Supporting Information

Eight-Electron Copper-Hydride Nanoclusters: Synthesis, Structure, Alloying Chemistry and Photoluminescence

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Materials

Copper(II) trifluoroacetate hydrate ($Cu(CF_3COO)_2$, 98%), silver trifluoroacetate (CF_3COOAg, 98%), phenylselenol (C_6H_6Se, 97%) and Bis-(triphenylphosphino)-cuprous borohydride ($(PPh_3)_2CuBH_4$, 98%) were purchased from Bide (Shanghai, China). Dichloromethane (CH_2Cl_2, A.R.), methanol (CH_3OH, A.R.), hexane (C_6H_{14}) and ether ($C_4H_{10}O$, A.R.) were purchased from Sinopharm Chemical Reagent Co. Ltd. (Shanghai, China). Water used in all experiments was ultrapure. All other reagents were used as received without further purification.

Synthesis of $[Cu_{47}(PhSe)_{15}(PPh_3)_5(CF_3COO)_{12}H_{12}]$ ($Cu_{47}H_{12}$)

The $Cu_{47}H_{12}$ was prepared using the direct reduction method. In a typical synthesis, 0.075 mmol of $Cu(CF_3COO)_2$ was suspended in a mixed solvent consisting of 1 mL of methanol and 2 mL of dichloromethane. The mixture was treated with sonication for 5 minutes, resulting in a clear solution. After stirring for 10 minutes, 10 μL of phenylselenol was added dropwise. The mixture was stirred for an additional 10 minutes, and then 40 mg of $(PPh_3)_2CuBH_4$ in dichloromethane was added. The reaction was allowed to continue for 12 hours at room temperature. The solvents were then removed using a rotary evaporator. To re-dissolve the solid, 2 mL of dichloromethane was used, and the resulting mixture was centrifuged at 10000 rpm for 3 minutes. Finally, the supernatant was subjected to diffusion using a mixture of hexane and ether. After 2 weeks, block-like black crystals were obtained. Yield: 58.3% based on Cu.

Synthesis of $[(CuAg)_{47}(PhSe)_{18}(PPh_3)_6(CF_3COO)_{12}H_6]^{3+}$ ($(CuAg)_{47}H_6$)

The $(CuAg)_{47}H_6$ was prepared using a similar method as $Cu_{47}H_{12}$, with the only difference being the addition of 0.025 mmol CF_3COOAg.

Characterizations

^1H, ^2H, and ^{31}P nuclear magnetic resonance (NMR) spectra were acquired at room temperature using a Bruker AV-600 spectrometer. Tetramethylsilane (TMS) was used

as an internal reference for chemical shifts, and a residual signal from the solvent was also utilized. The NMR data were processed using MestReNova software.

UV-Vis spectra were collected by Shimadzu UV-2550 Spectrophotometer using a quartz cuvette of 1 mm path length. The signal from the blank solvent was subtracted.

Mass spectra were recorded using an Agilent 6224 time-of-flight mass spectrometer in the positive mode and negetive mode. The cluster sample was first dissolved in dichloromethane and filtered. Subsequently, the solution was directly infused into the spectrometer at a flow rate of 1.2 mL/h using a syringe pump. The typical parameters for the measurements were as follows: capillary voltage of 4.0 kV, drying gas flow of 4 L/min, and nebulizer pressure of 20 psi.

Energy-dispersive X-ray spectroscopy analysis (EDS) was recorded on a Bruker XFlash6100 system.

X-ray photoelectron spectroscopy analysis (XPS) was performed through the X-ray photoelectron spectrometer (ESCALABX+) equipped with a monochromatic Al Ka X-ray source. The spectra were calibrated using the C 1s peak (284.8 eV).

Fluorescence spectra were measured using an Edinburgh FLS1000 fluorescence spectrometer that was equipped with an integrating sphere.

The X-ray diffraction (XRD) patterns of the samples were obtained using a Bruker D8 powder X-ray diffractometer from Germany. The instrument operated at 40 kV and 40 mA, with Cu Ka radiation.

The diffraction data of the single crystals nanocluster $[Cu_{47}(PhSe)_{15}(PPh_3)_5(CF_3COO)_{12}H_{12}]$ and $[(CuAg)_{47}(PhSe)_{18}(PPh_3)_6(CF_3COO)_{12}H_6]^{3+}$ was collected on an Agilent

Technologies SuperNova system X-ray single-crystal diffractometer using Cu Kα (λ= 1.54184 Å) at 100 K. The data were processed using CrysAlis^{Pro}. The structure was solved and refined using Full-matrix least-squares based on F^2 using ShelXT, ShelXL in Olex2. The thermal ellipsoids of the ORTEP diagram were done at 50% probability. Detailed crystal data and structure refinements for the compound are given in Table S1-S4. CCDC 2376750 and 2258390 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

DFT calculations

The geometry optimization of the isolated $Cu_{47}H_{12}$ cluster and $(CuAg)_{47}H_6$ cluster is calculated by using the Vienna ab initio simulation package (VASP) software. To save computational cost, we simplified ligands from PhSe to MeSe, from PPh_3 to PMe_3, from CF_3COO to CH_3COO, as done by others.[4-6] The Perdew–Burke–Ernzerhof (PBE) form of the generalized-gradient approximation (GGA) was used for electron exchange and correlation.[7] The projector-augmented-wave (PAW) method[8] was used to describe the electron-core interaction with the cutoff energy of 450 eV for the planewave bases. The projected density of states (PDOS) is obtained by the vaspkit package.[9]

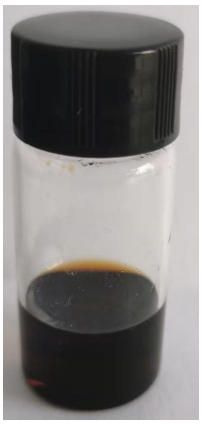

Figure S1. The digital image of raw product in the synthesis of the $Cu_{47}H_{12}$ cluster.

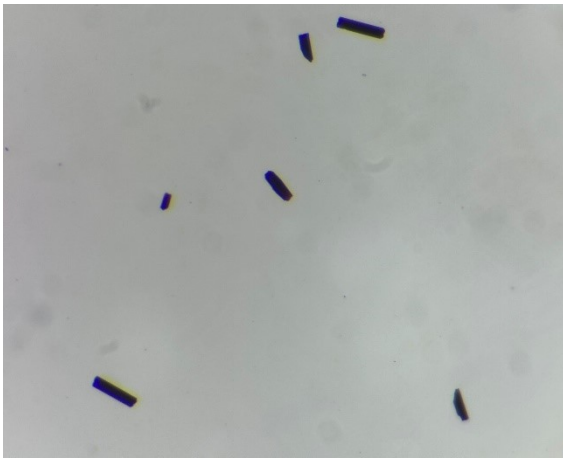

Figure S2. The digital image of $Cu_{47}H_{12}$ crystals.

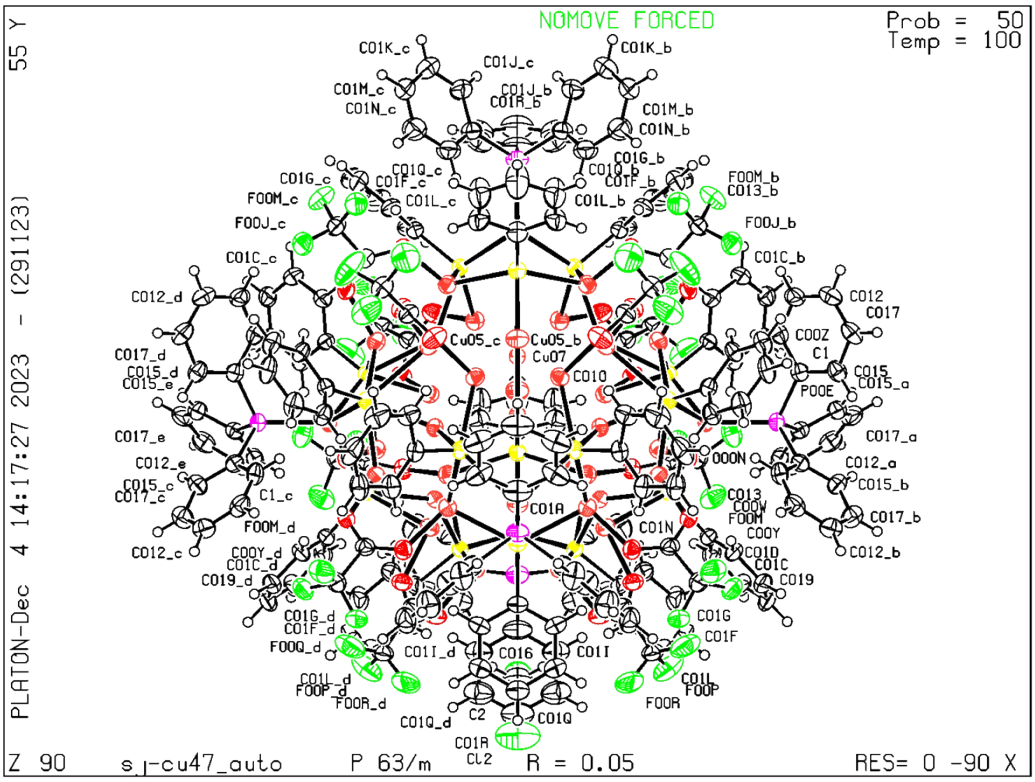

Figure S3. The thermal ellipsoids of the ORTEP diagram of the $Cu_{47}H_{12}$ cluster.

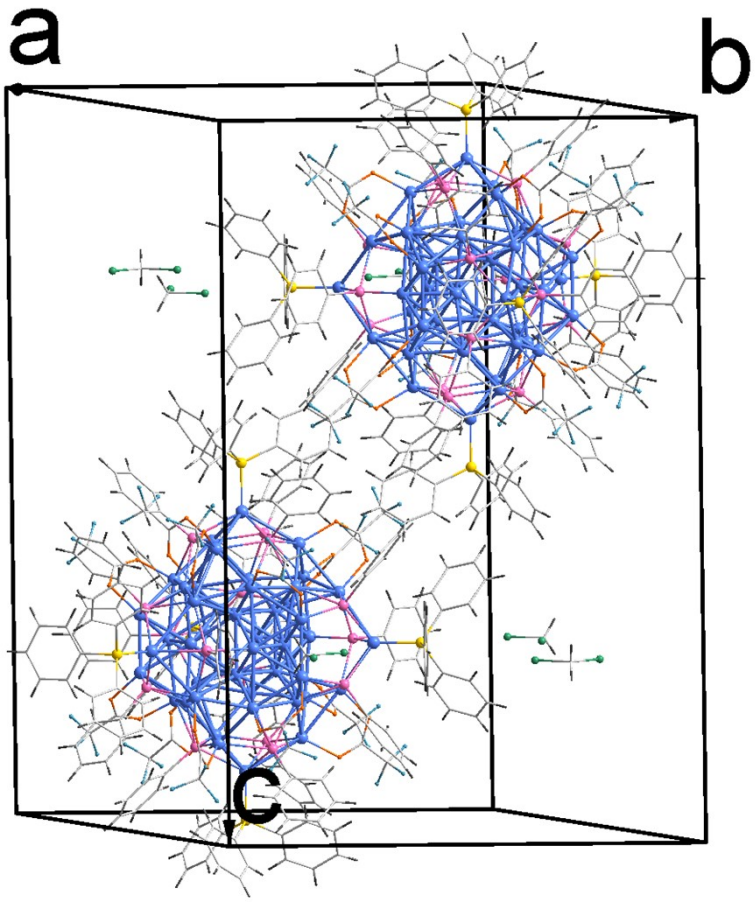

Figure S4. The packing structure of the $Cu_{47}H_{12}$ cluster in their single crystals. Color legends: Cu blue, Se pink, P yellow, O orange, F cyan, C grey, Cl green, C white and H grey.

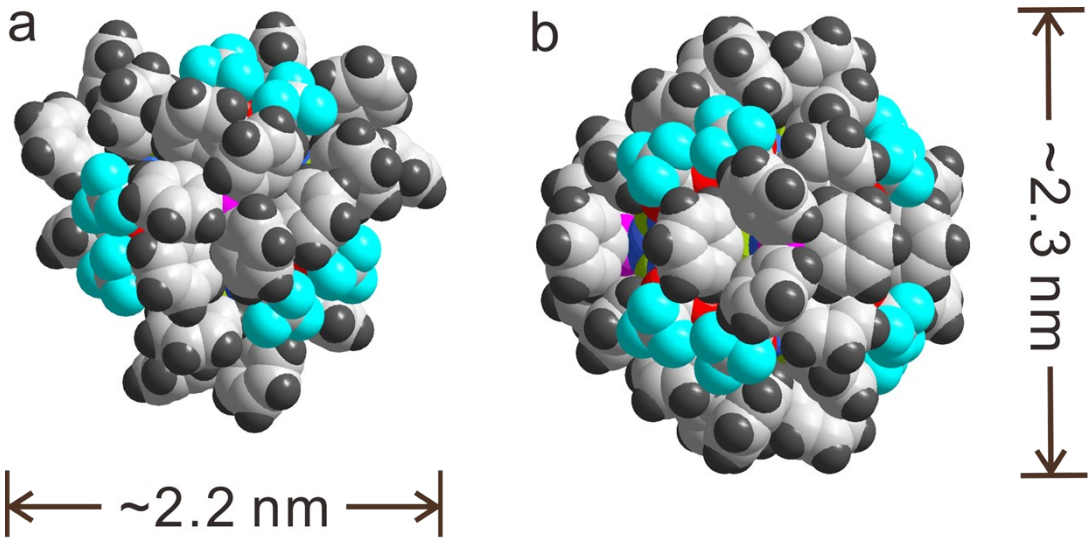

Figure S5. The diameter of the $Cu_{47}H_{12}$ cluster.

