Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Photodriven CO Dimerization on Cu_2O from an Electronic-Structure Perspective

Svante Hedström[†,‡], Joakim Halldin Stenlid[†], Chang Liu, Lars G. M. Pettersson*

Department of Physics, AlbaNova University Center, Stockholm University, 10691 Stockholm, Sweden

*Corresponding Author: lgm@fysik.su.se

Table of Contents

[†] Shared first authorship
[‡] Current address: Swedish Nuclear Fuel and Waste management Co, Evenemangsgatan 13, Box 3091, 169 03 Solna, Sweden

Excited state lifetime

The S1 excited state in the hydrated $Cu_{28}O_{14}(CO)_2$ cluster is of HOMO→LUMO character, and its radiative lifetime is estimated under the approximation of a dipole in a homogeneous medium (Cu_2O), according to the rate for spontaneous emission:

$$\Gamma_{\mathrm{rad}} = \frac{\omega^3 n^3 |\mu|^2}{3\pi\varepsilon_0 \hbar c^3} \qquad \text{(S1)}$$

Where Γ_{rad} is the radiative rate, ω is the light frequency, n is the refractive index which for Cu_2O is 2.78 for 656 nm light,[1] μ is the transition dipole moment, ε_0 is the vacuum permittivity, and c is the speed of light. The radiative lifetime τ_{rad} is then obtained from the calculated μ of the S1 state of $Cu_{28}O_{14}(CO)_2$ optimized with TD-DFT, which in atomic units becomes:

$$\tau_{\mathrm{rad}} = \frac{1}{\Gamma_{\mathrm{rad}}} = \frac{3c^3}{4\omega^3 n^3 |\mu|^2} = \frac{3 \times 137^3}{4(2.11 \times 10^{-4})^3 2.78^3 0.28^2} = 1.20 \times 10^{17}\ \mathrm{a.u.} = 2.90\ \mathrm{s}$$

Optical properties

Table S1. Full list of electronic excitations in hydrated $Cu_{28}O_{14}(H_2O)_5$ as calculated with TD-PBE0[2]/Def2-SVP[3]/SMD-H_2O[4]. The wavelengths λ, oscillator strengths f, and the dominant orbital configuration of the excitation and its contribution (in %).

Transition	λ [nm]	f	OriginMO	TargetMO	Contrib.%
1	726.46	0.0096	HOMO	LUMO	92.95
2	666.47	0.0254	HOMO−1	LUMO	40.30
3	654.51	0.0245	HOMO−7	LUMO	63.84
4	637.94	0.0023	HOMO−6	LUMO	32.77
5	613.36	0.0002	HOMO−3	LUMO	46.98
6	597.75	0.0019	HOMO−6	LUMO	37.35
7	579.35	0.0018	HOMO−4	LUMO	32.64
8	577.60	0.0031	HOMO−2	LUMO	29.44
9	563.53	0.0037	HOMO−10	LUMO	31.09
10	558.47	0.0002	HOMO−9	LUMO	26.43
11	521.49	0.0109	HOMO−11	LUMO	24.71
12	515.89	0.0031	HOMO−12	LUMO	29.07
13	487.75	0.0091	HOMO−11	LUMO	18.33
14	482.62	0.0026	HOMO−8	LUMO	13.76
15	477.91	0.0075	HOMO−17	LUMO	27.04
16	475.10	0.0010	HOMO−16	LUMO	46.66
17	470.83	0.0009	HOMO−13	LUMO	37.00
18	467.52	0.0090	HOMO−12	LUMO	24.90
19	459.16	0.0040	HOMO−30	LUMO	11.11
20	448.28	0.0024	HOMO	LUMO+1	78.35
21	446.06	0.0064	HOMO−48	LUMO	18.10
22	443.17	0.0040	HOMO−14	LUMO	19.35
23	441.33	0.0039	HOMO−32	LUMO	13.08
24	437.00	0.0019	HOMO−14	LUMO	16.35

25	433.62	0.0012	HOMO−30	LUMO	8.63
26	430.17	0.0022	HOMO−15	LUMO	12.77
27	429.43	0.0015	HOMO−1	LUMO+1	35.52
28	423.98	0.0052	HOMO−15	LUMO	14.10
29	422.94	0.0011	HOMO−19	LUMO	21.59
30	420.51	0.0046	HOMO−19	LUMO	11.71
31	418.49	0.0065	HOMO−3	LUMO+1	28.23
32	416.15	0.0006	HOMO−5	LUMO+1	40.64
33	414.72	0.0057	HOMO−18	LUMO	14.50
34	413.54	0.0020	HOMO−1	LUMO+1	12.29
35	409.68	0.0023	HOMO−4	LUMO+1	15.75
36	408.24	0.0003	HOMO−2	LUMO+1	23.17
37	405.71	0.0156	HOMO	LUMO+2	35.08
38	405.25	0.0031	HOMO−20	LUMO	14.17
39	401.02	0.0049	HOMO−21	LUMO	24.54
40	399.94	0.0070	HOMO−21	LUMO	14.13
41	396.00	0.0015	HOMO	LUMO+3	33.38
42	392.91	0.0039	HOMO−24	LUMO	24.54
43	389.92	0.0056	HOMO	LUMO+4	14.94
44	387.63	0.0045	HOMO−2	LUMO+2	15.93
45	386.43	0.0062	HOMO	LUMO+3	13.77
46	385.88	0.0002	HOMO−29	LUMO	16.50
47	385.01	0.0033	HOMO−2	LUMO+3	10.67
48	382.71	0.0047	HOMO−73	LUMO	12.39
49	380.62	0.0015	HOMO−31	LUMO	25.92
50	378.54	0.0005	HOMO−49	LUMO	7.35
51	378.07	0.0002	HOMO−8	LUMO+1	10.96
52	376.59	0.0041	HOMO−5	LUMO+2	13.55
53	375.48	0.0010	HOMO−6	LUMO+2	11.57
54	374.18	0.0003	HOMO−22	LUMO	10.09
55	372.93	0.0106	HOMO−4	LUMO+4	9.80
56	372.13	0.0041	HOMO	LUMO+5	20.82
57	371.68	0.0008	HOMO−3	LUMO+2	4.61
58	371.37	0.0017	HOMO−4	LUMO+3	12.54
59	370.06	0.0166	HOMO−3	LUMO+2	9.69
60	369.69	0.0021	HOMO−27	LUMO	11.81
61	368.93	0.0018	HOMO−2	LUMO+3	5.75
62	367.88	0.0075	HOMO	LUMO+5	9.71
63	367.63	0.0088	HOMO	LUMO+5	9.30
64	366.54	0.0003	HOMO−3	LUMO+3	8.85
65	365.84	0.0011	HOMO−10	LUMO+1	7.36
66	364.36	0.0009	HOMO−3	LUMO+3	9.00
67	362.56	0.0010	HOMO−1	LUMO+4	6.27
68	361.58	0.0016	HOMO−2	LUMO+3	6.02
69	360.21	0.0008	HOMO−33	LUMO	6.98
70	359.91	0.0005	HOMO−2	LUMO+3	18.44
71	359.06	0.0012	HOMO−7	LUMO+2	7.02
72	357.46	0.0015	HOMO−7	LUMO+2	17.90

