374 0.2995585881131243  
0.6789807641672403 0.1882787517275797 0.0436633689158005  
0.6741643289059838 0.4989932314565719 0.2483163579975051  
0.6827728388239875 0.9552732751021055 0.1123509613188161  
0.7948323393127242 0.5413328876589789 0.1712522462481201  
0.9183976993229175 0.3493545021334041 0.1476376125763215  
0.5577135717746352 0.9244788803460583 0.2041773752695585  
0.5625223203445785 0.3855723202840623 0.0629840981808369  
0.5531791138308074 0.6819208127617911 0.2692292246074376  
0.9271205096467130 0.8416471074076883 0.0138695695282605  
0.9241308146265153 0.1082502165759696 0.2148821870030992  
0.5550076001775384 0.9773621127882384 0.0253858373577550  
0.5502932785896095 0.3198639099586144 0.2273343825199798  
0.9243443508104906 0.7357700814645424 0.1803605541149251  
0.7331561959467855 0.2318519469015020 0.1887324641193766  
0.7893095925673365 0.3879652392956199 0.0616525163157735  
0.7376410285564042 0.8059009498981371 0.2413368076828894  
0.5479155989733209 0.1499022167258385 0.1269569548666291  
0.9263363393335963 0.5672966083897193 0.0790622336726605  
0.9316157855792561 0.8802237480602081 0.2826556870274984  
0.6132364949746094 0.6545401403786986 0.1242620525014718  
0.8593153006213672 0.0860970111651367 0.0722287510048083  
0.8536066808641597 0.3695072201396049 0.2980358703790945  
0.7820531653784732 0.8339907622842353 0.9714899813532497  
0.3144220363866144 0.5431135943111338 0.9472277930457713

0.2208402913739953 0.2143827586664819 0.3596778410276608  
0.9131090257158821 0.4069162898464212 0.3930315865154687  
0.3611752798311985 0.3556461273024957 0.3540766509471636  
0.4937442563994309 0.4162729871819166 0.4067010769771916  
0.4290489712126297 0.5756684127549220 0.3532916740291301  
0.5576939003251165 0.6393656656833037 0.3974128889874329  
0.5685367980001702 0.2407407934927598 0.5080114970597339

#### 4.18 Output file of the structure COOH\* on Cu<sub>4</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996

O Al H Cu C  
76 48 5 4 1

Direct

0.4341410122118122 0.3889243829227668 0.0613742958258704  
0.4348547023125003 0.6741377939724360 0.2582246588486601  
0.0311741354172788 0.8302860560902960 0.9901949148077005  
0.0444095478039625 0.1202847085146310 0.2119232835542269  
0.0408653270249561 0.3392206835781755 0.1458553371038830  
0.4380250472793384 0.9114338378671122 0.2026419964675298  
0.1836499687853766 0.7673358904321637 0.0827744537552022  
0.2656506353283840 0.1472517377469258 0.3613000599232576  
0.3005486656425825 0.2066331692171651 0.0351125172665028  
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0.7968661700087859 0.5378199458516814 0.1711919749686332  
0.9206136084868786 0.3455419023923103 0.1484913246734587  
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0.5570524966136627 0.6750359670498686 0.2603878848346060  
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0.7354524617035918 0.2277719706385700 0.1894749831772064  
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0.7397558912468503 0.8026296901550106 0.2409703159883324  
0.5491662850790853 0.1465267338113564 0.1283866528283928  
0.9288774734129941 0.5632444783343616 0.0795188734604022  
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0.7853965221980451 0.8315967992284873 0.9717586224285681

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0.5067811916658698 0.4996598692485508 0.3689807114097970  
0.3902519282853500 0.6420622244717271 0.3708287893368232  
0.5210908421838685 0.7657052191461903 0.3738568456289149  
0.6046685353721826 0.5346756255400553 0.4177075388919905

#### 4.19 Output file of the structure OCHO\* on Cu<sub>4</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.000000000000000  
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-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Cu C  
76 48 5 4 1  
Direct  
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0.0392061883258276 0.3436579737909211 0.1461625017937873  
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0.5483435957268062 0.1503914314039657 0.1283358079307220  
0.9266085651057970 0.5675435309255925 0.0805021063706379  
0.9318968221985781 0.8802524006037485 0.2841219291564385  
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0.8595433559778766 0.0862234311857221 0.0736765118884806



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0.8540441869203752 0.3703753837632124 0.2993991350104707
0.7824336856921565 0.8336383789198245 0.9727014302021080
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0.9120224553455248 0.4149080687970742 0.3946166152710547
0.6660090260345339 0.4165565769000454 0.5206802568924543
0.3578015139835159 0.3525015797431070 0.3549994098520474
0.4814730199717943 0.4032793798833829 0.4115001154916901
0.4238333447812832 0.5745552907473918 0.3559174555550701
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0.6226565859755436 0.4481117047797153 0.4839244533874164

```

## 4.20 Output file of the structure CO\* on Cu<sub>4</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