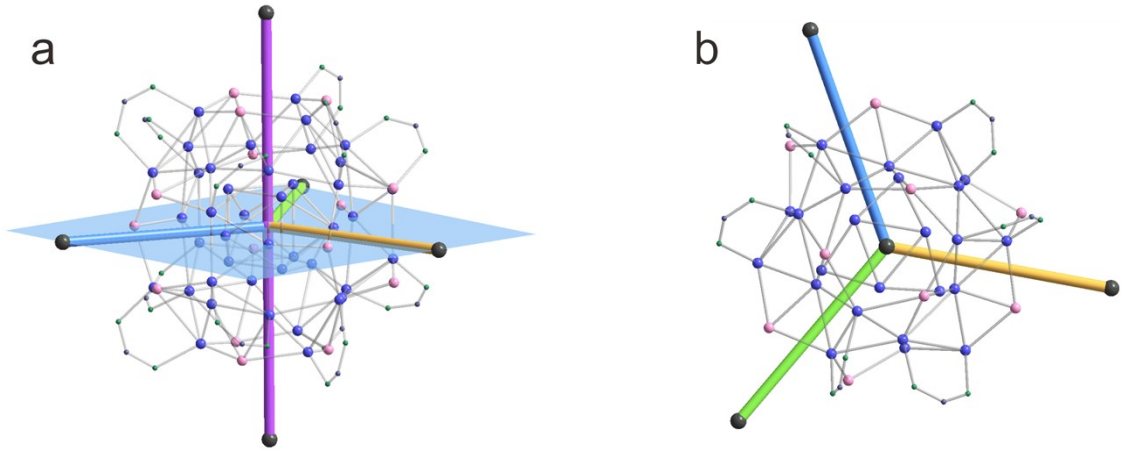

Figure S6. The crystallographic C_3 symmetry axis in the $Cu_{47}H_{12}$ cluster. Color legends: Cu blue, Se pink, P gray, O green and C blue gray. All other atoms are omitted for clarity.

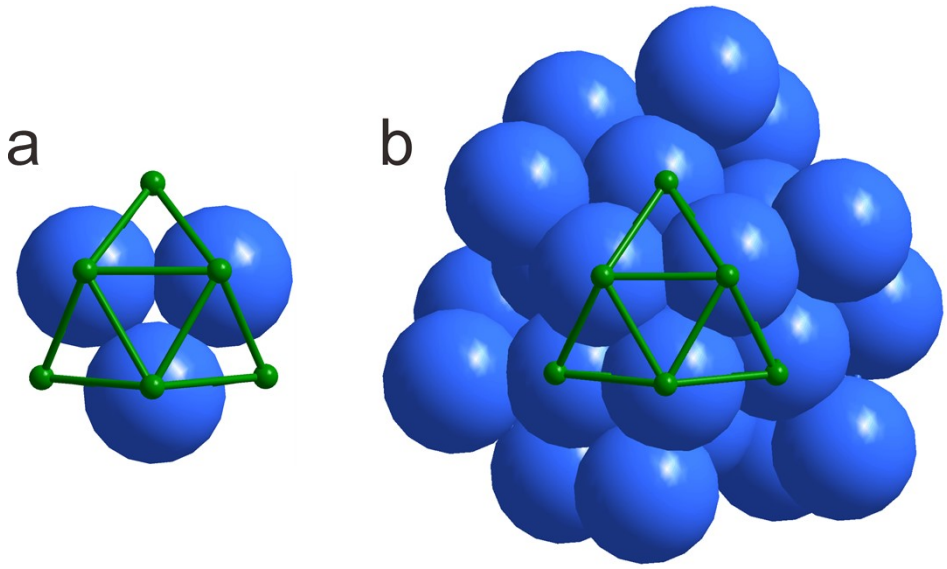

Figure S7. (a) Cu_9 kernel of the cluster $Cu_{47}H_{12}$. (b) Metal kernel of the Cu_{31} cluster.

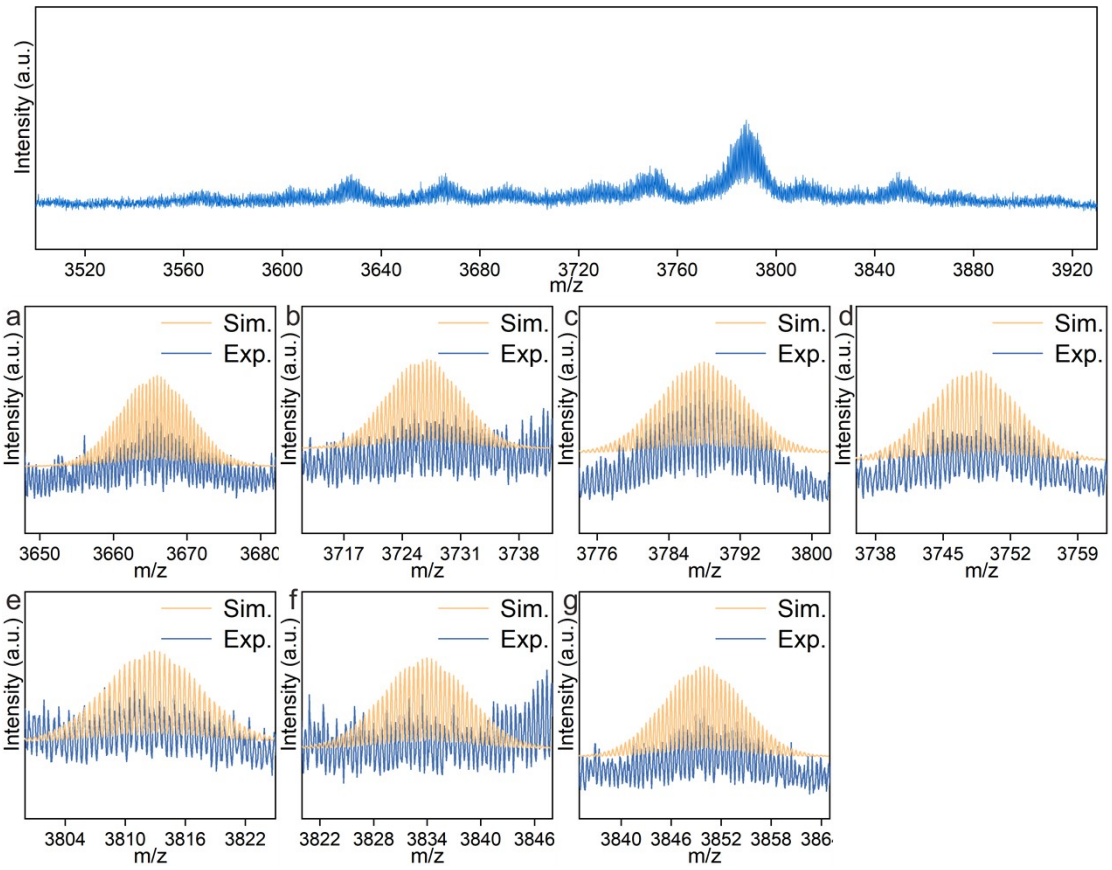

Figure S8. The ESI-MS spectroscopy of the $Cu_{47}H_{12}$ clusters in the range of 3500-3900 m/z. (a-g) The comparison between the simulated (orange) and experimental (blue) isotopic pattern of

(a) $[Cu_{47}(PPh_3)(CF_3COO)_{11}(PhSe)_{18}H_{12}(H_2O)]^{2-}$,

(b) $[Cu_{47}(PPh_3)_2(CF_3COO)_{15}(PhSe)_{14}H_{12}(CH_3OH)(H_2O)]^{2-}$,

(c) $[Cu_{47}(PPh_3)_2(CF_3COO)_{14}(PhSe)_{15}H_{12}(CH_3OH)(H_2O)]^{2-}$,

(d) $[Cu_{47}(PPh_3)_2(CF_3COO)_{11}(PhSe)_{18}H_{12}]^{2-}$,

(e) $[Cu_{47}(PPh_3)_2(CF_3COO)_{11}(PhSe)_{18}H_{12}(CH_3OH)(H_2O)]^{2-}$,

(f) $[Cu_{47}(PPh_3)_2(CF_3COO)_{11}(PhSe)_{18}H_{12}(C_4H_{10}O)(H_2O)]^{2-}$,

(g) $[Cu_{47}(PPh_3)_2(CF_3COO)_{11}(PhSe)_{18}H_{12}(C_4H_{10}O)(CH_3OH)(H_2O)]^{2-}$.

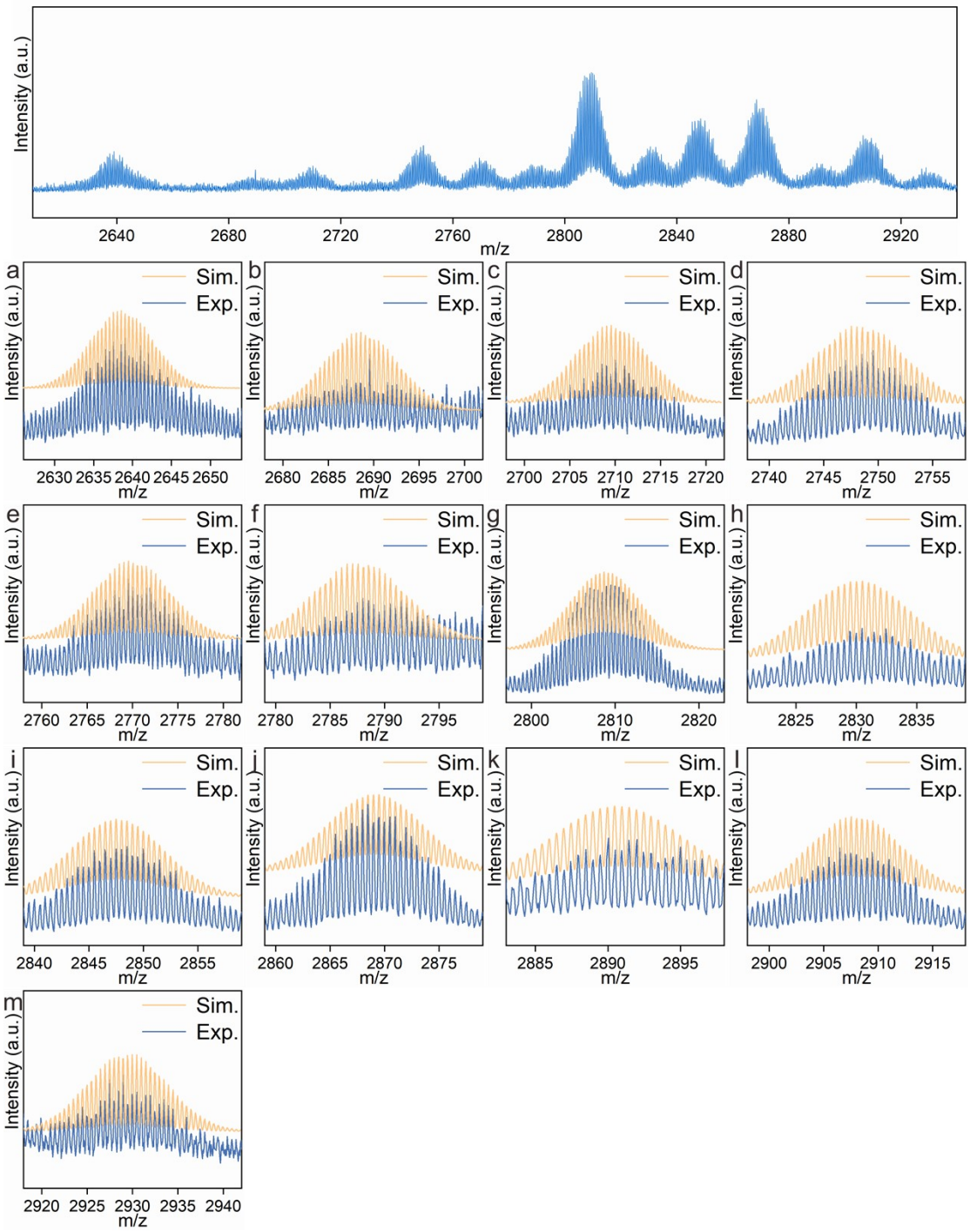

Figure S9. The ESI-MS spectroscopy of $Cu_{47}H_{12}$ clusters in the range of 2600-3000 m/z. (a-m) The comparison between the simulated (orange) and experimental (blue) isotopic pattern of

(a) $[Cu_{36}(PPh_3)_3(CF_3COO)_2(PhSe)_{12}H_{12}(C_4H_{10}O)(H_2O)]^{2-}$,

(b) $[Cu_{34}(PPh_3)_3(CF_3COO)_3(PhSe)_{13}H_{12}(CH_3OH)(H_2O)]^{2-}$,

(c) $[Cu_{34}(PPh_3)_3(CF_3COO)_3(PhSe)_{13}H_{12}(C_4H_{10}O)(H_2O)]^{2-}$,

(d) $[Cu_{36}(PPh_3)_3(CF_3COO)_3(PhSe)_{12}H_{12}Cl_3(C_4H_{10}O)(H_2O)]^{2-}$,

(e) $[Cu_{36}(PPh_3)_3(CF_3COO)_2(PhSe)_{13}H_{12}Cl_3(C_4H_{10}O)(H_2O)]^{2-}$,

(f) $[Cu_{36}(PPh_3)_3(CF_3COO)_3(PhSe)_{13}H_{12}Cl_2(CH_3OH)(H_2O)]^{2-}$,

(g) $[Cu_{36}(PPh_3)_3(CF_3COO)_3(PhSe)_{13}H_{12}Cl_2(C_4H_{10}O)(H_2O)]^{2-}$,

(h) $[Cu_{36}(PPh_3)_3(CF_3COO)_2(PhSe)_{14}H_{12}Cl_2(C_4H_{10}O)(H_2O)]^{2-}$,

(i) $[Cu_{36}(PPh_3)_3(CF_3COO)_3(PhSe)_{13}H_{12}Cl_2(CH_2Cl_2)_2]^{2-}$,

(j) $[Cu_{36}(PPh_3)_3(CF_3COO)_2(PhSe)_{14}H_{12}Cl_2(CH_2Cl_2)_2]^{2-}$,

(k) $[Cu_{36}(PPh_3)_3(CF_3COO)(PhSe)_{15}H_{12}Cl_2(CH_2Cl_2)_2]^{2-}$,

(l) $[Cu_{36}(PPh_3)_3(CF_3COO)_3(PhSe)_{14}H_{12}Cl(CH_2Cl_2)_2]^{2-}$,

(m) $[Cu_{36}(PPh_3)_3(CF_3COO)_2(PhSe)_{15}H_{12}Cl(CH_2Cl_2)_2]^{2-}$.