73	357.44	0.0035	HOMO−1	LUMO+5	20.22
74	356.09	0.0032	HOMO−1	LUMO+5	3.89
75	355.82	0.0001	HOMO−26	LUMO	10.62
76	355.18	0.0015	HOMO−7	LUMO+3	11.82
77	354.58	0.0092	HOMO−4	LUMO+3	9.87
78	354.02	0.0056	HOMO−6	LUMO+3	20.73
79	353.62	0.0009	HOMO−1	LUMO+5	8.18
80	352.69	0.0032	HOMO−28	LUMO	8.05
81	351.68	0.0027	HOMO−100	LUMO	8.73
82	351.00	0.0035	HOMO−3	LUMO+5	7.96
83	349.96	0.0002	HOMO	LUMO+6	12.83
84	349.35	0.0006	HOMO	LUMO+6	8.49
85	348.56	0.0040	HOMO−4	LUMO+3	4.23
86	348.06	0.0022	HOMO−3	LUMO+5	4.28
87	347.29	0.0008	HOMO−111	LUMO	6.40
88	347.20	0.0019	HOMO−36	LUMO	8.14
89	346.74	0.0069	HOMO−2	LUMO+5	14.42
90	346.11	0.0043	HOMO−6	LUMO+2	14.27
91	345.60	0.0048	HOMO−4	LUMO+2	7.41
92	345.16	0.0033	HOMO	LUMO+7	8.54
93	344.32	0.0016	HOMO−6	LUMO+4	4.84
94	343.91	0.0036	HOMO−6	LUMO+5	10.15
95	343.11	0.0002	HOMO−112	LUMO	7.51
96	342.73	0.0005	HOMO	LUMO+7	6.92
97	342.64	0.0014	HOMO−14	LUMO+1	7.98
98	341.04	0.0043	HOMO−10	LUMO+1	6.59
99	340.89	0.0020	HOMO−52	LUMO	7.56
100	340.69	0.0043	HOMO−39	LUMO	9.95
101	340.02	0.0001	HOMO−32	LUMO	6.38
102	339.47	0.0050	HOMO	LUMO+7	8.65
103	339.18	0.0029	HOMO−34	LUMO	18.19
104	338.59	0.0024	HOMO−5	LUMO+5	8.50
105	337.91	0.0019	HOMO−8	LUMO+2	7.50
106	337.61	0.0011	HOMO−1	LUMO+6	9.05
107	337.21	0.0013	HOMO−10	LUMO+2	17.26
108	336.97	0.0011	HOMO−5	LUMO+5	7.30
109	335.87	0.0021	HOMO−40	LUMO	10.11
110	335.60	0.0023	HOMO−10	LUMO+2	7.67
111	335.16	0.0000	HOMO−3	LUMO+5	19.90
112	334.47	0.0003	HOMO−1	LUMO+6	8.86
113	334.29	0.0001	HOMO−39	LUMO	9.48
114	333.86	0.0006	HOMO−10	LUMO+2	4.73
115	333.37	0.0051	HOMO	LUMO+8	7.05
116	332.79	0.0065	HOMO	LUMO+8	7.79
117	332.62	0.0028	HOMO−39	LUMO	5.83
118	331.95	0.0010	HOMO	LUMO+8	4.50
119	331.74	0.0013	HOMO−6	LUMO+5	6.39
120	331.14	0.0038	HOMO−6	LUMO+5	7.40

121	330.77	0.0030	HOMO−43	LUMO	7.41
122	330.12	0.0061	HOMO	LUMO+8	7.79
123	329.61	0.0035	HOMO−5	LUMO+6	7.55
124	329.16	0.0028	HOMO−109	LUMO	5.70
125	328.84	0.0009	HOMO−1	LUMO+7	5.54
126	328.14	0.0012	HOMO−1	LUMO+7	7.43
127	327.24	0.0053	HOMO−1	LUMO+7	6.07
128	326.99	0.0033	HOMO−8	LUMO+3	5.77
129	326.75	0.0044	HOMO−1	LUMO+8	5.44
130	326.53	0.0015	HOMO−4	LUMO+7	5.75
131	326.36	0.0000	HOMO−2	LUMO+6	8.24
132	325.91	0.0034	HOMO−1	LUMO+7	8.66
133	325.71	0.0006	HOMO−44	LUMO	20.51
134	324.94	0.0041	HOMO−5	LUMO+7	3.68
135	324.59	0.0006	HOMO−45	LUMO	5.27
136	324.46	0.0006	HOMO−3	LUMO+6	15.78
137	323.63	0.0033	HOMO−5	LUMO+6	5.56
138	323.42	0.0031	HOMO−3	LUMO+6	18.99
139	323.14	0.0038	HOMO−5	LUMO+6	10.46
140	323.09	0.0032	HOMO−118	LUMO	4.43
141	322.64	0.0131	HOMO−4	LUMO+6	5.61
142	322.26	0.0016	HOMO−1	LUMO+8	4.18
143	322.01	0.0019	HOMO−11	LUMO+2	5.00
144	321.82	0.0027	HOMO−4	LUMO+6	4.32
145	321.80	0.0019	HOMO−4	LUMO+8	5.51
146	321.42	0.0005	HOMO−46	LUMO	2.91
147	321.02	0.0051	HOMO−6	LUMO+6	8.30
148	320.31	0.0004	HOMO−72	LUMO	4.58
149	320.06	0.0042	HOMO−3	LUMO+7	9.64
150	319.81	0.0022	HOMO−63	LUMO	2.53
151	319.72	0.0022	HOMO−69	LUMO	4.92
152	318.98	0.0037	HOMO−5	LUMO+7	6.49
153	318.77	0.0035	HOMO−68	LUMO	5.01
154	318.49	0.0033	HOMO−69	LUMO	11.81
155	318.07	0.0025	HOMO	LUMO+9	4.73
156	317.70	0.0056	HOMO−4	LUMO+7	5.62
157	317.34	0.0007	HOMO−2	LUMO+7	15.18
158	317.19	0.0006	HOMO−8	LUMO+3	3.46
159	316.96	0.0132	HOMO−5	LUMO+8	12.38
160	316.46	0.0021	HOMO−5	LUMO+7	5.06
161	316.27	0.0010	HOMO−58	LUMO	6.79
162	315.88	0.0015	HOMO	LUMO+9	7.40
163	315.76	0.0041	HOMO−7	LUMO+5	5.70
164	315.49	0.0051	HOMO−12	LUMO+2	5.69
165	314.88	0.0118	HOMO−1	LUMO+8	6.97
166	314.25	0.0008	HOMO−10	LUMO+4	5.75
167	314.10	0.0012	HOMO−5	LUMO+7	9.01
168	313.88	0.0050	HOMO−22	LUMO+1	5.92

169	313.69	0.0038	HOMO	LUMO+10	4.10
170	313.29	0.0023	HOMO−6	LUMO+7	6.33
171	313.26	0.0075	HOMO−78	LUMO	3.43
172	312.87	0.0076	HOMO−1	LUMO+8	6.19
173	312.41	0.0024	HOMO−53	LUMO	3.05
174	312.06	0.0050	HOMO−5	LUMO+8	8.90
175	311.94	0.0022	HOMO−53	LUMO	4.41
176	311.51	0.0060	HOMO−2	LUMO+8	4.00
177	311.24	0.0021	HOMO−7	LUMO+5	3.48
178	311.10	0.0031	HOMO−4	LUMO+8	12.30
179	311.06	0.0005	HOMO−12	LUMO+2	5.14
180	310.62	0.0003	HOMO−3	LUMO+8	5.09

Table S2. Full list of electronic excitations in hydrated $Cu_{28}O_{14}(CO)_2$ as calculated with TD-PBE0[1]/Def2-SVP[2]/SMD-H_2O[4]. The wavelengths λ, oscillator strengths f, and the dominant orbital configuration of the excitation and its contribution (in %).