```

1.000000000000000
16.0489997863999996 0.0000000000000000 0.0000000000000000
-0.0582879140000000 10.0169307487000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.7133998870999996
O Al H Cu C
75 48 4 4 1
Direct
0.4315287849806325 0.3927301273420986 0.0589213953241344
0.4321046669125570 0.6754906294958676 0.2691004499478372
0.0287931777147623 0.8308803460528625 0.9875634560094553
0.0426345647171163 0.1224375149111210 0.2091524769420949
0.0387737875537303 0.3417701013212837 0.1433061416224783
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0.1962862192938796 0.1480318234150021 0.3637127532053466
0.9140108992288843 0.4065746919924367 0.3912193812735016
0.3878498027026477 0.3795717493560601 0.3608220480105815
0.5145679406383686 0.4585041969202066 0.4198867156526238
0.4564961289393833 0.5917512279015743 0.3512978661176322
0.5884344852251827 0.6666279329908777 0.3973108577124048
0.6938956283562421 0.7322412178666653 0.4159097786999094

```

#### 4.21 Output file of the structure CO<sub>2</sub>\* on Cu<sub>3</sub>Sn supported by γ-Al<sub>2</sub>O<sub>3</sub> (110) surface

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-0.0582879140000000 10.0169307487000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.7133998870999996
O Al H Cu Sn C
76 48 4 3 1 1
Direct
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0.4356116628573328 0.6756121531803528 0.2646023207614766
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0.0439281524884709 0.1211289769459740 0.2122065078654925
0.0400053967881313 0.3407261238504543 0.1466968941570667
0.4375104229707193 0.9162090439418346 0.2040643896804767
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0.2357448566260393 0.1206952173632414 0.3545073091209809
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0.1773783540509636 0.5410112076882974 0.1601117968364706
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0.3046654960013772 0.1291374036649376 0.2268235069167366
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0.5402312407087421 0.4232104514921589 0.3724298206580083  
0.3955586944532434 0.7283428415289658 0.4074307660981779

## 4.22 Output file of the structure OCHO\* on Cu<sub>3</sub>Sn supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
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-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Cu Sn C  
76 48 5 3 1 1

Direct  
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0.0399687256360217 0.3405927489657578 0.1469878798213484  
0.4370222395776714 0.9165828854016614 0.2050868134117329  
0.1827581616871470 0.7684663543974858 0.0843161352717289  
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0.0626185649919483 0.2106067878489319 0.0475531131248227  
0.0651096000287615 0.4953767730905935 0.2629063659302591  
0.4240134584088792 0.7473850217356136 0.0909536470720155  
0.4119102179071551 0.0554209507757477 0.3044136056768373  
0.4166664406254396 0.5320191343868550 0.1666461512582643  
0.0633457625755750 0.9731705396360324 0.1133763433284189  
0.3349602046711853 0.7688155464689984 0.9923872054332167  
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0.1821810685653774 0.3740388105491438 0.0420210445653747  
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0.3042523728883222 0.3503426781894259 0.1465193826253100  
0.4237654422532816 0.1536105970218320 0.1349771913970731  
0.0430106465531861 0.5569681798256807 0.0702774673404520  
0.0506247704081601 0.8630613253512003 0.2834584853212775  
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0.1651480262861155 0.3168755231699478 0.2380840862541514  
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0.9396555485214360 0.9187218271121687 0.1995012915662897  
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0.7982746072571253 0.2340209826381291 0.3322295509176533  
0.7932934313368709 0.2063703824866772 0.0420346404439550  
0.7904655220309494 0.4789895005134372 0.2556121458682578  
0.7977632668439683 0.9475542111689870 0.1015351073585000  
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0.5618841516472957 0.1983779336244995 0.0480720026826965

0.5612541146500929 0.4906339781129604 0.2635579807608884  
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0.9263923477568067 0.0539955569433484 0.3009010677644200  
0.9150923770844970 0.5385222411788482 0.1644058105950594  
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0.8230402734132173 0.7843669870603152 0.9991829834680410  
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0.8025757831002273 0.5695369075305445 0.0806464814618101  
0.8049440914966141 0.8933035841144347 0.2979549656928721  
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0.9167188151643645 0.4496500528562146 0.3556015963413451  
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0.3176961019001062 0.6579161218071071 0.4106678832200192  
0.2947908895411184 0.7594205556412973 0.0683475328562598  
0.2997499322576639 0.0496396825072492 0.3015170660145355  
0.1860197533503425 0.1900728527481571 0.0444790435881805  
0.1778937946084806 0.5025288631317703 0.2456549349931850  
0.1852133649299840 0.9501650659590265 0.1081358209938670  
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0.4186454031777752 0.3396885406412360 0.1453899427262696  
0.0625178090024735 0.9255431331851844 0.2031598734605893  
0.0770263313407782 0.3869040140187880 0.0677616039273310  
0.0529875547383734 0.6795513826975742 0.2643419932639408  
0.4319306713269037 0.8317178398048211 0.0084345260847012  
0.4184414695118491 0.1046576634432519 0.2220711573859974  
0.0543703313836535 0.9851188187489112 0.0262316305929563  
0.0517785746918494 0.3269198439458173 0.2329653168869319  
0.4227376724446602 0.7450595676478620 0.1767383598856757  
0.2366175859712637 0.2374771323770518 0.1878209976533107  
0.2984653479212216 0.3960254023378479 0.0328137331618483  
0.2381736481437563 0.7946171296211820 0.2334487345337238  
0.0525984719679550 0.1536618130666596 0.1291113865461565  
0.4340774663705490 0.5685957257377601 0.0803413042937815  
0.4254230756691320 0.8730759965821242 0.2947815486538824  
0.1133829208678008 0.6548007327289851 0.1192072091846044  
0.3618969674509276 0.0800794126605765 0.0697899153847827  
0.4021224492751214 0.4969471324740013 0.2561872848577386  
0.7937356943405146 0.7602399117339063 0.0863109112353387  
0.8160592144104178 0.0766432885482362 0.3030215308794794  
0.6802499056924831 0.1856971158023403 0.0469392907461530  
0.6784701448095770 0.4925351478089892 0.2499739765963374  
0.6839578078638542 0.9530953157013553 0.1148340253825875  
0.7974316116928927 0.5400006795928255 0.1732206336465718  
0.9202456211097902 0.3467474576173585 0.1501507796794185  
0.5584729337626179 0.9243467729041049 0.2075453528187722  
0.5617958533543744 0.3816645429074317 0.0657600347853316  
0.5531763934504991 0.6831455548991959 0.2664884055152125  
0.9279753298025574 0.8397556549573219 0.01534903503054931  
0.9262216482665455 0.1056246649608928 0.2175515564596023  
0.5557001701745750 0.9789764881192041 0.0284111281854227  
0.5520508692219461 0.3098471338933305 0.2303208645666315  
0.9267660558516038 0.7331333485825859 0.1829486971641057  
0.7357784628640893 0.2278213220090631 0.1911892864994422  
0.7902355440684242 0.3854067746193330 0.0643896469961857  
0.7419508244536812 0.8077622535752502 0.2428011694027041  
0.5478613737928655 0.1469951282474071 0.1303068021517315  
0.9282800201009261 0.5650724846964575 0.0813149112674929

0.9348359747871818 0.8775495342469775 0.2855047583374397  
0.6159726200483326 0.6522700269601401 0.1253023255153380  
0.8605213384026317 0.0837992496295733 0.0747533288464750  
0.8569108149949645 0.3679968047183842 0.3007739167207445  
0.7816132496317173 0.8292341158164807 0.9739703900862825  
0.3185457509416356 0.5384352534270439 0.9493482750491310  
0.1765698058108285 0.0890945934414318 0.3579627258070975  
0.9189261524230589 0.4049091757970306 0.3951337438617040  
0.2947874066150692 0.8574528531704499 0.4098412570195478  
0.3911762000882785 0.5158614681060130 0.3736720668402277  
0.6434109483839208 0.6301516596748435 0.3669519598064061  
0.5049663511869030 0.6756955560547788 0.3903450367559579  
0.5408830630263810 0.4227950277014328 0.3723785655807046  
0.3388924825145417 0.7758601977664843 0.4004946928801513

## 4.23 Output file of the structure COOH\* on Cu<sub>3</sub>Sn supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Cu Sn C  
76 48 5 3 1 1  
Direct  
0.4366460532340796 0.3895356961460461 0.0624786369201320  
0.4357744514418610 0.6780135469882895 0.2604709856234325  
0.0320169485073767 0.8306016347939538 0.9905510112358483  
0.0457062160814404 0.1207290130868216 0.2125474659530581  
0.0416775372188990 0.3400835166501879 0.1466380725398486  
0.4382556641777750 0.9153497086797941 0.2022356015681741  
0.1844753937402632 0.7681456981596828 0.0836052346888653  
0.2344423505998626 0.0932028604028145 0.3590196506360566  
0.3015004738181068 0.2077584432009490 0.0361255215521152  
0.2929717811598471 0.4983490248593488 0.2455516357736778  
0.2997370986477014 0.9445176890274665 0.0939361835426170  
0.1787506391787901 0.5389477405358235 0.1593070141827367  
0.0652737878862634 0.2106256731217289 0.0475518674810063  
0.0660912689795899 0.4950100479257927 0.2619045719176374  
0.4255257965011994 0.7453702328226484 0.0889755699116555  
0.4145327154959321 0.0484770937447505 0.3040846096341332  
0.4183440688089110 0.5305290402276436 0.1655329656663283  
0.0658218044634880 0.9728710759264060 0.1131888546191540  
0.3361026652833143 0.7682547293794882 0.9910811852183132  
0.3053225308027798 0.1268344558931815 0.2288637273173338  
0.1847030660552225 0.3737477576459969 0.0411719279522096  
0.1707491262000847 0.6762137410304824 0.2681091884298780  
0.1777110073679566 0.9109861703717204 0.1929800159194229  
0.3058194426379627 0.3481122134638809 0.1467707030207679  
0.4249947933854100 0.1526656503804653 0.1343924859093839  
0.0446444709997472 0.5562791770503508 0.0697075433866600  
0.0519834601360695 0.8625452419407502 0.2828070315805436  
0.1660699844542330 0.0206594840697753 0.0239725592830551  
0.1663533853888355 0.3159602175703044 0.2379630276018639  
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0.0468664622457165 0.7271977967745548 0.1760572371598526  
0.4427971857354007 0.0077516050055181 0.0247721627659608  
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0.9412324698453647 0.9182414480566103 0.1986629592127524  
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0.7996239682271958 0.9464940525743768 0.1001556707966375

0.6826893916954205 0.5446955112536812 0.1694638722001059  
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0.8101944203004279 0.1157631379785360 0.2198985742382979  
0.6781906531978117 0.3695259519316493 0.0459665705661126  
0.6738757619686983 0.6749644089830216 0.2769638168038314  
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0.5431857230751814 0.8576937330214002 0.2852946579116009  
0.6674728967900428 0.0129014720720568 0.0271908483303984  
0.6640306068162098 0.3090806105937058 0.2393980146451656  
0.8090236174550489 0.7267743056213436 0.1817545126477915  
0.5482155609677648 0.7264616174425415 0.1800472135831502  
0.9384884571415404 0.0150194369208137 0.0254089624940507  
0.9350047245514995 0.3037923594301895 0.2358745192708002  
0.8039769555332341 0.5689546907814458 0.0798307432661127  
0.8053791156598662 0.8926940841488858 0.2969511698978136  
0.6761630953455245 0.1468823392160676 0.1319663004313205  
0.3269160834630859 0.4448200914767629 0.9571111290552680  
0.9187373945405475 0.4477413029381180 0.3544994261760741  
0.3490621704642233 0.8935119416190900 0.4295310339870859  
0.3207554909893255 0.6792429593665632 0.4085142136841461  
0.2962955374043300 0.7582428919074112 0.0671534676153674  
0.3021052876497217 0.0429818822066019 0.3028643639300204  
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0.1876671103031299 0.9496979158021805 0.1078851026182799  
0.2924667294788674 0.5343456948507915 0.1580141888018030  
0.4199007859808609 0.3387476473292666 0.1446415133664795  
0.0646571855052638 0.9249625427470798 0.2026970494942002  
0.0800463142916765 0.3869528453592173 0.0678355740502460  
0.0542603475169494 0.6791159391488715 0.2634962265453568  
0.4332616233056614 0.8307590219802365 0.0069251317275970  
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0.0569963091133722 0.9849202998543369 0.0260073662292411  
0.0528328926809285 0.3263620892130611 0.2325703456920675  
0.4243242103084705 0.7423532058668394 0.1741050999212537  
0.2386439426890001 0.2353524920565426 0.1885895157517007  
0.3008630154932119 0.3952670316370723 0.0309031825373911  
0.2404592998050153 0.7919526160930789 0.2327531698451052  
0.0548132332116653 0.1533457547663923 0.1288817834135264  
0.4354344607707686 0.5664788876029416 0.0788171066223195  
0.4269467892950608 0.8683934268085569 0.2880236206552420  
0.1149051034994627 0.6548354284590883 0.1184555111068100  
0.3638119044449172 0.0792295060862155 0.0689370686585110  
0.4024722692125052 0.4950226290774504 0.2568381626702136  
0.7955378728122151 0.7592730293800933 0.0850489328992118  
0.8168155696019714 0.0755938766837636 0.3018201392317420  
0.6818088430649708 0.1850898281136231 0.0461568806499348  
0.6797555217121599 0.4926956273733401 0.2497762400252279  
0.6858498386154653 0.9521160530423040 0.1134453320910693  
0.7986269162802144 0.5391569410006073 0.1725607196177710  
0.9216799741025948 0.3459788213798174 0.1494295201286341  
0.5602155457474646 0.9237239465150577 0.2049409382446566  
0.5633362339313014 0.3804654165974638 0.0646560467112815  
0.5546581383541827 0.6817367431877855 0.2640303698532021  
0.9309383090953640 0.8389690363578950 0.0150203033164909  
0.9275781940644382 0.1047349278817497 0.2167138679064630  
0.5573314550003803 0.9776596289707546 0.0272065885538631  
0.5534932167435046 0.3097261203208873 0.2294327906981050  
0.9280784165603783 0.7328079131447758 0.1820990363251576  
0.7369010198264102 0.2272973882465557 0.1903940474286717  
0.7918392194386084 0.3847006422890659 0.0636535686156176  
0.7426556223628785 0.8061783165597181 0.2419700296006704



0.5490764815603827 0.1464255796007964 0.1293069492004342  
0.9299307925650966 0.5639762485071432 0.0807475782273894  
0.9362456566571611 0.8770622505256214 0.2846109361956604  
0.6178117020846272 0.6507383525035436 0.1235063952401898  
0.8625346821352250 0.0831573670483058 0.0739328242461767  
0.8579965755887022 0.3670975759290552 0.2999686090355455  
0.7859483628510736 0.8293540835683710 0.9722584892128544  
0.3189848481577048 0.5389656394688437 0.9478039349291921  
0.1748207717414470 0.0923792970548560 0.3521879940585224  
0.9192700305651288 0.4055683288659396 0.3946372320073586  
0.2885512369529575 0.8921162591946376 0.4382535354360147  
0.3841221028209705 0.5292380850248584 0.3696716682196329  
0.6255989775141181 0.6576608506346547 0.3681172649980560  
0.4867311265026387 0.7216246927465243 0.3897898323297742  
0.5331469967460768 0.4449147397711293 0.3746988203513290  
0.3735838875077889 0.7740768645801868 0.4089186052929965

#### 4.24 Output file of the structure CO\* on Cu<sub>3</sub>Sn supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996

O Al H Cu Sn C  
75 48 4 3 1 1

Direct

0.4357235989549054 0.3918104230921962 0.0629616233941731  
0.4349156030276596 0.6792544711323958 0.2635717936575761  
0.0319228224843610 0.8323563493963971 0.9922656261537600  
0.0455111183102606 0.1225740037789801 0.2143143196460283  
0.0414788893067302 0.3416395347950028 0.1483126689977363  
0.4373222082266146 0.9174583212370183 0.2030514846530589  
0.1841957369379763 0.7696960445803409 0.0848847726609507  
0.2408144052394190 0.1127448431988329 0.3598082354235697  
0.3006580539809903 0.2096039214501280 0.0372156391118105  
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0.0646542351452001 0.2115397834675838 0.0491941685449404  
0.0664697363536895 0.4964482618120015 0.2638320391817346  
0.4245228032711776 0.7475563616548783 0.0891140795303396  
0.4152307205710714 0.0506187554374906 0.3049337091245884  
0.4181459516966334 0.5333878922867845 0.1661785694113841  
0.0657658729588056 0.9743645739707909 0.1150001117797184  
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0.3056469782473993 0.1286026215039682 0.2295947470402366  
0.1835931128918997 0.3753852565167218 0.0428605034043504  
0.1710707309957893 0.6776212497570965 0.2703795412951631  
0.1778071846303504 0.9122641061772909 0.1947222594344580  
0.3053593390248482 0.3507691734039952 0.1473802677331042  
0.4244901630667887 0.1540899145284436 0.1348090655139935  
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0.5429810820705060 0.3318570815273746 0.1466080512221534  
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0.6840082094366754 0.7733500317791716 0.0923078129445698  
0.7979884863224771 0.2345058006844991 0.3324179004441519  
0.7949564317327958 0.2072892375613527 0.0427351328694640

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 0.9277124776975161 0.1620697290487045 0.1344803762611981  
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 0.8087419017797142 0.7286972384954032 0.1831594986627555  
 0.5466075881072691 0.7292337717342942 0.1800562904251241  
 0.9383004016563806 0.0166675086415790 0.0270761867802453  
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 0.9164662707032215 0.4509026004430442 0.3560765272497716  
 0.3881502209955640 0.8926070236687493 0.4457852334328158  
 0.2953631258080109 0.7603503864400178 0.0665947127177162  
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 0.1875018448420679 0.9512299179633005 0.1095050125707431  
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 0.4237652634094714 0.7459023525848790 0.1740205895795674  
 0.2386952536582410 0.2375449744979785 0.1897028627113129  
 0.2995966422719546 0.3972445656502448 0.0322913429791283  
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 0.4047854777087236 0.4983978039126715 0.2552042412143723  
 0.7953593422760361 0.7609163838231530 0.0864594409631540  
 0.8161586367214807 0.0771295099229358 0.3032020017946287  
 0.6818557407791297 0.1867779766451931 0.0471735259472584  
 0.6774677442731425 0.4943091565294713 0.2503210935526791  
 0.6853967698480927 0.9536934060157308 0.1142849969427436  
 0.7982143356665496 0.5409630750326857 0.1741577258921684  
 0.9214456792608255 0.3477021395852203 0.1512380308180078  
 0.5599647439228326 0.9257161034476737 0.2061606553829557  
 0.5632866107364930 0.3821317040520601 0.0653452122265398  
 0.5535708846533981 0.6806028306626254 0.2633733936552666  
 0.9308280383024258 0.8406227587074538 0.0166570457791227  
 0.9272816906434032 0.1066156435826292 0.2184443290384287  
 0.5569379783833236 0.9804771028002521 0.0279993790084286  
 0.5527194934188809 0.3160252925280261 0.2301836468830711  
 0.9278708609476242 0.7345606934609661 0.1836557487985346  
 0.7363041710516123 0.2289931331807895 0.1916921895897531  
 0.7918810286088739 0.3863778490346525 0.0650651317292872

0.7419892655595731 0.8079907378291379 0.2432229874894250  
0.5491858685366653 0.1482761491598303 0.1303682056537075  
0.9295759257548059 0.5657353619207739 0.0823524709960881  
0.9359653176908207 0.8785580884447042 0.2861810137916804  
0.6173140075167297 0.6525313726035709 0.1241799476578553  
0.8623439529906560 0.0848818155393558 0.0755590767397959  
0.8564701256405567 0.3692995003080699 0.3013713721775467  
0.7860202515319212 0.8313793825216304 0.9737314077430221  
0.3171651548311817 0.5409220266790743 0.9489165302337653  
0.1861962110646501 0.0777671756299037 0.3698319675363623  
0.9178397275262098 0.4076486301374916 0.3959571691574459  
0.4062867624869818 0.4512410841125416 0.3719013642931252  
0.6262161285624513 0.6477798499130545 0.3670597888782270  
0.4767806533442828 0.6655678322628978 0.3907256356442643  
0.5542143618399435 0.4446249608469505 0.4160986335209600  
0.4183930431901423 0.8178875999966423 0.4117966493817973

## 4.25 Output file of the structure CO<sub>2</sub>\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996

O Al H Sn Cu C  
76 48 4 2 2 1

Direct

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0.4328847364656454 0.6779723291964075 0.2591324390963692  
0.0265535734384272 0.8354284274437020 0.9886571069983958  
0.0408956122973123 0.1248390173381679 0.2106916348274268  
0.0368508974900408 0.3440614650948390 0.1447500926107281  
0.4336476160251479 0.9186544936639365 0.2023412666236482  
0.1795149588689284 0.7724658212387681 0.0817325700619804  
0.2348516661540856 0.1123220206885307 0.3574060341146321  
0.2967258827036616 0.2115551312724548 0.0345407296637177  
0.2869844555468788 0.5033054391023271 0.2435533724347252  
0.2947332501201672 0.9486691676483474 0.0924069048285219  
0.1732947939317029 0.5436173560303246 0.1571900800473998  
0.0605150875803631 0.2147290847225420 0.0456491142439575  
0.0608627459993301 0.4987409317063651 0.2600385544985642  
0.4202555921956446 0.7499176833378129 0.0875489793160469  
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0.4127862826723856 0.5347067356076991 0.1636454617098693  
0.0607143800918024 0.9770655987651509 0.1112597883117701  
0.3314218682953936 0.7725954198878213 0.9892014191283280  
0.3010644303470826 0.1308059434470366 0.2270545036383496  
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0.3008162524911242 0.3523179717827176 0.1450844208239630  
0.4202682375842031 0.1563894671676280 0.1332738886231581  
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0.0462894347557921 0.8661630222323922 0.2811380949004914  
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0.1615155232348968 0.3203473431055102 0.2357965739128005  
0.3041438657805955 0.7251484656129819 0.1729467636753910  
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 0.8053178194087423 0.1210682248734472 0.2183094625112574  
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 0.1824547049421099 0.9540305102718705 0.1060993702253015  
 0.2867569185516388 0.5389712221337533 0.1558416402803431  
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 0.2338045387114249 0.2390184313302939 0.1868363934360744  
 0.2963278618173959 0.3989886999216026 0.0293924746537826  
 0.2348819428972178 0.7966930042325586 0.2309485534177327  
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 0.3589730548963459 0.0833041679773459 0.0675948796697838  
 0.3953527763907587 0.5007603092656581 0.2531848952109215  
 0.7904547828974131 0.7635100419355680 0.0838925024632360  
 0.8121910099510217 0.0796596142528259 0.2999911761776559  
 0.6766571974748388 0.1893281531978559 0.0449501952729037  
 0.6761804733962649 0.4993905123126297 0.2496086862830325  
 0.6808788691134566 0.9562972621269026 0.1126945635753529  
 0.7934492827935955 0.5427509059865514 0.1707703098112177  
 0.9168135067035266 0.3502625121475447 0.1475626090021152  
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 0.5584856309922159 0.3847587458484156 0.0634566956705243  
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 0.9255521581625175 0.8437627541549233 0.0134527912729752  
 0.9226376538340446 0.1089820305733511 0.2149345250757833  
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0.7867783124674901 0.3889045803750193 0.0618810932751330  
0.7368411896927896 0.8083702030708295 0.2410647452857972  
0.5447334094242535 0.1511302585191956 0.1285872689087029  
0.9247369709487998 0.5679293353475998 0.0787387650659213  
0.9300366082858957 0.8808822383209503 0.2826754542287375  
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0.7801957211011796 0.8361388721973526 0.9716486722154372  
0.3142950634038968 0.5425865070791289 0.9463303815422321  
0.1769926143462328 0.0861256831422565 0.3619083052165806  
0.9147245354095972 0.4067296245960819 0.3931171439734555  
0.3912999546562972 0.6773909159980818 0.3900829527336143  
0.3609932901978326 0.4031169060921016 0.4115695552391259  
0.4902919871209406 0.5281851349120927 0.4585858860883931  
0.4900553680227375 0.4714758063428093 0.3472261274015906  
0.6755009602503321 0.5514180781987790 0.5144338370422190

#### 4.26 Output file of the structure OCHO\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Sn Cu C  
76 48 5 2 2 1

Direct

0.4320352957999916 0.3963889408016001 0.0607451722341636  
0.4332845354269210 0.6821722341646819 0.2626348957245099  
0.0279958255815913 0.8355834284644459 0.9890739576704419  
0.0417478607760486 0.1270118362798698 0.2104046061310996  
0.0378566138687617 0.3462498313899829 0.1444908569933148  
0.4337129491923122 0.9208717997341864 0.1994751708361591  
0.1805918939073976 0.7747063646927117 0.0819027492641666  
0.2413312629669093 0.1155917947123868 0.3587424054474440  
0.2973000842194864 0.2141570119060887 0.0342265699891797  
0.2878916346577540 0.5054426218493902 0.2435290418652798  
0.2957611074782278 0.9506061737998195 0.0917480109288107  
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 0.7940898785409942 0.5449353071020440 0.1705654285641032  
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 0.9234444713543297 0.7392269535108724 0.1798619885146522

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0.1823771052630363 0.1004759912636928 0.3653305006402263  
0.9096915957809912 0.4253127438233406 0.3938076524901319  
0.5754282462732618 0.4452037681568513 0.5898937068046592  
0.3724236255914732 0.5850906646071508 0.4089195017254497  
0.3869041936522919 0.3064683627614571 0.4067820654705159  
0.4985961113546864 0.4639178801220822 0.4613583306945088  
0.4905996377736628 0.4646153308612568 0.3459648641304653  
0.6267758151759892 0.4543426549828382 0.5554158587602771

#### 4.27 Output file of the structure COOH\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
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-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Sn Cu C  
76 48 5 2 2 1  
Direct  
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0.0416028805013768 0.1258604757767658 0.2100809727591521  
0.0377141453901756 0.3451767584985370 0.1441930099667645  
0.4341050305590955 0.9196274179699016 0.2013926304146426  
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0.2388073566483156 0.1168270293562866 0.3580662305380073  
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0.9232528497429827 0.1099331226965230 0.2142747637917214  
0.5530300999070484 0.9819431430085876 0.0259616099310163



0.5497647694157076	0.3168551333426645	0.2281957643331620
0.9234142231612844	0.7378545763777811	0.1795287823696462
0.7327225027380607	0.2340089836740252	0.1886213150039640
0.7876521366575276	0.3898052149370761	0.0612569622490842
0.7376949249435225	0.8095176266735133	0.2403905566492899
0.5456856691703483	0.1523737386866054	0.1279090343375703
0.9254825195813169	0.5690155591692144	0.0781468563074525
0.9304735599599626	0.8820075431682808	0.2821145763497721
0.6140573097280055	0.6546992646485797	0.1213928361834391
0.8582173417396572	0.0882407199623473	0.0716961088614379
0.8548446747615936	0.3715416292167003	0.2976028277011489
0.7815419579059664	0.8343638185451985	0.9698910540748464
0.3149726142355685	0.5437159852791121	0.9453904218244967
0.1809668008042140	0.0928620023983433	0.3644981609905291
0.9122333083686648	0.4150929701548860	0.3931582640491157
0.6047991780499081	0.3105064357463090	0.5761698473988062
0.3991698103476613	0.6839173464778533	0.3956539827402745
0.3567791039794361	0.4089617150399875	0.4079310103980148
0.4897279892808595	0.5076442414799350	0.4618399099401358
0.4910723934476203	0.4753993366418846	0.3476056581945308
0.5689563283170032	0.4507771413786454	0.5231169741510892

#### 4.28 Output file of the structure CO\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

