Supplementary Information for

Insight into the Structure and Bonding of Copper (I) Iodide Clusters and a Cluster-Based Coordination Polymer

Turbasu Sengupta, Thanh Truong Dang, Jin Suk Chung,* and Sung Gu Kang*

School of Chemical Engineering, University of Ulsan, 93 Daehakro, Nam-Gu, Ulsan 44610, South Korea

*(J.S.C.) E-mail: jschung@mail.ulsan.ac.kr.
*(S.G.K.) E-mail: sgkang@mail.ulsan.ac.kr.

***To whom correspondence should be addressed**

Content Index

1. Cartesian Coordinates, Energies and Normal Modes of Vibration for Ground State Cu_4 and $[Cu_4I_j]^{+(4-j)}$Clusters [B3LYP-D3(BJ)/def2-TZVP]

(Spin Multiplicities (M=2S+1=1), energies are in kcal/mol)
Only the first six normal vibrational modes are included

1.Cu_4

Energy: -4117940.5613724

Cu	-0.00004	1.15809	-0.00003
Cu	-2.16343	-0.00004	0.00003
Cu	2.16342	0.00001	0.00003
Cu	0.00004	-1.15805	-0.00003

Frequencies --	54.7586	114.7687	128.1257
Frequencies --	147.4252	218.0635	252.1752

2.$[Cu_4I_2]^{2+}$(I)

Energy: -4491396.9789878

Cu	-3.82884	0.91817	-0.00001
Cu	-0.00000	0.00001	1.27153
Cu	0.00000	-0.00001	-1.27153
Cu	3.82885	-0.91817	0.00001
I	2.10476	0.91392	-0.00000
I	-2.10476	-0.91392	0.00000

Frequencies --	19.0099	22.3032	31.7592
Frequencies --	46.1159	62.1650	88.6354

3.$[Cu_4I_2]^{2+}$(II)

Energy: -4491395.6967475

Cu	-0.00039	-0.29888	-1.27573
Cu	-0.00031	-0.30332	1.27619
Cu	3.65243	1.46210	0.00146
Cu	-3.65041	1.46346	0.00116
I	2.26868	-0.63552	-0.00099
I	-2.26940	-0.63575	-0.00070

Frequencies --	19.9940	26.8963	34.0194
Frequencies --	36.3507	55.8813	89.2285

4.$[Cu_4I_4]^{0}$(I)

Energy: -4865684.2836168

Cu	-1.90762	-0.00019	-0.00088
Cu	0.00030	-1.90396	0.00043
Cu	-0.00030	1.90396	0.00043
Cu	1.90762	0.00019	-0.00088
I	-1.90001	-1.89870	1.60727
I	1.90001	1.89870	1.60727
I	1.90001	-1.90035	-1.60703
I	-1.90001	1.90035	-1.60703

Frequencies --	18.0509	29.0601	30.7837
Frequencies --	44.4314	52.1131	52.1334

5.$[Cu_4I_4]^0$(II).log

Energy: -4865677.7900422

Cu	0.93743	0.93787	0.93766
Cu	0.93743	-0.93787	-0.93766
Cu	-0.93743	0.93787	-0.93766
Cu	-0.93743	-0.93787	0.93766
I	1.58385	1.58348	-1.58338
I	1.58385	-1.58348	1.58338
I	-1.58385	-1.58348	-1.58338
I	-1.58385	1.58348	1.58338
Frequencies --	43.9275	43.9407	68.0429
Frequencies --	68.0706	68.0963	93.9999

6.$[Cu_4I_6]^{2-}$

Energy: -5239587.8795401

Cu	-1.03884	0.92099	0.98460
Cu	0.87632	1.03824	-1.02475
Cu	1.08256	-0.87646	0.97553
Cu	-0.92064	-1.08258	-0.93549
I	3.21957	0.26821	-0.07671
I	0.07282	0.07172	3.22639
I	-0.26867	3.21913	-0.06792
I	-3.21951	-0.26609	0.07985
I	0.26909	-3.21975	0.06455
I	-0.07297	-0.07334	-3.22610
Frequencies --	27.3256	27.3916	27.4331
Frequencies --	36.1664	36.5400	42.0236