Transition	λ [nm]	f	OriginMO	TargetMO	Contrib.%
1	626.45	0.0001	HOMO	LUMO	92.87
2	589.25	0.0015	HOMO−1	LUMO	55.32
3	576.43	0.0010	HOMO	LUMO+1	84.74
4	557.03	0.0019	HOMO−4	LUMO	51.75
5	550.96	0.0029	HOMO−1	LUMO+1	50.01
6	544.28	0.0038	HOMO	LUMO+2	74.18
7	538.86	0.0006	HOMO−5	LUMO	46.60
8	532.90	0.0020	HOMO	LUMO+3	28.11
9	532.08	0.0098	HOMO	LUMO+3	21.98
10	528.98	0.0061	HOMO−4	LUMO+1	16.61
11	526.26	0.0029	HOMO−2	LUMO	40.37
12	524.72	0.0103	HOMO−1	LUMO+2	27.66
13	523.85	0.0010	HOMO−1	LUMO+2	20.90
14	519.28	0.0028	HOMO−1	LUMO+3	33.06
15	512.16	0.0005	HOMO−6	LUMO	15.31
16	510.81	0.0023	HOMO−2	LUMO+1	21.52
17	507.37	0.0035	HOMO−2	LUMO+1	22.85
18	503.20	0.0023	HOMO−3	LUMO+1	31.19
19	501.51	0.0035	HOMO	LUMO+4	33.13
20	497.05	0.0027	HOMO−8	LUMO	39.12
21	493.77	0.0033	HOMO−6	LUMO+1	20.02
22	491.60	0.0037	HOMO−4	LUMO+2	29.05
23	488.84	0.0003	HOMO−5	LUMO+2	17.55
24	488.30	0.0159	HOMO−4	LUMO+2	23.80
25	486.37	0.0074	HOMO−2	LUMO+4	12.57
26	485.20	0.0105	HOMO−5	LUMO+3	19.01
27	484.70	0.0140	HOMO−5	LUMO+2	12.55
28	479.91	0.0040	HOMO−5	LUMO+2	11.57
29	476.67	0.0096	HOMO−5	LUMO+3	21.51
30	475.30	0.0004	HOMO−4	LUMO+3	21.80

31	474.93	0.0098	HOMO−4	LUMO+3	25.36
32	469.21	0.0010	HOMO−2	LUMO+3	30.06
33	468.67	0.0046	HOMO−8	LUMO+1	8.69
34	467.52	0.0038	HOMO−3	LUMO+3	36.96
35	464.95	0.0019	HOMO−3	LUMO+3	19.04
36	463.87	0.0068	HOMO−15	LUMO	16.43
37	460.78	0.0049	HOMO−8	LUMO+1	12.05
38	457.97	0.0048	HOMO−3	LUMO+4	8.36
39	454.80	0.0083	HOMO−10	LUMO	13.20
40	449.24	0.0014	HOMO−6	LUMO+2	55.08
41	447.58	0.0047	HOMO−6	LUMO+3	26.41
42	445.72	0.0087	HOMO−6	LUMO+3	38.02
43	443.97	0.0065	HOMO−2	LUMO+4	25.43
44	440.36	0.0041	HOMO−16	LUMO	13.74
45	439.61	0.0123	HOMO−16	LUMO	11.57
46	436.19	0.0053	HOMO−5	LUMO+4	19.11
47	436.14	0.0109	HOMO−4	LUMO+4	30.62
48	432.78	0.0022	HOMO−11	LUMO	19.32
49	431.02	0.0151	HOMO−7	LUMO+1	13.61
50	428.67	0.0086	HOMO−9	LUMO+1	27.16
51	423.85	0.0061	HOMO−6	LUMO+4	18.52
52	421.81	0.0031	HOMO−10	LUMO+1	31.02
53	421.51	0.0083	HOMO−12	LUMO	23.58
54	419.34	0.0073	HOMO−7	LUMO+2	20.97
55	417.74	0.0006	HOMO−28	LUMO	12.44
56	416.38	0.0041	HOMO−15	LUMO+1	10.67
57	415.14	0.0032	HOMO−14	LUMO	17.70
58	414.25	0.0005	HOMO−6	LUMO+4	5.68
59	412.84	0.0112	HOMO−9	LUMO+1	4.62
60	412.21	0.0044	HOMO−7	LUMO+3	11.99
61	411.47	0.0087	HOMO−7	LUMO+3	10.24
62	409.29	0.0006	HOMO−7	LUMO+3	7.74
63	408.87	0.0067	HOMO−8	LUMO+2	40.93
64	407.95	0.0016	HOMO−1	LUMO+5	27.03
65	406.90	0.0044	HOMO−8	LUMO+2	12.75
66	406.18	0.0100	HOMO−8	LUMO+2	8.09
67	405.59	0.0016	HOMO−8	LUMO+3	9.82
68	404.53	0.0015	HOMO−8	LUMO+3	34.91
69	402.65	0.0005	HOMO−3	LUMO+6	10.54
70	402.07	0.0015	HOMO−3	LUMO+6	11.14
71	401.78	0.0014	HOMO−2	LUMO+5	15.34
72	400.86	0.0019	HOMO−11	LUMO+1	13.04
73	399.34	0.0214	HOMO−9	LUMO+2	30.33
74	398.75	0.0012	HOMO	LUMO+7	10.13
75	398.51	0.0043	HOMO	LUMO+7	40.46
76	397.99	0.0013	HOMO−10	LUMO+3	10.13
77	396.79	0.0049	HOMO−10	LUMO+2	31.07
78	396.61	0.0016	HOMO−8	LUMO+4	8.45

79	395.91	0.0020	HOMO	LUMO+7	5.51
80	394.93	0.0003	HOMO−9	LUMO+2	15.31
81	394.75	0.0036	HOMO−1	LUMO+6	30.98
82	393.52	0.0087	HOMO−61	LUMO	9.20
83	393.16	0.0019	HOMO−9	LUMO+3	21.29
84	392.16	0.0029	HOMO−9	LUMO+3	12.87
85	389.33	0.0041	HOMO−10	LUMO+3	11.58
86	388.65	0.0069	HOMO−21	LUMO	9.68
87	387.69	0.0013	HOMO−12	LUMO+1	30.62
88	387.13	0.0107	HOMO−13	LUMO+1	14.87
89	386.25	0.0026	HOMO−5	LUMO+5	15.88
90	384.99	0.0016	HOMO−3	LUMO+5	14.25
91	384.92	0.0014	HOMO−1	LUMO+7	34.70
92	383.63	0.0032	HOMO−7	LUMO+6	10.19
93	382.23	0.0090	HOMO−12	LUMO+2	17.73
94	381.03	0.0026	HOMO−17	LUMO+1	10.29
95	380.11	0.0011	HOMO−3	LUMO+6	9.58
96	379.23	0.0003	HOMO−12	LUMO+2	11.35
97	378.49	0.0074	HOMO−7	LUMO+6	8.70
98	378.17	0.0017	HOMO−14	LUMO+2	10.55
99	377.52	0.0039	HOMO−4	LUMO+7	12.32
100	376.76	0.0039	HOMO−2	LUMO+7	13.19
101	375.95	0.0043	HOMO−2	LUMO+6	11.46
102	375.55	0.0035	HOMO−4	LUMO+7	21.11
103	375.37	0.0077	HOMO−4	LUMO+6	17.60
104	374.92	0.0036	HOMO−2	LUMO+7	13.51
105	374.37	0.0009	HOMO−6	LUMO+6	8.88
106	374.26	0.0066	HOMO−3	LUMO+7	24.26
107	372.90	0.0014	HOMO−11	LUMO+2	16.59
108	372.08	0.0017	HOMO−3	LUMO+7	10.25
109	370.89	0.0019	HOMO−5	LUMO+7	9.95
110	370.51	0.0036	HOMO−3	LUMO+7	20.93
111	369.44	0.0019	HOMO−13	LUMO+3	11.53
112	369.09	0.0022	HOMO−6	LUMO+6	10.03
113	368.56	0.0052	HOMO−11	LUMO+4	15.20
114	368.41	0.0097	HOMO−20	LUMO	13.94
115	367.35	0.0076	HOMO−13	LUMO+3	10.88
116	366.69	0.0038	HOMO−14	LUMO+3	6.83
117	365.01	0.0002	HOMO−15	LUMO+2	4.39
118	364.46	0.0046	HOMO−14	LUMO+3	11.76
119	363.89	0.0027	HOMO−12	LUMO+3	20.18
120	362.85	0.0067	HOMO−20	LUMO	8.10
121	362.31	0.0020	HOMO−14	LUMO+3	11.48
122	361.67	0.0014	HOMO−18	LUMO+1	7.37
123	361.29	0.0034	HOMO−14	LUMO+3	11.82
124	360.89	0.0064	HOMO−21	LUMO	8.00
125	359.58	0.0038	HOMO−13	LUMO+4	19.12
126	358.83	0.0011	HOMO	LUMO+8	11.91