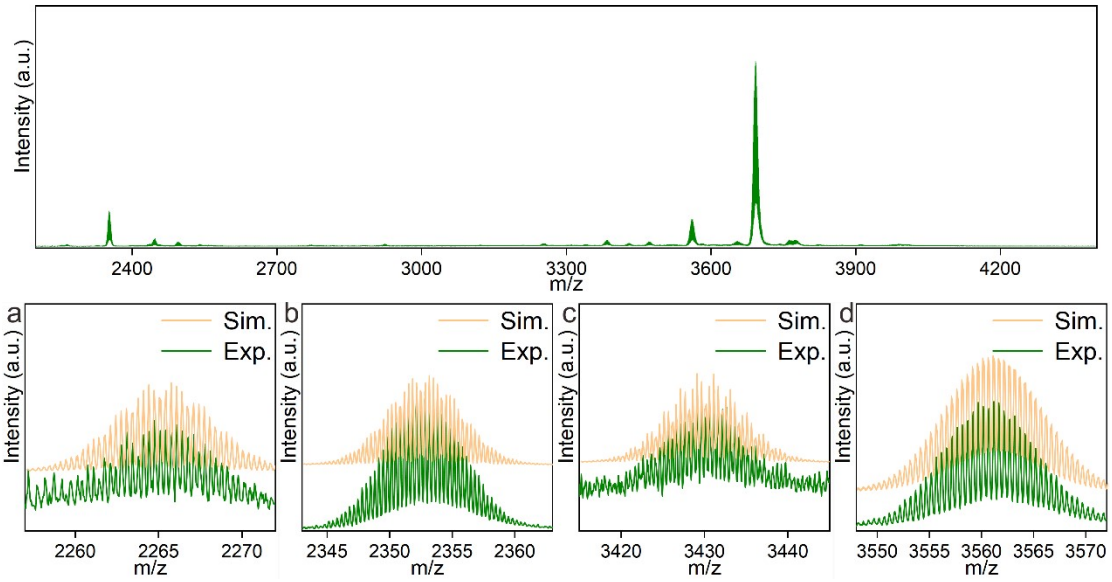

Figure S10. The ESI-MS spectroscopy of $Cu_{47}D_{12}$ clusters in the range of 2200-4400 m/z. (a-d) The comparison between the simulated (orange) and experimental (green) isotopic pattern of

(a) $[Cu_{47}(PPh_3)(CF_3COO)_{13}(PhSe)_{11}D_{12}Cl_6(C_4H_{10}O)(CH_3OH)(H_2O)]^{3-}$,

(b) $[Cu_{47}(PPh_3)_2(CF_3COO)_{13}(PhSe)_{11}D_{12}Cl_6(C_4H_{10}O)(CH_3OH)(H_2O)]^{3-}$,

(c) $[Cu_{47}(CF_3COO)_{13}(PhSe)_{14}D_{12}Cl_2(C_4H_{10}O)(CH_3OH)(H_2O)]^{2-}$,

(d) $[Cu_{47}(PPh)_3(CF_3COO)_{13}(PhSe)_{14}D_{12}Cl_2(C_4H_{10}O)(CH_3OH)(H_2O)]^{2-}$.

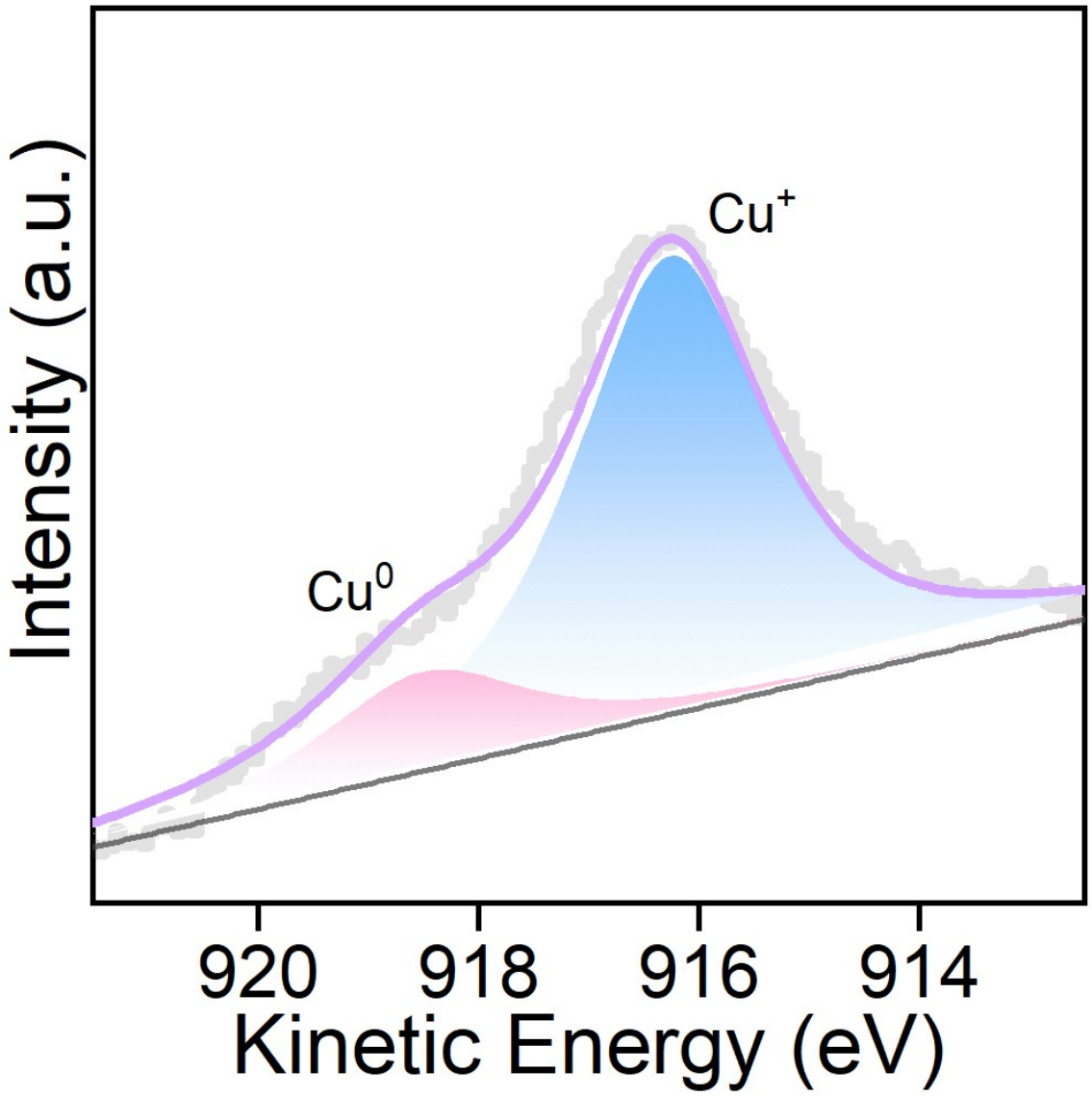

Figure S11. Cu LMM Auger spectrum of the $Cu_{47}H_{12}$ cluster.

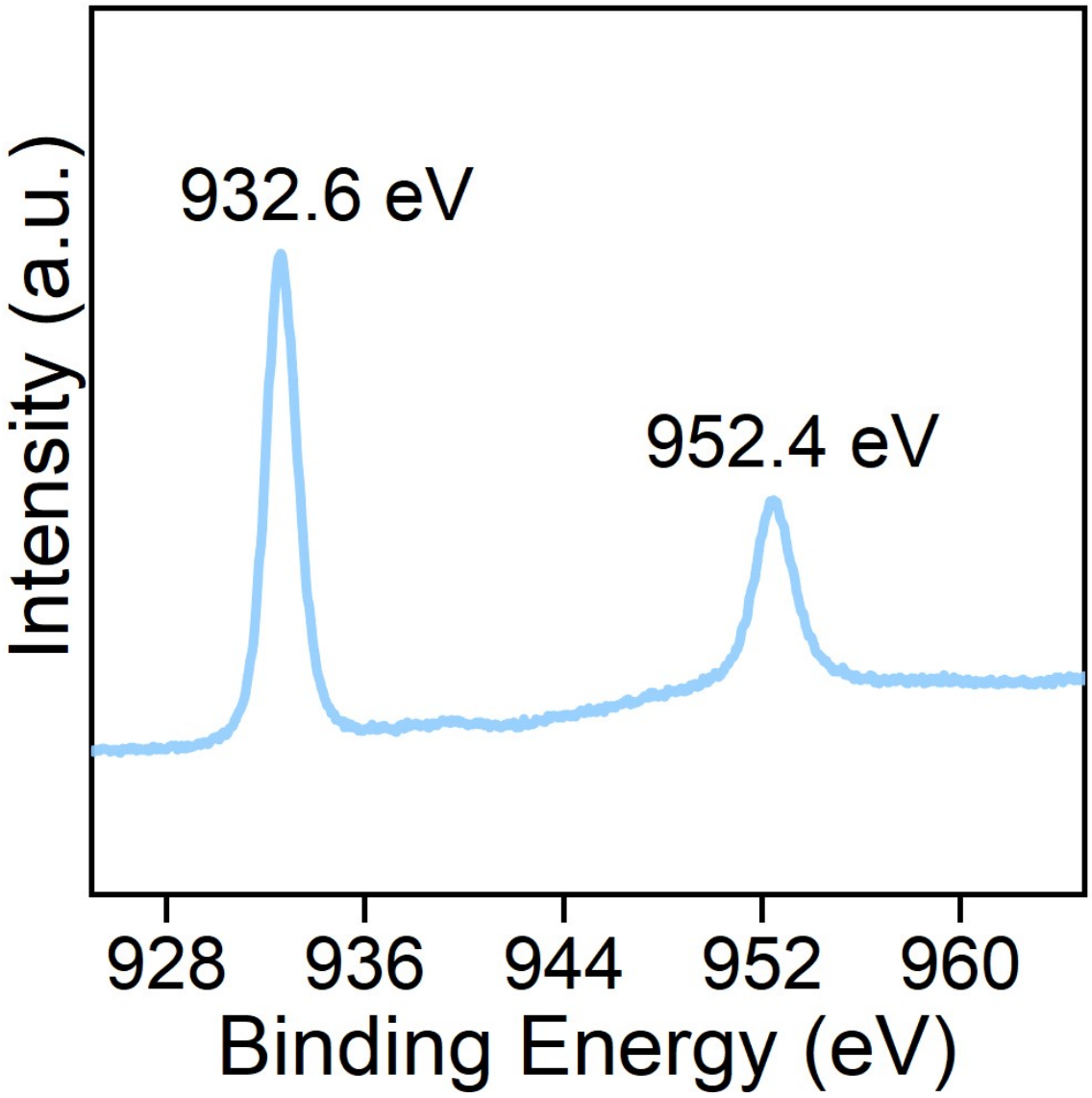

Figure S12. X-ray photoelectron spectroscopy (XPS) of the $Cu_{47}H_{12}$ cluster.

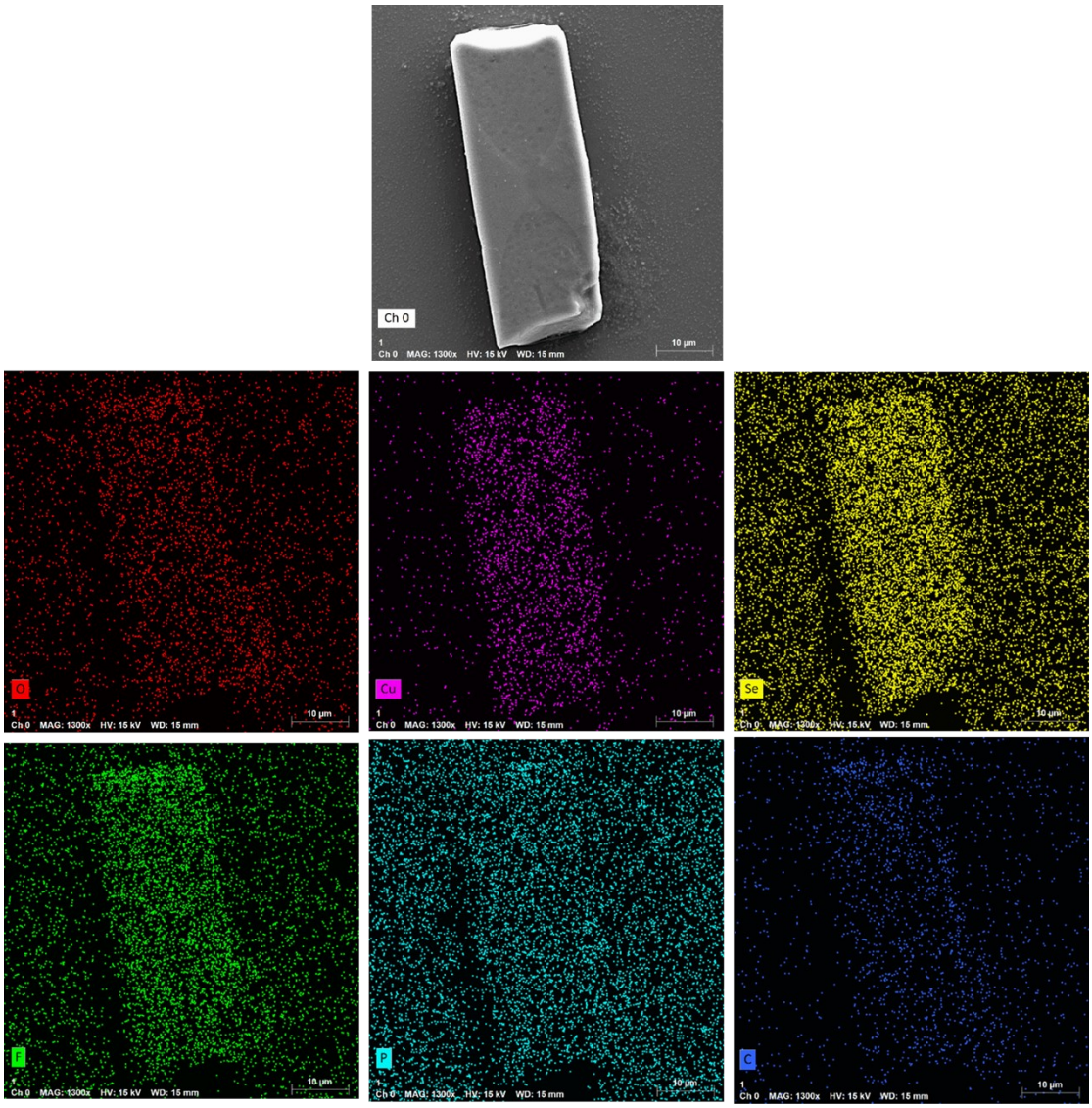

Figure S13. The energy-dispersive X-ray spectroscopy (EDS) mapping of the $Cu_{47}H_{12}$ crystals.

