Supporting Information

Glutathione-Coated $Au_{29}(SG)_{27}$: Structural Determination Based on Different Combination Styles Confirmed by Experiments

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1 Table S1. Part R and Part CS of $Au_{29}(SCH_3)_{27}$ in different divisions

N[a]	Part R[b]	Part CS[c]
N=3	$Au_3(SCH_3)_3$	$Au_{26}(SCH_3)_{24}$
N=4	$Au_4(SCH_3)_4$	$Au_{25}(SCH_3)_{23}$
N=5	$Au_5(SCH_3)_5$	$Au_{24}(SCH_3)_{22}$
N=6	$Au_6(SCH_3)_6$	$Au_{23}(SCH_3)_{21}$
N=7	$Au_7(SCH_3)_7$	$Au_{22}(SCH_3)_{20}$
N=8	$Au_8(SCH_3)_8$	$Au_{21}(SCH_3)_{19}$
N=9	$Au_9(SCH_3)_9$	$Au_{20}(SCH_3)_{18}$
N=10	$Au_{10}(SCH_3)_{10}$	$Au_{19}(SCH_3)_{17}$

[a]N represents the number of Au or S atoms in the ring motif, [b]Part R represents the ring motif, [c]Part CS represents the Au_4 core and staple motif structure.

2 Structural divisions of $Au_{29}(SCH_3)_{27}$ based on the "divide and protect" method

We take the Part CS as $Au_{26}(SCH_3)_{24}$ as an example when the Part R is $Au_3(SCH_3)_3$.

According to the general structural formula, we expand $Au_{26}(SCH_3)_{24}$ to $[Au]_{a+a'}[Au(SCH_3)_2]_b[Au_2(SCH_3)_3]_c[Au_3(SCH_3)_4]_d[Au_4(SCH_3)_5]_e[Au_5(SCH_3)_6]_f[Au_6(SCH_3)_7]_g[Au_7(SCH_3)_8]_h[Au_8(SCH_3)_9]_i[Au_9(SCH_3)_{10}]_j[Au_{10}(SCH_3)_{11}]_k[Au_{11}(SCH_3)_{12}]_l[Au_{12}(SCH_3)_{13}]_m[Au_{13}(SCH_3)_{14}]_n[Au_{14}(SCH_3)_{15}]_p[Au_{15}(SCH_3)_{16}]_q$…where a represents the internal gold atom, a' represents the surface gold atom, b, c, d, e, f, g…denote the number of different staple motifs with an increasing length. And the numbers satisfy the following equations

$$a+a'+b+2c+3d+4e+5f+6g+7h+8i+9j+10k+11l+12m+13n+14p+15q = 26 \quad (1)$$

$$2b+3c+4d+5e+6f+7g+8h+9i+10j+11k+12l+13m+14n+15p+16q=24 \quad (2)$$

The above two equations are subtracted to obtain the equation (3)

$$a+a'-(b+c+d+e+f+g+h+i+j+k+l+m+n+p+q)=2 \quad (3)$$

Each of the surface gold atom binds with a sulfur atom of the staple motif, i.e.

$$a'=2(b+c+d+e+f+g+h+i+j+k+l+m+n+p+q) \quad (4)$$

Then we get the relationship of a and a',

$$a+a'/2=2 \quad (5)$$

If a'=2, a=1, then b+c+d+e+f+g+h+i+j+k+l+m+n+p+q =1, the Equation (2) does not establish.

If a'=4, a=0, then b+c+d+e+f+g+h+i+j+k+l+m+n+p+q =2, so the size of the gold core is determined as Au_4. And the different division are $Au_4[Au_{11}(SCH_3)_{12}]_2$, $Au_4Au_{10}(SCH_3)_{11}Au_{12}(SCH_3)_{13}$, $Au_4Au_9(SCH_3)_{10}Au_{13}(SCH_3)_{14}$, $Au_4Au_8(SCH_3)_9Au_{14}(SCH_3)_{15}$, $Au_4Au_7(SCH_3)_8Au_{15}(SCH_3)_{16}$.