7.$[Cu_4I_8]^{4-}$

Energy: -5613241.9878642

Cu	1.72819	-1.07052	0.94356
Cu	-1.11058	1.15348	1.56794
Cu	-1.37805	-1.49376	-0.94485
Cu	0.76062	1.41033	-1.56657
I	-2.00070	1.23918	-1.09280
I	1.59553	1.72897	1.09435
I	-3.07520	-3.33292	-2.10793
I	1.69681	3.14807	-3.49526
I	-0.88050	-1.63304	1.81401
I	3.85643	-2.38871	2.10490
I	-2.47823	2.57419	3.49829
I	1.28576	-1.33548	-1.81560
Frequencies --	14.5588	14.6029	22.3810
Frequencies --	22.3962	22.4335	39.1709

2. Cartesian Coordinates, Energies and Normal Modes of Vibration for Ground State Cu_4 and $[Cu_4I_j]^{+(4-j)}$Clusters [B3LYP-D3(BJ)/def2-TZVPD]

(Spin Multiplicities (M=2S+1=1) , energies are in kcal/mol)

Only the first six normal vibrational modes are included

1.Cu_4

Energy: -4117940.9527500

Cu	-0.00004	1.15787	-0.00003
Cu	-2.16366	-0.00004	0.00003
Cu	2.16365	0.00001	0.00003
Cu	0.00004	-1.15784	-0.00003
Frequencies --	53.9080	114.5127	128.1582
Frequencies --	147.2401	217.9913	252.3383

2.$[Cu_4I_2]^{2+}$(I)

Energy: -4491398.2382738

Cu	3.84746	0.90533	0.00001
Cu	0.00000	0.00001	-1.27131
Cu	-0.00000	-0.00001	1.27131
Cu	-3.84746	-0.90533	-0.00001
I	-2.10541	0.90524	0.00000
I	2.10541	-0.90525	-0.00000
Frequencies --	19.2466	22.7680	32.1862
Frequencies --	47.1290	62.2599	88.7535

3.$[Cu_4I_2]^{2+}$(II)

Energy: -4491397.0006432

Cu	0.00000	-0.29846	-1.27501
Cu	-0.00000	-0.29845	1.27501
Cu	3.66529	1.45223	-0.00001
Cu	-3.66529	1.45223	-0.00000
I	2.26656	-0.63131	0.00001
I	-2.26655	-0.63131	-0.00000
Frequencies --	19.8858	27.6525	34.5976
Frequencies --	37.0356	56.4214	89.1436

4.$[Cu_4I_4]_0$(I)

Energy: -4865685.7544551

Cu	0.00000	-1.90630	0.00000
Cu	-1.90630	0.00000	0.00000
Cu	1.90630	0.00000	0.00000
Cu	-0.00000	1.90630	0.00000
I	-1.89794	-1.89794	-1.60804
I	1.89794	1.89794	-1.60804
I	-1.89794	1.89794	1.60804
I	1.89794	-1.89794	1.60804

Frequencies --	17.8970	28.9506	30.6624
Frequencies --	44.7586	52.1885	52.1886

5.$[Cu_4I_4]^0$(II)

Energy: -4865679.0193019

Cu	-0.93868	0.93866	0.93865
Cu	-0.93868	-0.93866	-0.93865
Cu	0.93868	-0.93866	0.93865
Cu	0.93868	0.93866	-0.93865
I	-1.58225	-1.58224	1.58221
I	-1.58225	1.58224	-1.58221
I	1.58225	-1.58224	-1.58221
I	1.58225	1.58224	1.58221
Frequencies --	43.7153	43.7170	67.7135
Frequencies --	67.7150	67.7170	94.1840