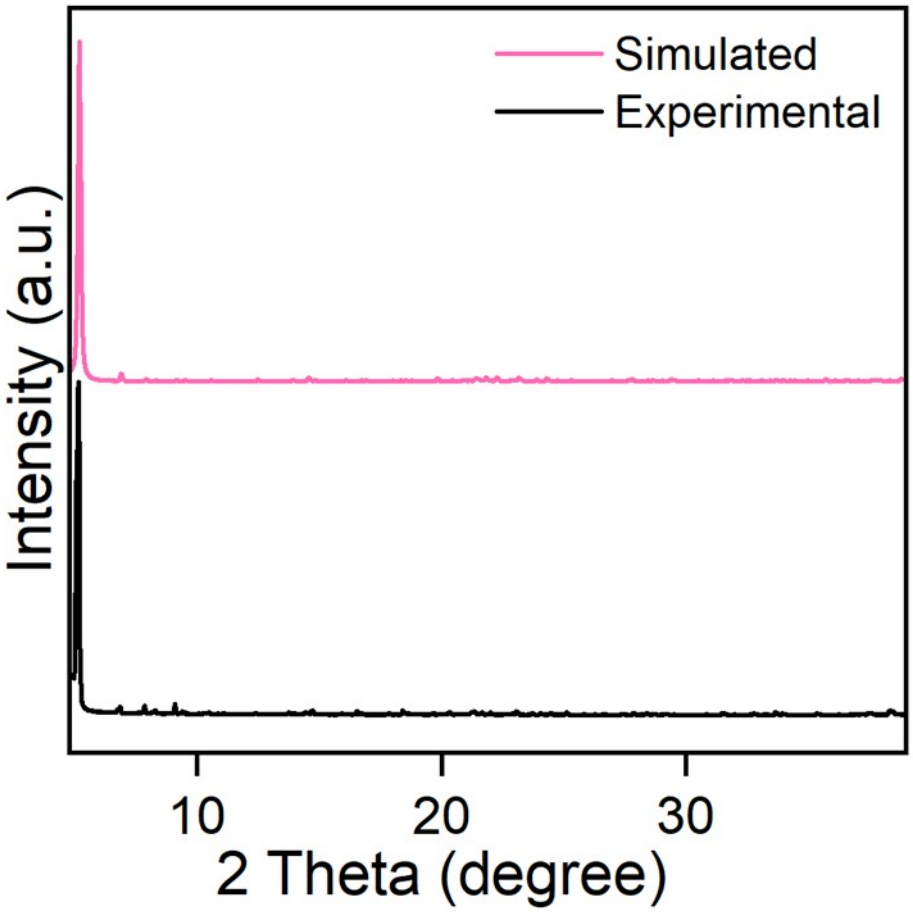

Figure S14. PXRD spectra of the $Cu_{47}H_{12}$ cluster.

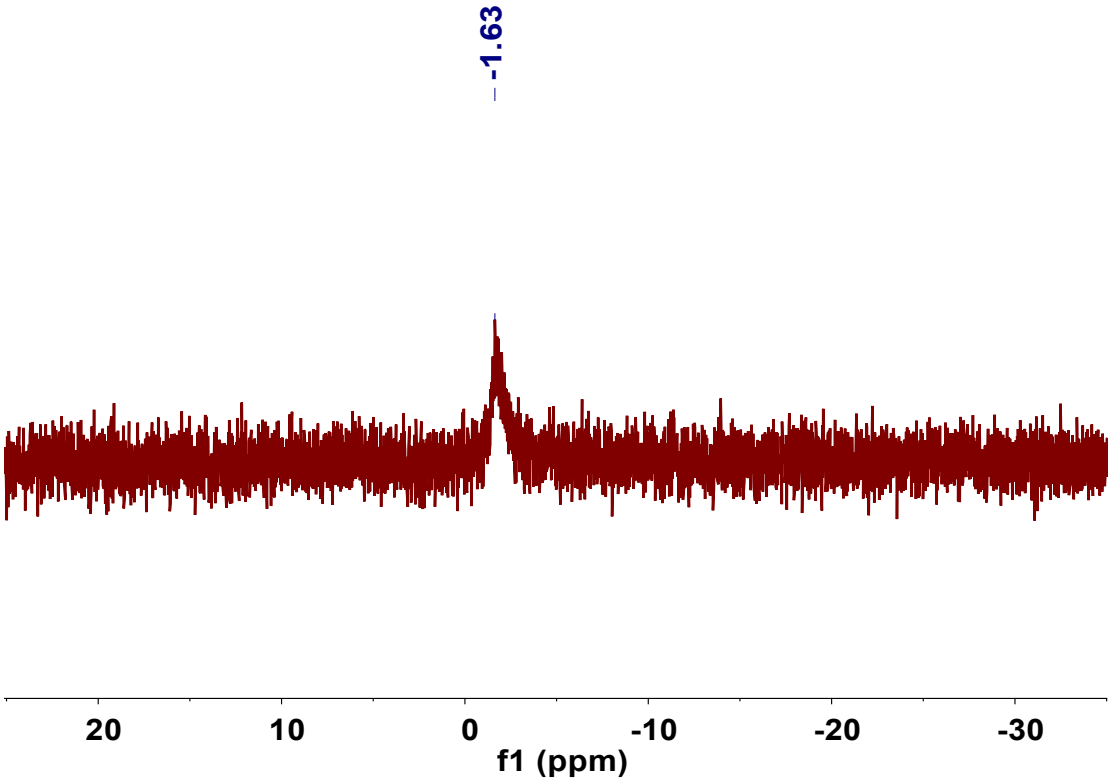

Figure S15. Proton-decoupled ^{31}P NMR spectra of the $Cu_{47}H_{12}$ in d_6-DMSO.

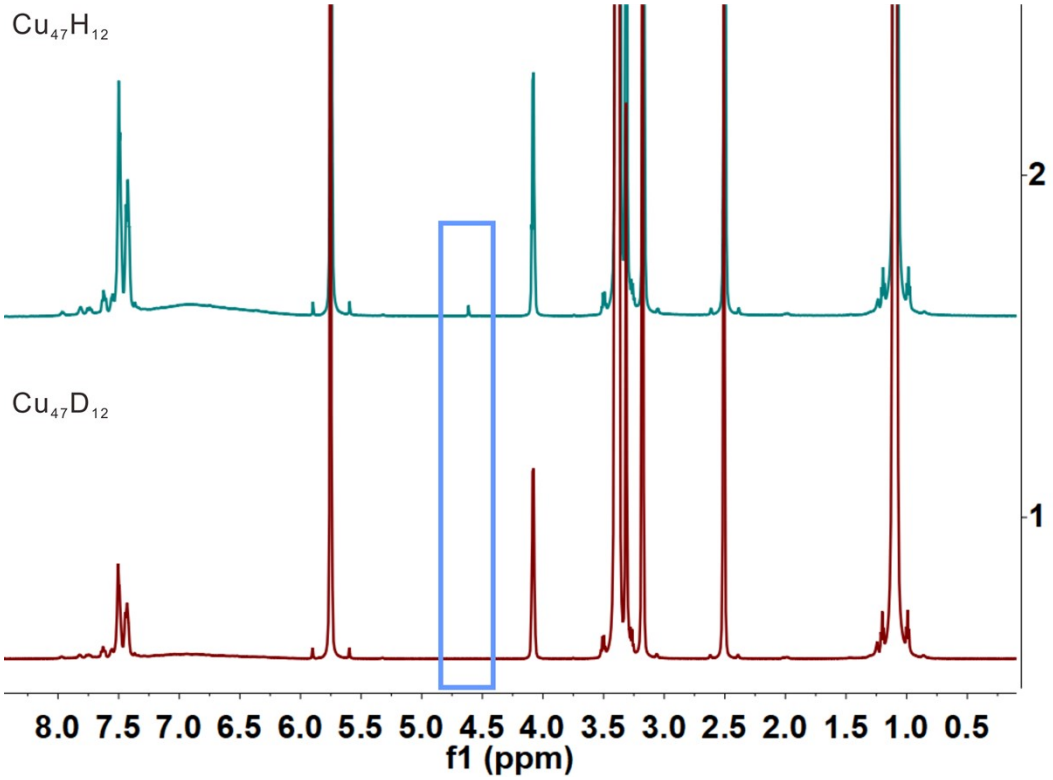

Figure S16. ^{1}H NMR spectrum of $Cu_{47}H_{12}$ and $Cu_{47}D_{12}$ in d_6-DMSO.

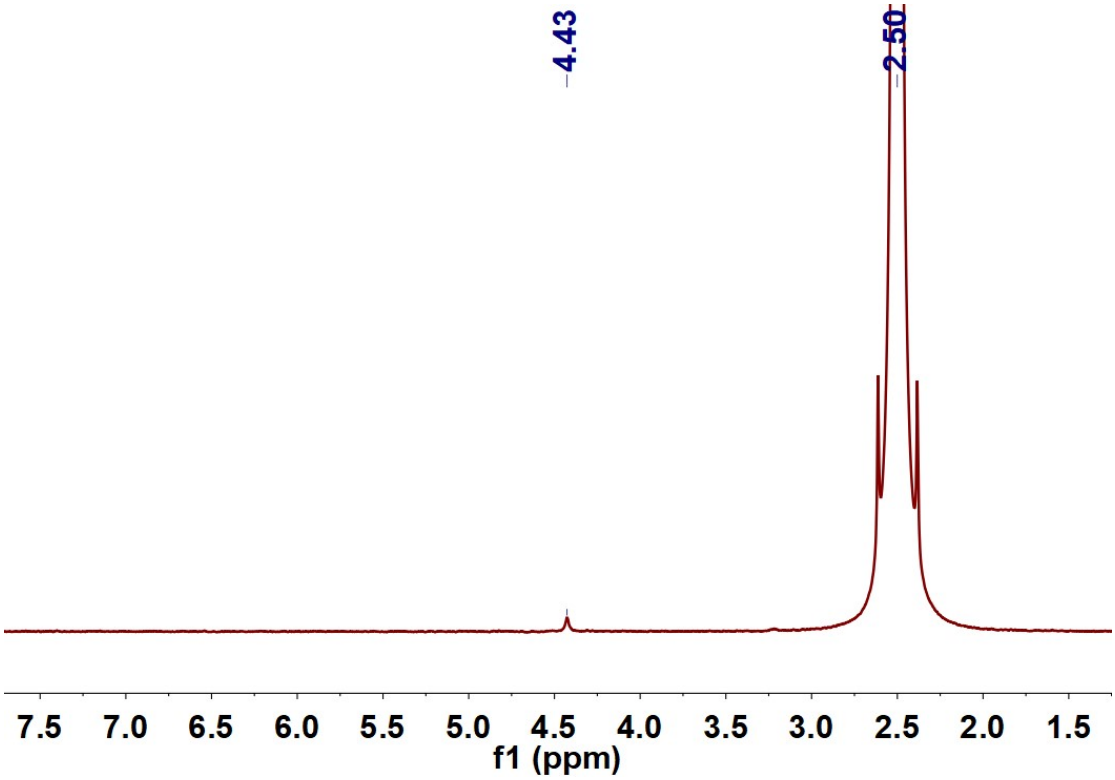

Figure S17. ^{2}H NMR spectrum of $Cu_{47}D_{12}$ in d_6-DMSO.