The other Part CS are also divided according to the above methods.

3 Comparison of energies of four different combination styles

Table S2. The relative energies for four combination styles of every isomer

isomers	a[a]	b[b]	c[c]	d[d]
$Au_5(SR)_5+Au_4$ $Au_5(SR)_6+Au_{15}(SR)_{16}$	0.198 eV	0 eV	0.448 eV	0.161 eV
$Au_5(SR)_5+Au_4$ $Au_6(SR)_7+Au_{14}(SR)_{15}$	0.247 eV	0 eV	0.405 eV	1.51 eV
$Au_5(SR)_5+Au_4$ $Au_9(SR)_{10}+Au_{11}(SR)_{12}$	0.153 eV	0 eV	1.533 eV	0.711 eV

$Au_5(SR)_5+Au_4$ $Au_8(SR)_9+Au_{12}(SR)_{13}$	0.062 eV	0 eV	1.263 eV	0.980 eV
$Au_5(SR)_5+Au_4$ $Au_7(SR)_8+Au_{13}(SR)_{14}$	0 eV	0.325 eV	0.843 eV	0.938 eV
$Au_6(SR)_6+Au_4$ $Au_9(SR)_{10}+Au_{10}(SR)_{11}$	0 eV	0.347 eV	0.248 eV	0.370 eV
$Au_6(SR)_6+Au_4$ $Au_4(SR)_5+Au_{15}(SR)_{16}$	0.016 eV	0.075 eV	0 eV	0.540 eV
$Au_6(SR)_6+Au_4$ $Au_8(SR)_9+Au_{11}(SR)_{12}$	0.249 eV	0.264 eV	0.277 eV	0 eV
$Au_6(SR)_6+Au_4$ $Au_5(SR)_6+Au_{14}(SR)_{15}$	0 eV	0.360 eV	0.187 eV	0.646 eV
$Au_6(SR)_6+Au_4$ $Au_7(SR)_8+Au_{12}(SR)_{13}$	0.188 eV	0 eV	0.312 eV	0.534 eV
$Au_6(SR)_6+Au_4$ $Au_6(SR)_7+Au_{13}(SR)_{14}$	0.067 eV	0 eV	0.149 eV	0.198 eV
$Au_7(SR)_7+Au_4$ $[Au_9(SR)_{10}]_2$	0.454 eV		0 eV	0.430 eV
$Au_7(SR)_7+Au_4$ $Au_6(SR)_7+Au_{12}(SR)_{13}$	0.494 eV	0.472 eV	0 eV	0.022 eV
$Au_7(SR)_7+Au_4$ $Au_4(SR)_5+Au_{14}(SR)_{15}$	0.301 eV	0.746 eV	0 eV	0.161 eV
$Au_8(SR)_8+Au_4$ $Au_7(SR)_8+Au_{10}(SR)_{11}$	0.112 eV	0.489 eV	0 eV	0.523 eV
$Au_9(SR)_9+Au_4$ $[Au_8(SR)_9]_2$	0.477 eV		0 eV	0.301 eV
$Au_9(SR)_9+Au_4$ $Au_4(SR)_5+Au_{12}(SR)_{13}$	0.495 eV	0.143 eV	0 eV	0.313 eV

[a] The first combination style: the Part R goes through the smaller staple motif; [b] The second combination style: the Part R goes through the larger staple motif; [c] The third combination style: the Part R goes through both staple motifs with crossing the gold core; [d] The fourth combination style: the Part R goes through neither staple motif with crossing the gold core.