```

1.000000000000000
16.0489997863999996 0.0000000000000000 0.0000000000000000
-0.0582879140000000 10.0169307487000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.713399870999996
O Al H Sn Cu C
75 48 4 2 2 1

```

Direct

0.43225019484544710	0.3936796232911593	0.0608645514102026
0.4342372500680053	0.6773156107780588	0.2593943628110014
0.0278501195453818	0.8353606084089344	0.9880271509117108
0.04192335646933094	0.1250044426917040	0.2099537077321069
0.0379623454033141	0.3443257975779165	0.1440751866762142
0.4346485557355652	0.9179974307144569	0.2018157289793570
0.1807296648549022	0.7728198774148536	0.0812980443625160
0.2358748066538379	0.1117932692585497	0.3569742324096077
0.2979570915704958	0.2118325307034883	0.0340522165844276
0.2876213777400032	0.5037182947166196	0.2427155885800559
0.2958499153065249	0.9490455204813883	0.0919901880247029
0.1743063944640276	0.5437223669972846	0.1564516021525416
0.0617927612342431	0.2151348460585682	0.0450288686299257
0.0617407299209699	0.4990499463608962	0.2591462171785038
0.4212382282268424	0.7500765815867426	0.0869762028062250
0.4107411131780920	0.0521812603074965	0.3027939176382315
0.4138146136948061	0.5357485228176292	0.1632586433064568
0.0619440413625355	0.9772772328458025	0.1106149772048609
0.3323071491714292	0.7732144991986164	0.9886858178894365
0.3021318193549301	0.1308546420731632	0.2266767159578645
0.1813493918201246	0.3779809526216085	0.0388514786581320
0.1662204875889797	0.6805455576103454	0.2657824678151810
0.1734334160457529	0.9156833353889363	0.1907100912497150
0.3020066133909160	0.3524697196009183	0.1447533855839490
0.4212563636505907	0.1567976904093306	0.1330835126648096
0.0407291004044782	0.5606116901789908	0.0668960071632060
0.0473083740511112	0.8663749279077292	0.2804680987175857
0.1623076557120811	0.0249268087325586	0.0215165751315910
0.1624655251343719	0.3204310135581870	0.2352371096722411
0.3052406620524555	0.7253578656882217	0.1725764417080503
0.0427831881112477	0.7317255584321378	0.1734325772539319
0.4389997898680255	0.0121410732898788	0.0230972454857932
0.4349481921398830	0.3273886717512551	0.2335144895511947
0.3103315356138515	0.5665553656236321	0.0721149203019005
0.3038427945695397	0.8697169431591908	0.2860055763587747
0.1761960285248262	0.1561827096442466	0.1269272593108482
0.9077104375590451	0.3963112929712669	0.0605663414644758
0.9336646992456653	0.7041880665055918	0.2632056923237516
0.5342089939527531	0.8309507869562615	0.9871498626361265
0.5350525446889205	0.1237692967988440	0.2149792395534901

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0.7954697892111792 0.2373361283806318 0.3288405591145835  
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0.7893270076702146 0.4824862706578931 0.2526102909862196  
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0.6785632437707770 0.5453064203641047 0.1668719386113071  
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0.5603082879627495 0.9727878803803744 0.1157740908569468  
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0.9241772576080711 0.1648988173474530 0.1302539047307607  
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0.6631828249210020 0.0172559910297447 0.0257908884425618  
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0.8000212540616644 0.5731918375046511 0.0770904517699897  
0.8032497935968202 0.8967540368123560 0.2937671551773716  
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0.3242447129483578 0.4488023551080805 0.9551309149530006  
0.9177487533753408 0.4483839022575501 0.3520201080701109  
0.6084093488736300 0.5256908908812302 0.5688857405513288  
0.2924395218872909 0.7632371583315460 0.0646947059503857  
0.2983201685069187 0.0474690516087158 0.3007164229682037  
0.1847871159227311 0.1941218854935791 0.0419240238752164  
0.1739068273281602 0.5062843503021066 0.2414953495835949  
0.1836117763345141 0.9544165012434304 0.1056151337455001  
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0.4160869459343714 0.3433163939006655 0.1430662778168436  
0.0602459262944394 0.9293686100485060 0.2004657316390394  
0.0766060773632151 0.3914799550151949 0.0654960242918074  
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0.2976071894945114 0.3991993535858268 0.0288678636665190  
0.2358709448617615 0.7966979840261093 0.2304698564134746  
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0.6778376068383073 0.4996328970745313 0.2491215436666314  
0.6819578133984170 0.9564837612309115 0.1121689130220034  
0.7946619760331858 0.5429249691703963 0.1700382666991703  
0.9179137489000510 0.3504415755416401 0.1468443785310645  
0.5568004045297541 0.9281776533903194 0.2042439586562957  
0.5594695845867819 0.3848350729390004 0.0630460641322009  
0.5561513185398733 0.6870129396470908 0.2605578016767889  
0.9267522184583256 0.8437412902695577 0.0126665695872589  
0.9236841819218272 0.1091353947526305 0.2141929236069025

0.5533142778414026	0.9815595218698923	0.0261059014970619
0.5501851612018080	0.3159368258682842	0.2284187086983705
0.9238310704856008	0.7370585001215064	0.1793670865972244
0.7330992890873590	0.2330230300308600	0.1885395980123949
0.7878454288931191	0.3889766121401311	0.0612397960885403
0.7381990711771822	0.8087401607829706	0.2403660853995267
0.5457943359228324	0.1513579180722061	0.1281960942667499
0.9258231654767387	0.5681018496911756	0.0779859469731426
0.9310131573915874	0.8811641191235211	0.2819697097615846
0.6145137544975032	0.6536822845897964	0.1214141161089769
0.8584391089610872	0.0875158758376819	0.0716994456987215
0.8553266318762127	0.3706087083398184	0.2975675274648020
0.7814127702438468	0.8353710633757508	0.9705127827296535
0.3157639678615216	0.5427826174048008	0.9457383976459789
0.1779501140466908	0.0861856481840172	0.3615551254787947
0.9157954981989734	0.4077169412310409	0.3924691945906967
0.3946703087592293	0.6723370725476033	0.3888113153442699
0.3619242924616232	0.3987986166709502	0.4028111359233095
0.4889122921305746	0.5009877498792696	0.4632664154792281
0.4981585705111318	0.4721185876700844	0.3484461686605078
0.5651452652977293	0.5170889867832859	0.5268160468528745

## 4.29 Output file of the structure CO<sub>2</sub>\* on CuSn<sub>1</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

```

1.000000000000000
16.0489997863999996 0.0000000000000000 0.0000000000000000
-0.0582879140000000 10.0169307487000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.7133998870999996
O Al H Sn Cu C
76 48 4 3 1 1

```

Direct

0.4359584803836954	0.3988363592061856	0.0617740598852143
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0.0320626281629574	0.8403597283207911	0.9905556641979452
0.0447086268752031	0.1309530731020609	0.2128213205186728
0.0412832421698705	0.3492059848602876	0.1465945218421267
0.4361235463572344	0.9240027855615514	0.2002831047387053
0.1842115278027381	0.7775233040490070	0.0837215316616772
0.2328571777299700	0.1067321425287176	0.3557768348564491
0.3003915179562230	0.2171091750540514	0.0353127128433199
0.2940057352943157	0.5083001663565258	0.2452627464487412
0.2993398847190349	0.9538764311376504	0.0932075813843751
0.1789136078442327	0.5492840718989761	0.1598791088882751
0.0644010898975791	0.2186656261838816	0.0474900694649001
0.0661899611713960	0.5035878759234533	0.2625415785090475
0.4243548600947189	0.7544327105929421	0.0873526724346858
0.4144994302442234	0.0560726005941965	0.3030981369100963
0.4181190532946382	0.5421770414283736	0.1647072751804809
0.0655879210774096	0.9821149314393752	0.1136280689737446
0.3349774246430576	0.7780200530577115	0.9897772242681642
0.3050714887451866	0.1351949079051709	0.2278655778824475
0.1832459737056174	0.3827071369755791	0.0410774479671557
0.1702883740101698	0.6856378843283444	0.2687601326282795
0.1775974463323196	0.9201826915410656	0.1935391987710798
0.3055085862065818	0.3579002728244385	0.1456157653835860
0.4242909226844344	0.1614055263854525	0.1323517024332427
0.0445283868651006	0.5658419651369259	0.0695398461523926
0.0504422303074514	0.8720537665021496	0.2830503108352729
0.1655931736085210	0.0297133994761813	0.0240807680530344
0.1666542525091561	0.3255383887566531	0.2376405428903194
0.3089556481604279	0.7304176774982299	0.1741062610931689
0.0466047114288606	0.7364502275485619	0.1761184700358555
0.4420312147112679	0.0170570617409307	0.0228912483637439
0.4359214727715209	0.3235097096955171	0.2312897787547164
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0.3091905208898031	0.8735286383355839	0.2880625741793699
0.1792768031770166	0.1615168686631459	0.1292830763171761
0.9129704424296544	0.4011933715823621	0.0622175058225829
0.9373106158888350	0.7088535084375670	0.2654403676396439
0.5373728623530168	0.8354379416210557	0.9877430974474617
0.5384335633195755	0.1253122406618810	0.2146594208849599

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0.9215070405965199 0.3556376557315467 0.1483753188842773  
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0.5635856524044658 0.3899603436098664 0.0646162111603842  
0.5564573183070910 0.6914641892191160 0.2636478488436440  
0.9308730155758639 0.8486961914119245 0.0146904215216785

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0.9274007834935880 0.7417779078525937 0.1813556846238049  
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0.7919819613288580 0.3941548354530967 0.0618424263426818  
0.7396730650925953 0.8117948951605787 0.2406268965194490  
0.5493930673094283 0.1564677005331281 0.1284452675881855  
0.9296450824115103 0.5736915634284616 0.0797713872876686  
0.9343137760111471 0.8859788125087498 0.2839802090565648  
0.6170832378566204 0.6601974219193616 0.1225879169412355  
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0.8562001053695811 0.3761843754388351 0.2970495256233900  
0.7859655091341610 0.8405133627580120 0.9719613965438331  
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0.3985721939402428 0.3943982851933003 0.3664553362042999  
0.2018194431376748 0.3412638811039378 0.4133151144884773

### 4.30 Output file of the structure OCHO\* on CuSn<sub>1</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Sn Cu C  
76 48 5 3 1 1

Direct  
0.4353965195431890 0.3959776607414869 0.0630595108926074  
0.4338674345902309 0.6841398407734997 0.2633110871598247  
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0.0465098489587291 0.1299995702873565 0.2133184924613686  
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0.6863586604517785 0.9611596248824545 0.1143008537166333  
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0.5593469460572618 0.9299837735623275 0.2044542279652867  
0.5648453282783862 0.3884889811634925 0.0663405917001724  
0.5558646150020448 0.6895536304685673 0.2632373484249224

0.9304259912569744	0.8460550886324325	0.0167355748405946
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0.5580651511306359	0.9800843593727968	0.0276325307395360
0.5511047144538224	0.3154976262182691	0.2343591405910242
0.9278095710108807	0.7398215723902831	0.1823342857309355
0.7358771858983778	0.2376650121320232	0.1896879666298284
0.7920164918646473	0.3923328500294706	0.0640535441108252
0.7394676855239896	0.8094602962818520	0.2425881989441710
0.5496655707663832	0.1551532348660562	0.1293865988668380
0.9300792945586085	0.5699763350421415	0.0799231613519608
0.9385033117143963	0.8840773841575800	0.2847587845810818
0.6167708865023821	0.6591481759638707	0.1230620172719069
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0.8564703142168062	0.3740612481815861	0.2985165877653073
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0.3286234288792350	0.5520923337078568	0.9456134782946237
0.1861149449309269	0.0826713245681686	0.3712358337519712
0.9604997602253404	0.4773445188796409	0.3604385316972062
0.2223403752775578	0.3936662758030774	0.4430409382520502
0.6674460892654438	0.2489016460557879	0.3839971884696200
0.4947893604260796	0.1721366649415008	0.3741456735769514
0.5121819334053347	0.4721877640427422	0.3760884154288155
0.3602931713492320	0.4070439934195142	0.3563788062040844
0.1869469544447153	0.4386138984328060	0.4043905494353009

### 4.31 Output file of the structure COOH\* on CuSn<sub>1</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

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0.0000000000000000 0.0000000000000000 21.7133998870999996
O Al H Sn Cu C
76 48 5 3 1 1