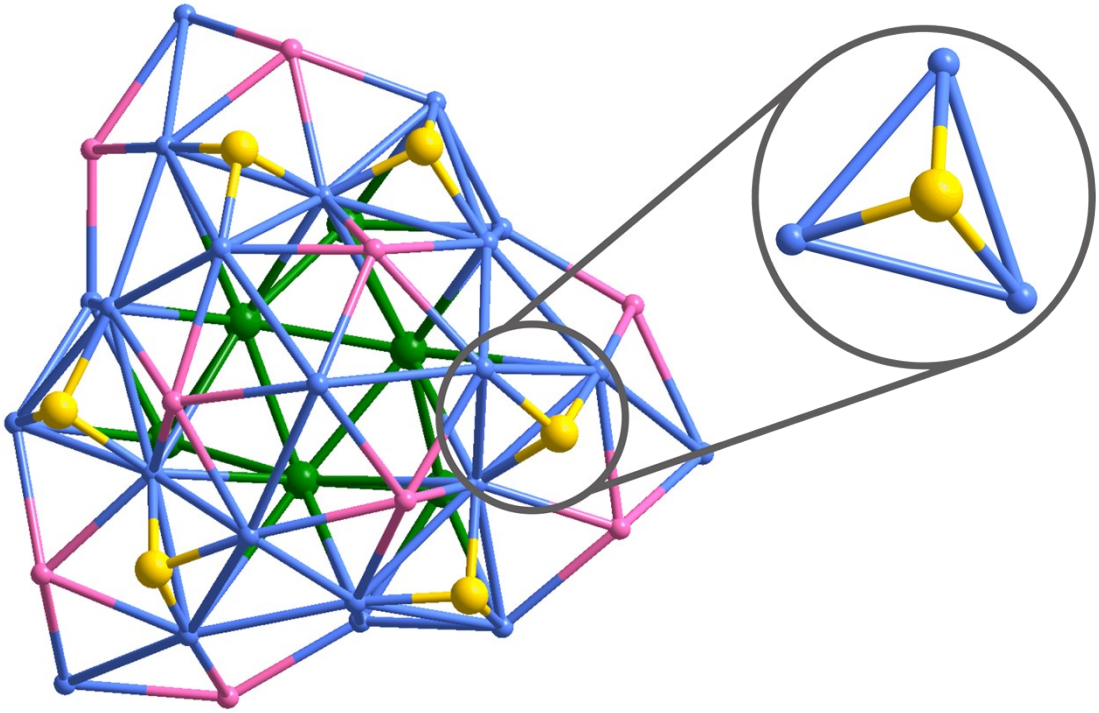

Figure S18. Proposed position of 12 hydrides in $Cu_{47}H_{12}$ cluster. The illustration depicts the precise coordination mode of hydride. Color codes for atoms: blue and green spheres, Cu; pink spheres, Se; yellow spheres, H.

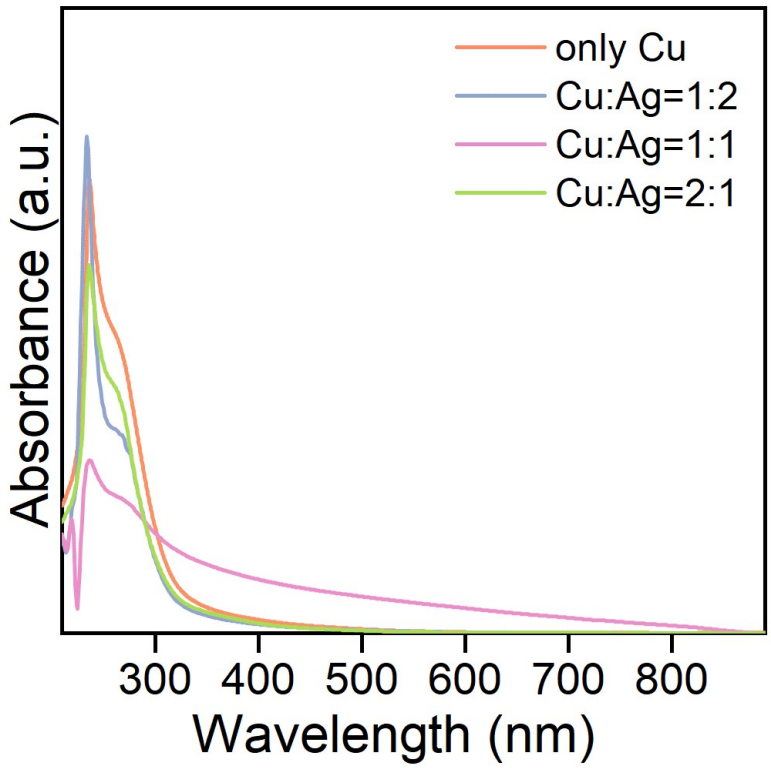

Figure S19. UV-Vis spectra of crude products synthesized using varying ratios of Ag and Cu salts.

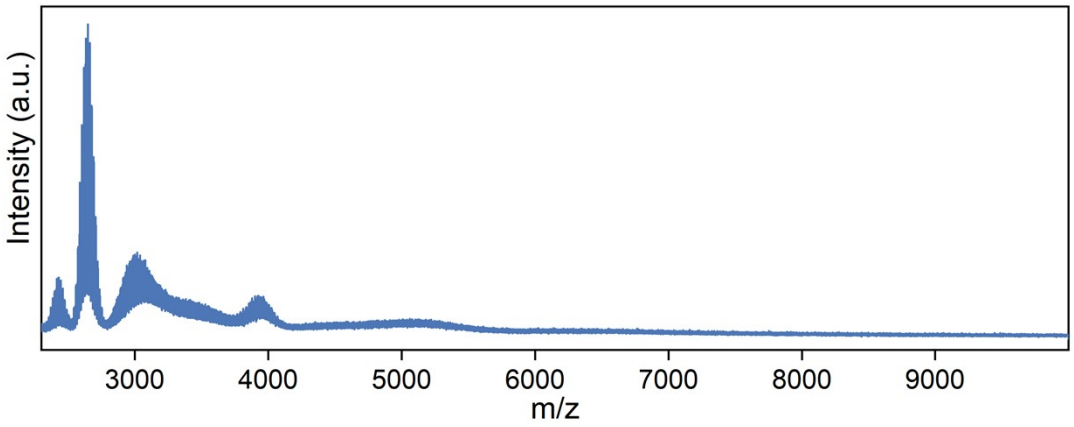

Figure S20. The ESI-MS spectroscopy of $(CuAg)_{47}H_6$ clusters in the wide range.

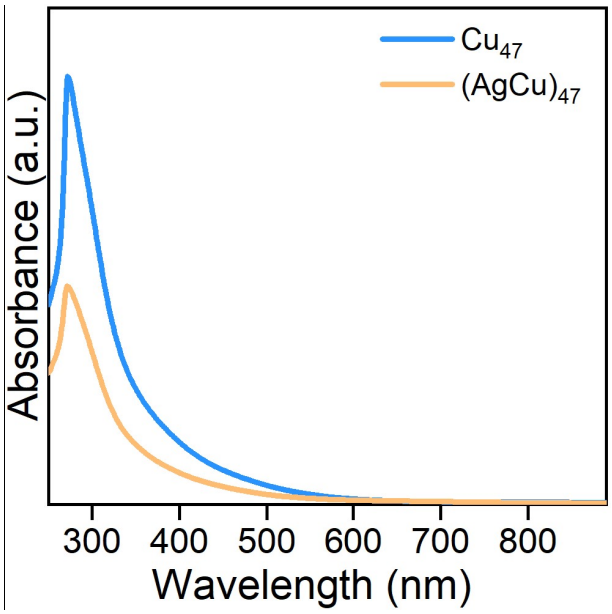

Figure 21. UV-Vis spectra of two clusters under the same measurement conditions. The cluster solutions in DMF were measured in air at room temperature.

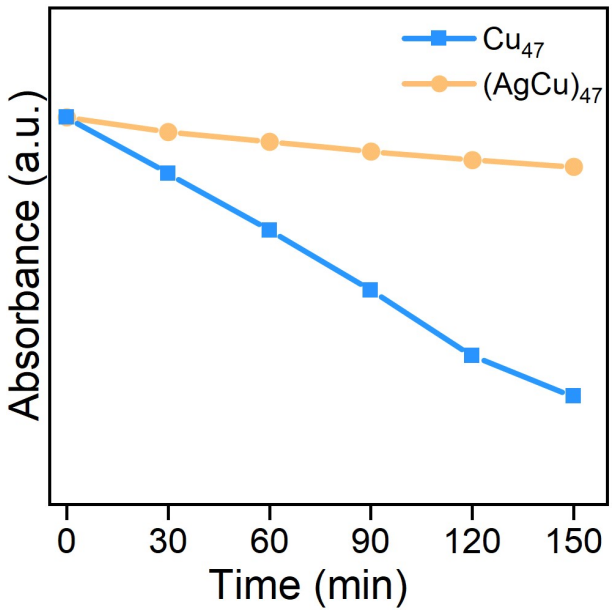

Figure 22. The stability evaluation of two clusters by UV-Vis spectra. The cluster solutions in DMF were stored in air at room temperature.

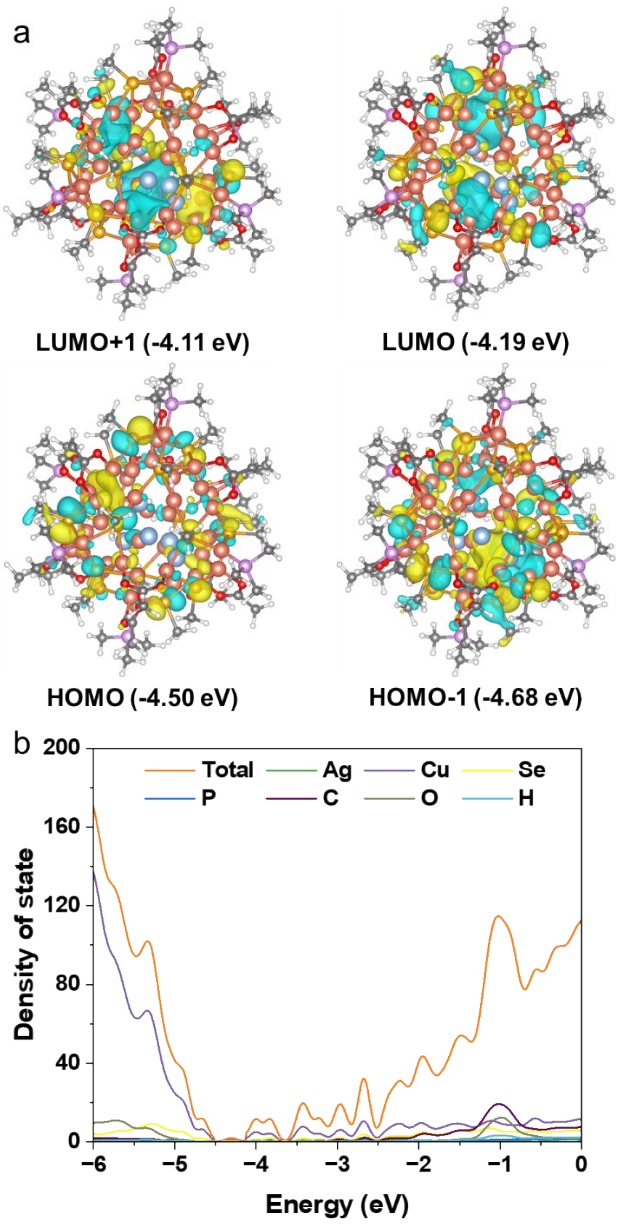

Figure S23. (a) Frontier orbitals of $(CuAg)_{47}H_6$ cluster. (b) The projected density of states of $(CuAg)_{47}H_6$ cluster.

Table S1. Crystallographic data of $Cu_{47}H_{12}$.

identification code	$[Cu_{47}(PhSe)_{15}(PPh_3)_5(CF_3COO)_{12}H_{12}]$
formula	$C_{207}H_{168}Cl_6Cu_{47}F_{36}O_{24}P_5Se_{15}$
formula weight	8261.73
Temperature/K	100.15
crystal system	hexagonal
space group	$P6_3/m$
a (Å)	21.8398(5)
b (Å)	21.8398(5)
c (Å)	33.3259(5)
α (˚)	90
β (˚)	90
γ (˚)	120
V (Å3)	13766.0(6)
Z	2
Dc/(g·cm^{-3})	1.993
Radiation	Cu Kα (λ= 1.54184 Å)
Theta (˚) range	4.672 to 153.354
Index ranges	$-26 \le h \le 23$, $-26 \le k \le 22$, $-41 \le l \le 23$
Refls. Total	30008
restraints	48
parameters	535
Rint	0.0501
R1/wR2 [I>2σ(I)]	0.0479/0.1282
R1/wR2 (all data)	0.0617/0.1355
completeness	0.936
GooF	1.0274

Table S2 Selected bond lengths (Å) for cluster $Cu_{47}H_{12}$.

Parameter	value	Parameter	value
Se1-Cu05	2.4610(9)	Cu05-Cu07[1]	2.6678(8)
Se1-Cu08	2.4114(10)	Cu05-Cu08	2.5757(11)
Se1-Cu08[1]	2.5257(10)	Cu05-Cu09	2.6038(11)
Se1-Cu0A	2.5561(8)	Cu05-Cu0B	2.6530(12)
Se1-Cu0B	2.6746(10)	Cu06-Cu08	2.8859(12)
Se1-C00W	1.933(5)	Cu06-Cu0B[3]	2.7170(12)
Se02-Cu05	2.4699(10)	Cu06-Cu0C	3.0291(12)
Se02-Cu06	2.5019(10)	Cu06-O00L	2.017(4)
Se02-Cu09	2.4352(10)	Cu07-Cu09[3]	2.7021(13)
Se02-Cu0C	2.5183(10)	Cu07-Cu09[4]	2.7021(13)
Se02-C00V	1.944(5)	Cu07-Cu0D	2.4292(18)
Se03-Cu06[2]	2.4946(9)	Cu08-Cu0A	2.9964(11)
Se03-Cu06	2.4947(9)	Cu08-Cu0B[3]	2.5815(12)
Se03-Cu0C	2.5467(15)	Cu08-O00N	1.993(4)
Se03-Cu0D	2.3808(16)	Cu09-Cu09[2]	2.6795(15)
Se03-C010	1.941(7)	Cu09-Cu0B	2.7332(12)
Cu04-Cu04[3]	2.6282(14)	Cu09-Cu0D[1]	2.5942(15)
Cu04-Cu04[2]	2.7861(14)	Cu09-O00O	2.036(4)
Cu04-Cu04[1]	2.6281(14)	Cu0A-P00E	2.238(2)
Cu04-Cu05	2.9979(11)	Cu0B-Cu0D[1]	2.7950(8)
Cu04-Cu05[1]	2.6226(11)	Cu0B-O00K	1.973(4)
Cu04-Cu07[1]	2.6057(12)	Cu0C-P00F	2.244(3)
Cu04-Cu07[3]	2.6168(13)	Cu04-Cu0D[1]	2.7577(14)
Cu04-Cu0B	2.4954(11)	Cu05-Cu06	2.6145(12)

[1]1-Y,+X-Y,+Z; [2]+X,+Y,3/2-Z; [3]1+Y-X,1-X,+Z; [4]1+Y-X,1-X,3/2-Z.