4 The relative energies of all isomers of $Au_{29}(SCH_3)_{27}$ (arranged from low to high energy)

Table S3. Relative energies of various isomers of $Au_{29}(SCH_3)_{27}$

isomers	∆ E(Ha)	∆ E(eV)
$Au_7(SR)_7+Au_4+Au_8(SR)_9+Au_{10}(SR)_{11}$	0.0000000	0.00000000
$Au_6(SR)_6+Au_4+Au_7(SR)_8+Au_{12}(SR)_{13}$	0.0039509	0.10751051
$Au_7(SR)_7+Au_4+Au_4(SR)_5+Au_{14}(SR)_{15}$	0.0041932	0.11410389
$Au_7(SR)_7+Au_4+[Au_9(SR)_{10}]_2$	0.0046285	0.12594912
$Au_6(SR)_6+Au_4+Au_9(SR)_{10}+Au_{10}(SR)_{11}$	0.0049161	0.13377519
$Au_7(SR)_7+Au_4+Au_6(SR)_7+Au_{12}(SR)_{13}$	0.0054367	0.14794158
$Au_6(SR)_6+Au_4+Au_5(SR)_6+Au_{14}(SR)_{15}$	0.0061272	0.16673122
$Au_{10}(SR)_{10}+Au_4+Au_3(SR)_4+Au_{12}(SR)_{13}$	0.0063827	0.17368380
$Au_8(SR)_8+Au_4+Au_6(SR)_7+Au_{11}(SR)_{12}$	0.0066553	0.18110169
$Au_9(SR)_9+Au_4+Au_4(SR)_5+Au_{12}(SR)_{13}$	0.0076959	0.20941814
$Au_7(SR)_7+Au_4+Au_7(SR)_8+Au_{11}(SR)_{12}$	0.0078792	0.21440603

$Au_9(SR)_9+Au_4+Au_5(SR)_6+Au_{11}(SR)_{12}$	0.0083686	0.22772341
$Au_8(SR)_8+Au_4+Au_7(SR)_8+Au_{10}(SR)_{11}$	0.0084071	0.22877106
$Au_6(SR)_6+Au_4+Au_6(SR)_7+Au_{13}(SR)_{14}$	0.0085469	0.23257525
$Au_6(SR)_6+Au_4+Au_4(SR)_5+Au_{15}(SR)_{16}$	0.0087221	0.23734273
$Au_8(SR)_8+Au_4+Au_8(SR)_9+Au_9(SR)_{10}$	0.0087848	0.23904890
$Au_7(SR)_7+Au_4+Au_5(SR)_6+Au_{13}(SR)_{14}$	0.0091571	0.24917980
$Au_6(SR)_6+Au_4+Au_8(SR)_9+Au_{11}(SR)_{12}$	0.0094615	0.25746303
$Au_8(SR)_8+Au_4+Au_4(SR)_5+Au_{13}(SR)_{14}$	0.0099427	0.27055727
$Au_7(SR)_7+Au_4+Au_3(SR)_4+Au_{15}(SR)_{16}$	0.0106612	0.29010884
$Au_{10}(SR)_{10}+Au_4+Au_6(SR)_7+Au_9(SR)_{10}$	0.0111379	0.30308064
$Au_{10}(SR)_{10}+Au_4+Au_7(SR)_8+Au_8(SR)_9$	0.0113948	0.31007131
$Au_9(SR)_9+Au_4+Au_6(SR)_7+Au_{10}(SR)_{11}$	0.0122408	0.33309237
$Au_5(SR)_5+Au_4+Au_7(SR)_8+Au_{13}(SR)_{14}$	0.0125207	0.34070891
$Au_5(SR)_5+Au_4+[Au_{10}(SR)_{11}]_2$	0.0125897	0.34258651
$Au_9(SR)_9+Au_4+[Au_8(SR)_9]_2$	0.0139681	0.38009505
$Au_{10}(SR)_{10}+Au_4+Au_4(SR)_5+Au_{11}(SR)_{12}$	0.0163176	0.44402882
$Au_8(SR)_8+Au_4+Au_5(SR)_6+Au_{12}(SR)_{13}$	0.0166031	0.45179775
$Au_5(SR)_5+Au_4+Au_6(SR)_7+Au_{14}(SR)_{15}$	0.0171615	0.46699273
$Au_{10}(SR)_{10}+Au_4+Au_5(SR)_6+Au_{10}(SR)_{11}$	0.0184905	0.50315701
$Au_9(SR)_9+Au_4+Au_7(SR)_8+Au_9(SR)_{10}$	0.0195180	0.53111698
$Au_5(SR)_5+Au_4+Au_5(SR)_6+Au_{15}(SR)_{16}$	0.0195379	0.53165850
$Au_5(SR)_5+Au_4+Au_9(SR)_{10}+Au_{11}(SR)_{12}$	0.0206728	0.56254100
$Au_9(SR)_9+Au_4+Au_3(SR)_4+Au_{13}(SR)_{14}$	0.0208475	0.56729487
$Au_5(SR)_5+Au_4+Au_8(SR)_9+Au_{12}(SR)_{13}$	0.0213343	0.58054150
$Au_8(SR)_8+Au_4+Au_3(SR)_4+Au_{14}(SR)_{15}$	0.0353828	0.96282437
$Au_4+Au_{12}(SR)_{13}+Au_{13}(SR)_{14}$	0.0382575	1.04104970
$Au_3(SR)_3+Au_4+[Au_{11}(SR)_{12}]_2$	0.0428944	1.16722740
$Au_4(SR)_4+Au_4+Au_{10}(SR)_{11}+Au_{11}(SR)_{12}$	0.0433357	1.17923590
$Au_4(SR)_4+Au_4+Au_8(SR)_9+Au_{13}(SR)_{14}$	0.0458761	1.24836438
$Au_4+Au_{11}(SR)_{12}+Au_{14}(SR)_{15}$	0.0470502	1.28031357
$Au_4+Au_{10}(SR)_{11}+Au_{15}(SR)_{16}$	0.0480938	1.30871165
$Au_4(SR)_4+Au_4+Au_7(SR)_8+Au_{14}(SR)_{15}$	0.0487952	1.32779790
$Au_4(SR)_4+Au_4+Au_9(SR)_{10}+Au_{12}(SR)_{13}$	0.0514653	1.40045573
$Au_4(SR)_4+Au_4+Au_6(SR)_7+Au_{15}(SR)_{16}$	0.0515715	1.40334561
$Au_3(SR)_3+Au_4+Au_7(SR)_8+Au_{15}(SR)_{16}$	0.0530704	1.44413315
$Au_3(SR)_3+Au_4+Au_9(SR)_{10}+Au_{13}(SR)_{14}$	0.0536188	1.45905602
$Au_3(SR)_3+Au_4+Au_8(SR)_9+Au_{14}(SR)_{15}$	0.0596708	1.62374092
$Au_3(SR)_3+Au_4+Au_{10}(SR)_{11}+Au_{12}(SR)_{13}$	0.0751228	2.04421534