127	358.10	0.0064	HOMO	LUMO+8	7.29
128	357.53	0.0077	HOMO−12	LUMO+3	13.93
129	357.24	0.0052	HOMO−13	LUMO+3	10.11
130	356.21	0.0014	HOMO−19	LUMO+1	26.25
131	356.06	0.0028	HOMO−8	LUMO+5	10.60
132	355.07	0.0054	HOMO−14	LUMO+4	9.88
133	354.80	0.0086	HOMO−16	LUMO+4	9.22
134	353.31	0.0012	HOMO−6	LUMO+7	31.64
135	352.70	0.0010	HOMO−6	LUMO+7	10.43
136	351.89	0.0039	HOMO−1	LUMO+8	11.77
137	350.64	0.0052	HOMO−17	LUMO+2	7.02
138	350.56	0.0048	HOMO−1	LUMO+8	15.76
139	349.94	0.0007	HOMO−24	LUMO	11.43
140	349.05	0.0079	HOMO−9	LUMO+5	5.74
141	348.35	0.0028	HOMO−16	LUMO+3	7.93
142	347.80	0.0017	HOMO−8	LUMO+6	8.07
143	347.12	0.0008	HOMO−17	LUMO+3	24.51
144	346.90	0.0027	HOMO−15	LUMO+2	7.87
145	346.21	0.0064	HOMO−8	LUMO+6	5.31
146	345.59	0.0028	HOMO	LUMO+9	8.35
147	345.15	0.0048	HOMO−10	LUMO+5	8.85
148	344.49	0.0009	HOMO−18	LUMO+2	7.22
149	344.20	0.0016	HOMO−18	LUMO+2	9.08
150	343.39	0.0047	HOMO−31	LUMO	5.09
151	343.35	0.0035	HOMO	LUMO+10	11.92
152	342.55	0.0017	HOMO−23	LUMO+1	7.23
153	342.45	0.0019	HOMO	LUMO+10	8.85
154	342.01	0.0021	HOMO−4	LUMO+8	8.28
155	341.52	0.0034	HOMO−20	LUMO+2	6.15
156	341.34	0.0021	HOMO	LUMO+10	9.81
157	341.28	0.0043	HOMO−19	LUMO+2	5.72
158	340.34	0.0144	HOMO−9	LUMO+5	9.95
159	340.17	0.0072	HOMO−7	LUMO+7	8.36
160	340.02	0.0022	HOMO−18	LUMO+2	7.47
161	339.87	0.0013	HOMO−3	LUMO+8	18.22
162	339.58	0.0026	HOMO−15	LUMO+2	6.22
163	338.91	0.0020	HOMO−15	LUMO+3	5.27
164	338.69	0.0011	HOMO−1	LUMO+9	13.40
165	338.04	0.0019	HOMO−30	LUMO	13.48
166	337.64	0.0013	HOMO−15	LUMO+3	9.81
167	337.41	0.0033	HOMO	LUMO+9	5.32
168	336.95	0.0014	HOMO−7	LUMO+6	7.20
169	336.84	0.0020	HOMO−18	LUMO+3	11.12
170	336.57	0.0095	HOMO−25	LUMO	9.89
171	336.07	0.0011	HOMO−1	LUMO+10	6.23
172	335.20	0.0013	HOMO−16	LUMO+3	4.70
173	334.63	0.0010	HOMO−10	LUMO+6	11.29
174	334.33	0.0054	HOMO−20	LUMO+3	14.84

175	334.11	0.0014	HOMO−10	LUMO+5	4.48
176	333.85	0.0023	HOMO−33	LUMO	5.50
177	333.69	0.0011	HOMO−8	LUMO+7	4.21
178	333.17	0.0010	HOMO−10	LUMO+6	9.69
179	332.81	0.0004	HOMO−15	LUMO+5	4.61
180	332.53	0.0011	HOMO−6	LUMO+8	7.57

Example input files

Periodic DFT (structural optimization)

VASP INCAR-file:

```
ENCUT  =  400
EDIFF  = 1E-06
EDIFFG = -0.03
LWAVE  = .FALSE.
ISMEAR = -5
LREAL  = Auto
LPLANE = .TRUE.
NSIM = 1
IVDW = 12
NSW = 300
IBRION=2
ISIF=2
NCORE  = 12
LCHARG = .FALSE.
NELM = 140
NBANDS = 648
LMAXMIX=4
ALGO = FAST
LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = 2 -1 -1 -1
LDAUU = 3.6 0 0 0
LDAUJ = 0.0 0 0 0
LDAUPRINT= 0
GGA = PE
```

Cluster DFT, uDFT and TD-DFT

Gaussian Route section, S0 DFT:

```
#p opt=(maxstep=10) freq pbe1pbe/Def2SVP
scrf=(smd,solvent=water) empiricaldispersion=gd3bj scf=(xqc,maxconv=150)

Comment

0 1
```

Gaussian Route section, 1-electron reduced uDFT:

```
#p opt freq upbe1pbe/Def2SVP scrf=(smd,solvent=water)
empiricaldispersion=gd3bj scf=(xqc,maxconv=150)

Comment
```

-1 2

Gaussian Route section, UV-vis calculation TD-DFT:

#p td=(nstates=180,maxdavidson=1000) pbe1pbe/Def2SVP scrf=(smd,solvent=water) guess=read scf=(xqc,maxconv=150) geom=check

Comment

0 1

Gaussian Route section, S1 TD-DFT:

#p opt=(maxstep=5) td=(nstates=3) pbe1pbe/Def2SVP scrf=(smd,solvent=water) guess=read empiricaldispersion=gd3bj scf=(xqc,maxconv=150)

Comment

0 1

DFT-optimized coordinates in xyz-format

*Periodic DFT, 2*CO*

128
One *CO at Cu_{CUS}, one at $Cu@V_{OCUS}$, Lattice="9.1556186 -5.28599886 0.0 9.1556186 5.28599886 0.0 0.0 0.0 36.5"

Cu	6.51242000	2.63894000	0.95584000
Cu	1.81262000	0.67594000	0.92707000
Cu	12.53893000	-1.91472000	0.91711000
Cu	5.14726000	0.52580000	1.09465000
Cu	6.67500533	3.43143422	15.24196118
Cu	1.61796093	0.80255986	15.24669808
Cu	12.08810393	-1.82780338	15.18333337
Cu	4.64188377	0.85113835	15.23420607
Cu	-0.00855027	0.02813862	13.06131032
Cu	4.43507910	2.55746353	12.93146213
Cu	3.08842637	-0.09242865	12.93468428
Cu	10.61031200	-2.63414881	12.96385253
Cu	12.20748860	-3.52399886	10.59034000
Cu	4.57781000	-0.88100000	10.59034000
Cu	6.10375000	1.76200000	10.59034000
Cu	1.52594140	-0.88099886	10.59034000
Cu	6.10375000	3.52400000	8.09849000
Cu	1.52594140	0.88099886	8.09849000
Cu	12.20749000	-1.76200000	8.09849000
Cu	4.57781000	0.88100000	8.09849000
Cu	0.00000000	0.00000000	5.60665000
Cu	13.73342860	-2.64299886	5.60665000
Cu	3.05187000	0.00000000	5.60665000
Cu	10.68156000	-2.64300000	5.60665000
Cu	3.18367000	1.68599000	3.11608000
Cu	4.48621000	-0.91652000	3.35390000
Cu	6.09437000	1.86182000	3.34665000
Cu	10.69796000	4.35285000	3.23245000
Cu	10.13726000	-2.30772000	1.26673000
Cu	10.29222146	1.07910176	15.46422962
Cu	6.41062000	-1.57531000	1.11247000
Cu	8.00337000	-4.45575000	0.98164000
Cu	8.89897187	-1.75688120	15.37850653
Cu	6.12122382	-0.04615898	13.07241568
Cu	6.12614312	-1.91794039	15.22041726
Cu	16.63355284	0.76794088	15.23536006
Cu	10.78022062	2.59397374	12.93474693
Cu	7.64839737	-2.64987795	12.93001832
Cu	9.12940694	0.09800842	12.98176287
Cu	13.77821246	2.55150266	12.94319002
Cu	6.10375000	-3.52400000	10.59034000
Cu	16.78529860	-0.88099886	10.59034000
Cu	9.15562000	-3.52400000	10.59034000