6.$[Cu_4I_6]^{2-}$

Energy: -5239592.2711714

Cu	-1.18343	0.61415	1.06661
Cu	1.08516	1.24761	-0.42551
Cu	0.85678	-1.26248	0.76628
Cu	-0.75860	-0.59946	-1.40754
I	3.17757	-0.02432	0.55742
I	-0.53438	-1.06084	2.99939
I	-0.16078	3.04647	1.04891
I	-3.17755	0.02421	-0.55748
I	0.16082	-3.04650	-1.04893
I	0.53437	1.06108	-2.99923
Frequencies --	27.3528	27.4261	27.4958
Frequencies --	35.6458	35.6681	42.0869

7.$[Cu_4I_8]^{4-}$

Energy: -5613253.5462498

Cu	-0.92436	1.51910	1.32966
Cu	1.58829	0.95557	-1.22325
Cu	-1.55295	-0.85456	-1.33765
Cu	0.88913	-1.62005	1.23107
I	1.07954	-1.77490	-1.55503
I	1.81398	0.99859	1.56407
I	-3.47397	-1.91126	-2.99070
I	1.98904	-3.62324	2.75271
I	-1.03829	1.89282	-1.43989
I	-2.06776	3.39767	2.97359
I	3.55243	2.13689	-2.73508
I	-1.85503	-1.11662	1.43042
Frequencies --	14.4343	14.4554	22.1909
Frequencies --	22.1965	22.2154	38.5132

3. Cartesian Coordinates, Energies and Normal Modes of Vibration for Ground State Cu_4 and $[Cu_4I_j]^{+(4-j)}$Clusters [B3LYP-D3(BJ)/def2-QZVPP]

(Spin Multiplicities (M=2S+1=1) , energies are in kcal/mol)
Only the first six normal vibrational modes are included

1.Cu_4

Energy: -4118048.0346054

Cu	-0.00069	-1.15362	-0.00065
Cu	-2.15853	0.00102	0.00065
Cu	2.15847	0.00025	0.00065
Cu	0.00075	1.15234	-0.00065

Frequencies --	54.3584	112.1328	124.8108
Frequencies --	144.4554	212.8647	248.4194

2.$[Cu_4I_2]^{2+}$(I)

Energy: -4491508.6458101

Cu	-3.83563	0.89530	-0.00001
Cu	-0.00000	0.00000	1.26655
Cu	0.00000	-0.00001	-1.26655
Cu	3.83563	-0.89529	0.00001
I	2.09706	0.89601	-0.00000
I	-2.09707	-0.89601	0.00000

Frequencies --	19.5762	22.5126	33.1390
Frequencies --	46.9925	63.6446	87.5740

3.$[Cu_4I_2]^{2+}$(II)

Energy: -4491507.4186652

Cu	0.00004	-0.30045	-1.27021
Cu	-0.00006	-0.30146	1.27065
Cu	3.64709	1.44372	-0.00005
Cu	-3.64709	1.44378	0.00060
I	2.25597	-0.62527	0.00003
I	-2.25596	-0.62533	-0.00057

Frequencies --	20.1704	27.6479	35.0920
Frequencies --	37.0153	57.3992	87.8728

4.$[Cu_4I_4]^{0}$(I)

Energy: -4865797.2965787

Cu	-0.00000	-1.91602	0.00000
Cu	1.91603	-0.00000	0.00000
Cu	-1.91603	0.00000	0.00000
Cu	0.00000	1.91602	0.00000
I	1.91057	-1.91058	1.57535
I	-1.91057	1.91058	1.57535
I	1.91057	1.91057	-1.57535

I	-1.91057	-1.91057	-1.57535	
Frequencies --	17.5481	28.2757		32.9596
Frequencies --	44.8084	52.0670		52.0673

5.$[Cu_4I_4]^0$(II)