5 Table S4. The structures and energies of $Au_{29}(SCH_3)_{27}$ without Part R

isomers	energy(Ha)
$Au_4Au_{12}(SCH_3)_{13}Au_{13}(SCH_3)_{14}$	-15752.3412025
$Au_4Au_{11}(SCH_3)_{12}Au_{14}(SCH_3)_{15}$	-15752.3324098
$Au_4Au_{10}(SCH_3)_{11}Au_{15}(SCH_3)_{16}$	-15752.3313662

6 Table S5. Comparison of energies of isomers with different method

isomers	Method D (Ha)	Method S(Ha)	△ E(eV)
$Au_5(SCH_3)_5+Au_4[Au_{10}(SCH_3)_{11}]_2$	-15752.3668703	-15752.3632843	0.098
$Au_5(SCH_3)_5+Au_4Au_5(SCH_3)_6Au_{15}(SCH_3)_{16}$	-15752.3599221	-15752.3026017	1.560
$Au_7(SCH_3)_7+Au_4[Au_9(SCH_3)_{10}]_2$	-15752.3748315	-15752.3136644	1.664
$Au_7(SCH_3)_7+Au_4Au_5(SCH_3)_6Au_{13}(SCH_3)_{14}$	-15752.3703029	-15752.2469400	3.357
$Au_7(SCH_3)_7+Au_4Au_6(SCH_3)_7Au_{12}(SCH_3)_{13}$	-15752.3740233	-15752.2942265	2.171