```

Direct

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0.4349051188655393	0.9216559184095673	0.2014918186936027
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0.3048396757020894	0.2155674385261336	0.0333842241018865
0.2923688268556030	0.5092699286325552	0.2432236759796960
0.3018033517601849	0.9557830336298041	0.0942325039797071
0.1705394848350624	0.5342033855532075	0.1398757121649247
0.0752995518349523	0.2470564309688241	0.0539899474737244
0.0684368261440541	0.5032521861976458	0.2702015121532552
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0.3063360853228003	0.1340859540006400	0.2295768264118687
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0.2689614604507370 0.4204962494512543 0.3853508399870171

### 4.32 Output file of the structure CO\* on CuSn<sub>1</sub> supported by $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (110) surface

1.0000000000000000  
16.0489997863999996 0.0000000000000000 0.0000000000000000  
-0.0582879140000000 10.0169307487000001 0.0000000000000000  
0.0000000000000000 0.0000000000000000 21.7133998870999996  
O Al H Sn Cu C  
75 48 4 3 1 1

Direct

0.4343317861656696 0.3979639513080210 0.0615226884249019  
0.4343945027437342 0.6851056395211640 0.2633366104314493  
0.0309086128252368 0.8394542277844029 0.9900030587820315  
0.0433295488437877 0.1299796950195456 0.2123788752675070  
0.0398754475887353 0.3480789183789584 0.1460628402119414  
0.4351294445188750 0.9225498782456585 0.1999640379866808  
0.1829925813091708 0.7764720388612733 0.0833236444986141  
0.2347423078349024 0.1108975783939748 0.3561072475615458  
0.2992740001152940 0.2159070494437215 0.0351889469385963  
0.2928706397602079 0.5071601940819114 0.2454048068902267  
0.2981461356539863 0.9525735307574121 0.0928161095120449  
0.1778864034963596 0.5485094293948838 0.1596617675248106  
0.0632507216582882 0.2175886213610496 0.0470427080554747  
0.0644872844345003 0.5028906124033633 0.2615579650379862  
0.4230122060999334 0.7536781232536779 0.0869579496213418  
0.4138040014709316 0.0550412459899492 0.3027116481337851  
0.4169248952453364 0.5418238762321268 0.1643537214055705  
0.0642733778723159 0.9810504587505173 0.1131810792640341  
0.3337320749870789 0.7766733268888296 0.9892257846577727  
0.3040763627779294 0.1340175707055243 0.2274715415425315  
0.1821923283998215 0.3815396178751365 0.0408359851259848  
0.1689235290973388 0.6847619799778151 0.2683849242638084  
0.1763030326253189 0.9191837130375948 0.1931288159831719  
0.3042893079038220 0.3572348994992324 0.1454184099804239  
0.4231340465030715 0.1605830093888411 0.1322058934962292  
0.0435503898029394 0.5648477100688676 0.0691455590453485  
0.0490191896168789 0.8712332640963782 0.2824858861243221  
0.1644513500992961 0.0285913008995288 0.0237034291749837  
0.1653847522890784 0.3247795312291203 0.2369126916590686  
0.3078375101094739 0.7294965038053601 0.1743379630082200  
0.0452940652168366 0.7357304228631074 0.1756006659650716  
0.4407386351226815 0.0159178022892684 0.0226173493191185  
0.4348558778734342 0.3236525477115678 0.2312638834178432  
0.3118953132956340 0.5708834002698875 0.0739453610105395  
0.3081188948779454 0.8729395713716986 0.2879242404593622  
0.1780558693554407 0.1603722022678429 0.1289102768789275  
0.9117948297654277 0.4003445928435456 0.0615208614836025  
0.9358791159903087 0.7079523886871845 0.2648934276705965

0.5360189057952757 0.8343346840312676 0.9872757487763116  
 0.5372823699314261 0.1247562082735795 0.2142697532136263  
 0.5421833080440338 0.3378886639286967 0.1455623126756743  
 0.9390330483971246 0.9272871603720492 0.1981043680658242  
 0.6826288463343949 0.7803985930249508 0.0899140741611476  
 0.7888994429865068 0.2381258179836850 0.3299478891644370  
 0.7935657449384154 0.2139199745050983 0.0391626317994779  
 0.7891575869035595 0.4858505419769121 0.2523273982282747  
 0.7978943419108127 0.9556876244119460 0.0988720051174130  
 0.6820083104945923 0.5506975627236846 0.1649759370401491  
 0.5617382748867137 0.2070791643940769 0.0455273101510241  
 0.5590384617944872 0.5018206480042923 0.2565022629386212  
 0.9163003741076583 0.7540227211680222 0.0870858800232926  
 0.9220573244211130 0.0627919762940822 0.2994500450947715  
 0.9148010419942048 0.5455344784035793 0.1621706025088882  
 0.5626393609287352 0.9768597238237233 0.1149341398516662  
 0.8250464279675103 0.7932535592575899 0.9968752468355080  
 0.8075257558076596 0.1293004872644175 0.2190652541325795  
 0.6770224237627336 0.3780637290083645 0.0440437715564325  
 0.6701019894157004 0.6831531653247830 0.2709479479463187  
 0.6725018590325627 0.9226502478620143 0.1982895490721926  
 0.8003578500922529 0.3593218297596288 0.1464023032350961  
 0.9258767246218006 0.1688808946147312 0.1319918651847984  
 0.5489553250473470 0.5675804177023190 0.0716522628301562  
 0.5399094851680781 0.8651671039050565 0.2843816305407830  
 0.6655513515620485 0.0213703344965758 0.0251232698499463  
 0.6629036436845234 0.3190537706327341 0.2367528729811396  
 0.8073459485220243 0.7345608338484896 0.1794584081187134  
 0.5453963897553795 0.7367350414754120 0.1781972952242693  
 0.9372626668956368 0.0238653995553765 0.0245962047542178  
 0.9324198285632390 0.3124116577787020 0.2353183595659210  
 0.8040248496957858 0.5773734549715316 0.0768944471004731  
 0.8029422294503877 0.8982971289294154 0.2938560427222933  
 0.6746511705675281 0.1552528075036301 0.1295412445320667  
 0.3242902947965308 0.4534144929134059 0.9570958223133409  
 0.9110584187638161 0.4466102240091461 0.3552613115414937  
 0.2162409601697591 0.4283024090026099 0.3873355858661842  
 0.2945254511323700 0.7664283905509675 0.0654231499153637  
 0.2997556280565717 0.0506500878266223 0.3009022083124036  
 0.1866362208556865 0.1979420132965907 0.0437277624219106  
 0.1781559503506473 0.5101068889501725 0.2445052942653095  
 0.1863567608278424 0.9576435652590219 0.1075029171524219  
 0.2919885572872866 0.5433581226819844 0.1581448908518428  
 0.4188853781911521 0.3479565189738782 0.1435839341809989  
 0.0629682236225367 0.9331282362987383 0.2022935032206070  
 0.0771913413820386 0.3945773695193213 0.0666141670487829  
 0.0523199314315653 0.6871818350423624 0.2627459649942888  
 0.4311505333896574 0.8388744610316317 0.0049561649863453  
 0.4182592750722707 0.1149527777257871 0.2184050855829272  
 0.0554289094575955 0.9938590645366834 0.0255785769035628  
 0.0519041722674828 0.3343085156180420 0.2319354808101875  
 0.4234558158365596 0.7467134644271617 0.1721467965051200  
 0.2375547419050611 0.2445821191523703 0.1874831314098445  
 0.2986802016702213 0.4036166714900715 0.0310025977333929  
 0.2390372447534656 0.7991169882205339 0.2324639655961906  
 0.0534888857170174 0.1614423369816494 0.1285040389990197  
 0.4333043100009996 0.5747268593261345 0.0770174270341273  
 0.4250583531750127 0.8732152630773120 0.2827023919726384  
 0.1138216859555550 0.6626291695374373 0.1181450686705692  
 0.3620753987573304 0.0871365736449528 0.0671584416661519  
 0.4026931896580095 0.5020334558243437 0.2592146726975634  
 0.7940141122855343 0.7681600223341409 0.0838066464865978  
 0.8115260424378343 0.0781246555998879 0.2984501004720022  
 0.6799761637983510 0.1937037221453278 0.0437835184357147  
 0.6760758623983429 0.5050138619991499 0.2466513077696526  
 0.6838722662019652 0.9608598296713224 0.1116703959536137  
 0.7966950207649546 0.5471715149257274 0.1698070997202438  
 0.9202835838126729 0.3546220561797555 0.1476830158429029  
 0.5585184661785026 0.9315900021754385 0.2034592798932380  
 0.5621730190813105 0.3891130468363280 0.0640172676824623  
 0.5554928666375073 0.6906532226199810 0.2630299560008187

0.9296981260244073 0.8478698514772226 0.0140630115794729  
0.9254508210705062 0.1136555111143937 0.2156356409914606  
0.5553137223920676 0.9855977491348266 0.0256146367890201  
0.5512318080223290 0.3192971485858525 0.2309371272954510  
0.9261715915642065 0.7408532828442081 0.1807884627382487  
0.7341357123255958 0.2384334520210088 0.1870591956331893  
0.7907886157587909 0.3932093407994517 0.0610696256017581  
0.7384490410974407 0.8107479911701927 0.2398448801377172  
0.5478290381118884 0.1555213195990386 0.1279288769003435  
0.9286555659417253 0.5728144486115438 0.0791208233584658  
0.9331060929751538 0.8850332014221656 0.2834604582470807  
0.6156852361267052 0.6594526050972151 0.1218652563268251  
0.8607858046801735 0.0920296908885576 0.0725162873283786  
0.8549293692988172 0.3758657189659436 0.2960842468688282  
0.7847375360865310 0.8399810374799752 0.9713794482287157  
0.3159701753973193 0.5474133680734548 0.9476807121176342  
0.1826077696498654 0.0674419355165709 0.3665340649969624  
0.9130509974542389 0.4009565061301756 0.3944788643751421  
0.6804582872065050 0.2854378000841198 0.3967789839193350  
0.5085597368877299 0.1906653916091031 0.3813055165098972  
0.5418497755029225 0.4941943465714400 0.3750314245177759  
0.3992074159339099 0.3857919836928078 0.3715996987790460  
0.2861030085818851 0.4023708545363597 0.3836569690404312

### 4.33 Output file of the structure CO<sub>2</sub>\* on Cu<sub>4</sub> supported by graphene surface

1.0000000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000

C Cu O  
51 4 2

Direct

0.0034867983105798 0.0038712244473642 0.9949729563134110  
0.0699340546563984 0.1370681428318938 0.9952174266910343  
0.2035980193621467 0.0040521942348998 0.9953931931139571  
0.2701826679058503 0.1371921454930147 0.9960639071656333  
0.4035208897162352 0.0038714062344588 0.9943401127311271  
0.4702931145640347 0.1370387960963000 0.9942879652128647  
0.6034729259511082 0.0038381718550474 0.9944301566903663  
0.6701798928993440 0.1370648769029953 0.9940041508420254  
0.8035105622773084 0.0038446539712706 0.9947142768043299  
0.8700590421515688 0.1370755356501209 0.9943687905691272  
0.0033840365329455 0.2038059745960743 0.9946589439036408  
0.0699667799629308 0.3370702458257367 0.9941977616480936  
0.2032029054642116 0.2037269238704850 0.9961328787081670  
0.2690477099290007 0.3366029552469839 0.9973867996607522  
0.4036949847725919 0.2036984178818951 0.9952318391643967  
0.4707900009495739 0.3365750408794967 0.9962952956366937  
0.6035651412994929 0.2037659508770219 0.9938519755855911  
0.6702825057860702 0.3370513573252891 0.9932128836861761  
0.8034925683512784 0.2038155247935483 0.9938487887354597  
0.8701628442173709 0.3371279342701520 0.9933018438492552  
0.0034379830368967 0.4039008336515297 0.9934026375443404  
0.0700573058271574 0.5371781270883588 0.9932583246090064  
0.2031273712386704 0.4037044239118446 0.9951845492664220  
0.2699287374592431 0.5373877514891438 0.9947080638529933  
0.4032406051944741 0.4031997540996640 0.0014720093270688  
0.4705496602927622 0.5379681517731378 0.0010985482796852  
0.6037612940603131 0.4036630592162088 0.9938885477093390  
0.6706269602458539 0.5373729976041455 0.9940812843924893  
0.8036400950295526 0.4039051730845121 0.9929418427346972  
0.8702676708485092 0.5371754796945652 0.9929371983126012  
0.0035501015502615 0.6039668180333798 0.9932001027697608  
0.0701981276109432 0.7372703037735545 0.9938348696725890  
0.2033977511456109 0.6040126039351849 0.9937065131302214  
0.2701042525770876 0.7372991133427103 0.9940406899112180  
0.4028924507897056 0.6045307398965141 0.9965302651338704  
0.4700040598427790 0.7374218967049799 0.9950042510047448  
0.6047567371904746 0.6045408132336491 0.9962835560388613  
0.6705608602487770 0.7374203365409356 0.9950397942246282  
0.8037619469388778 0.6040238094621415 0.9933388209304489  
0.8703306945723902 0.7372931520844228 0.9940431584178470  
0.0036399473297308 0.8040220015643875 0.9942764693946755

```

0.0701873062626970 0.9372527263941028 0.9950074889441898
0.2035023922205837 0.8040254643256658 0.9941473134284338
0.2702160775152429 0.9372587502273411 0.9946650159454322
0.4033895518492713 0.8040555619976004 0.9942690466902456
0.4701602653422765 0.9372282961289128 0.9942449421149475
0.6035306063658140 0.8039153478244678 0.9953283141070375
0.6701065996007168 0.9370633714638714 0.9948999808514688
0.8037989126538593 0.8040546777497712 0.9944291215302019
0.8702180446891564 0.9372352038578853 0.9946754104566716
0.5332496642801142 0.6248626599027686 0.4547270612070837
0.3736720857143919 0.2868459160349294 0.2223476441836870
0.4587495116368608 0.4827697032289303 0.2915358157853476
0.4430752439990582 0.4749426368230013 0.1379895767538409
0.5255180346613388 0.6722677423484031 0.2156377907247810
0.5768046252519569 0.7286377740703966 0.4787826083415914
0.4889160958665327 0.5181801291529193 0.4337895235654390