Energy: -4865787.9411091

Cu	-0.94215	0.94217	0.94187	
Cu	-0.94215	-0.94217	-0.94187	
Cu	0.94215	-0.94217	0.94187	
Cu	0.94215	0.94217	-0.94187	
I	-1.57596	-1.57543	1.57504	
I	-1.57596	1.57543	-1.57504	
I	1.57596	-1.57543	-1.57504	
I	1.57596	1.57543	1.57504	
Frequencies --	43.9077	43.9341		66.0501
Frequencies --	66.0887	66.0890		90.8159

6.$[Cu_4I_6]^{2-}$

Energy: -5239702.6501247

Cu	1.30533	-0.83063	0.75631	
Cu	-0.54868	1.26620	1.03031	
Cu	0.53373	0.66709	-1.49527	
Cu	-1.29025	-1.10278	-0.29118	
I	-0.02419	3.12632	-0.75208	
I	2.97354	-0.26468	-1.19509	
I	1.22381	0.70465	2.88883	
I	0.02416	-3.12624	0.75217	
I	-1.22383	-0.70437	-2.88892	
I	-2.97356	0.26438	1.19500	
Frequencies --	28.1606	28.1769		28.1906
Frequencies --	34.8844	34.8947		42.8562

7.$[Cu_4I_8]^{4-}$

Energy: -5613360.7887977

Cu	-0.50004	1.09112	1.89537	
Cu	2.22801	-0.19121	-0.18749	
Cu	-0.80275	1.14339	-1.75552	
Cu	-0.92475	-2.04340	0.04733	
I	0.57640	-1.25802	-2.18404	
I	0.92518	-1.31761	2.02285	
I	-1.77795	2.53198	-3.88690	
I	-2.04854	-4.52489	0.10548	
I	1.06591	2.35463	-0.05511	
I	-1.10766	2.41701	4.19653	
I	4.93316	-0.42366	-0.41467	
I	-2.56676	0.22061	0.21603	
Frequencies --	14.6974	14.7432		22.4820
Frequencies --	22.5101	22.5294		39.2988

4. Cartesian Coordinates, Energies and Normal Modes of Vibration for Ground State Cu_4 and $[Cu_4I_j]^{+(4-j)}$Clusters [MN15/aug-cc-pVTZ-PP]

(Spin Multiplicities (M=2S+1=1), energies are in kcal/mol)
Only the first six normal vibrational modes are included

1.Cu_4

Energy: -496149.0754785

Cu	0.00006	1.14256	0.00006
Cu	-2.14989	0.00005	-0.00006
Cu	2.14989	-0.00001	-0.00006
Cu	-0.00006	-1.14260	0.00006
Frequencies --	55.7913	116.4491	131.1097
Frequencies --	147.9745	214.9401	252.4301

2.$[Cu_4I_2]^{2+}$(I)

Energy: -866072.2314718

Cu	3.95267	0.83071	0.00001
Cu	0.00000	0.00001	-1.25513
Cu	-0.00000	-0.00001	1.25513
Cu	-3.95267	-0.83070	-0.00001
I	-2.10535	0.85337	0.00000
I	2.10535	-0.85337	-0.00000
Frequencies --	18.1766	21.5997	31.2887
Frequencies --	44.7686	60.2466	93.0027

3.$[Cu_4I_2]^{2+}$(II)

Energy: -866071.1559519

Cu	0.00009	-0.26492	-1.26019
Cu	-0.00007	-0.26644	1.26017
Cu	3.80957	1.35153	0.00038
Cu	-3.80977	1.35141	0.00060
I	2.24481	-0.59412	-0.00014
I	-2.24471	-0.59410	-0.00039
Frequencies --	20.2677	27.9775	33.1384
Frequencies --	34.8190	54.4137	92.6670

4.$[Cu_4I_4]^{0}$(I)

Energy: -1236801.4316650

Cu	1.88627	-0.00000	-0.00000
Cu	-0.00000	1.88584	0.00000
Cu	0.00000	-1.88584	0.00000
Cu	-1.88627	0.00000	-0.00000
I	1.86084	1.86080	1.62868
I	-1.86084	-1.86080	1.62868
I	-1.86084	1.86081	-1.62868
I	1.86084	-1.86081	-1.62868