7 The specific energies of Iso1-3 isomers with different basis settings

We utilized multi-functions and multi-basis groups for Iso1, Iso2 and Iso3 to confirm whether Iso1 is the most optimized geometry. The multi-functions are set as PBE and TPSS. The multi-basis groups are 6-31(G) for C, H, S atoms and LANL2DZ for Au atoms (basis group 1) and 6-311(G) for C, H, S atoms and LANL2MB for Au atoms (basis group 2). Then the basis settings are PBE+ basis group 1, TPSS+ basis group 1 and PBE+ basis group 2 for the top three isomers. As a result, the isomer 1 remains the lowest energy as the most optimized geometry after confirmation.

Table S6. The relative energies of isomers with multi-functions and multi-basis groups

	PBE+basis group 1	TPSS+ basis group 1	PBE+basis group 2
isomer	ΔE (eV)	ΔE (eV)	ΔE (eV)
Iso1	0.0000000	0.0000000	0.0000000
Iso2	0.1075105	0.0021848	0.9462824
Iso3	0.1141039	0.0027776	0.5552483

8 Rationality confirmation of the simplifying from -SG to -SCH_3

To consider the ligand effect and verify the reasonability of simplification from -SG to -SCH_3, we replaced one -SG ligand (noted as confirmation 1) and all -SG ligands of the ring motif (noted as confirmation 2) for verification calculations. Figure S1 shows the initial atomic structure/backbone structure and the optimized atomic structure/backbone structure of confirmation 1. Figure S2 shows the initial atomic structure/backbone structure and the optimized atomic structure/backbone structure of confirmation 2. Both confirmation 1 and confirmation 2 show no drastic changes after -SG ligand replacement. The root mean square deviations (RMSDs) of Au-S backbone structures of confirmation1 and confirmation 2 are 1.537 Å and 2.087 Å respectively which are below the threshold of confirmation change as 3.000 Å.