Table S3. Optimized fractional atomic coordinates for $Cu_{47}H_{12}$ cluster. Box size is 30×30×30 Å^3.

Atom		x	y	z	Atom		x	y	z
1	Se	0.48375	0.32958	0.35265	143	H	0.48413	0.4792	0.22658
2	Se	0.39363	0.25164	0.45986	144	H	0.53341	0.36132	0.1774
3	Se	0.55883	0.42655	0.35273	145	H	0.52493	0.32697	0.22549
4	Se	0.67163	0.38758	0.45973	146	H	0.56666	0.36825	0.22664
5	Se	0.43812	0.44339	0.35317	147	H	0.79621	0.36611	0.48448
6	Se	0.41458	0.56039	0.46	148	H	0.82809	0.34379	0.52969
7	Se	0.48373	0.32918	0.68438	149	H	0.78086	0.37906	0.53985
8	Se	0.39301	0.25098	0.57699	150	H	0.76386	0.28737	0.44033
9	Se	0.55863	0.42635	0.68541	151	H	0.76085	0.23833	0.47285
10	Se	0.67205	0.38734	0.57727	152	H	0.81192	0.26913	0.47069
11	Se	0.43799	0.44305	0.68439	153	H	0.81036	0.26837	0.56782
12	Se	0.41516	0.56092	0.57685	154	H	0.75828	0.23936	0.56598
13	Se	0.33158	0.35008	0.51892	155	H	0.76287	0.28874	0.59774
14	Se	0.6178	0.28507	0.51906	156	H	0.36786	0.57601	0.3905
15	Se	0.53084	0.56563	0.51924	157	H	0.42188	0.60256	0.38594
16	Cu	0.52323	0.36065	0.47688	158	H	0.37902	0.62645	0.4209
17	Cu	0.45239	0.32305	0.43396	159	H	0.58432	0.62083	0.48396
18	Cu	0.36481	0.3324	0.4466	160	H	0.60842	0.59416	0.53238
19	Cu	0.41242	0.36962	0.37417	161	H	0.56939	0.63948	0.53956
20	Cu	0.47471	0.24718	0.47725	162	H	0.37512	0.57347	0.65132
21	Cu	0.53524	0.29141	0.43544	163	H	0.37227	0.62226	0.61665
22	Cu	0.51285	0.44532	0.47686	164	H	0.42312	0.60952	0.64658
23	Cu	0.5807	0.40259	0.43368	165	H	0.37591	0.44868	0.74059
24	Cu	0.61659	0.32215	0.44651	166	H	0.37206	0.49465	0.70212
25	Cu	0.56032	0.34437	0.37374	167	H	0.41325	0.49621	0.7458
26	Cu	0.63526	0.46023	0.47731	168	H	0.24665	0.34093	0.52886
27	Cu	0.56702	0.4898	0.43512	169	H	0.26058	0.37963	0.48461
28	Cu	0.44487	0.39428	0.47671	170	H	0.26582	0.39644	0.54236
29	Cu	0.44761	0.47569	0.43461	171	H	0.38622	0.18096	0.41354
30	Cu	0.50065	0.54522	0.44695	172	H	0.38905	0.22874	0.37718
31	Cu	0.508	0.48573	0.37416	173	H	0.338	0.21652	0.40598
32	Cu	0.37048	0.49231	0.4772	174	H	0.62627	0.20852	0.48509
33	Cu	0.37903	0.41818	0.43507	175	H	0.61192	0.20512	0.54361
34	Cu	0.52299	0.3606	0.56053	176	H	0.66878	0.21629	0.52722
35	Cu	0.45161	0.32292	0.60247	177	H	0.51295	0.26691	0.73245
36	Cu	0.36434	0.33249	0.59123	178	H	0.46256	0.24867	0.70495
37	Cu	0.41245	0.36916	0.66358	179	H	0.45864	0.28539	0.75225
38	Cu	0.47435	0.24742	0.56059	180	H	0.39484	0.18494	0.63028

39	Cu	0.53461	0.29166	0.60266	181	H	0.33907	0.20727	0.62597
40	Cu	0.513	0.44527	0.56068	182	H	0.37955	0.23481	0.66044
41	Cu	0.58063	0.4025	0.60343	183	H	0.74435	0.40359	0.61882
42	Cu	0.61621	0.32203	0.5915	184	H	0.71766	0.35418	0.64122
43	Cu	0.56035	0.34479	0.6637	185	H	0.69776	0.40878	0.65616
44	Cu	0.6353	0.45996	0.56059	186	H	0.6963	0.40462	0.37931
45	Cu	0.56721	0.48965	0.60232	187	H	0.72211	0.35452	0.39969
46	Cu	0.44493	0.39441	0.56054	188	H	0.74219	0.40864	0.41774
47	Cu	0.44778	0.47528	0.60285	189	H	0.59311	0.46254	0.28505
48	Cu	0.50043	0.54516	0.59147	190	H	0.62989	0.41965	0.30618
49	Cu	0.50822	0.48548	0.66328	191	H	0.62715	0.47347	0.33335
50	Cu	0.3708	0.49255	0.56054	192	H	0.63218	0.46618	0.70239
51	Cu	0.37935	0.41833	0.60268	193	H	0.6242	0.4192	0.73921
52	Cu	0.43981	0.46622	0.51871	194	H	0.59334	0.47047	0.74799
53	Cu	0.33818	0.26509	0.51783	195	H	0.36851	0.44998	0.30656
54	Cu	0.37092	0.42013	0.51886	196	H	0.41182	0.48676	0.28518
55	Cu	0.46301	0.32048	0.5184	197	H	0.37967	0.50284	0.33312
56	Cu	0.6886	0.33381	0.51802	198	H	0.49446	0.24787	0.33146
57	Cu	0.53727	0.28354	0.51903	199	H	0.49466	0.28369	0.28313
58	Cu	0.5777	0.41348	0.5186	200	H	0.44244	0.26891	0.3092
59	Cu	0.45346	0.60213	0.51742	201	O	0.54988	0.23411	0.40524
60	Cu	0.57215	0.49628	0.51871	202	O	0.31576	0.32927	0.39816
61	Cu	0.49339	0.39948	0.31104	203	O	0.35726	0.35473	0.33922
62	Cu	0.49258	0.39847	0.72639	204	O	0.49864	0.19254	0.44297
63	H	0.25056	0.35037	0.34773	205	O	0.60903	0.53126	0.4048
64	H	0.28423	0.3625	0.29957	206	O	0.64395	0.2812	0.39827
65	H	0.27486	0.30647	0.31629	207	O	0.60164	0.30484	0.33912
66	H	0.50648	0.14564	0.36876	208	O	0.6705	0.50816	0.44298
67	H	0.55865	0.17097	0.35383	209	O	0.322	0.43372	0.40492
68	H	0.55521	0.13307	0.39957	210	O	0.52115	0.58975	0.39839
69	H	0.48258	0.27702	0.43074	211	O	0.52225	0.54106	0.33944
70	H	0.40308	0.33113	0.4095	212	O	0.31198	0.49926	0.44211
71	H	0.65827	0.21428	0.34791	213	O	0.55	0.23429	0.63228
72	H	0.63079	0.2373	0.29978	214	O	0.31579	0.32879	0.63993
73	H	0.68415	0.25706	0.3162	215	O	0.35725	0.35475	0.69867
74	H	0.70737	0.53837	0.36874	216	O	0.4982	0.19285	0.59524
75	H	0.6593	0.57084	0.35379	217	O	0.60893	0.53156	0.63234
76	H	0.69378	0.5868	0.39964	218	O	0.64419	0.28198	0.64011
77	H	0.60584	0.45153	0.43068	219	O	0.60063	0.30428	0.69883
78	H	0.59792	0.35555	0.40948	220	O	0.67056	0.50814	0.59466
79	H	0.57216	0.63544	0.34787	221	O	0.32206	0.43368	0.63251
80	H	0.56578	0.60004	0.29982	222	O	0.52041	0.58982	0.63989

81	H	0.52206	0.63643	0.31629	223	O	0.52257	0.54075	0.69851
82	H	0.26695	0.51572	0.36838	224	O	0.31175	0.49902	0.59506
83	H	0.26272	0.45788	0.35336	225	C	0.32116	0.34182	0.35796
84	H	0.2321	0.47971	0.39948	226	C	0.50803	0.45419	0.2147
85	H	0.3929	0.47093	0.4307	227	C	0.52779	0.19843	0.41287
86	H	0.47985	0.51339	0.40977	228	C	0.37447	0.21515	0.40785
87	H	0.25063	0.35044	0.69	229	C	0.47795	0.27576	0.3146
88	H	0.28412	0.36259	0.73829	230	C	0.28007	0.34068	0.32848
89	H	0.27469	0.30651	0.72159	231	C	0.24175	0.22006	0.47096
90	H	0.50643	0.14589	0.66917	232	C	0.53765	0.1599	0.38167
91	H	0.55859	0.17123	0.68412	233	C	0.63057	0.27978	0.35796
92	H	0.55514	0.13341	0.63827	234	C	0.43933	0.38578	0.2146
93	H	0.48191	0.27697	0.60719	235	C	0.65092	0.53029	0.41271
94	H	0.40281	0.33082	0.628	236	C	0.71297	0.38896	0.40786
95	H	0.65802	0.21446	0.68987	237	C	0.60855	0.44805	0.31479
96	H	0.63082	0.2372	0.73829	238	C	0.65193	0.24461	0.32856
97	H	0.68408	0.25709	0.72157	239	C	0.77539	0.27183	0.47132
98	H	0.70779	0.53878	0.66828	240	C	0.67936	0.55819	0.38165
99	H	0.65916	0.5701	0.68415	241	C	0.52928	0.57875	0.35813
100	H	0.69304	0.58731	0.63825	242	C	0.53319	0.36068	0.21397
101	H	0.60611	0.45128	0.60756	243	C	0.30231	0.47086	0.41221
102	H	0.59827	0.35597	0.62834	244	C	0.3935	0.59548	0.40789
103	H	0.57205	0.63518	0.68993	245	C	0.39413	0.4747	0.31478
104	H	0.56583	0.60008	0.73819	246	C	0.54898	0.61475	0.32862
105	H	0.52209	0.63647	0.72162	247	C	0.46475	0.70724	0.46995
106	H	0.26702	0.5156	0.66904	248	C	0.2639	0.48155	0.38121
107	H	0.26282	0.45779	0.68409	249	C	0.32117	0.34169	0.68003
108	H	0.23198	0.47963	0.63813	250	C	0.50845	0.45494	0.82105
109	H	0.39296	0.47135	0.60721	251	C	0.52766	0.1987	0.62509
110	H	0.47943	0.51312	0.62831	252	C	0.3745	0.21535	0.62988
111	H	0.23062	0.18797	0.5761	253	C	0.47875	0.27587	0.72328
112	H	0.2144	0.24314	0.56086	254	C	0.28002	0.34072	0.70941
113	H	0.26076	0.23528	0.59637	255	C	0.24299	0.22136	0.56765
114	H	0.22768	0.18684	0.4648	256	C	0.53758	0.16021	0.65626
115	H	0.2599	0.23119	0.44125	257	C	0.63024	0.27989	0.68015
116	H	0.2145	0.24376	0.47664	258	C	0.43938	0.38599	0.82402
117	H	0.30831	0.15305	0.48382	259	C	0.65087	0.53039	0.6248
118	H	0.28163	0.13947	0.53533	260	C	0.7128	0.38853	0.62966
119	H	0.3361	0.1641	0.53466	261	C	0.60832	0.44807	0.72335
120	H	0.43699	0.34978	0.82868	262	C	0.65175	0.2447	0.7094
121	H	0.41318	0.39553	0.80032	263	C	0.77397	0.27236	0.56703
122	H	0.43345	0.40279	0.85598	264	C	0.67923	0.55819	0.65595

123	H	0.52813	0.47314	0.79621	265	C	0.52908	0.57861	0.67998
124	H	0.5273	0.45285	0.85234	266	C	0.53398	0.35994	0.82235
125	H	0.47781	0.47411	0.82677	267	C	0.30223	0.47071	0.62509
126	H	0.5604	0.35402	0.79772	268	C	0.39404	0.59569	0.62925
127	H	0.5171	0.32793	0.82794	269	C	0.39452	0.47469	0.72297
128	H	0.549	0.37129	0.85373	270	C	0.54892	0.61464	0.70938
129	H	0.36769	0.65432	0.53185	271	C	0.46492	0.70549	0.56815
130	H	0.37213	0.68926	0.48457	272	C	0.26388	0.48144	0.65621
131	H	0.37409	0.7132	0.53903	273	C	0.2681	0.36874	0.51867
132	H	0.43638	0.71988	0.45065	274	C	0.30336	0.16359	0.51848
133	H	0.48442	0.68543	0.44823	275	C	0.63353	0.22082	0.51872
134	H	0.48551	0.73559	0.47998	276	C	0.79445	0.35278	0.51846
135	H	0.48802	0.73218	0.55865	277	C	0.57899	0.61098	0.51876
136	H	0.48223	0.68262	0.59074	278	C	0.38389	0.68436	0.51882
137	H	0.43683	0.72043	0.5862	279	P	0.28039	0.22061	0.51879
138	H	0.43152	0.35103	0.22295	280	P	0.75563	0.3053	0.5187
139	H	0.43796	0.39032	0.17832	281	P	0.44476	0.67455	0.51851
140	H	0.41379	0.40649	0.23058	282	P	0.49355	0.39997	0.23911
141	H	0.5085	0.45404	0.17811	283	P	0.49358	0.39965	0.79836
142	H	0.54089	0.46419	0.22723					

Table S4. Frontier orbitals for $Cu_{47}H_{12}$ cluster. Gap=0.1807 eV.

