Crystal structure prediction and properties calculation of copper-oxygen compounds by an innovative search software from first principles

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1. Supporting Information:

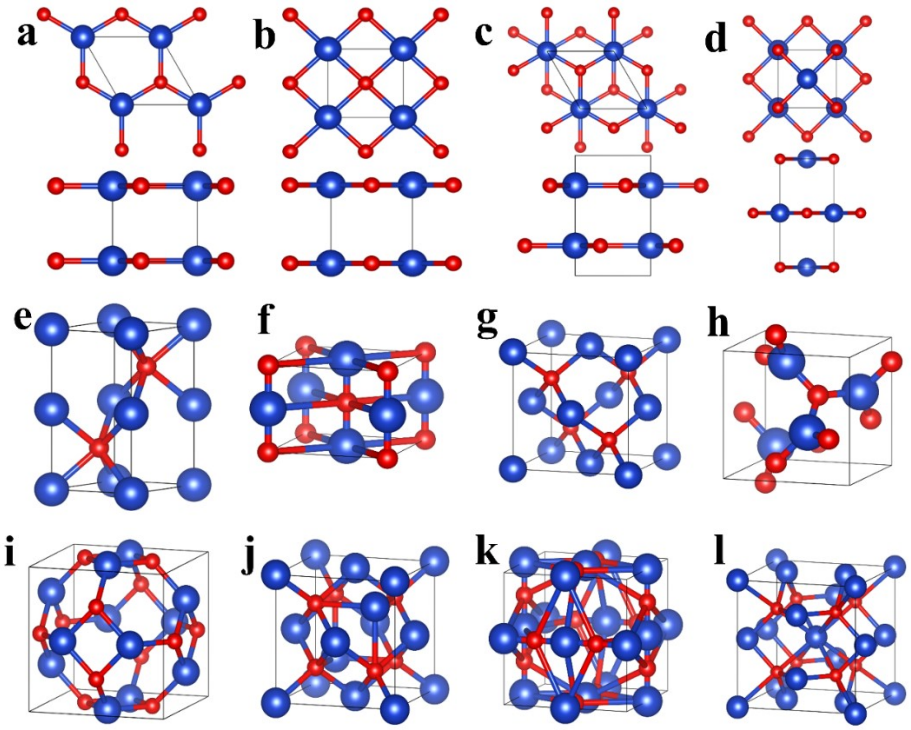

Figure. S 1 Crystal structure diagram of 12 predicted structures of CuxOy(x=y=1-10).

Table. S 1 Crystallographic information for 12 predicted structures of CuxOy(x=y=1-10).

Structure Name	Constituent atom	Crystal system	Space group	Coordination number of copper	Coordination number of oxygen	a=b/ Å	a=b/ Å	c/ Å
4303	2	Tetragonal	P-6M2(187)	3	3	3.29	3.29	2.52

						9	9	0
4103	2	Tetragonal	P4-MMM(123)	4	4	2.828	2.828	2.985
4739	4	Tetragonal	P63/MMC(194)	3	3	3.371	3.371	4.688
4834	4	Tetragonal	I4/MMM(139)	4	4	2.871	2.871	5.863
2316	4	Tetragonal	P63/MMC(194)	6	6	2.462	2.462	4.887
5594	4	Tetragonal	I4/MMM(139)	6	6	3.443	3.443	2.491
4603	8	Cubic	F-43M(216)	4	4	4.446	4.446	4.446
1026	8	Cubic	P4332(212)	3	3	3.625	3.625	3.625
5310	12	Cubic	PM-3N(223)	3	3	5.275	5.275	5.275
4841	12	Cubic	PN-3M(224)	3	5	4.340	4.340	4.340
4345	12	Cubic	PM-3N(223)	6	6	4.360	4.360	4.360
962	16	Cubic	PM-3N(223)	8	5	5.656	5.656	5.656

Continuation table:

Structure	α=β	Υ	Volume/ Å^3	Cu-O bond length/Å	Cu-Cu bond length/Å	O-O bond length/Å	Cu-O-Cu 键角
4303	90	120	23.762	1.905	3.299	3.299	120
4103	90	90	23.872	1.999	2.828	2.828	90
4739	90	120	46.130	1.946	3.371	3.371	120
4834	90	90	48.338	2.030	2.871	2.871	90
2316	90	120	25.668	1.875	2.444	2.828	82.098
5594	90	90	29.525	2.434	2.735	2.735	90