Cu	7.50435656	2.65528958	12.80023708
Cu	9.15562000	-1.76200000	8.09849000
Cu	9.15562000	1.76200000	10.59034000
Cu	6.10375000	-1.76200000	8.09849000
Cu	16.78529860	0.88099886	8.09849000
Cu	10.68156000	-0.88100000	10.59034000
Cu	7.62968000	-2.64300000	5.60665000
Cu	12.20749000	1.76200000	10.59034000
Cu	13.73342860	2.64299886	5.60665000
Cu	6.24637000	-3.55500000	3.12397000
Cu	7.66403000	4.41214000	3.21853000
Cu	9.11715000	-3.48901000	3.36623000
Cu	7.62968000	-0.88100000	10.59034000
Cu	12.20749000	0.00000000	5.60665000
Cu	7.62968000	0.88100000	8.09849000
Cu	9.15562000	3.52400000	8.09849000
Cu	10.68156000	0.88100000	8.09849000
Cu	6.10375000	0.00000000	5.60665000
Cu	4.02916000	-1.75439000	0.98206000
Cu	10.68156000	2.64300000	5.60665000
Cu	9.15562000	0.00000000	5.60665000
Cu	7.62968000	2.64300000	5.60665000
Cu	11.43506219	3.44485086	15.27452422
Cu	9.24700000	1.64658000	3.12561000
Cu	10.62760000	-0.86474000	3.37468000
Cu	12.21628000	1.72608000	3.23534000
Cu	7.56822000	-0.84915000	3.31770000
Cu	15.16904406	-0.08955739	12.90169567
Cu	12.20748860	3.52399886	8.09849000
Cu	15.25936000	-0.00000000	5.60665000
Cu	13.93726000	0.87034000	0.98019000
Cu	13.73343000	-0.88100000	10.59034000
Cu	13.73343000	0.88100000	8.09849000
Cu	13.53276677	0.87773330	15.21480869
Cu	13.79082000	-0.87593000	3.22582000
Cu	7.60473000	0.51677000	1.11259000
Cu	9.26183000	3.34007000	0.98544000
Cu	10.89852000	0.56775000	0.98241000
Cu	12.08492321	0.00055972	13.06024952
Cu	7.76268429	1.18434480	14.99731826
Cu	9.05761410	3.25578698	14.95371030
O	3.10239807	1.72297784	15.75987433
O	9.43241000	5.09326000	0.45011000
O	5.94391788	3.46001310	13.45816572
O	9.14369856	5.26924048	14.91918834
O	0.00000000	0.00000000	11.21330000
O	2.91277094	1.66043414	12.39904680
O	12.20748860	-3.52399886	8.72145000
O	6.10375000	3.52400000	9.96738000

O	6.10375000	3.52400000	6.22961000
O	0.00000000	0.00000000	7.47553000
O	0.04002000	-0.00673000	3.79081000
O	12.20748860	-3.52399886	4.98369000
O	3.45087000	1.52809000	1.24982000
O	15.30456000	-1.71354000	2.59094000
O	15.11226618	1.63446882	15.76940811
O	9.11068201	-1.67111597	13.51803345
O	15.31700644	1.67096705	12.40521177
O	6.10375000	-3.52400000	8.72145000
O	9.15562000	-1.76200000	9.96738000
O	9.15562000	-1.76200000	6.22961000
O	6.10375000	-3.52400000	4.98369000
O	6.40274000	-3.50301000	1.25437000
O	9.08783000	-1.72539000	2.77166000
O	6.27259037	-0.07316443	14.94441000
O	6.10375000	0.00000000	11.21330000
O	9.15367646	1.84281243	12.38957436
O	9.15562000	1.76200000	8.72145000
O	12.20749000	0.00000000	7.47553000
O	6.10375000	0.00000000	7.47553000
O	6.01436000	0.05399000	3.80318000
O	9.15562000	1.76200000	4.98369000
O	9.27614000	1.47989000	1.25712000
O	12.50222000	-0.14949000	0.44081000
O	12.23680000	-0.03920000	3.78953000
O	11.88686056	0.02067992	14.91651672
O	3.15686521	-1.81984814	13.57239227
O	12.20749000	0.00000000	11.21330000
O	12.20748860	3.52399886	9.96738000
O	12.20748860	3.52399886	6.22961000
O	12.18354000	3.45987000	2.61609000
C	9.08860209	-1.81029560	17.15906472
C	9.41262182	1.05722159	17.12637893
O	9.23691957	-1.95175980	18.29004870
O	8.81285979	1.49074170	18.02345672

Cluster, S0 2*CO

76
Cu28O14hyd9OH9H1H2O_2CO_S0_pcm

O	5.59540	1.01660	0.73960
Cu	-1.22860	-3.34500	-1.40780
Cu	-0.83410	-4.91660	0.77310
Cu	1.00030	-5.44770	-1.45800
O	0.46890	-3.77980	-1.90410
Cu	4.77850	1.00820	-0.97710
Cu	-2.45750	1.83340	-1.22630
Cu	4.67550	-1.72010	-1.15760

Cu	-4.03630	2.36460	0.92200
Cu	-1.97760	0.08370	0.66650
Cu	0.73500	2.36070	-0.80890
Cu	-0.80840	-0.78630	-1.62330
Cu	2.90600	-1.36010	0.93430
Cu	1.60450	-2.50570	-1.22950
Cu	1.75430	3.77740	1.33170
Cu	-0.12090	-2.01600	0.68220
Cu	0.78490	0.74040	1.25160
Cu	2.11150	-4.20700	0.85310
Cu	3.91310	1.47030	1.30690
Cu	-0.86280	1.26960	3.33740
Cu	1.25600	-0.99440	3.31290
Cu	1.32200	4.71020	-0.93870
Cu	-1.40780	4.77980	-1.09270
Cu	-1.13860	2.97090	0.98060
Cu	2.28890	0.58080	-0.76650
Cu	3.18750	2.98600	-0.83560
O	-3.66930	0.63210	1.39460
O	-0.24480	-0.26010	0.08910
O	0.41370	-3.73420	1.34300
O	-0.46740	-0.48990	3.89790
O	2.91350	-1.21050	-0.95070
O	2.88570	-1.42520	2.77150
O	2.17920	2.00690	1.70890
O	-1.06430	2.98080	-0.89920
O	-1.19010	2.92990	2.81820
O	-1.16750	-0.45490	-4.53060
O	1.27740	1.18150	-3.44480
C	-0.97440	-0.56440	-3.41330
C	1.28470	1.23220	-2.29250
O	1.41120	5.49080	0.78930
Cu	-2.95460	-2.77860	0.62420
O	-3.01390	-2.81840	-1.21830
Cu	-3.42890	-1.00270	-1.38680
Cu	-5.37310	1.36710	-1.38580
Cu	-4.94010	-0.52380	0.81700
O	-3.74990	0.72720	-1.85300
O	5.05410	4.07700	-0.18620
H	5.54350	3.48000	-0.77770
O	4.07590	1.96460	-2.49910
H	4.79420	2.58080	-2.70100
O	3.83780	-4.68960	0.29560
H	3.61590	-4.92660	-0.61660
O	1.69370	-7.07990	-0.89740
H	2.37280	-6.73690	-0.29810
O	-2.27150	-5.95800	0.19940
H	-2.86440	-5.24460	-0.07720
O	-6.10850	-1.84710	0.21410