Frequencies --	16.9630	20.0606	27.8229
Frequencies --	40.0118	47.8556	47.8577

5.$[Cu_4I_4]^0$ (II)

Energy: -1236806.0120385

Cu	-0.92415	0.92330	0.92368
Cu	-0.92415	-0.92330	-0.92368
Cu	0.92415	-0.92330	0.92368
Cu	0.92415	0.92330	-0.92368
I	-1.57133	-1.57134	1.56968
I	-1.57133	1.57134	-1.56968
I	1.57133	-1.57134	-1.56968
I	1.57133	1.57134	1.56968
Frequencies --	46.0163	46.0559	73.7580
Frequencies --	73.8149	73.8463	105.6571

6.$[Cu_4I_6]^{2-}$

Energy: -1607160.2388280

Cu	0.07676	-0.74538	1.51720
Cu	0.99524	-0.83025	-1.08712
Cu	-1.59623	-0.02850	-0.56212
Cu	0.52350	1.60466	0.13123
I	-0.98431	-1.40769	-2.71307
I	-2.49561	-1.27596	1.56776
I	1.76357	-2.58888	0.70771
I	0.97642	1.41538	2.71200
I	-1.76244	2.58843	-0.71199
I	2.50277	1.26843	-1.56197
Frequencies --	24.2010	24.4032	24.7590
Frequencies --	34.8296	34.8812	39.3509

7.$[Cu_4I_8]^{4-}$

Energy: -1977273.1010091

Cu	0.20622	1.93233	-0.93968
Cu	-1.50230	0.10895	1.54629
Cu	1.89056	-0.58217	0.86893
Cu	-0.59199	-1.45904	-1.47580
I	-0.24830	-2.33709	1.13771
I	-2.28410	0.70506	-1.05260
I	4.29638	-1.32484	1.97559
I	-1.35068	-3.31841	-3.35566
I	0.71696	1.76395	1.78713
I	0.46938	4.39477	-2.13603
I	-3.41809	0.24795	3.51618
I	1.81710	-0.13142	-1.87217
Frequencies --	13.4295	13.4477	19.6036
Frequencies --	19.6507	19.7414	32.1880

5. Cartesian Coordinates, Energies and Normal Modes of Vibration for the Cluster Model of a Coordination Polymer [B3LYP-D3(BJ)/def2-SVP(C,H,N,P,Cu)+def2-SVPD(I)]

(Energy are in kcal/mol)

Only the first six normal vibrational modes are included

Energy: -10811251.3866686

I	-4.58261	-0.69264	2.66038
Cu	-3.22231	-0.62007	0.25618
P	-0.98821	-0.83173	0.11074
N	0.08890	0.04352	1.13313
C	-0.48944	-2.51724	0.13183
C	-0.36087	-3.73258	0.11488
C	-0.17389	-5.14333	0.08460
C	-1.29027	-6.00446	0.03369
H	-2.29387	-5.57500	0.02125
C	-1.10423	-7.38473	-0.00128
H	-1.97140	-8.04759	-0.04124
C	0.18817	-7.92078	0.01551
H	0.32932	-9.00380	-0.01098
C	1.29978	-7.07282	0.06636
H	2.30847	-7.49152	0.07993
C	1.12635	-5.69077	0.09981
H	1.98663	-5.02064	0.14027
C	-0.05316	0.35150	2.56844
C	-0.43248	-0.95183	3.28314
H	-1.39908	-1.33719	2.92295
H	-0.53136	-0.77753	4.36493
H	0.33485	-1.72120	3.11292
C	1.29989	0.85191	3.08193
H	2.08506	0.09964	2.92198
H	1.23500	1.06862	4.15839
H	1.60303	1.78063	2.57612
C	-1.13226	1.42562	2.77627
H	-0.84130	2.36804	2.29179
H	-1.29379	1.61532	3.84853
H	-2.08619	1.10227	2.33943
P	0.98892	0.83281	-0.11049
N	-0.08808	-0.04260	-1.13288
C	0.48959	2.51818	-0.13158
C	0.35996	3.73340	-0.11452
C	0.17155	5.14397	-0.08408
C	1.28705	6.00637	-0.03595
H	2.29116	5.57806	-0.02579
C	1.09953	7.38643	-0.00082
H	1.96603	8.05028	0.03698
C	-0.19350	7.92103	-0.01466
H	-0.33581	9.00389	0.01196
C	-1.30425	7.07179	-0.06272