4603	90	90	87.902	1.925	3.144	3.144	109.471
1026	90	90	47.647	1.282	2.220	2.220	120
5310	90	90	146.817	1.865	2.638	2.638	120
4841	90	90	81.725	1.879	3.069	2.170	109.471
4345	90	90	82.908	2.437	2.180	2.670	126.870
962	90	90	180.971	2.449	3.162	2.828	90

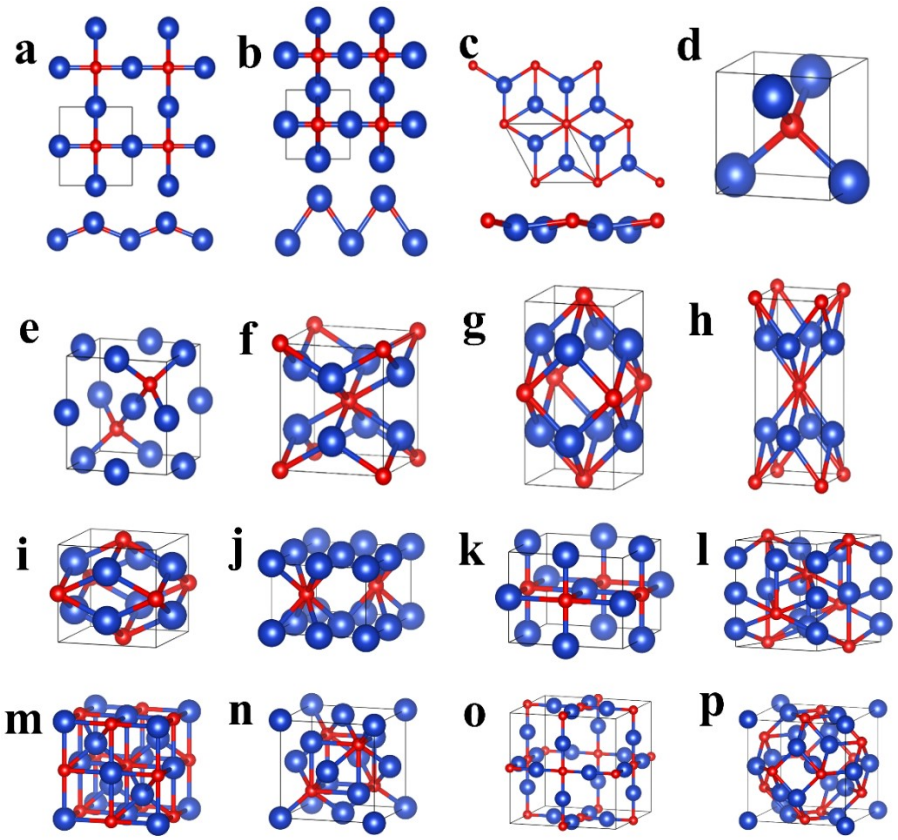

Figure. S 2 Crystal structure diagram of 16 predicted structures of Cu_2xOx(x=1-6).

Table. S 2 Crystallographic information for 16 predicted structures of Cu_2xOx(x=1-6).

Structure Name	Constituent atom	Crystal system	Space group	Coordination number of copper	Coordination number of oxygen	a/ Å	b/ Å	c/ Å
3831	3	Tetragonal	PMM2(25)	2	4	3.474	3.474	5.785
3848	3	Tetragonal	PMM2(25)	2	4	2.558	2.558	8.562
5046	3	Tetragonal	P3M1(156)	3	6	3.906	3.906	3.419

4739	3	Tetragonal	PMM2(25)	4	8	2.966	2.966	2.816
560	6	Cubic	PN-3M(224)	2	4	4.263	4.263	4.263
2574	6	Tetragonal	I4/MMM(139)	4	8	3.862	3.862	4.219
2447	6	Tetragonal	I4/MMM(139)	4	8	3.116	3.116	5.706
2457	6	Tetragonal	I4/MMM(139)	4	8	2.911	2.911	7.185
2603	6	Tetragonal	I4/MMM(139)	4	8	3.599	3.599	3.442
2695	6	Orthorhombic	CMMM(65)	4	8	5.232	3.672	2.606
2733	6	Tetragonal	P4/MMM(123)	4	8	4.552	4.552	3.472
3814	9	Tetragonal	P6422(181)	4	8	3.758	3.758	4.742
497	12	Cubic	F-43M(216)	6	12	4.288	4.288	4.288
1975	12	Cubic	F-43M(216)	3	6	4.363	4.363	4.363
781	18	Cubic	IM-3M(229)	2	4	7.133	7.133	7.133
2441	18	Cubic	P4232(208)	4	6	5.674	5.674	5.674