H	-5.80740	-1.89210	-0.70480
O	-7.02180	2.00960	-0.81590
H	-7.00470	1.69870	0.09960
O	-4.12440	4.20420	0.54430
H	-3.74790	4.17660	-0.34840
O	1.43120	4.25300	-2.73690
H	2.19710	3.67610	-2.87130
O	-2.57220	-2.55300	2.47350
H	-1.72070	-3.01340	2.50640
H	5.72830	0.08730	0.97810
H	0.47710	5.63710	1.00590
H	-2.10610	3.14970	3.04340
H	3.06460	-2.34760	3.00450
H	0.40000	-3.64870	2.30870
H	-3.54600	0.59810	2.35510
H	-1.07230	-1.04880	3.37560
H	2.14110	1.96070	2.68050
H	-3.66450	-3.43100	-1.58410
H	5.05410	3.57340	0.64400

Cluster, S1 2 *CO

76

Cu28O14hyd9OH9H1H2O_2CO_S1_pcm

O	2.65740	5.01100	0.73228
Cu	1.86299	-3.06057	-1.36910
Cu	3.32246	-3.71207	0.82797
Cu	4.89529	-2.61727	-1.39732
O	3.26104	-2.00218	-1.86075
Cu	2.17147	4.35387	-0.98430
Cu	-2.95747	-0.81491	-1.22470
Cu	4.24900	2.57960	-1.13600
Cu	-4.37603	-1.70637	0.90012
Cu	-1.46938	-1.32427	0.70136
Cu	-1.36432	2.00732	-0.80028
Cu	0.33069	-0.71238	-1.76626
Cu	2.85163	1.42854	0.95199
Cu	2.98167	-0.30557	-1.25625
Cu	-1.89551	3.71455	1.29500
Cu	1.60388	-1.16470	0.66159
Cu	-0.11265	1.05326	1.23194
Cu	4.59230	-0.96099	0.90081
Cu	1.25336	3.97651	1.29461
Cu	-1.56859	0.11929	3.32704
Cu	1.52157	0.37666	3.32654
Cu	-2.87679	3.93897	-0.98518
Cu	-4.62310	1.84031	-1.13976
Cu	-3.05466	0.94288	0.95235
Cu	0.95977	2.15544	-0.79746

Cu	-0.36762	4.33337	-0.86368
O	-2.79338	-2.49006	1.39102
O	0.00945	-0.44376	0.10765
O	3.16414	-1.99634	1.38556
O	0.05201	-0.65826	3.90606
O	2.76912	1.50480	-0.93405
O	2.87484	1.38422	2.78970
O	-0.24642	2.95194	1.69097
O	-3.00149	0.99196	-0.92385
O	-3.06950	0.88910	2.79032
O	0.23935	-1.93702	-4.45924
O	-0.24556	1.75414	-3.43445
C	0.24449	-1.61053	-3.36302
C	-0.12833	1.38955	-2.30637
O	-3.44732	4.50480	0.73469
Cu	0.33134	-4.05017	0.65656
O	0.34103	-4.13333	-1.18549
Cu	-1.33906	-3.33359	-1.37296
Cu	-4.40375	-3.38863	-1.39708
Cu	-2.67031	-4.20758	0.82561
O	-2.89107	-2.51537	-1.85740
O	-0.20745	6.39244	-0.01275
H	0.73730	6.31885	-0.22806
O	1.04953	4.48894	-2.53351
H	1.01913	5.44482	-2.67799
O	5.99360	0.16467	0.36147
H	5.97936	-0.03524	-0.58510
O	6.60421	-3.06477	-0.81862
H	6.78111	-2.27166	-0.29218
O	3.24562	-5.48570	0.26069
H	2.34434	-5.48076	-0.09254
O	-2.34895	-5.95905	0.27057
H	-2.07255	-5.77073	-0.63764
O	-5.93607	-4.27191	-0.83401
H	-5.63184	-4.59108	0.02647
O	-5.86253	-0.65365	0.45077
H	-5.60117	-0.41321	-0.45031
O	-2.48113	3.84662	-2.80194
H	-1.59969	3.45568	-2.87626
O	0.37106	-3.51357	2.47662
H	1.32448	-3.45976	2.63040
H	3.47028	4.54432	0.97618
H	-4.14801	3.87090	0.95222
H	-3.81180	0.31041	3.01824
H	3.70607	0.95039	3.03132
H	3.05221	-1.94053	2.34691
H	-2.71194	-2.42156	2.35484
H	0.13071	-1.50930	3.43368
H	-0.24120	2.88647	2.66267

H	0.41380	-5.03412	-1.52591
H	-0.24809	6.01127	0.87980

Cluster, S1 *OCCO

76
Cu28O14hyd9OH9H1H2O_OCCO_S1_pcm

O	-4.51336	-3.37477	0.89680
Cu	-0.39451	3.54193	-1.43619
Cu	-1.40999	4.80407	0.74967
Cu	-3.32823	4.42488	-1.44207
O	-2.11775	3.16269	-1.89280
Cu	-3.81644	-3.03460	-0.84420
Cu	3.02447	-0.54282	-1.21607
Cu	-4.95371	-0.54588	-1.03123
Cu	4.71002	-0.28141	0.86641
Cu	1.92737	0.58728	0.66093
Cu	0.35627	-2.45849	-1.13977
Cu	0.05239	1.06392	-1.74392
Cu	-3.16121	-0.04314	1.01388
Cu	-2.52278	1.53042	-1.21064
Cu	0.17105	-4.12262	1.41331
Cu	-0.82633	1.81327	0.68253
Cu	-0.12116	-1.11972	1.12585
Cu	-3.72261	2.85454	0.89380
Cu	-2.79329	-3.02167	1.42701
Cu	1.42468	-0.68014	3.34470
Cu	-1.48136	0.39969	3.35695
Cu	0.92412	-4.79605	-0.85954
Cu	3.39747	-3.64661	-1.07206
Cu	2.39054	-2.10805	0.98933
Cu	-1.77049	-1.56117	-0.76949
Cu	-1.51712	-4.09532	-0.71473
O	3.61552	1.11591	1.32847
O	0.21547	0.40116	0.08828
O	-1.98629	3.19522	1.35226
O	0.29620	0.72672	3.90448
O	-3.08170	-0.16420	-0.82514
O	-3.14335	0.04853	2.85140
O	-0.99417	-2.72239	1.78594
O	2.26646	-2.18621	-0.87465
O	2.45013	-2.02986	2.82764
O	1.02334	-0.66975	-3.81296
O	-1.48863	-2.06124	-3.48598
C	0.17567	-0.39455	-2.99490
C	-0.82320	-1.62402	-2.56464
O	1.23400	-5.51139	0.87320
Cu	1.43901	3.83351	0.56103
O	1.43989	3.86627	-1.27977

Cu	2.62024	2.42599	-1.44990
Cu	5.41631	1.17471	-1.47950
Cu	4.22720	2.70640	0.72222
O	3.67157	1.01115	-1.91747
O	-2.83714	-5.71361	-0.45652
H	-3.44942	-5.56731	-1.19512
O	-4.55451	-2.15622	-2.42720
H	-5.30646	-2.70442	-2.68394
O	-5.42793	2.18499	0.46204
H	-5.23807	1.87536	-0.43670
O	-4.46190	5.79115	-0.88986
H	-3.92689	6.15407	-0.17041
O	-1.01913	6.47034	0.00262
H	-1.65655	6.42555	-0.72583
O	5.03554	4.23870	0.03422
H	5.38657	3.85190	-0.78101
O	7.16087	1.48492	-0.91712
H	6.98639	2.19290	-0.28115
O	5.58868	-1.87366	0.41091
H	5.21887	-1.99292	-0.47692
O	0.64942	-4.32517	-2.64669
H	-0.29561	-4.25732	-2.83721
O	1.20572	3.42635	2.39402
H	0.28855	3.70370	2.52541
H	-4.98789	-2.54296	1.04687
H	2.14155	-5.21777	1.05075
H	3.37065	-1.82672	3.04892
H	-3.71056	0.79892	3.07972
H	-1.91545	3.11935	2.31630
H	3.50567	1.09969	2.29247
H	0.57705	1.51134	3.39694
H	-0.95707	-2.57973	2.74735
H	1.74355	4.68825	-1.68551
H	-3.30139	-5.28984	0.28626