```

#### 4.34 Output file of the structure OCHO\* on Cu<sub>4</sub> supported by graphene surface

```

1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
C Cu O H
51 4 2 1
Direct
0.0005956778420332 0.0020699143580906 0.9987910050348667
0.0670870439048499 0.1353191822151980 0.9987457445066424
0.2005412151783496 0.0019828927992907 0.9996477389808283
0.2671535946771428 0.1352733220559365 0.9997950143680348
0.4005664886026442 0.0021514670647250 -0.0000980753457882
0.4672281892763077 0.1353961232400595 0.0002051743506810
0.6005908371647036 0.0022204420002114 0.9995853758265943
0.6672119566608150 0.1355197496292722 0.9998537602716969
0.8006891581016077 0.0021752630950433 0.9987188117048498
0.8671693713411882 0.1354275980299161 0.9988893122966106
0.0004482700636737 0.2019430028701728 0.9987452929878570
0.0669725259695373 0.3352774779446044 0.9990556039143643
0.2004124243837621 0.2018090401129057 0.9992942287470249
0.2668904707711967 0.3349394694235416 0.0000759305990398
0.4004390858650005 0.2018241751993199 0.0003201308845823
0.4670512587744437 0.3350451702603990 0.0012462465115373
0.6005121720302341 0.2020718885196309 0.0004622608981205
0.6671586294279724 0.3354563831994817 0.0010397881691977
0.8005191436639576 0.2020994606435710 0.9995423843272674
0.8671127521629177 0.3354116880573667 -0.0001060454813339
0.0003809434180341 0.4020266755405977 0.9995733568644140
0.0668846433121027 0.5353115470683660 0.9997703266400444
0.2000156808707247 0.4016818957717410 0.9996646146355456
0.2660635887734728 0.5349026934319961 0.0011025243839811
0.3999739334785264 0.4008751528487732 0.0022327732503768
0.4674600602921442 0.5351149697713941 0.0060688843022558
0.6005748557091645 0.4020049000040150 0.0016061490070063
0.6676780323902537 0.5355488038063211 0.0014585888928585
0.8005634325314601 0.4021338526028620 0.0005174387769806
0.8672601670622563 0.5354064681942237 0.0002384119136053
0.0005160079953842 0.6021047098122987 0.9999021854250864
0.0672129495216312 0.7354095568164511 0.9999208263596739
0.2001363215603794 0.6020670900449472 0.0001320842153612
0.2671576456194948 0.7354888855957536 0.0001836417645848
0.4001081918472179 0.6024783999894869 0.0042324923804839
0.4676739830269168 0.7365507499523055 0.0011889836062838
0.6018590362081686 0.6027991598722618 0.0023817540954380
0.6677397337474851 0.7357806523670176 0.9998368324620469
0.8009108828573738 0.6022342053954038 0.0004100713280868
0.8674149955780345 0.7355236814229398 0.9997910646397845
0.0006908374727254 0.8021423675730227 0.9996572089335134
0.0672582369639079 0.9354183284991554 0.9993092741353586
0.2005703476283105 0.8020918597513333 0.000088171339114
0.2672482386115743 0.9354548592092593 0.9998959457430016

```

0.4006393461262384 0.8024896505515483 0.0001913572891166  
0.4673316298757657 0.9357244766077361 0.9998147690900780  
0.6009007038501917 0.8025729928636115 0.9998142210073566  
0.6673267629909648 0.9356349395530351 0.9991396656768265  
0.8008659689066661 0.8022607314992604 0.9991170086881879  
0.8673336140269179 0.9355588423754823 0.9986445442892887  
0.6163302893626315 0.5251525782992883 0.3941610852002186  
0.5705385346277743 0.5184929652170419 0.2133734283611992  
0.4467991140108050 0.5783803193311001 0.3022414780430199  
0.4298230104743481 0.5706330544307653 0.1421734467889983  
0.3093467483930578 0.6265088812635868 0.2308857611600184  
0.5312535587494500 0.5567332858831129 0.3995488007956369  
0.6765039090015178 0.5120712115564282 0.4533421737310178  
0.6380951622645648 0.5063286855073303 0.3202584274366990

### 4.35 Output file of the structure COOH\* on Cu<sub>4</sub> supported by graphene surface

1.0000000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Cu O H  
51 4 2 1  
Direct  
0.9985492531547340 0.0128597399450402 0.0033059770828683  
0.0649413369126209 0.1460905591722767 0.0039664838202804  
0.1984405341956531 0.0127051920491205 0.0048559083010267  
0.2648283205307831 0.1455651282090604 0.0061177722021867  
0.3984925645802949 0.0127248209547908 0.0057108448388672  
0.4653472068207514 0.1458946315109273 0.0067353632985223  
0.5987252195701496 0.0132398520633916 0.0053248705744649  
0.6653849228092441 0.1464440813938825 0.0057470736997572  
0.7987804183146003 0.0132218186835084 0.0037172274063136  
0.8652268244336041 0.1464016868281160 0.0042013545020176  
0.9984555509490709 0.2129046168130922 0.0043474967240916  
0.0648608163012650 0.3461237289651147 0.0055242143379269  
0.1980494534780408 0.2124888539364161 0.0058409499705384  
0.2636376533091331 0.3452263870105297 0.0091750091226784  
0.3981151805652177 0.2116187935594033 0.0082640760816800  
0.4657158523754224 0.3452155903426323 0.0130854492631173  
0.5987025775192867 0.2129511650278301 0.0068901804663174  
0.6656884057016641 0.3463876508841134 0.0073798639722696  
0.7986974003250951 0.2131163725352078 0.0051737347916435  
0.8653220893002970 0.3463445691220792 0.0054707103330700  
0.9984758083402260 0.4130493753896973 0.0056103662351165  
0.0649878799360480 0.5461986662402839 0.0060900050785736  
0.1978695321785653 0.4125859024065001 0.0077567493066425  
0.2641941736210337 0.5460418525474032 0.0094668252780494  
0.3977848677811409 0.4122053761903374 0.0170734854723013  
0.4664312444627004 0.5477591101293143 0.0142947150255477  
0.5997712513443004 0.4133322510586895 0.0095232166113686  
0.6659693060662373 0.5466990756278998 0.0074810439374087  
0.7989682264844161 0.4131663721241832 0.0060181454672194  
0.8654314999081690 0.5463149644218742 0.0055118194441229  
0.9986237179768082 0.6130236394082406 0.0054109745862949  
0.0652292843622802 0.7462240088988082 0.0050902721179666  
0.1982989614178845 0.6129451219772576 0.0073494443488066  
0.2652834316198484 0.7464079690346366 0.0066682286544301  
0.3984617619932211 0.6141311902077304 0.0117023987390055  
0.4659118643351683 0.7477857256214501 0.0075625491204159  
0.6000168774156960 0.6141010453069896 0.0079607752785941  
0.6658718400466672 0.7469965384810066 0.0049519184378451  
0.7989676056734105 0.6131882089779327 0.0053586553474416  
0.8654399537746184 0.7464502768406205 0.0041120978318980  
0.9986645156331377 0.8129481413209094 0.0041424722617085  
0.0651268096278864 0.9461502622213196 0.0038675596510574  
0.1985720787910996 0.8128861291644601 0.0056743662570624  
0.2652359318192311 0.9461110206471723 0.0054159849509230  
0.3986172027604475 0.8134695011990442 0.0064384677256941  
0.4654313050911773 0.9465748909799181 0.0056157725882747  
0.5990994790428124 0.8137867727638775 0.0052182358552551

0.6655308374059014 0.9467327282631386 0.0044428896326771  
 0.7989678453543840 0.8133044199824153 0.0036020512731683  
 0.8653872128330937 0.9465133810745034 0.0031709281689122  
 0.4563379419838793 0.3554161882574688 0.3337884161126700  
 0.4284585568448768 0.3760446254819900 0.1494697003669875  
 0.4363833101483761 0.4914096597082142 0.2917972968080071  
 0.4295367628811059 0.5785884358730812 0.1498843992116308  
 0.4154153018736193 0.6708455506428694 0.2798851097939482  
 0.4332172557838287 0.2759135563038527 0.2520956167517233  
 0.4873955451993150 0.3220209866351720 0.3995532453480466  
 0.4560220580404670 0.2107608675832008 0.2620633451335890

#### 4.36 Output file of the structure CO\* on Cu<sub>4</sub> supported by graphene surface

1.0000000000000000  
 12.3386001587000003 0.0000000000000000 0.0000000000000000  
 -6.1693000793000001 10.6855411845999999 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 15.0000000000000000

C Cu O

51 4 1

Direct

0.9984571755658598 0.9988649347013501 0.9943337079921524  
 0.0650338325487311 0.1321401347999432 0.9941049373500056  
 0.1984302409154877 0.9988584259104586 0.9940829446625460  
 0.2650826960290633 0.1321156885278121 0.9939309833240402  
 0.3984221382263342 0.9988618025228170 0.9932007386272718  
 0.4651561273797719 0.1321289654946272 0.9928005411636316  
 0.5984418462617085 0.9989081864306116 0.9932142028872915  
 0.6651506240351720 0.1322091167153988 0.9929881041745510  
 0.7984931075920748 0.9989055729140918 0.9940134036491072  
 0.8651393987326034 0.1322205770713763 0.9937110605627215  
 0.9984419011866478 0.1988428950073158 0.9938852979684574  
 0.0651007883954182 0.3321995013825416 0.9936870783726505  
 0.1983130231418647 0.1987039446413007 0.9942114997722282  
 0.2647175535650302 0.3318419890586554 0.9947819156015305  
 0.3984126571054959 0.1986638911360861 0.9931029775407465  
 0.4652132709302094 0.3317807742139922 0.9935768833975718  
 0.5984428758197505 0.1988003606502613 0.9926350191196680  
 0.6651860413867785 0.3321506043870199 0.9924108400119902  
 0.7984663730368768 0.1988764084815337 0.9932268959834081  
 0.8651488488988280 0.3322031332200291 0.9931763114881098  
 0.9984436761134092 0.3989020468787893 0.9934314902328560  
 0.0650380786082288 0.5321849837091005 0.9934704074785492  
 0.1983026990034865 0.3988463905323953 0.9940659866171968  
 0.2646855698562572 0.5321725183526511 0.9939585744437013  
 0.3980168035348066 0.3979587605692436 0.9962177448420100  
 0.4649692252355244 0.5321839347933628 0.9984923427923632  
 0.5985947320238170 0.3987046299542878 0.9927387313998676  
 0.6655315379788562 0.5320527325209435 0.9945012066665981  
 0.7985306919341906 0.3988902469678715 0.9929673872749302  
 0.8652048144631531 0.5321667663404540 0.9934386161070986  
 0.9984652180852119 0.5989017227920814 0.9936766532681254  
 0.0651078708687483 0.7322046978646466 0.9941235139054994  
 0.1983118776916344 0.5988905332461568 0.9935616960925721  
 0.2650675798988362 0.7322571675989725 0.9938242055859666  
 0.3979650826943240 0.5993386554287438 0.9959299098548849  
 0.4651740290942739 0.7326776264285231 0.9938887886540281  
 0.5992752151480584 0.5992278081052077 0.9972656688484977  
 0.6654753692661478 0.7326702957551834 0.9956868149430608  
 0.7986379475761034 0.5988869496463547 0.9940926751819897  
 0.8651956919555750 0.7322388888352293 0.9947827201633169  
 0.9984489896902595 0.7988815377872495 0.9945165053725807  
 0.0651059526617524 0.9322102126868652 0.9944449871579829  
 0.1984362159872196 0.7988791772310887 0.9939993506138950  
 0.2651202954004580 0.9322134555362355 0.9937769545162959  
 0.3984425605281893 0.7990258371832630 0.9933589485988273  
 0.4651617429111731 0.9323092907139586 0.9931629750694896  
 0.5984843784721550 0.7990706158586756 0.9942395273710647  
 0.6651486781362209 0.9322678459649701 0.9936989890883409  
 0.7986092665355889 0.7990192231960083 0.9950184542543966

0.8651918932021211 0.9323109479233656 0.9944447658440163  
0.4523616072409505 0.4985984588741650 0.4186677589585702  
0.5467964812714967 0.4089329358079569 0.2169918736510853  
0.4644686279018420 0.5148872198603867 0.2992201904240357  
0.4749464611960360 0.5307325813253090 0.1426035865730535  
0.3975337418797254 0.6407396080585653 0.2254249462703311  
0.4442159302004521 0.4872534524045180 0.4954117862332638

### 4.37 Output file of the structure CO<sub>2</sub>\* on Cu<sub>3</sub>Sn supported by graphene surface

1.0000000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Cu Sn O  
51 3 1 2  
Direct  
0.0136439170801982 0.0132314419694002 0.0050455725882321  
0.0801855926420986 0.1464686941835610 0.0040717540618671  
0.2135528792940837 0.0131345940451357 0.0042429686213224  
0.2800898678235262 0.1463691146503095 0.0024815957632347  
0.4135083578597604 0.0130645224068984 0.0051594375789431  
0.4802075989107247 0.1464005776776028 0.0037273006545612  
0.6135512151881688 0.0132443294881845 0.0059907423369757  
0.6802653434838847 0.1464807826454534 0.0050247928174586  
0.8135792413169851 0.0132823469349544 0.0062386930563588  
0.8801983206851047 0.1465550405819329 0.0055910862508250  
0.0134961805999475 0.2131293391358610 0.0046858266111038  
0.0800909442717658 0.3464682600154226 0.0042122976867552  
0.2134391953660663 0.2129843247881568 0.0023778378616014  
0.2800218966981169 0.3463007362636943 0.0016895170144172  
0.4133748813753095 0.2129185275527813 0.0015380417297656  
0.4799541051154992 0.3460139552251665 0.0003147523818857  
0.6135569039387972 0.2129936533980914 0.0036045592649462  
0.6802393173690668 0.3461896513070768 0.0026728302095525  
0.8135267776160107 0.2131713493261843 0.0052332538847725  
0.8801821962927938 0.3465213114030947 0.0048888424006413  
0.0135229415820222 0.4132096826867565 0.0047243725881888  
0.0802344089750503 0.5464835802790046 0.0047433505091828  
0.2134413383280393 0.4131297525679512 0.0032164763690623  
0.2800114119986842 0.5464843582675167 0.0041431624781424  
0.4131138138405926 0.4127649238882485 0.0013076232648512  
0.4793453915364153 0.5461949833806582 0.0044902308059164  
0.6131826901018556 0.4121217948333855 0.0022016722339495  
0.6805603606781808 0.5461330456244401 0.0072698727003041  
0.8136060694231908 0.4131302931052880 0.0041979189818952  
0.8805212334750395 0.5465164420523659 0.0046895745361014  
0.0137459484775027 0.6132287470623181 0.0049957903955075  
0.0803011183083570 0.7464932777905965 0.0054059043814901  
0.2134665277619109 0.6131934229190749 0.0049001042290129  
0.2801841646125907 0.7464717736929919 0.0056491528412491  
0.4132413691090749 0.6132345671135605 0.0049401056290087  
0.4801711461242814 0.7465850400322990 0.0062705317703998  
0.6132650641289258 0.6135437758797060 0.0079281021915706  
0.6805808669266972 0.7474363827745046 0.0075817724841712  
0.8145419484127718 0.6135611015309844 0.0057841389810876  
0.8805562752109454 0.7467116973983808 0.0058542341517301  
0.0137489414060421 0.8132723281289765 0.0054278995721492  
0.0802911273648475 0.9465782268210208 0.0049510294067996  
0.2135917429315990 0.8131685210782118 0.0055788680714562  
0.2802182211715945 0.9464621029658461 0.0051107827234935  
0.4135395276425906 0.8131750414897742 0.0061694562048163  
0.4802377645108060 0.9465115767383517 0.0060241081779228  
0.6135610322597945 0.8135059223238196 0.0069944108742975  
0.6802943148293428 0.9467373730084192 0.0065760178926005  
0.8138297470761486 0.8135248935399680 0.0066422657331950  
0.8803255396635478 0.9466806282816039 0.0060973501735065  
0.2047917619485936 0.4134071230797924 0.2247158425359674  
0.4552661846653837 0.3910159458564214 0.2276488681960877  
0.5132993151245000 0.2324716880736583 0.2335580453723101  
0.6258575112706662 0.5544459948141840 0.1478982484072608