Continuation table:

Structure	α=β	ϒ	Volume/ Å^3	Cu-O bond length/Å	Cu-Cu bond length/Å	O-O bond length/Å	Cu-O-Cu 键角
3831	90	90	69.799	1.739	2.565	3.474	139.140
3848	90	90	56.045	2.159	2.441	2.558	72.643
5046	90	120	45.175	2.282	2.257	3.906	59.445
4739	90	90	24.775	2.185	2.966	2.966	85.515

560	90	90	77.448	1.846	3.014	3.691	109.471
2574	90	90	62.940	2.200	2.731	3.451	76.716
2447	90	90	55.389	2.112	2.203	3.116	84.968
2457	90	90	60.899	2.312	2.059	2.911	52.874
2603	90	90	44.585	1.995	1.721	3.072	51.108
2695	90	90	50.055	2.062	1.836	3.196	78.383
2733	90	90	71.956	1.736	3.219	3.219	90
3814	90	120	57.984	2.038	1.879	2.455	134.373
497	90	90	78.856	2.144	3.032	3.032	90
1975	90	90	83.034	1.889	3.085	3.085	109.471
781	90	90	362.948	1.783	2.522	3.567	90
2441	90	90	182.650	2.006	2.837	2.837	120

The elastic constants of these stable copper oxide structures are calculated as follows:

S. 3 Elastic tensor for T-CuO in the unit of GPa:

153.182	107.264	118.177	-0.000	-0.000	0.000
107.264	181.455	133.689	-0.001	-0.000	0.000
118.177	133.689	139.149	-0.000	-0.000	0.000
-0.000	-0.001	-0.000	36.536	0.000	-0.000
-0.000	-0.000	-0.000	0.000	30.935	-0.000
0.000	0.000	0.000	-0.000	-0.000	6.751

S. 4 Elastic tensor for C1-CuO in the unit of GPa:

181.926	163.401	163.405	-0.021	-0.014	0.004
163.401	181.936	163.412	-0.021	-0.012	0.002
163.405	163.412	181.949	-0.024	-0.012	0.004
-0.021	-0.021	-0.024	46.713	-0.003	-0.003
-0.014	-0.012	-0.012	-0.003	46.709	0.000
0.004	0.002	0.004	-0.003	0.000	46.723

S. 5 Elastic tensor for C2-CuO in the unit of GPa:

207.480	87.564	87.450	-0.035	-0.032	-0.026
87.564	207.900	87.572	-0.020	-0.035	-0.039
87.450	87.572	207.494	-0.032	-0.020	-0.042
-0.035	-0.020	-0.032	44.014	-0.001	-0.002
-0.032	-0.035	-0.020	-0.001	44.014	0.000

-0.026	-0.039	-0.042	-0.002	0.000	44.016

S. 6 Elastic tensor for C3-CuO in the unit of GPa:

295.178	126.634	126.634	0.000	0.000	0.000
126.634	295.178	126.634	0.000	0.000	0.000
126.634	126.634	295.178	0.000	0.000	0.000
0.000	0.000	0.000	68.259	0.000	0.000
0.000	0.000	0.000	0.000	68.259	0.000
0.000	0.000	0.000	0.000	0.000	68.259

S. 7 Elastic tensor for D1-Cu_2O in the unit of GPa:

162.326	125.582	124.626	10.568	-3.140	-0.859
125.582	165.635	126.554	10.241	-3.243	-0.877
124.626	126.554	166.186	10.162	-3.213	-0.880
10.568	10.241	10.162	16.770	-0.004	0.055
-3.140	-3.243	-3.213	-0.004	16.870	-0.100
-0.859	-0.877	-0.880	0.055	-0.100	16.635

S. 8 Elastic tensor for D2-Cu_2O in the unit of GPa:

50.553	36.833	40.967	0.934	0.497	-1.431
36.833	42.802	35.462	0.505	0.831	-1.410
40.967	35.462	53.475	0.711	0.647	-1.472
0.934	0.505	0.711	5.038	-0.199	-0.036
0.497	0.831	0.647	-0.199	5.294	-0.004
-1.431	-1.410	-1.472	-0.036	-0.004	6.266