Cluster, 1-electron reduced 2*CO

76
Cu28O14hyd9OH9H1H2O_2CO_1red_pcm

O	4.59632	-3.36628	0.70432
Cu	-3.27832	-1.40409	-1.38003
Cu	-4.13129	-2.76488	0.81145
Cu	-3.27717	-4.46843	-1.42319
O	-2.43318	-2.93800	-1.88008
Cu	4.01470	-2.78140	-1.00864
Cu	-0.36207	3.01384	-1.21379
Cu	1.95868	-4.58085	-1.16748
Cu	-1.03473	4.56273	0.91674
Cu	-1.36306	1.46429	0.67222

Cu	2.20838	1.05985	-0.83860
Cu	-0.93147	0.06389	-1.69852
Cu	1.02366	-3.04207	0.92894
Cu	-0.72534	-2.88338	-1.21599
Cu	3.97136	1.32353	1.29099
Cu	-1.62498	-1.24388	0.68918
Cu	1.08100	-0.05354	1.25466
Cu	-1.59242	-4.41914	0.87345
Cu	3.77576	-1.83025	1.27514
Cu	0.36866	1.50914	3.32715
Cu	0.17703	-1.58576	3.31160
Cu	4.33344	2.27257	-0.98494
Cu	2.50842	4.30508	-1.12801
Cu	1.39593	2.87224	0.95829
Cu	2.01841	-1.27326	-0.81739
Cu	4.36130	-0.26704	-0.87613
O	-2.03838	3.10752	1.40132
O	-0.38058	-0.00016	0.10861
O	-2.40996	-2.85903	1.36671
O	-0.63430	0.01495	3.89980
O	1.11354	-2.95959	-0.95646
O	0.97807	-3.06769	2.76672
O	2.97932	-0.20007	1.68029
O	1.44072	2.82079	-0.91904
O	1.34659	2.88582	2.79635
O	-1.93928	0.12918	-4.47959
O	1.76814	-0.09148	-3.46339
C	-1.61217	0.10804	-3.38640
C	1.44293	-0.06270	-2.31749
O	4.97670	2.74823	0.73652
Cu	-4.03396	0.24437	0.65464
O	-4.11937	0.25590	-1.18715
Cu	-3.08583	1.80391	-1.36818
Cu	-2.69759	4.84442	-1.37763
Cu	-3.75616	3.23655	0.83815
O	-2.05251	3.22396	-1.84657
O	6.35935	-0.72431	0.23131
H	5.99078	-1.62463	0.19603
O	4.39269	-1.65847	-2.53455
H	5.34653	-1.78142	-2.63336
O	-0.70731	-5.99302	0.34991
H	-0.84117	-5.90035	-0.60402
O	-3.96038	-6.09796	-0.84248
H	-3.20618	-6.35660	-0.29267
O	-5.88268	-2.42111	0.26357
H	-5.74482	-1.53150	-0.09246
O	-5.53044	3.15829	0.26171
H	-5.36721	2.88244	-0.65145
O	-3.35527	6.48461	-0.80585

H	-3.40312	6.30762	0.14365
O	0.23555	5.89045	0.51719
H	0.49348	5.56727	-0.35957
O	4.16811	1.93708	-2.81816
H	3.75550	1.06412	-2.87490
O	-3.67954	0.11995	2.51491
H	-3.43322	-0.81522	2.55010
H	4.02207	-4.10566	0.95115
H	4.44175	3.52692	0.95670
H	0.87633	3.70174	3.02281
H	0.42231	-3.82551	3.00008
H	-2.34232	-2.77992	2.33049
H	-1.96484	2.99682	2.36119
H	-1.44159	0.05993	3.35645
H	2.93173	-0.20556	2.65335
H	-5.02435	0.31223	-1.51945
H	5.87998	-0.33679	0.98323

Cluster, 1-electron reduced HS-*OCCO

76

Cu28O14hyd9OH9H1H2O_OCCO_1red_pcm

O	-4.77093	-2.94957	0.95132
Cu	-0.06264	3.55190	-1.45843
Cu	-0.94649	4.91590	0.72350
Cu	-2.90478	4.69479	-1.45498
O	-1.81535	3.32566	-1.90323
Cu	-4.05785	-2.68631	-0.79652
Cu	2.97287	-0.85867	-1.25286
Cu	-4.96789	-0.10695	-0.99605
Cu	4.69210	-0.69768	0.84503
Cu	1.98047	0.66824	0.61179
Cu	0.11675	-2.37810	-1.07897
Cu	-0.05422	0.75954	-1.71735
Cu	-3.12470	0.24781	1.03487
Cu	-2.38669	1.77134	-1.20274
Cu	-0.16955	-4.11149	1.44800
Cu	-0.62323	1.93890	0.68316
Cu	-0.27261	-1.03034	1.17775
Cu	-3.42393	3.18330	0.89469
Cu	-3.02271	-2.74835	1.46898
Cu	1.40007	-0.78206	3.34496
Cu	-1.39723	0.55498	3.36504
Cu	0.50477	-4.86661	-0.82278
Cu	3.07092	-3.94551	-1.05832
Cu	2.21933	-2.30752	0.99528
Cu	-1.93228	-1.37444	-0.80603
Cu	-1.86214	-3.94895	-0.67261
O	3.73238	0.79495	1.30464

O	0.23174	0.43404	0.13912
O	-1.66191	3.37027	1.34183
O	0.40583	0.72489	3.90011
O	-3.09484	0.15262	-0.80693
O	-3.08686	0.35077	2.87142
O	-1.20362	-2.60892	1.81595
O	2.02531	-2.41797	-0.87903
O	2.29693	-2.22195	2.83300
O	0.46208	-0.74389	-4.14192
O	-1.72156	-2.35833	-3.46306
C	-0.20979	-0.52383	-3.12966
C	-1.05854	-1.74466	-2.61802
O	0.76250	-5.59417	0.91226
Cu	1.80211	3.69209	0.52641
O	1.79492	3.71106	-1.31432
Cu	2.83985	2.16949	-1.48007
Cu	5.51201	0.67171	-1.51511
Cu	4.47864	2.32001	0.68034
O	3.75715	0.66299	-1.94320
O	-3.31756	-5.43444	-0.37777
H	-3.89690	-5.25540	-1.13571
O	-4.84641	-1.72552	-2.34269
H	-5.67814	-2.18716	-2.50504
O	-5.18045	2.69063	0.45290
H	-5.02441	2.34379	-0.43851
O	-3.87657	6.17877	-0.90201
H	-3.24613	6.54155	-0.26371
O	-0.41190	6.55234	0.00267
H	-0.95854	6.53779	-0.79673
O	5.39597	3.78223	-0.02988
H	5.64409	3.37841	-0.87427
O	7.28053	0.83260	-0.95665
H	7.16424	1.56914	-0.33981
O	5.41778	-2.38216	0.42208
H	5.01633	-2.46308	-0.45685
O	0.10725	-4.74737	-2.65090
H	-0.56534	-4.06232	-2.76775
O	1.48958	3.34673	2.36756
H	0.55280	3.58190	2.42158
H	-5.17778	-2.08231	1.09698
H	1.68984	-5.38889	1.10794
H	3.23517	-2.09307	3.03698
H	-3.59203	1.14197	3.10593
H	-1.61461	3.27979	2.30655
H	3.61240	0.79440	2.26639
H	0.75150	1.46838	3.37084
H	-1.14500	-2.47959	2.77834
H	2.17308	4.50348	-1.71552
H	-3.75417	-4.94239	0.33977