0.6777685619745367 0.4508171215130112 0.2765277807843471  
 0.1557086675105185 0.4737019981818195 0.2230395618362646  
 0.2549299387094270 0.3529981492261396 0.2276330027395050

#### 4.38 Output file of the structure OCHO\* on Cu<sub>3</sub>Sn supported by graphene surface

```

1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
C Cu Sn O H
51 3 1 2 1
Direct
0.0062306687751322 0.0036306435777948 0.0072067520001903
0.0727162104013021 0.1367812902753123 0.0059751916885894
0.2060359711544657 0.0034774440173480 0.0068920099984828
0.2725716512978144 0.1367097028551950 0.0056052267495489
0.4060250932640400 0.0034182560733506 0.0073855486162184
0.4726935015772452 0.1366885905544394 0.0065083742316064
0.6060698526985315 0.0035086701280606 0.0081319237880769
0.6728113511188275 0.1367696209608648 0.0076335484304124
0.8062343151634905 0.0036016308085101 0.0083432181580721
0.8729249568393608 0.1368493901144726 0.0075503227624523
0.0061335782991475 0.2034052996030462 0.0063641638778112
0.0726724542672946 0.3366146919280162 0.0061756180904435
0.2058522899965594 0.2032044080578284 0.0048409711765528
0.2723551009681994 0.3363987796369783 0.0044772076041772
0.4058967766023748 0.2032265009780658 0.0053251016344185
0.4725685028785580 0.3363901534490565 0.0045129491865542
0.6060302296423653 0.2032768228392804 0.0067031947547826
0.6728072278072493 0.3365601275111202 0.0060977176520155
0.8061660608050253 0.2034002882649842 0.0075918274636395
0.8728297445827820 0.3366904956281606 0.0073790905877375
0.0061348788229606 0.4033444255347658 0.0070539880462224
0.0727095174716830 0.5366698629341288 0.0073173562748861
0.2058677671434694 0.4032469377235955 0.0055998037029784
0.2724007581534770 0.5365994563382439 0.0066457573598050
0.4054635819675623 0.4027106640833755 0.0047410847740065
0.4718064102755264 0.5362457758106857 0.0075339932490877
0.6060876751463408 0.4029586297183542 0.0051088243166312
0.6732904036553856 0.5362295443627064 0.0070367793986081
0.8061765108481209 0.4033397910096195 0.0070854558504051
0.8729324692579272 0.5366671519920259 0.0072407441788518
0.0061952585302541 0.6034339562113891 0.0075751794119337
0.0727677329463024 0.7367645751652905 0.0077976969787407
0.2059627882316286 0.6034249571986510 0.0073060041536453
0.2726553117860676 0.7367433193442671 0.0077885759225011
0.4055673145141696 0.6035163587039896 0.0073698742445344
0.4726155907722147 0.7369064422157819 0.0081538397401293
0.6062557895554387 0.6034603190027465 0.0097736884612720
0.6732492038795245 0.7376832078226780 0.0097349544195293
0.8064971962147109 0.6034352155280021 0.0072976026135076
0.8729284727707043 0.7368650447415892 0.0080387310734153
0.0061706827872549 0.8035359566488439 0.0078838333929466
0.0727637252355788 0.9368953487782734 0.0074332915202448
0.2060660805795970 0.8034716976747952 0.0077957343966733
0.2726895094042599 0.9368064419743940 0.0074401038933947
0.4059941754627189 0.8034936974719512 0.0080398480031445
0.4727491213074773 0.9368333744211046 0.0080024012752318
0.6060705906398804 0.8038350987544097 0.0089291231894612
0.6728735538289388 0.9370201306761942 0.0086295860236482
0.8065365987484435 0.8038657398182013 0.0088296445661006
0.8730032880470231 0.9370686966933400 0.0082748809339740
0.2045502177769900 0.3003923643397741 0.2246533584353916
0.4621886105302067 0.3811009853999740 0.2284570658988976
0.6459891144137569 0.3800794688622001 0.2756562768477361
0.5788805910618520 0.5783012331421507 0.1537556496875562
0.6356320113989630 0.5720674542787140 0.3161216905209865
0.2911906858836234 0.2689326408166280 0.2345082560156619
0.0932309406689677 0.2254708254707000 0.2110593772847509

```



0.2389269381412230 0.4030852990745944 0.2290866130417440

### 4.39 Output file of the structure COOH\* on Cu<sub>3</sub>Sn supported by graphene surface

```
1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
C Cu Sn O H
51 3 1 2 1
Direct
-0.0024209078653837 0.0048289947064473 0.0037030314778145
0.0642927330877016 0.1381211241754874 0.0028412086266727
0.1975378040268237 0.0048213965060734 0.0030517904803032
0.2640532329689276 0.1380409515623704 0.0016386767829072
0.3973994597323097 0.0046666788033271 0.0019586855988992
0.4639949950520694 0.1379540222867971 0.0004020867986266
0.5974158328707915 0.0046622672854021 0.0016980796825889
0.6641279287052358 0.1379390946607043 0.0006671137017922
0.7974647450332107 0.0047627233299388 0.0026196815158426
0.8642178531564130 0.1380393604673839 0.0022066461601725
-0.0024482100031196 0.2046912034186667 0.0025360963463870
0.0642186046472030 0.3379908721078568 0.0023407576894505
0.1975153706916891 0.2047216679418619 0.0017829359702796
0.2640977355059251 0.3379648982381471 0.0011635589866406
0.3972313673913997 0.2044753345379051 0.0001788368642991
0.4637691170607152 0.3377449427891252 0.9992767348856605
0.5973618408908100 0.2045081699844344 -0.0005923065782014
0.6640342752178277 0.3376704063293495 0.9985258683236427
0.7974519831566392 0.2045615394325646 0.0010630303047353
0.8642142141818970 0.3378775814133343 0.0008533636458532
-0.0024299246969664 0.4046325886890139 0.0021221789677327
0.0642513045884625 0.5379287818460640 0.0027739331379568
0.1975078734120024 0.4046403168980229 0.0019925768187331
0.2640680088105963 0.5379499164748516 0.0021825625873713
0.3972600189162957 0.4046265107136479 0.0002660030052959
0.4637944779216702 0.5379763594364246 0.0007493345508349
0.5969343023888972 0.4039167193448374 0.9988958691586334
0.6634372235116457 0.5376903443359143 0.0024684493357384
0.7975140860264308 0.4043512553571464 0.0000762429955418
0.8645943085393483 0.5376539428230154 0.0027582199505967
-0.0023004597265615 0.6046500987456082 0.0033923809967978
0.0642011724732194 0.7380715271222821 0.0042967922878172
0.1975054436457712 0.6046604601631355 0.0029070698998816
0.2641006212503499 0.7379918443983623 0.0032210482999995
0.3973087635119952 0.6047091610883897 0.0017105085520498
0.4640277361239824 0.7380214746831701 0.0022194442243832
0.5969182883630865 0.6049733408584529 0.0014345111978131
0.6640108573911884 0.7382514544665451 0.0022102255276177
0.7978293369699677 0.6048229361606474 0.0051901634009121
0.8645489064003128 0.7388153261608760 0.0050644294255729
-0.0022563262238348 0.8050039316801173 0.0047954686659322
0.0642880663378119 0.9382532640083119 0.0040792885474782
0.1974578952314596 0.8047112051594441 0.0037869887330920
0.2641052427161035 0.9380832378319519 0.0031114523050744
0.3974033320286912 0.8046961798622060 0.0026750721144964
0.4640842234801998 0.9380252572080076 0.0021357880928513
0.5973596895880986 0.8047859049108878 0.0021848590971476
0.6641444369160351 0.9381031768020568 0.0022642317554084
0.7974630662523560 0.8050282102704787 0.0035903491568035
0.8642324799893275 0.9382327565549429 0.0034762263684364
0.3747379925151353 0.3403856117800252 0.2617125814492652
0.5414743195338515 0.4061049384388893 0.2217776473514533
0.7192226383451606 0.3748507437011790 0.2317884579088578
0.7276261316664790 0.5640695276438662 0.1499482506184082
0.7230249783515071 0.5499530231901292 0.3214378326100649
0.2863426705952611 0.2760255020713248 0.2122760292849905
0.3561416585738639 0.3677122658124873 0.3468522434126026
0.2646710287717147 0.3264540163301310 0.3555673959420032
```

### 4.40 Output file of the structure CO\* on Cu<sub>3</sub>Sn supported by graphene surface

```

1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000

```

```

C Cu Sn O
51 3 1 1

```

Direct

```

0.0033391744052306 0.0045412254138284 0.9997235188127476
0.0698669817806134 0.1377859362193850 0.9997045371293238
0.2031915906832658 0.0043626703114859 0.9985146307608053
0.2697111210584810 0.1376139768597678 0.9976889663738234
0.4031479735089076 0.0042676339773618 0.9995369237941367
0.4697271536485822 0.1374275777183867 -0.0010580120963182
0.6032074269863160 0.0043881632445168 0.0015309281388734
0.6699416137730249 0.1375667603798120 0.0018134292107523
0.8033493850202788 0.0045919150637618 0.0015233008418181
0.8699906379185316 0.1378826738648389 0.0016439617807247
0.0033254283035577 0.2045256405012000 0.0008104746307057
0.0700042070284874 0.3378148015198743 0.0007756755777782
0.2030861517179872 0.2043031905561214 0.9983297124091942
0.2695836194102710 0.3375636555148758 0.9985027665575281
0.4029511773347497 0.2041208742745955 0.9969846762806258
0.4691639001361130 0.3372269461138810 0.9962424237398513
0.6029265740414606 0.2036467531629083 0.0011057468689798
0.6701704454655714 0.3374624484844382 0.0021129214520913
0.8033541652283670 0.2044748359161468 0.0020838425893615
0.8702559708004818 0.3378403950504889 0.0016884606505671
0.0034842059677363 0.4045795726545761 0.0010350814226100
0.0700128475391254 0.5378250157535267 0.0003359539589895
0.2032033597980673 0.4044845989646099 0.0002212732870339
0.2697246739100918 0.5377903158902559 0.0010228870140971
0.4026305275277829 0.4038557147766662 0.9978381343549790
0.4692742550360502 0.5374756722898015 0.0018850989060257
0.6030565816942230 0.4043664325873436 0.9988619700430044
0.6709090884798243 0.5382944184940678 0.9977837100467162
0.8041033988945387 0.4048126954166867 0.0012017842500083
0.8703987482436603 0.5379670456458756 0.9986924907626845
0.0035245771867951 0.6045953722375684 0.9991496719354097
0.0700100014887868 0.7378532256302837 0.9988345971123785
0.2032450505102172 0.6045471850554311 0.0007094732252446
0.2698978179388528 0.7377923034019124 0.0004784949492345
0.4028778627811526 0.6046969559922160 0.0018792806025664
0.4698901309431780 0.7380170696720809 0.0018300175294796
0.6037245331412393 0.6049451336688900 0.0022158030850423
0.6704745169737306 0.7388204642265520 0.0015857280979156
0.8037833304513050 0.6047771227503571 0.9974036417854952
0.8701873150200021 0.7380937687347693 0.9986166855451405
0.0033581394601479 0.8045609589739567 0.9987880014787102
0.0699247187980837 0.9378519726248814 0.9990355729361351
0.2032577742754359 0.8044524799856275 0.9994454253444618
0.2698462386921058 0.9377117552196176 0.9989743538771556
0.4032211503601405 0.8045088266731303 0.0011442020421509
0.4699278624052438 0.9377785709268923 0.0008248181791855
0.6033343137595265 0.8048795708217396 0.0018185271846986
0.6700443938611760 0.9379912066894737 0.0017538044298247
0.8036473045519144 0.8048907392065605 0.0001919630234328
0.8700997647157266 0.9380630272806402 0.0005719440360482
0.2973963102582560 0.2603419580958426 0.2711154041343347
0.4515636203042029 0.3729666831100491 0.2301339924181282
0.6256601462378724 0.3821067254898258 0.1517665969982581
0.5588646859707764 0.5670590930173286 0.1513217716435887
0.6800843656573766 0.5385730597584965 0.2793431058514389
0.2012125479153732 0.1915224301348081 0.3021398580050313

```

#### 4.41 Output file of the structure CO<sub>2</sub>\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by graphene surface

```

1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000

```

C Sn Cu O  
51 2 2 2

Direct

0.9912948281400509 0.9973874760029926 0.9941800803696141  
0.0577725799608837 0.1306283302772064 0.9943159688728876  
0.1913754072948100 0.9974520642604793 0.9947624308926876  
0.2579477121719029 0.1306548185627500 0.9950090615714706  
0.3913579195005115 0.9973653244752554 0.9947831218028670  
0.4580801158798004 0.1306064586140827 0.9948030208963999  
0.5913326330369392 0.9974240514658947 0.9945667132323365  
0.6580237743560433 0.1307247648425889 0.9943663474578076  
0.7913485727374793 0.9974357135549448 0.9942050220250708  
0.8579458649112900 0.1307297099944637 0.9941422530313149  
0.9912212588514943 0.1973757286829817 0.9940109467954075  
0.0577484681638226 0.3306859420728510 0.9935008868813393  
0.1909621227849793 0.1970854927736186 0.9947017150285610  
0.2569137918957750 0.3301986144911757 0.9950239238828629  
0.3913277018944890 0.1970513245346123 0.9950893277350166  
0.4584715956709150 0.3302483393318442 0.9951728270661911  
0.5913703530163996 0.1973355728083173 0.9943217178312712  
0.6581537590283466 0.3306871687323036 0.9933140155780634  
0.7913442190909656 0.1974193565648037 0.9939023673286095  
0.8580219268569669 0.3307188227372614 0.9931586556120885  
0.9912647307776793 0.3974599929597935 0.9930925811299640  
0.0579745421463713 0.5307329795789433 0.9931261181913908  
0.1908832458762818 0.3973978142833445 0.9936244840986871  
0.2577713158346573 0.5308505463408780 0.9934940956870418  
0.3911248565582117 0.3971275222529785 0.9966480057195597  
0.4584425970556897 0.5316455244205532 0.9948493986182235  
0.5917932397226351 0.3974641118294227 0.9932115979936644  
0.6583856932195610 0.5309648635508475 0.9921306880055575  
0.7914635954820128 0.3974239486799053 0.9926564190785602  
0.8581054237192657 0.5307948628475914 0.9922257140294527  
0.9914733313409267 0.5975141981247394 0.9929441645410404  
0.0580996308091832 0.7308646473257292 0.9936211146485417  
0.1912953748830417 0.5975075855990618 0.9935148294469200  
0.2580545421416951 0.7308642221899448 0.9940169982913610  
0.3911471825914084 0.5979542896516984 0.9938468126076684  
0.4580536560661508 0.7310748529469835 0.9939471165351396  
0.5921115726215115 0.5980369837711371 0.9928178921368618  
0.6582881220556925 0.7310843863104258 0.9930572284303579  
0.7915329918558743 0.5976140779815843 0.9918453005436918  
0.8581351669750634 0.7309185179151496 0.9927153635527127  
0.9914417863984610 0.7975326948993700 0.9935705139730049  
0.0580282286072155 0.9308221047948259 0.9942776815948171  
0.1914240341217002 0.7975180254628677 0.9942074096783126  
0.2580781628462002 0.9308073775146525 0.9947003127303178  
0.3913243412443753 0.7975725983254680 0.9941908518210756  
0.4580389179415161 0.9308106777031367 0.9945750422753034  
0.5913980734575564 0.7975704066466631 0.9939388990861761  
0.6580226238655452 0.9307939215946710 0.9943292017756408  
0.7915440668080158 0.7976022338756285 0.9931558757080686  
0.8580490977949032 0.9308357077464203 0.9938952922605392  
0.8545151874571157 0.5157844713323554 0.2104423067548210  
0.4308617180547810 0.5928283964568678 0.2682598823186677  
0.4061673306764960 0.3586468718917794 0.3023755728647760  
0.4149687724944603 0.4378888510696077 0.1390484532132814  
0.6104154183749047 0.5456652937103827 0.2368383490236272  
0.9019918676268035 0.4540402600353943 0.2122958622117733  
0.8059140422531580 0.5777504445987761 0.2099233665315424