LUMO+1	-2.5714 eV
LUMO	-2.5805 eV
HOMO	-2.7612 eV
HOMO-1	-2.7735 eV

Table S5. Crystallographic data of $(CuAg)_{47}H_6$.

identification code	$[(CuAg)_{47}(PhSe)_{18}(PPh_3)_6(CF_3COO)_{12}H_6]^{3+}$
formula	$C_{241}H_{183}Ag_{7.17}Cl_2Cu_{39.83}F_{36}O_{24}P_6Se_{18}$
formula weight	9128.98
Temperature/K	100.00(10)
crystal system	monoclinic
space group	Cc
a (Å)	21.2386(2)
b (Å)	36.7068(3)
c (Å)	38.4701(3)
α (˚)	90
β (˚)	98.3450(10)
γ (˚)	90
V (Å3)	29673.8(4)
Z	4
Dc / (g·cm-3)	2.043
Radiation	Cu Kα (λ= 1.54184 Å)
Theta (˚) range	7.124 to 130.896
Index ranges	$-25 \le h \le 23$, $-42 \le k \le 42$, $-39 \le l \le 45$
Refls. Total	101155
restraints	530
parameters	3452
Rint	0.0572
R1/wR2 [I>2σ(I)]	0.0592/0.1494
R1/wR2 (all data)	0.0743/0.1617
completeness	99.96
GooF	1.026

Table S6. Selected bond lengths (Å) for cluster $(CuAg)_{47}H_6$.

Parameter	value	Parameter	value
Se13-Cu26	2.569(3)	Se4-Cu47	2.611(3)
Se13-Cu39	2.613(3)	Se4-Cu49	2.484(3)
Se13-Cu46	2.545(3)	Se4-Cu63	2.604(4)
Se13-Cu57	2.426(3)	Se4-Cu64	2.544(4)
Se5-Cu27	2.478(3)	Se10-Cu2	2.419(3)
Se5-Cu47	2.589(3)	Se10-Cu27	2.405(3)
Se5-Cu49	2.440(3)	Se10-Cu47	2.548(3)
Se5-Cu62	2.636(4)	Se10-Cu72	2.340(6)
Se5-Cu25	2.526(7)	Se10-Cu8	2.358(8)
Se8-Cu33	2.504(3)	Se17-Cu24	2.454(3)
Se8-Cu41	2.569(4)	Se17-Cu35	2.428(3)
Se8-Cu50	2.766(4)	Se17-Cu59	2.544(3)
Se8-Cu58	2.436(3)	Se17-Cu	2.483(5)
Se8-Cu72	2.438(5)	Se2-Cu28	2.421(3)
Se16-Ag32	2.785(3)	Se2-Cu31	2.534(3)
Se16-Cu43	2.542(3)	Se2-Cu37	2.453(3)
Se16-Cu48	2.435(3)	Se2-Cu38	2.530(3)
Se16-Cu51	2.430(3)	Se2-Cu45	2.893(4)
Se16-Cu56	2.712(3)	Se12-Cu26	2.421(3)
Se16-Cu32	2.785(3)	Se12-Cu29	2.436(3)
Se3-Cu29	2.448(3)	Se12-Cu34	2.549(3)
Se3-Cu31	2.535(3)	Se12-Cu39	2.540(4)
Se3-Cu39	2.481(3)	Se1-Ag32	2.629(3)
Se3-Cu46	2.415(3)	Se1-Cu37	2.418(3)
Se18-Ag26	3.090(3)	Se1-Cu38	2.533(3)
Se18-Cu28	2.509(3)	Se1-Cu42	2.450(3)
Se18-Cu38	2.593(3)	Se1-Cu32	2.629(3)

Se18-Cu42	2.506(3)	Se11-Cu24	2.441(3)
Se18-Cu58	2.450(3)	Se11-Ag52	2.611(4)
Se18-Cu8	2.409(7)	Se11-Cu55	2.832(5)
Se6-Cu35	2.498(3)	Se11-Cu59	2.558(3)
Se6-Ag53	2.727(3)	Se11-Cu60	2.423(3)
Se6-Cu54	2.811(5)	Se11-Ag3	3.070(11)
Se6-Cu59	2.634(3)	Se14-Cu43	2.606(3)
Se6-Cu60	2.409(4)	Se14-Cu44	2.431(3)
Se6-Cu25	2.565(8)	Se14-Cu51	2.479(3)
Se9-Cu33	2.416(3)	Se14-Cu57	2.394(4)
Se9-Cu34	2.577(3)	Se7-Cu40	2.438(3)
Se9-Cu40	2.489(3)	Se7-Cu41	2.438(3)
Se9-Cu45	2.936(4)	Se7-Cu50	2.509(4)
Se9-Cu50	2.444(3)	Se7-Ag52	2.565(4)
Se4-Cu2	2.479(3)	Se7-Ag3	2.691(8)
Ag24-Ag23	2.906(3)	Ag24-Ag26	2.786(3)
Ag24-Ag1	2.964(4)	Ag24-Ag22	3.049(4)
Ag24-Cu31	2.760(4)	Cu2-O52	2.004(14)
Ag24-Cu34	3.135(4)	Cu26-Cu55	2.780(4)
Ag24-Ag36	2.786(4)	Cu26-O34	1.999(14)
Ag24-Cu45	2.681(3)	Cu26-Cu1	2.694(13)
Ag24-Cu58	2.687(4)	Cu27-Cu41	2.880(4)
Se15-Cu43	2.579(3)	Cu27-Cu47	2.868(4)
Se15-Cu44	2.441(3)	Cu27-Ag61	2.969(4)
Se15-Cu48	2.423(3)	Cu27-Cu62	2.669(4)
Se15-Cu64	2.458(4)	Cu27-Cu72	2.544(6)
Se15-Cu6	2.757(6)	Cu27-O10	2.013(13)
Ag26-Ag23	2.774(3)	Cu28-Cu33	2.786(4)
Ag26-Cu2	2.813(3)	Cu28-Cu38	2.905(4)

Ag26-Ag36	2.827(3)	Cu28-Cu45	2.696(4)
Ag26-Cu42	2.763(3)	Cu28-Cu58	2.547(4)
Ag26-Cu58	2.648(3)	Cu28-O87	2.033(13)
Ag26-Cu63	2.858(3)	Cu29-Cu31	2.661(3)
Ag26-Cu72	2.843(6)	Cu29-Cu34	2.674(4)
Ag22-Ag23	2.855(3)	Cu29-Cu39	2.870(4)
Ag22-Ag1	2.742(3)	Cu29-Cu45	2.715(4)
Ag22-Cu34	3.084(4)	Cu29-O94	2.005(12)
Ag22-Ag36	2.904(4)	Ag1-Cu31	2.815(3)
Ag22-Ag52	2.754(4)	Ag1-Ag32	3.239(4)
Ag22-Ag53	2.950(4)	Ag1-Cu56	2.662(3)
Ag22-Cu55	2.752(4)	Ag1-Cu57	2.520(5)
Ag22-Cu5	2.538(8)	Ag1-Cu5	2.754(8)
Ag22-Cu1	1.985(15)	Ag1-Cu1	2.678(13)
Ag23-Ag1	2.842(3)	Cu31-Cu37	2.626(4)
Ag23-Ag32	3.012(4)	Cu31-Cu45	2.705(4)
Ag23-Ag36	2.798(3)	Cu31-Cu56	2.785(4)
Ag23-Ag53	2.875(4)	Cu31-Ag7	3.084(6)
Ag23-Cu63	3.214(4)	Ag32-Cu37	2.723(4)
Ag23-Cu64	2.620(5)	Ag32-Cu48	2.758(4)
Ag23-Cu5	2.101(9)	Ag32-Cu56	2.775(4)
Cu24-Cu26	2.796(4)	Ag32-Cu63	2.697(4)
Cu24-Cu55	2.618(4)	Cu33-Cu45	2.724(4)
Cu24-Cu59	2.821(4)	Cu33-Cu50	2.959(4)
Cu24-O47	1.992(13)	Cu33-Cu58	2.531(3)
Cu24-Cu1	2.752(13)	Cu33-O88	2.000(15)
Cu2-Cu42	2.867(4)	Cu34-Cu40	2.663(4)
Cu2-Cu47	2.879(4)	Cu34-Cu45	2.756(4)
Cu2-Cu63	2.644(4)	Cu34-Cu55	2.699(5)

Cu2-Cu8	2.504(8)	Cu48-Cu64	2.676(5)
Cu34-Ag67	2.764(6)	Cu48-Cu6	2.561(7)
Cu34-Cu4	2.676(6)	Cu48-O85	2.009(15)
Cu35-Cu44	2.862(4)	Cu48-Cu32	2.758(4)
Cu35Cu54	2.712(4)	Cu49-Ag53	3.116(4)
Cu35-O92	1.976(12)	Cu49-Cu54	2.673(4)
Cu35-Ag2	2.880(3)	Cu49-Cu64	2.504(5)
Ag36-Cu41	3.067(4)	Cu49-Cu6	3.049(8)
Ag36-Ag52	2.805(5)	Cu49-Cu25	2.454(7)
Ag36-Ag53	2.839(4)	Cu49-O5	1.997(12)
Ag36-Cu62	2.613(4)	Cu50-P2	2.238(6)
Ag36-Cu72	2.553(7)	Cu51-Cu56	2.709(4)
Cu37-Cu38	3.002(4)	Cu51-Cu57	2.538(4)
Cu37-Cu56	2.727(4)	Cu51-O90	1.979(13)
Cu37-O37	2.012(13)	Ag52-Ag53	3.063(5)
Cu37-Cu32	2.723(4)	Ag52-Cu55	2.976(5)
Cu38-P69	2.260(6)	Ag52-Cu60	2.600(5)
Cu39-Cu46	3.037(4)	Ag52-Cu62	2.636(6)
Cu39-P68	2.237(6)	Ag53-Cu54	2.698(4)
Cu40-Cu50	2.806(4)	Ag53-Cu60	2.582(4)
Cu40-Ag52	2.889(5)	Ag53-Cu62	2.604(4)
Cu40-Cu55	2.639(4)	Ag53-Cu5	2.668(9)
Cu40-O43	2.033(12)	Cu54-Cu64	2.641(5)
Cu40-Ag3	2.586(10)	Cu54-Cu6	2.817(7)
Cu41-Ag61	2.718(4)	Cu54-Cu25	2.536(8)
Cu41-Cu62	2.817(5)	Cu54-O8	1.997(12)
Cu41-Cu72	2.462(6)	Cu54-Ag2	2.790(3)
Cu41-O14	2.001(12)	Cu54-Cu5	2.555(8)
Cu42-Cu63	2.997(4)	Cu55-Ag67	2.591(6)

Cu42-Cu8	2.503(8)	Cu55-O6	2.024(12)
Cu42-O84	1.987(13)	Cu55-Cu1	2.932(13)
Cu43-Cu48	2.961(4)	Cu55-Ag3	2.708(10)
Cu43-Cu51	2.888(4)	Cu56-Ag7	2.733(6)
Cu43-P4	2.242(5)	Cu56-O27	1.979(13)
Cu44-Cu54	2.865(4)	Cu56-Cu32	2.775(4)
Cu44-O91	1.989(12)	Cu57-Cu	2.459(5)
Cu44-Ag2	2.870(3)	Cu57-Ag7	3.047(9)
Cu45-Cu4	2.706(6)	Cu57-Ag2	2.711(4)
Cu45-O93	2.006(12)	Cu57-Cu1	2.724(13)
Cu46-Cu51	2.848(4)	Cu58-Ag61	2.657(4)
Cu46-Cu56	2.759(4)	Cu58-Cu72	2.464(6)
Cu46-Cu57	2.562(4)	Cu58-Cu4	2.767(6)
Cu46-O89	2.002(13)	Cu58-Cu8	2.443(8)
Cu47-P65	2.253(5)	Cu59-Cu60	2.930(4)
Cu48-Cu63	2.747(4)	Ag7-Cu4	3.014(7)
Cu59-P1	2.259(6)	Ag7-Cu6	3.135(10)
Cu60-Cu62	2.855(5)	Ag7-Ag2	2.772(5)
Cu60-Cu25	2.720(7)	Ag7-Cu32	2.489(7)
Cu60-O25	1.992(12)	Cu6-Ag2	3.169(7)
Cu60-Ag3	3.215(12)	Cu5-Cu1	2.745(14)
Ag61-Cu62	2.890(5)	Cu70-Cu71	2.806(7)
Ag61-Cu70	2.831(5)	Cu70-Ag7	2.906(9)
Ag61-Cu71	2.767(7)	Cu70-Cu4	2.730(7)
Ag61-Cu4	2.780(6)	Cu70-Cu6	2.933(8)
Ag61-Cu8	2.807(9)	Cu70-Cu8	2.512(11)
Ag61-Ag3	3.158(11)	Cu70-Cu32	2.583(5)
Cu62-Cu25	2.578(8)	Cu71Ag7	2.873(7)
Cu62-O42	1.999(14)	Cu71-Cu4	2.916(7)

Cu62-Ag3	2.972(10)	Cu71-Cu6	2.852(7)
Cu63-Cu64	2.676(5)	Cu71-Cu25	2.535(10)
Cu63-Cu70	2.557(5)	Cu71-Ag2	2.814(6)
Cu63-Cu6	2.547(7)	Cu71-Ag3	2.870(9)
Cu63-O86	2.024(14)	Ag67-Ag2	2.909(5)
Cu63-Cu32	2.697(4)	Ag67-Ag3	2.998(10)
Ag67-Cu71	2.824(7)	Ag67-Cu4	2.919(9)
Ag67-Cu	2.222(9)	Ag67-Ag7	2.738(7)

Table S7. Optimized fractional atomic coordinates for $(CuAg)_{47}H_6$ cluster. Box size is 30×30×30 Å^3.