H	-2.31344	7.48935	-0.07399
C	-1.12933	5.68994	-0.09634
H	-1.98894	5.01883	-0.13468
C	0.05393	-0.35056	-2.56821
C	0.43312	0.95279	-3.28294
H	1.39970	1.33824	-2.92277
H	0.53199	0.77847	-4.36473
H	-0.33427	1.72209	-3.11272
C	-1.29909	-0.85111	-3.08164
H	-2.08433	-0.09891	-2.92170
H	-1.23419	-1.06784	-4.15810
H	-1.60212	-1.77985	-2.57580
C	1.13309	-1.42460	-2.77608
H	0.84230	-2.36698	-2.29141
H	1.29445	-1.61443	-3.84835
H	2.08708	-1.10113	-2.33945
I	-3.20465	2.19167	-0.80830
Cu	-4.94765	1.26514	0.90825
I	-4.58536	-2.24890	-1.59014
I	-7.37483	0.96453	-0.34196
Cu	-4.94703	0.37084	-1.51240
Cu	-5.87898	-1.10548	0.39633
Cu	3.22306	0.62143	-0.25582
I	3.20400	-2.19169	0.80712
I	4.58319	0.69443	-2.66005
I	4.58719	2.24772	1.59147
Cu	4.94692	-1.26475	-0.90921
Cu	4.94726	-0.37217	1.51203
Cu	5.88009	1.10482	-0.39582
I	7.37465	-0.96652	0.34088

Frequencies --	2.6848	8.5994	8.7898
Frequencies --	9.7723	11.2959	15.3149

6. Energies of the Different Spin States of Cu_4 Clusters [B3LYP-D3(BJ)/def2-QZVPP]

M=2S+1	E+ZPE (a.u)
1	**-6562.525277**
3	-6562.499088
5	-6562.410313
7	-6562.243528
9	-6562.067059
11	-6561.876911
13	-6561.669227

7. Energies of the Different Spin States of $[Cu_4I_4]^0$ (I) Clusters [B3LYP-D3(BJ)/def2-TZVP]

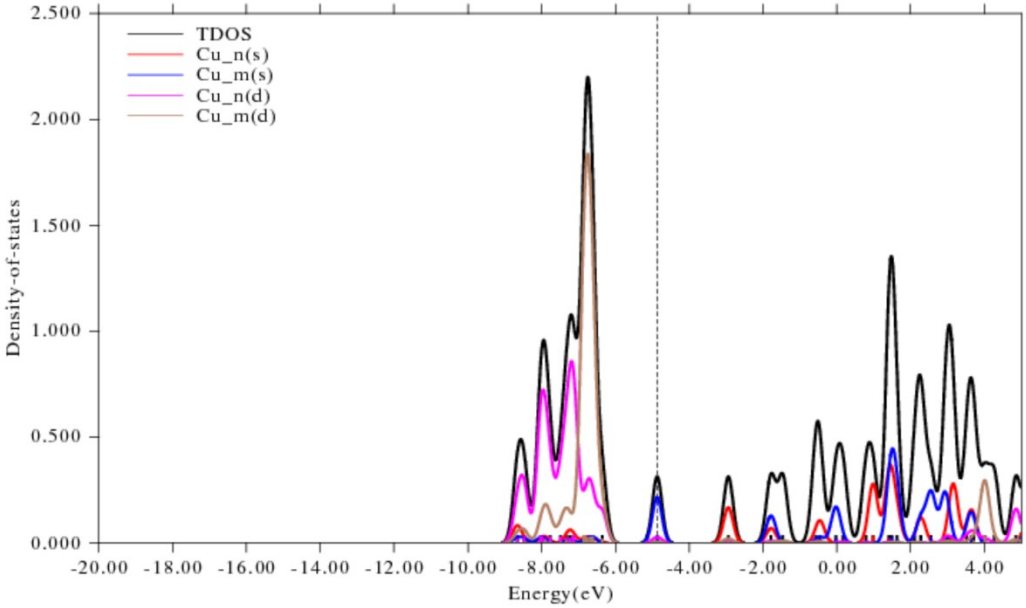
M=2S+1	E+ZPE (a.u)
1	**-7753.956769**
3	-7753.876834
5	-7753.740442
7	-7753.620319
9	-7753.481288
11	-7753.301855