#### 4.42 Output file of the structure OCHO\* on Cu2Sn2 supported by graphene surface

1.00000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Sn Cu O H  
51 2 2 2 1

Direct

0.9861222552392682 0.9967808393873532 0.0035434875221555

0.0525628639272586 0.1300643515834461 0.0039385858633829  
0.1860921723839208 0.9967973105617728 0.0041340784470336  
0.2526870477170651 0.1300106679254598 0.0044272821687681  
0.3861093138134539 0.9968080844131770 0.0049314194228433  
0.4529271120206750 0.1301049057133449 0.0048028607147523  
0.5861987171306496 0.9969848009308178 0.0051082200134590  
0.6529022012512440 0.1303299371744118 0.0047294147668755  
0.7862280730610557 0.9969469652835035 0.0043343942033151  
0.8527861987365608 0.1302913472396266 0.0043331568923576  
0.9860676904139222 0.1969121261648512 0.0040926985350455  
0.0525537959829102 0.3302677775776995 0.0039142888822097  
0.1857404987725055 0.1965101619853037 0.0041902050659457  
0.2517303550364232 0.3297404697643539 0.0051025161916621  
0.3861156247605266 0.1964372099967642 0.0047993718399991  
0.4534759169747404 0.3299125743703464 0.0050652304053668  
0.5863297707655801 0.1970430631669620 0.0044885183386326  
0.6532286946948405 0.3304270939226168 0.0031908649095585  
0.7862316885357070 0.1970662997320143 0.0042641093581743  
0.8528719783225793 0.3304233305684499 0.0034504468562885  
0.9861235421591691 0.3971109441979324 0.0034862532514314  
0.0527282616522834 0.5304173784532296 0.0033115601265080  
0.1857417511042857 0.3969664030724635 0.0042553049168594  
0.2526825451748240 0.5304263226355365 0.0045480881050381  
0.3860506225663536 0.3969067533789231 0.0066090952752808  
0.4534580953811899 0.5313144714293805 0.0051448836163105  
0.5869769083898788 0.3972665159104402 0.0028441151968940  
0.6534788426592536 0.5306276195278179 0.0014258238139934  
0.7864888990352762 0.3972773857821202 0.0025207579902793  
0.8530445825798352 0.5304949483474272 0.0013986989178154  
0.9862100286874592 0.5971072675961362 0.0022330995673227  
0.0528076090107832 0.7302845669809120 0.0026468554553567  
0.1860862889006927 0.5970395329264993 0.0042461522700782  
0.2527831481195539 0.7303596315760907 0.0045262117324814  
0.3861187447503500 0.5974075496780338 0.0049120927141529  
0.4529126144801873 0.7305676272806966 0.0049407450401347  
0.5869478344222515 0.5974609170506223 0.0029627569291268  
0.6532043087629523 0.7305724546459841 0.0033754769866658  
0.7865440146725490 0.5971619954593037 0.0008001866734109  
0.8530454095017120 0.7303204563534353 0.0015012668863994  
0.9862251886707334 0.7968825390029470 0.0023015758686831  
0.0527383176679554 0.9300800063482165 0.0033308574344565  
0.1860159493037680 0.7968874614074672 0.0039354564099457  
0.2527889409456011 0.9301774003407606 0.0044533299750748  
0.3861046516012012 0.7970458551434708 0.0050024029551612  
0.4528560401641544 0.9303028131361344 0.0051192075840429  
0.5863085567329718 0.7970529383389060 0.0046674939497285  
0.6528923642836137 0.9303445578759845 0.0048414107202673  
0.7864702268728008 0.7969920927940505 0.0026885256946307  
0.8528761026484560 0.9302412593203044 0.0035387044298665  
0.8747311983918536 0.6468316577186189 0.2452283159407801  
0.4104453312833235 0.5192191307119510 0.2985231103563994  
0.4061061795330504 0.2923861704712206 0.2982086419497703  
0.4046629143186645 0.4046430030408784 0.1502928305992506  
0.6050842376310975 0.5017862366286379 0.2502557903345748  
0.7677667302311678 0.5813685567536842 0.2032805807240078  
0.9779461189342751 0.6978456144552554 0.2086554674636848  
0.8674495842335763 0.6547602387662620 0.3190263077463201

#### 4.43 Output file of the structure COOH\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by graphene surface

1.0000000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Sn Cu O H  
51 2 2 2 1  
Direct  
0.9941516271397551 0.9975708848375162 0.0007154740299471  
0.0605933976611360 0.1307990096331356 0.0010245350698112  
0.1941844578764910 0.9976286690160739 0.0015828255402612

0.2607975356043574 0.1308452628740747 0.0019651276565216  
0.3942266653611531 0.9976101030681906 0.0021681026264584  
0.4609944439138443 0.1308624384070277 0.0022424059756264  
0.5942407536555659 0.9977079345569102 0.0020740816101672  
0.6609096735694295 0.1310161600319162 0.0018163289329468  
0.7942679048874810 0.9976662578076665 0.0012836199479741  
0.8608079121800220 0.1309707505390756 0.0013006867083765  
0.9940879421832123 0.1976089514102737 0.0009514615870894  
0.0605704608705608 0.3309234163556356 0.0004220830690721  
0.1937900671701627 0.1972665968446031 0.0014447431254603  
0.2597354033439191 0.3304029761069315 0.0018051899418240  
0.3942311791646172 0.1972884596643022 0.0023844107811545  
0.4614569143996149 0.3305391472453234 0.0024543292177147  
0.5943310079771186 0.1977069384215051 0.0017362190842590  
0.6611128327917863 0.3310255869501389 0.0005631692317223  
0.7942173373465136 0.1977025447953115 0.0012600372286086  
0.8608124434007345 0.3310365695431843 0.0004023873416643  
0.9940957476114950 0.3977312420929833 0.0002118326887144  
0.0607679264093129 0.5310309517799137 0.0001541257240928  
0.1937074130199361 0.3976307728783739 0.0003963919864493  
0.2606141272776826 0.5310961450307294 0.0005510345380255  
0.3940258926407891 0.3973566117013169 0.0036701186056869  
0.4614299679792275 0.5319195005789524 0.0021560350243695  
0.5947751606341932 0.3977966832279360 0.0005532201096454  
0.6613891525472644 0.5312543582847604 -0.0007736577208383  
0.7943382122541498 0.3977944030346424 -0.0003018344627179  
0.8609185285264361 0.5310839306636780 -0.0012473625602254  
0.9941992359680824 0.5977755055977136 0.9996428365468134  
0.0608465139959199 0.7311103923080766 0.0001562746783139  
0.1941242816102431 0.5977635763210686 0.0005768620097050  
0.2608659643988555 0.7311041437837995 0.0011878627712931  
0.3940325395264975 0.5981983005814168 0.0011621501515293  
0.4609406050147734 0.7313348913755904 0.0013193723050725  
0.5950841825485516 0.5982720029388137 0.0001244792968787  
0.6612689934076288 0.7313414672367116 0.0001062609244900  
0.7945026492009855 0.5979141147061824 0.9981464676610431  
0.8610123426140311 0.7311362395816513 0.9985675971810579  
0.9942158940786548 0.7977347963408441 0.9996185500004396  
0.0608184554063482 0.9309591237908476 0.0006437209885219  
0.1941861768739285 0.7977224863424209 0.0011701945036040  
0.2609126508672688 0.9310087746252774 0.0017701533291319  
0.3941802067946809 0.7978311250398837 0.0016041468766899  
0.4609212720713483 0.9310659690451593 0.0020663692447747  
0.5943401331736117 0.7978103307742057 0.0012567658089604  
0.6609225518570350 0.9310565162266492 0.0016643239873287  
0.7944998866925596 0.7978056123766081 0.9994977460400676  
0.8609080192635465 0.9309923483085117 0.0005060432470697  
0.7730461510825243 0.5907441343824698 0.2242593348075006  
0.4092946110608837 0.5819028340608238 0.2728600798221407  
0.3906132834404263 0.3512081695583489 0.3087166790928305  
0.4110771589964132 0.4340715005832593 0.1457800980082989  
0.6008084850360327 0.5385329867668133 0.2519951671165168  
0.8025129348444161 0.4967302146233321 0.2214163516819811  
0.8539481275232886 0.6995349564203280 0.2094527221043569  
0.8925932732534946 0.5372798589211114 0.2069647921737390

#### 4.44 Output file of the structure CO\* on Cu<sub>2</sub>Sn<sub>2</sub> supported by graphene surface

1.0000000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Sn Cu O  
51 2 2 1  
Direct  
0.9933055507082850 0.9973697506478093 0.9964839315848033  
0.0597637346583970 0.1306150760079292 0.9965856578730342  
0.1933664022063267 0.9974463268330823 0.9968980203442169  
0.2599500707910256 0.1306585049728483 0.9971239674574651  
0.3933391864118900 0.9973805804767114 0.9968516714153809  
0.4600871653235324 0.1306208328309303 0.9968405373178700

0.5933260871036480 0.9974173384549740 0.9967443479885341  
0.6600288579747587 0.1307224500920526 0.9965474682558575  
0.7933487216429586 0.9974233470495554 0.9964568563341338  
0.8599430971262481 0.1307177482869568 0.9963686171825396  
0.9932166068959769 0.1973543390928645 0.9962626020029296  
0.0597414324136214 0.3306859549970990 0.9956723781055635  
0.1929646213183776 0.1970745717182049 0.9969141878008034  
0.2589266051277338 0.3301823014815120 0.9969946306482410  
0.3933214980552152 0.1970633183069368 0.9970219396077344  
0.4604221334427848 0.3301943791661844 0.9969485225537744  
0.5933846032402125 0.1973425438398429 0.9964681650747329  
0.6601957660932518 0.3306895102631893 0.9956366033201511  
0.7933378341456331 0.1974186876674137 0.9961758806728692  
0.8600119659575686 0.3307392057018610 0.9955655228915146  
0.9932646543006525 0.3974813551748715 0.9953371942289053  
0.0599291207574687 0.5307524690565363 0.9951763679707061  
0.1928572125696937 0.3973999882157557 0.9956583812627056  
0.2596887364195067 0.5308766621965627 0.9953901870984307  
0.3930735133363798 0.3969593981634290 0.9983161000781267  
0.4604113200817346 0.5315888295578526 0.9971359026770160  
0.5937341021750000 0.3973717838413481 0.9954814443410197  
0.6604181105164137 0.5309017893031510 0.9947921040288085  
0.7935064700380782 0.3974886678210064 0.9951050837808628  
0.8601703860236973 0.5307803015848982 -0.0054596887909312  
0.9934179077428310 0.5974905531180683 0.9950364570675198  
0.0600766463648408 0.7308089406266247 0.9956903791619043  
0.1932415476437025 0.5975323479870872 0.9954036956795282  
0.2600324383570217 0.7308789249451521 0.9959431954108704  
0.3930581367165348 0.5980171144675028 0.9959692787942424  
0.4600499006970087 0.7311216146268403 0.9961010530621121  
0.5942074095424654 0.5980399448039959 0.9954031608216682  
0.6603370446478811 0.7311213099171004 0.9955917936676980  
0.7936374254363044 0.5975694691383017 0.9945305817050587  
0.8601831168163003 0.7309057683634369 0.9952688637182603  
0.9934748010037232 0.7975104440476404 0.9958479933770584  
0.0600340779388409 0.9308094184230100 0.9964952272286303  
0.1933906175492588 0.7975033233746489 0.9961807700001649  
0.2600612570846366 0.9308012347454787 0.9967392166879240  
0.3933024121158687 0.7975968994507646 0.9962702186724756  
0.4600443828696309 0.9308375338492354 0.9966923725709902  
0.5934155430868346 0.7975715638593636 0.9962582447959005  
0.6600255392425080 0.9307941958900311 0.9965685845425231  
0.7935751839357185 0.7976009724535811 0.9956683906154468  
0.8600560763100277 0.9308385073179065 0.9962352301922361  
0.7750042989589916 0.5425328353312017 0.2172737942950554  
0.4669826698549885 0.6123320844314838 0.2713910174319388  
0.3837463573491187 0.3621189203495632 0.3016412436067544  
0.4203304330437014 0.4513205796876249 0.1391580984546037  
0.6118660402805434 0.5065205743250236 0.2340664495170356  
0.8774999785546435 0.5651374366659603 0.2216499728146089

#### 4.45 Output file of the structure CO<sub>2</sub>\* on CuSn<sub>3</sub> supported by graphene surface

```

1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
C Sn Cu O
51 3 1 2
Direct
0.0056432794739718 -0.0121189061049702 0.9882862375778264
0.0723462975481071 0.1212122111999773 0.9877020582000262
0.2056592324913740 -0.0120785863744632 0.9879043956948860
0.2723101154949933 0.1212098937184312 0.9868382576674927
0.4056112470419118 -0.0121052704344133 0.9873782943892954
0.4722404138754721 0.1212198465341007 0.9871184861827020
0.6055638915745899 -0.0121390118926576 0.9871256538924268
0.6722306132335043 0.1211991807919814 0.9878156870309184
0.8056035629464282 -0.0121420727792100 0.9879092959527960
0.8722797047096238 0.1212034409864090 0.9882469598347141