Cluster, 1-electron reduced LS-*OCCO

76
Cu28O14hyd9OH9H1H2O_OCCOlsgeom_1red_pcm

O	-4.23429	-3.64175	0.95033
Cu	-0.62577	3.52744	-1.46367
Cu	-1.70996	4.73208	0.72179
Cu	-3.61343	4.20365	-1.45247
O	-2.32123	3.02538	-1.90478
Cu	-3.57647	-3.26815	-0.79795
Cu	3.07797	-0.34148	-1.30412
Cu	-4.88449	-0.86577	-0.99374
Cu	4.74991	0.08680	0.82483
Cu	1.87092	0.84486	0.58614
Cu	0.54484	-2.38528	-0.61858
Cu	0.00093	-0.26426	-1.72001
Cu	-3.11802	-0.22307	1.03399
Cu	-2.69211	1.41899	-1.19941
Cu	0.49478	-4.05739	1.43528
Cu	-1.02309	1.75836	0.64999
Cu	-0.25416	-0.89412	1.20873
Cu	-3.88003	2.62705	0.89684
Cu	-2.53858	-3.16490	1.46440
Cu	1.51920	-0.52160	3.33205
Cu	-1.45499	0.35308	3.35986
Cu	1.27479	-4.69316	-0.83877
Cu	3.66138	-3.37646	-1.07625
Cu	2.56487	-1.89673	0.97870
Cu	-1.76969	-1.68585	-0.67334
Cu	-1.20702	-4.16372	-0.68252
O	3.56599	1.40759	1.28787
O	0.14239	0.53159	-0.02128
O	-2.16878	3.09163	1.33974
O	0.29929	0.80747	3.89108
O	-3.14034	-0.30797	-0.83234
O	-3.09191	-0.11612	2.86983
O	-0.76415	-2.73894	1.80654
O	2.43522	-2.02333	-0.90221
O	2.63239	-1.80001	2.81667
O	0.73935	-2.29117	-3.72478
O	-2.19433	-0.02318	-3.84938
C	-0.13264	-1.38855	-3.33348
C	-1.18072	-0.69914	-3.63675
O	1.64931	-5.37261	0.89610
Cu	1.19776	3.96116	0.51714
O	1.18321	3.97990	-1.32355
Cu	2.45968	2.62419	-1.49349
Cu	5.33591	1.57075	-1.53577
Cu	4.05879	3.03226	0.66370
O	3.60373	1.28306	-1.95988

O	-2.40720	-5.86299	-0.38487
H	-3.00958	-5.77772	-1.14092
O	-3.13764	-3.22967	-2.61021
H	-2.21223	-2.94301	-2.67153
O	-5.53679	1.86177	0.45849
H	-5.32972	1.54482	-0.43368
O	-4.80762	5.51378	-0.89589
H	-4.24138	5.97183	-0.25866
O	-1.44428	6.43313	0.00130
H	-1.98364	6.33236	-0.79684
O	4.73013	4.62220	-0.04720
H	5.03733	4.26352	-0.89254
O	7.05767	2.01050	-0.98120
H	6.82719	2.71876	-0.36334
O	5.73331	-1.46053	0.39851
H	5.34779	-1.60368	-0.47961
O	0.08348	-4.41953	-2.29051
H	0.32221	-3.60725	-2.81836
O	0.94854	3.56935	2.35866
H	-0.01361	3.65245	2.41504
H	-4.77341	-2.85036	1.09761
H	2.53282	-5.02246	1.08970
H	3.53880	-1.52398	3.01864
H	-3.71591	0.58382	3.10632
H	-2.10568	3.00953	2.30462
H	3.45013	1.38728	2.25012
H	0.52104	1.59686	3.36171
H	-0.72447	-2.60224	2.76954
H	1.42955	4.82270	-1.72471
H	-2.91454	-5.44721	0.33464

Cluster, 1-electron reduced LS-*HOCCO

76

Cu28O14hyd10OH9H_OCCOHfront_1red_pcm

O	-4.16666	-3.70284	1.03348
Cu	-0.63731	3.47575	-1.46835
Cu	-1.72861	4.69423	0.70614
Cu	-3.63157	4.12238	-1.45766
O	-2.32841	2.95262	-1.90136
Cu	-3.51901	-3.34520	-0.75096
Cu	3.09893	-0.37575	-1.28154
Cu	-4.85159	-0.95073	-0.91905
Cu	4.77817	0.11540	0.84524
Cu	1.90399	0.90052	0.59114
Cu	0.50651	-2.45605	-1.28832
Cu	-0.16608	-0.08933	-1.61294
Cu	-3.08614	-0.27127	1.07085
Cu	-2.63385	1.32570	-1.19111

Cu	0.56714	-4.06320	1.51245
Cu	-1.07031	1.67914	0.70280
Cu	0.00804	-1.13522	1.03705
Cu	-3.87672	2.56957	0.90917
Cu	-2.47569	-3.20115	1.53854
Cu	1.55924	-0.49743	3.36678
Cu	-1.42352	0.34799	3.39193
Cu	1.34867	-4.71920	-0.75252
Cu	3.72018	-3.37935	-1.01859
Cu	2.61352	-1.88718	1.02643
Cu	-1.72644	-1.74998	-0.56397
Cu	-1.30484	-4.27888	-0.56946
O	3.58203	1.42897	1.29633
O	0.16942	0.50068	0.11521
O	-2.16931	3.05595	1.34291
O	0.32761	0.82571	3.91379
O	-3.10684	-0.40318	-0.82120
O	-3.05618	-0.14411	2.91114
O	-0.70466	-2.75667	1.87053
O	2.42442	-2.05165	-0.84348
O	2.68443	-1.77065	2.86300
O	1.21338	-1.28670	-3.90261
O	-2.36505	-1.21794	-4.00560
C	0.00447	-1.09135	-3.23808
C	-1.20654	-1.16775	-3.70450
O	1.73193	-5.37340	0.98482
Cu	1.18621	3.95044	0.50301
O	1.16737	3.94816	-1.33763
Cu	2.45708	2.60390	-1.49558
Cu	5.34370	1.57872	-1.53329
Cu	4.05693	3.05185	0.65301
O	3.61353	1.26915	-1.94997
O	-2.43243	-4.04510	-2.24115
O	-6.52812	-1.72235	-1.02662
H	-6.72199	-1.95396	-0.10907
O	-5.52677	1.78269	0.48378
H	-5.31864	1.45810	-0.40531
O	-4.83752	5.42672	-0.91294
H	-4.27456	5.89734	-0.28201
O	-1.48159	6.38965	-0.03402
H	-2.02178	6.27460	-0.82967
O	4.71059	4.64042	-0.07719
H	5.01945	4.27545	-0.91923
O	7.06217	2.04197	-0.98768
H	6.82598	2.75474	-0.37720
O	5.77601	-1.42658	0.43372
H	5.38990	-1.58340	-0.44182
O	0.73689	-4.24377	-2.47806
H	-0.20630	-4.44077	-2.58998

O	0.94533	3.57647	2.34929
H	-0.01750	3.65056	2.40706
H	-4.71409	-2.91376	1.17392
H	2.61314	-5.01258	1.17212
H	3.58823	-1.48285	3.05966
H	-3.68690	0.55298	3.14128
H	-2.10302	2.98557	2.30881
H	3.46851	1.41870	2.25902
H	0.53998	1.61111	3.37523
H	-0.66595	-2.60495	2.83258
H	1.40432	4.78919	-1.74861
H	-2.82176	-4.92117	-2.36870
H	1.89996	-1.20803	-3.21524

Supporting References

(1) Abu-Zeid, M. E.; Rakhshani, A. E.; Al-Jassar, A. A.; Youssef, Y. A. Determination of the Thickness and Refractive Index of Cu2O Thin Film Using Thermal and Optical Interferometry. *Phys. Status Solidi A* **1986**, *93* (2), 613–620.

(2) Adamo, C.; Barone, V. Toward Reliable Density Functional Methods without Adjustable Parameters: The PBE0 Model. *J. Chem. Phys.* **1999**, *110* (13), 6158–6170.

(3) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7* (18), 3297–3305.

(4) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113* (18), 6378–6396.