8. Energies of the Different Spin States of $[Cu_4I_6]^{2-}$ Clusters [B3LYP-D3(BJ)/def2-TZVP]

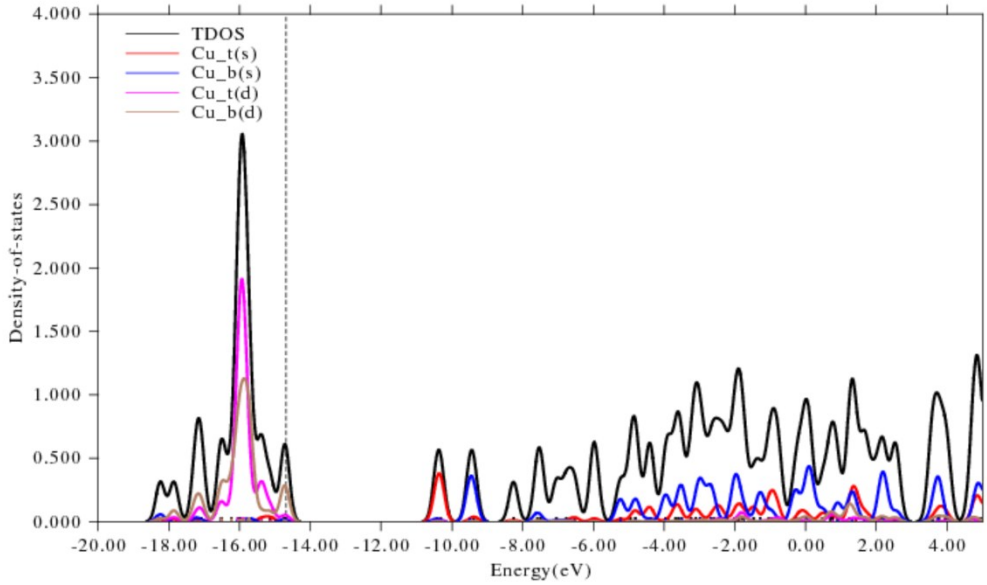
M=2S+1	E+ZPE (a.u)
1	**-8349.809841**
3	-8349.718862
5	-8349.593123
7	-8349.466181
9	-
11	-