```

0.0056417820780387 0.1878488484525850 0.9878527780083936  
0.0722888416414856 0.3211808994699311 0.9870880719220895  
0.2056565129368272 0.1878348558101220 0.9865600049558353  
0.2722862572316586 0.3211154454159738 0.9851616238604047  
0.4055864655119991 0.1878559824211383 0.9862329183449212  
0.4722659737223815 0.3211210982240755 0.9850465829634160  
0.6055537484543185 0.1878551284447738 0.9874168370886237  
0.6722074897404462 0.3211691337354323 0.9871885369184479  
0.8055861548543962 0.1878607877318951 0.9881943745246593  
0.8722661522226715 0.3212047209725386 0.9881251362219042  
0.0056225062463932 0.3878589435908694 0.9876196355530503  
0.0723092955600526 0.5211886254645526 0.9873367905290206  
0.2056298612705786 0.3878201117083697 0.9854913088891037  
0.2722980206493313 0.5211991268594512 0.9845815040621135  
0.4056192280035367 0.3877640389727565 0.9842142074083420  
0.4722088022103216 0.5211043655123521 0.9838706384646398  
0.6055464192526296 0.3877822022414127 0.9859469346256629  
0.6722372638350634 0.5210890961244519 0.9861260834937791  
0.8055463537103537 0.3878297732697327 0.9878602286206032  
0.8722585874534148 0.5211554034955579 0.9879725113538205  
0.0056139982418626 0.5878363961981137 0.9880636469540928  
0.0722813212668635 0.7211862804009893 0.9882167717174345  
0.2056360303425283 0.5878550274309344 0.9859981199337801  
0.2722896356611023 0.7211886176423570 0.9863662035754760  
0.4055886472744540 0.5878384623050937 0.9836056631178600  
0.4722360044253736 0.7211544096793051 0.9844018512470717  
0.6055889907833191 0.5877856386878567 0.9851428400370817  
0.6722849514111425 0.7211799450195377 0.9859418598434515  
0.8055701931467509 0.5878096439651818 0.9874874350616635  
0.8722642399288570 0.7211654392473825 0.9879238382394887  
0.0056309408799282 0.7878783416400580 0.9884532522198286  
0.0723246899957402 0.9212309173256814 0.9883481954705793  
0.2056292496217170 0.7878851989558824 0.9877041426526985  
0.2722995382245956 0.9212300599605809 0.9877890406557572  
0.4056163362141009 0.7878583552501860 0.9856125542872058  
0.4722374781993174 0.9211848401709040 0.9867328675195096  
0.6055848239710979 0.7878603708071178 0.9855239945542302  
0.6722531075451658 0.9212137811077230 0.9868939744453524  
0.8055958598503280 0.7878449287321680 0.9873991863592969  
0.8722930049562767 0.9212000979050186 0.9880498579098300  
0.4292865593443163 0.3511039859550648 0.2081489736171595  
0.3405024954856667 0.4929978181819333 0.2369024627670089  
0.2650271517615417 0.6738146545248689 0.2536611610169930  
0.5275377955031849 0.7679529440862910 0.2361208746013976  
0.5845882949813824 0.6038096634296265 0.2118667914994386  
0.3585726290046796 0.2399537710675895 0.2025982498348422  
0.5455226580028331 0.4269140757593782 0.2021283186295706

#### 4.46 Output file of the structure OCHO\* on CuSn<sub>3</sub> supported by graphene surface

1.00000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Sn Cu O H  
51 3 1 2 1  
Direct  
0.0110408415050847 0.0010674961214802 0.9888311582347807  
0.0774657243654928 0.1343063017952197 0.9886198108275680  
0.2110627826862313 0.0010919189662500 0.9888255540445339  
0.2776737442088964 0.1342924619974095 0.9890050309317781  
0.4110250654747458 0.0010412043354984 0.9884086860808352  
0.4778350269811875 0.1342628836090174 0.9881791382508863  
0.6110297674761630 0.0011061246858937 0.9886180453088041  
0.6777841210538398 0.1343986085749262 0.9879859255195776  
0.8111119547406415 0.0011407536050116 0.9886414544572004  
0.8776731902745120 0.1344189680080283 0.9879661075712817  
0.0109512935194089 0.2010708172605101 0.9877427111628473  
0.0774302684452299 0.3343989170016549 0.9864431137633474  
0.2107224967619367 0.2007952278576789 0.9889357712194800  
0.2767444248183666 0.3338550094579889 0.9887633115502342

0.4110736760555417 0.2007251850908702 0.9884069645648853  
0.4781331465988248 0.3337803862876021 0.9882097082158090  
0.6111320523991460 0.2010207087233030 0.9876409064574150  
0.6779755787035299 0.3343298290759632 0.9867229827198761  
0.8111089276979764 0.2011679007246026 0.9873634137216323  
0.8777968679639212 0.3344700753645385 0.9861194408061438  
0.0109713795308793 0.4012115140485027 0.9852627336514289  
0.0775609016734496 0.5344130534770178 0.9848001808915609  
0.2105855067398249 0.4010283194834648 0.9869785953337695  
0.2772347726236306 0.5345346443745452 0.9863162737807442  
0.4106668372860575 0.4003497889732416 0.9900682447003293  
0.4779026306297345 0.5350067153258694 0.9899128580244795  
0.6114684479179986 0.4009096898815525 0.9868114137443056  
0.6783106693496822 0.5344937000915898 0.9870127953959181  
0.8112900664287455 0.4011644792020785 0.9861272298907739  
0.8779350417222676 0.5344070612013991 0.9860510444657314  
0.0111267640188788 0.6011249051037659 0.9856757723289885  
0.0777316888191289 0.7343855048324383 0.9869391352475961  
0.2107936318335361 0.6011955281928800 0.9854124860932130  
0.2775981095885995 0.7344767369890816 0.9867844531374620  
0.4104652779212765 0.6016623273631567 0.9881611970324967  
0.4776507080807623 0.7348071390209193 0.9885129655685820  
0.6121340674426623 0.6017091204357177 0.9884309605192910  
0.6781614060048413 0.7348739667255740 0.9884933940383722  
0.8114224830800468 0.6011933505894095 0.9868175459253630  
0.8778916431636113 0.7345105198714394 0.9877677310872094  
0.0111674277299151 0.8011304810711971 0.9879212899434250  
0.0777123496312654 0.9344147137644784 0.9887240530163965  
0.2110049473534631 0.8011104244559868 0.9873570793208434  
0.2777214181380121 0.9343926803929443 0.9883482298399255  
0.4108355281316720 0.8012728616200312 0.9880041724626148  
0.4777111733100839 0.9344859718123456 0.9884967978768470  
0.6111782654419439 0.8012886140830728 0.9888235626146924  
0.6777549328516841 0.9344758617208848 0.9888091574989598  
0.8113636284336183 0.8012948254681658 0.9883996205764604  
0.8778033442893580 0.9345304424439111 0.9887341037659784  
0.1597955878657285 0.5067972539735023 0.2023183227595476  
0.3131304182841750 0.3325734502809805 0.2641141314525536  
0.5669694959504917 0.4994574453426534 0.2849454445093994  
0.4524283472442413 0.6608552405680382 0.2461648672228374  
0.4634415649724904 0.4783328733242429 0.1298045900891081  
0.0580804252990228 0.4992646630940694 0.1928603294280957  
0.2672406104696699 0.6131316215833533 0.2119016859338351  
0.1694230230168742 0.4205616532730348 0.2033711494219625

#### 4.47 Output file of the structure COOH\* on CuSn3 supported by graphene surface

```

1.0000000000000000
12.3386001587000003 0.0000000000000000 0.0000000000000000
-6.1693000793000001 10.6855411845999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
C Sn Cu O H
51 3 1 2 1
Direct
0.0120144764554292 0.0009618766064606 0.9839494496089647
0.0786411238474530 0.1342993613510709 0.9832626087686488
0.2119820194048949 0.0009029347416744 0.9839906074289553
0.2785962352646636 0.1342566975839591 0.9831800664607674
0.4120063080246390 0.0008968553287781 0.9839853039099794
0.4787013687997356 0.1342380272059378 0.9835725739215467
0.6119777617062673 0.0009112502368152 0.9840286619187424
0.678698487767265 0.1342664312885924 0.9840075423416107
0.8120020417299320 0.0009508228254293 0.9840250332684708
0.8787141980731570 0.1342997594422316 0.9838281222675703
0.0120290223102645 0.2009973377641467 0.9830718653781620
0.0786767253569998 0.3342631158565843 0.9820205730106404
0.2119402175435883 0.2009504358685071 0.9825147751577641
0.2785605858555421 0.3342828548302029 0.9811862962593750
0.4120009797162537 0.2009160017273820 0.9827722218455552
0.4786969576226398 0.3343255323338756 0.9814312835596473

```



0.6120274328027367 0.2009278819100433 0.9835174574516846  
0.6786978058338548 0.3342653305130163 0.9827826230517336  
0.8120393924366975 0.2009411747125604 0.9837798446276530  
0.8787464418684579 0.3342630689662571 0.9832675814686136  
0.0120350173212225 0.4008699873723358 0.9825099783469439  
0.0786823962858242 0.5341767364545974 0.9823874625728680  
0.2119124577950564 0.4009056508645039 0.9808613202119403  
0.2786033694040524 0.5341946389195568 0.9806211422534422  
0.4119461048575234 0.4009600702633189 0.9806378975982024  
0.4786109717693278 0.5342522336153303 0.9803486035490221  
0.6120362635048358 0.4009423789040508 0.9815531208804674  
0.6786462814342706 0.5342055976616370 0.9814583137851817  
0.8120277551542906 0.4008927604121462 0.9830826105298701  
0.8786655173726942 0.5342216043265983 0.9830607064073658  
0.0120163914965064 0.6008529083318253 0.9831969340701368  
0.0786616123546956 0.7342050834976863 0.9836849907309586  
0.2119857603284645 0.6008548592494015 0.9816150576927989  
0.2786636301982648 0.7341815795253746 0.9826691342913941  
0.4119053307226228 0.6009024331583130 0.9807749788981766  
0.4785702845357281 0.7342060664880454 0.9820649034758985  
0.6119142435958271 0.6008095086773814 0.9810605152556060  
0.6786318248439637 0.7342274698481269 0.9824194551532102  
0.8119956489706467 0.6008799319423620 0.9826820004503614  
0.8786639017456356 0.7342122339327498 0.9833765258298752  
0.0119901771846749 0.8008880822696492 0.9839500170996777  
0.0786476231456151 0.9342450601905035 0.9840977664859494  
0.2120186059789098 0.8008780987397169 0.9836628374411851  
0.2786753354823684 0.9342471960298158 0.9840578258102990  
0.4119682820530208 0.8008687408117661 0.9829130877110470  
0.4786431142243766 0.9341872207382145 0.9838125272139941  
0.6118946391133356 0.8009062546027315 0.9828108183770736  
0.6786441860861246 0.9342573978812213 0.9838227327582274  
0.8120277478357253 0.8009156660672346 0.9833563576866251  
0.8786691534483254 0.9342674420530735 0.9839426499202786  
0.2617341151523849 0.5212566696171922 0.2041515586954608  
0.4103355086298212 0.2943962487147213 0.2269143994996729  
0.6578462279212574 0.4732550265755233 0.2418095772349126  
0.6209688177799207 0.6750140233035300 0.2283924486398917  
0.4029290346981751 0.4945226946884956 0.2155363382490054  
0.1521711642531471 0.4398146779383852 0.1965516821483544  
0.2957336812960328 0.6459899781334032 0.2045012160951032  
0.2175263185954105 0.6487362531059835 0.1973954732434305

#### 4.48 Output file of the structure CO\* on CuSn<sub>3</sub> supported by graphene surface

1.0000000000000000  
12.3386001587000003 0.0000000000000000 0.0000000000000000  
-6.1693000793000001 10.6855411845999999 0.0000000000000000  
0.0000000000000000 0.0000000000000000 15.0000000000000000  
C Sn Cu O  
51 3 1 1  
Direct  
0.0047086307482507 0.0012216064100587 0.9869818828470683  
0.0714081039291166 0.1345763383185894 0.9867550362386776  
0.2047241958986350 0.0012483449187831 0.9870527325293433  
0.2714017872879833 0.1345874309496213 0.9862490363931710  
0.4047295117792943 0.0012476013235914 0.9869837340164861  
0.4713972575650565 0.1345838650319453 0.9862799203822151  
0.6047139464624984 0.0012260972126879 0.9868612849197819  
0.6713740479785264 0.1345783887703472 0.9868531044245219  
0.8047009079357135 0.0012080774930814 0.9868453948696320  
0.8713770420735314 0.1345459783610369 0.9870920093235201  
0.0047273222458116 0.2012284019299844 0.9867790020494555  
0.0713786251677623 0.3345599019854182 0.9861479084764739  
0.2047465755001388 0.2012667622025387 0.9859396757402461  
0.2714078032856704 0.3345626546005114 0.9847463147390574  
0.4047242352062186 0.2012435139413355 0.9855340865200944  
0.4714231322814563 0.3346167410134822 0.9841213412607768  
0.6047239899238229 0.2012732547419248 0.9861845968151165  
0.6713788778322007 0.3345902517033341 0.9852049766593620  
0.8047196742181727 0.2012378665068384 0.9869051444896066

0.8713821275984471 0.3345708611940277 0.9865401012219085  
0.0047102233417841 0.4012244480236067 0.9863669170305481  
0.0713723237303679 0.5345461211676616 0.9863344271386033  
0.2047127009574564 0.4012022773064282 0.9851533150434463  
0.2714090439270374 0.5345780859230781 0.9849647444375983  
0.4047374193175198 0.4012821340831775 0.9835997031316499  
0.4714183708112658 0.5345747428406624 0.9829545208872453  
0.6047562980671810 0.4012790371445720 0.9837882646997994  
0.6713399254701149 0.5345365342355151 0.9833734135009503  
0.8046967318071152 0.4012226166577285 0.9858059035807357  
0.8713573487118977 0.5345487991140335 0.9857734712626833  
0.0046884630535749 0.6012037586966245 0.9864916665240143  
0.0713616809294386 0.7345420768416441 0.9869057616090305  
0.2047081027121236 0.6012196082144686 0.9859742666107878  
0.2713899100545895 0.7345530281191294 0.9865778849514941  
0.4047604978866819 0.6012467035619723 0.9840719912480637  
0.4713707237068977 0.7345501014958838 0.9850279526549204  
0.6046688861247780 0.6011572873466964 0.9830291288680193  
0.6713649289100835 0.7345258061644143 0.9844762847789827  
0.8046548440048529 0.6012039545573247 0.9849387572045295  
0.8713458000569385 0.7345494715057639 0.9856938559597801  
0.0046765936568738 0.8012118741605938 0.9867567118541306  
0.0713767139777451 0.9345550239528341 0.9870706714668095  
0.2047076028566976 0.8012190066980501 0.9871463302856406  
0.2713833207630446 0.9345709474109488 0.9871958108802056  
0.4047228501700657 0.8012047585872336 0.9862769936340067  
0.4713817138978922 0.9345538692261701 0.9868537820927845  
0.6046947211567453 0.8012136782174816 0.9852512561977743  
0.6713700630791830 0.9345406464282462 0.9864453764111543  
0.8047045082259354 0.8012056500456934 0.9855318795800641  
0.8713655216719681 0.9345260233777021 0.9866087923992365  
0.2061350217690263 0.4766793315943546 0.2131106203334304  
0.4508692740369742 0.3481030977170366 0.2370176470138765  
0.7044539418872808 0.5236692348125663 0.2467793690613547  
0.5866764522631048 0.6651830943780219 0.2373466389841562  
0.3606225546455428 0.4923517871949840 0.2212261081857258  
0.1076264074419168 0.4660929085885424 0.2090873215802742