Atom		x	y	z	Atom		x	y	z
1	Ag	0.450605	0.459223	0.42348	154	H	0.585741	0.43514	0.731771
2	Ag	0.559539	0.424081	0.542209	155	H	0.550595	0.483614	0.731001
3	Ag	0.48339	0.539881	0.463701	156	H	0.423502	0.469806	0.753915
4	Ag	0.501818	0.469712	0.600989	157	H	0.404623	0.526213	0.743228
5	Ag	0.545503	0.458388	0.454751	158	H	0.463272	0.514711	0.750124
6	Se	0.469459	0.673395	0.561486	159	H	0.497764	0.266426	0.30326
7	Se	0.583948	0.650701	0.549018	160	H	0.488462	0.209125	0.317133
8	Se	0.586327	0.610258	0.412735	161	H	0.531686	0.240395	0.344023
9	Se	0.334134	0.502624	0.58331	162	H	0.400239	0.224945	0.328787
10	Se	0.393191	0.398414	0.59027	163	H	0.401671	0.284271	0.321375
11	Se	0.399208	0.361323	0.446127	164	H	0.377629	0.261334	0.370223
12	Se	0.599791	0.36227	0.593715	165	H	0.736097	0.493671	0.383145
13	Se	0.58317	0.469467	0.653889	166	H	0.733923	0.471293	0.438613
14	Se	0.670265	0.476767	0.554869	167	H	0.734115	0.531085	0.430659
15	Se	0.436194	0.491194	0.672488	168	H	0.560488	0.258476	0.423421
16	Se	0.536503	0.331396	0.461314	169	H	0.543044	0.248614	0.480295
17	Se	0.657341	0.498691	0.414318	170	H	0.596965	0.273142	0.468496
18	Se	0.564999	0.511738	0.331273	171	H	0.565377	0.480223	0.252324
19	Se	0.424899	0.517722	0.318545	172	H	0.559437	0.540259	0.25133
20	Se	0.354234	0.518166	0.431633	173	H	0.512142	0.505746	0.264693
21	Se	0.429749	0.618904	0.404565	174	H	0.427113	0.498725	0.235235
22	Se	0.481596	0.390908	0.353589	175	H	0.404924	0.553885	0.243354
23	Se	0.524709	0.610285	0.656011	176	H	0.370601	0.5054	0.254189
24	Cu	0.535848	0.447517	0.368108	177	H	0.25597	0.598901	0.385051
25	Cu	0.390507	0.541262	0.626978	178	H	0.251054	0.649882	0.354749
26	Cu	0.54303	0.517083	0.529667	179	H	0.29127	0.644564	0.39884
27	Cu	0.401343	0.498822	0.495495	180	H	0.2858	0.506177	0.480759
28	Cu	0.473677	0.551305	0.633001	181	H	0.271313	0.502591	0.422481
29	Cu	0.554693	0.371934	0.395561	182	H	0.281082	0.556619	0.44821
30	Cu	0.415887	0.411954	0.508519	183	H	0.372683	0.680918	0.404455
31	Cu	0.613708	0.431809	0.401576	184	H	0.420274	0.695451	0.369509
32	Cu	0.447342	0.414199	0.648382	185	H	0.423926	0.699833	0.429174
33	Cu	0.598137	0.614809	0.6213	186	H	0.480199	0.406642	0.269779
34	Cu	0.631426	0.557293	0.463238	187	H	0.457494	0.352329	0.281634
35	Cu	0.552248	0.592884	0.488773	188	H	0.517332	0.360921	0.282951
36	Cu	0.467251	0.607953	0.514804	189	H	0.672646	0.525671	0.257967
37	Cu	0.635816	0.529533	0.616616	190	H	0.717138	0.514809	0.295477
38	Cu	0.627242	0.467037	0.485224	191	H	0.724356	0.554813	0.25172
39	Cu	0.404724	0.397606	0.374028	192	H	0.629001	0.615995	0.258082

40	Cu	0.520364	0.671374	0.498738	193	H	0.685202	0.63497	0.249493
41	Cu	0.536607	0.68245	0.611604	194	H	0.651388	0.657809	0.293071
42	Cu	0.632161	0.557591	0.363479	195	H	0.279271	0.370473	0.659842
43	Cu	0.647518	0.401319	0.545252	196	H	0.251033	0.420703	0.646079
44	Cu	0.53952	0.397541	0.635785	197	H	0.241914	0.395084	0.699225
45	Cu	0.427336	0.609906	0.590803	198	H	0.489874	0.205659	0.425713
46	Cu	0.374729	0.56944	0.357972	199	H	0.446211	0.181362	0.393203
47	Cu	0.370112	0.478964	0.363774	200	H	0.433496	0.217817	0.438872
48	Cu	0.612227	0.571037	0.546109	201	H	0.270677	0.544256	0.306172
49	Cu	0.545839	0.590127	0.346964	202	H	0.302642	0.567301	0.261925
50	Cu	0.363562	0.456149	0.645758	203	H	0.253456	0.595446	0.28045
51	Cu	0.398376	0.583697	0.470838	204	H	0.301913	0.67256	0.285617
52	Cu	0.341237	0.441666	0.532934	205	H	0.355268	0.648301	0.273834
53	Cu	0.653991	0.440367	0.626435	206	H	0.347844	0.680836	0.322722
54	Cu	0.45711	0.590292	0.33497	207	H	0.571247	0.631935	0.723852
55	Cu	0.362823	0.436385	0.444315	208	H	0.550313	0.576174	0.729849
56	Cu	0.600351	0.386123	0.469623	209	H	0.513703	0.622927	0.739389
57	Cu	0.507852	0.627519	0.420644	210	H	0.518695	0.732505	0.719739
58	Cu	0.498241	0.523991	0.373338	211	H	0.47921	0.758209	0.683755
59	Cu	0.554817	0.544228	0.61296	212	H	0.522377	0.791024	0.708792
60	Cu	0.477055	0.325312	0.404288	213	H	0.509505	0.798144	0.599007
61	Cu	0.463638	0.341901	0.494899	214	H	0.566404	0.79435	0.582939
62	Cu	0.47737	0.386707	0.569248	215	H	0.551195	0.826599	0.630824
63	Cu	0.375359	0.563071	0.546599	216	H	0.655303	0.366652	0.720561
64	Cu	0.454176	0.536122	0.551918	217	H	0.674027	0.417731	0.744365
65	Cu	0.481594	0.460016	0.516095	218	H	0.71055	0.370625	0.742913
66	P	0.458654	0.25975	0.373979	219	H	0.742711	0.362733	0.613692
67	P	0.704154	0.406825	0.669882	220	H	0.701224	0.331208	0.641749
68	P	0.316209	0.606588	0.331448	221	H	0.753497	0.34174	0.668715
69	P	0.313434	0.43451	0.69624	222	O	0.28823	0.40789	0.515221
70	P	0.679665	0.584614	0.313268	223	O	0.65158	0.345251	0.461554
71	P	0.55018	0.74634	0.646292	224	O	0.298829	0.415323	0.440812
72	H	0.498655	0.792817	0.409388	225	O	0.451937	0.369972	0.696566
73	H	0.526048	0.767912	0.362777	226	O	0.527239	0.365147	0.691421
74	H	0.557296	0.78822	0.409791	227	O	0.452151	0.288073	0.532334
75	H	0.205005	0.410029	0.470448	228	O	0.511147	0.693075	0.398475
76	H	0.227622	0.370411	0.432573	229	O	0.64122	0.401581	0.350343
77	H	0.222843	0.357779	0.49114	230	O	0.530455	0.725557	0.463861
78	H	0.750633	0.649187	0.501534	231	O	0.483074	0.322779	0.591962
79	H	0.772516	0.594832	0.506166	232	O	0.698064	0.368875	0.516137
80	H	0.754562	0.623452	0.555391	233	O	0.589828	0.346384	0.344626
81	H	0.488977	0.343452	0.779372	234	O	0.35885	0.583496	0.66837

82	H	0.4612	0.30187	0.748018	235	O	0.39455	0.642527	0.637531
83	H	0.521198	0.303972	0.749002	236	O	0.347814	0.630656	0.473657
84	H	0.360721	0.656702	0.728645	237	O	0.324315	0.605161	0.540448
85	H	0.342116	0.690204	0.68338	238	O	0.650817	0.626912	0.657678
86	H	0.308999	0.644151	0.703031	239	O	0.679214	0.556553	0.656582
87	H	0.720018	0.282103	0.472802	240	O	0.545042	0.628467	0.293798
88	H	0.676736	0.320519	0.312192	241	O	0.470053	0.629992	0.284585
89	H	0.758612	0.327119	0.474404	242	O	0.326139	0.447617	0.326671
90	H	0.48503	0.693212	0.230172	243	O	0.358384	0.379427	0.331555
91	H	0.544199	0.694844	0.240151	244	O	0.678071	0.59032	0.54806
92	H	0.724728	0.317393	0.425755	245	O	0.688629	0.591444	0.473343
93	H	0.259606	0.388028	0.309012	246	C	0.509572	0.641819	0.274221
94	H	0.285784	0.407417	0.259968	247	C	0.515159	0.673241	0.235217
95	H	0.297731	0.352324	0.280281	248	C	0.606448	0.752526	0.669176
96	H	0.520939	0.653558	0.204801	249	C	0.735934	0.473608	0.544757
97	H	0.63238	0.325651	0.273421	250	C	0.284794	0.480065	0.725173
98	H	0.673281	0.369367	0.278994	251	C	0.275854	0.403589	0.474592
99	H	0.253165	0.649606	0.499753	252	C	0.489864	0.355071	0.709008
100	H	0.281092	0.679609	0.542025	253	C	0.284833	0.666036	0.508286
101	H	0.290831	0.692927	0.484341	254	C	0.522379	0.726612	0.421877
102	H	0.750312	0.601371	0.681369	255	C	0.526602	0.771431	0.399092
103	H	0.71655	0.596304	0.729349	256	C	0.230246	0.383701	0.466463
104	H	0.719154	0.648615	0.700919	257	C	0.32791	0.405973	0.317997
105	H	0.493883	0.223337	0.584278	258	C	0.680015	0.59766	0.667904
106	H	0.472714	0.249975	0.633056	259	C	0.689389	0.345998	0.48139
107	H	0.435621	0.22709	0.59177	260	C	0.747512	0.617738	0.520056
108	H	0.425333	0.464971	0.530581	261	C	0.36695	0.625006	0.665042
109	H	0.457543	0.523321	0.407571	262	C	0.342898	0.656179	0.696577
110	H	0.473957	0.398057	0.510977	263	C	0.753118	0.440733	0.683425
111	H	0.593953	0.52614	0.576112	264	C	0.73087	0.60929	0.335517
112	H	0.503012	0.542539	0.582846	265	C	0.701322	0.598412	0.51352
113	H	0.587869	0.545597	0.498304	266	C	0.420373	0.717112	0.551987
114	H	0.630944	0.750925	0.642044	267	C	0.273472	0.527012	0.594928
115	H	0.613575	0.725032	0.692245	268	C	0.61555	0.669528	0.406952
116	H	0.610009	0.784484	0.686753	269	C	0.635077	0.689705	0.532571
117	H	0.744447	0.498816	0.519797	270	C	0.36912	0.337734	0.601766
118	H	0.74443	0.439983	0.533452	271	C	0.33334	0.399164	0.741847
119	H	0.751872	0.481512	0.576607	272	C	0.347374	0.320106	0.453088
120	H	0.260541	0.466995	0.749353	273	C	0.591288	0.299108	0.57524
121	H	0.267274	0.500985	0.70078	274	C	0.72577	0.316771	0.462297
122	H	0.309124	0.501147	0.742563	275	C	0.582556	0.469604	0.720314
123	H	0.771705	0.448157	0.652786	276	C	0.431294	0.501817	0.738259

124	H	0.775257	0.42322	0.706798	277	C	0.497715	0.241979	0.330488
125	H	0.742356	0.472457	0.698153	278	C	0.404533	0.25714	0.345767
126	H	0.753099	0.619703	0.308288	279	C	0.723708	0.498867	0.417064
127	H	0.748258	0.584996	0.356642	280	C	0.562194	0.270116	0.457892
128	H	0.722701	0.63843	0.356099	281	C	0.548405	0.509104	0.266795
129	H	0.401772	0.718678	0.583343	282	C	0.404315	0.519326	0.254938
130	H	0.399357	0.704663	0.52491	283	C	0.274649	0.627187	0.371247
131	H	0.435402	0.749196	0.54331	284	C	0.289816	0.521202	0.447773
132	H	0.250222	0.499039	0.597537	285	C	0.40898	0.681717	0.401316
133	H	0.265132	0.549126	0.567183	286	C	0.490499	0.323703	0.7485
134	H	0.27554	0.546034	0.625982	287	C	0.484509	0.375791	0.288758
135	H	0.60656	0.683262	0.374414	288	C	0.700591	0.540982	0.275967
136	H	0.651378	0.663205	0.40987	289	C	0.659599	0.627313	0.274598
137	H	0.603636	0.690807	0.434033	290	C	0.290811	0.386846	0.289803
138	H	0.652008	0.674613	0.504039	291	C	0.266898	0.402147	0.673345
139	H	0.657297	0.691245	0.561435	292	C	0.467427	0.288536	0.572233
140	H	0.621527	0.722479	0.524004	293	C	0.456738	0.211429	0.411324
141	H	0.380789	0.327282	0.634705	294	C	0.625926	0.365618	0.333119
142	H	0.381649	0.315529	0.575694	295	C	0.282305	0.575572	0.291211
143	H	0.332731	0.340181	0.600437	296	C	0.331576	0.656892	0.300379
144	H	0.357138	0.417855	0.76241	297	C	0.542085	0.610345	0.720208
145	H	0.350881	0.370105	0.72816	298	C	0.51428	0.758377	0.694219
146	H	0.305546	0.38797	0.762961	299	C	0.543788	0.796258	0.611641
147	H	0.361265	0.286397	0.454571	300	C	0.684294	0.388619	0.724706
148	H	0.325682	0.324738	0.424158	301	C	0.321826	0.631737	0.507346
149	H	0.330265	0.328535	0.484145	302	C	0.653489	0.344291	0.296692
150	H	0.563583	0.297603	0.551648	303	C	0.467145	0.244779	0.597362
151	H	0.583448	0.280444	0.605606	304	C	0.727962	0.355762	0.64646
152	H	0.622429	0.287518	0.560175	305	C	0.718872	0.612404	0.696511
153	H	0.610319	0.490308	0.731784					

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