9. Sample DOS Plots

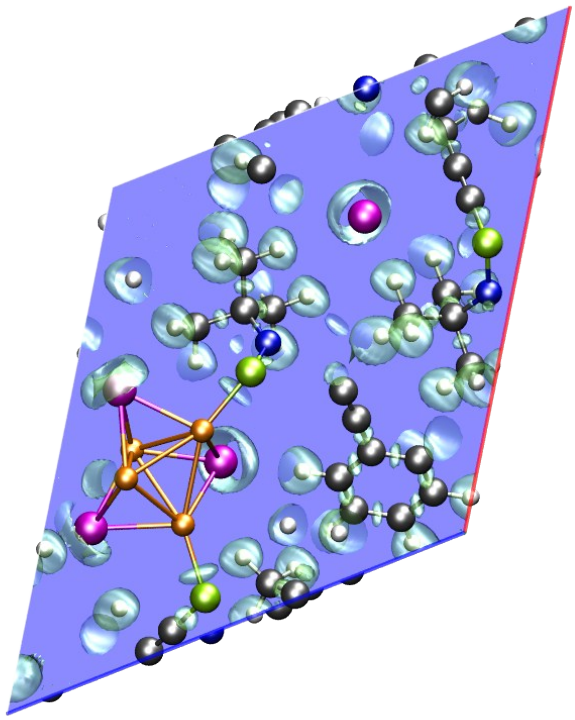
Cu_4



$[Cu_4I_2]^{2+}$ (I)



10. ELF Plot of The Periodic Model



11. Calculated Results with B3LYP-D3(BJ)/def2-TZVP Level of Theory

Cu_4 Cluster	Cluster		Cu	ΔE_b (a.u)	ΔE_b (eV)	H-L gap(eV)
E	-6562.353966	--	-1640.542211	-0.0462805	-1.259338685	
U	-6562.347256	--	-1640.540794	-0.04602	-1.25225022	1.92
H	-6562.346312	--	-1640.53985	-0.046728	-1.271515608	
G	-6562.388733	--	-1640.55872	-0.03846325	-1.046623496	
$[Cu_4I_2]^{2+}$ (I)	**Cluster**	I^-	Cu^+	ΔE_b (a.u)	ΔE_b (eV)	H-L gap(eV)
E	-7157.493947	-297.896556	-1640.24661	-0.119065833	-3.239900391	4.27
U	-7157.482259	-297.89514	-1640.245194	-0.118533833	-3.225424139	
H	-7157.481315	-297.894195	-1640.24425	-0.119320833	-3.246839196	
G	-7157.541222	-297.913404	-1640.262465	-0.110759	-3.013863149	
$[Cu_4I_2]^{2+}$ (II)						
E	-7157.491918	-297.896556	-1640.24661	-0.118727667	-3.230698538	4.19
U	-7157.480218	-297.89514	-1640.245194	-0.118193667	-3.216167864	
H	-7157.479273	-297.894195	-1640.24425	-0.1189805	-3.237578386	
G	-7157.539252	-297.913404	-1640.262465	-0.110430667	-3.004928871	
$[Cu_4I_4]^0$ (I)						
E	-7753.956769	-297.896556	-1640.24661	-0.173013125	-4.707860144	4.92
U	-7753.94104	-297.89514	-1640.245194	-0.172463	-4.692890693	
H	-7753.940096	-297.894195	-1640.24425	-0.1732895	-4.715380585	
G	-7754.010325	-297.913404	-1640.262465	-0.163356125	-4.445083517	
$[Cu_4I_4]^0$ (II)						
E	-7753.946739	-297.896556	-1640.24661	-0.171759375	-4.673744353	4.96
U	-7753.930912	-297.89514	-1640.245194	-0.171197	-4.658441567	
H	-7753.929968	-297.894195	-1640.24425	-0.1720235	-4.680931459	
G	-7753.996897	-297.913404	-1640.262465	-0.161677625	-4.399409854	
$[Cu_4I_6]^{2-}$						
E	-8349.809841	-297.896556	-1640.24661	-0.1444065	-3.929445272	3.86
U	-8349.788879	-297.89514	-1640.245194	-0.1437263	-3.910936349	
H	-8349.787935	-297.894195	-1640.24425	-0.1445765	-3.934071142	
G	-8349.873276	-297.913404	-1640.262465	-0.1342992	-3.654415531	
$[Cu_4I_8]^{4-}$						
E	-8945.266295	-297.896556	-1640.24661	-0.092283917	-2.511137656	4.62
U	-8945.23915	-297.89514	-1640.245194	-0.091437833	-2.488114883	
H	-8945.238206	-297.894195	-1640.24425	-0.092303833	-2.511679609	
G	-8945.346038	-297.913404	-1640.262465	-0.082412167	-2.242517467	