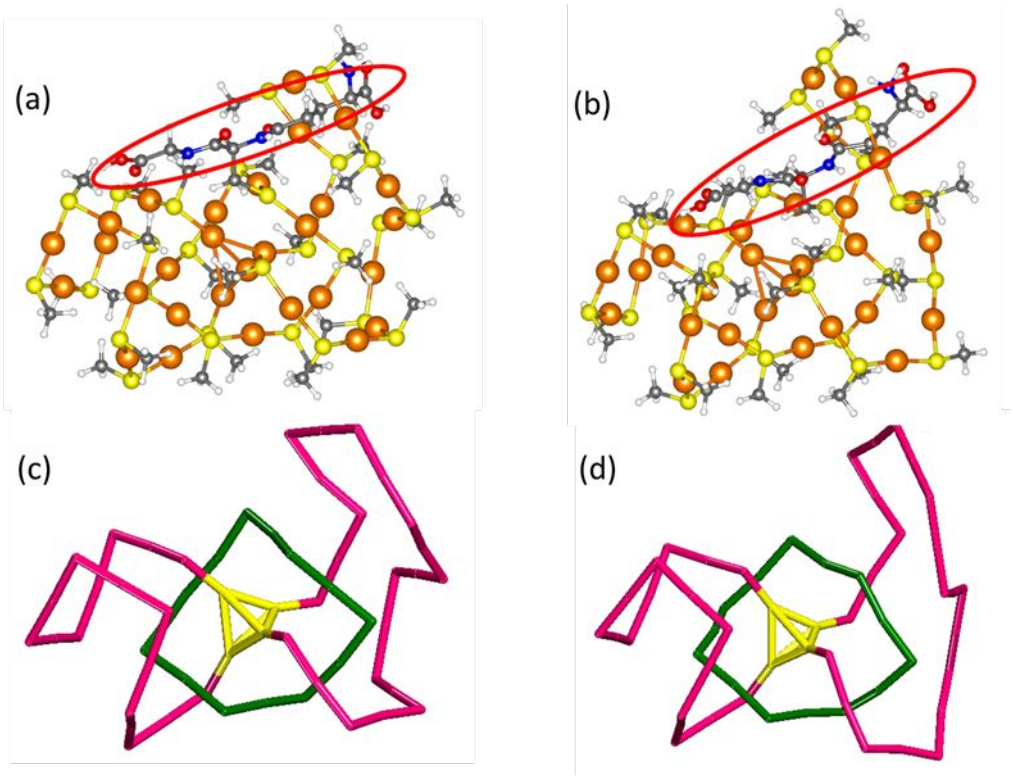

Figure S1. The initial atomic structure (a) and initial backbone structure (c) of confirmation 1. The optimized atomic structure (b) and optimized backbone structure (d) of confirmation 1. The replaced -SG is marked with a red oval.

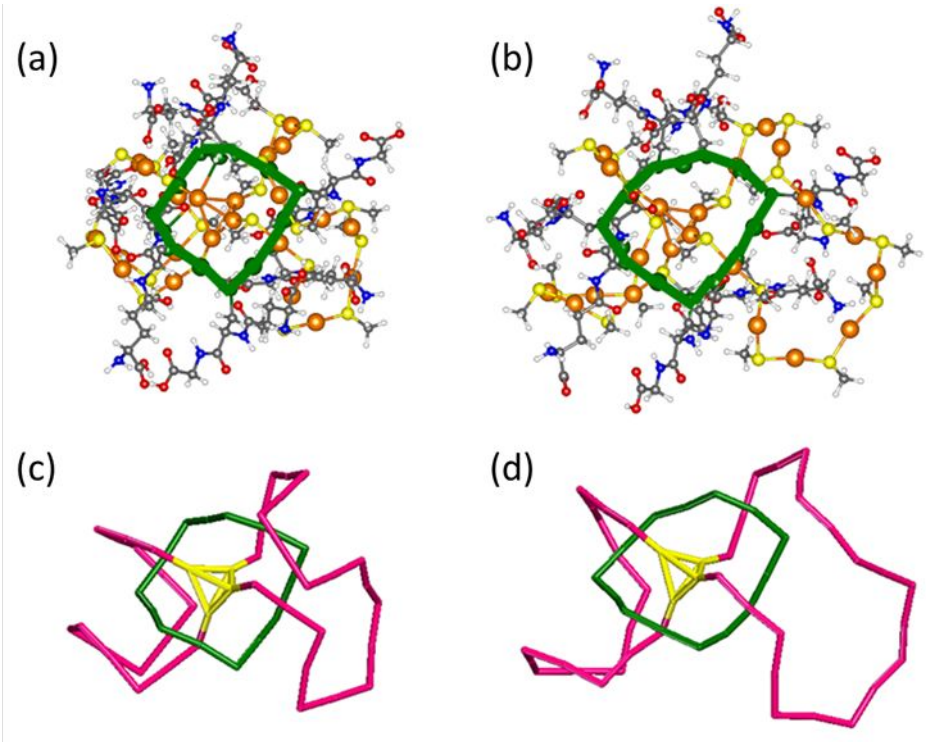

Figure S2. The initial atomic structure (a) and initial backbone structure (c) of confirmation 2. The optimized atomic structure (b) and optimized backbone structure (d) of confirmation 2. The Au-S ring motif with replacing -SG ligands are marked in green.

9 Table S7. The orbital energies of isomer 1.

orbit	Energy(eV)	orbit	energy(eV)
HOMO	-4.86	LUMO+9	-1.65
HOMO-1	-5.02	LUMO+8	-1.75
HOMO-2	-5.18	LUMO+7	-1.77
HOMO-3	-5.23	LUMO+6	-1.84
HOMO-4	-5.33	LUMO+5	-1.87
HOMO-5	-5.38	LUMO+4	-1.97
HOMO-6	-5.45	LUMO+3	-2.03
HOMO-7	-5.49	LUMO+2	-2.10
HOMO-8	-5.52	LUMO+1	-2.35
HOMO-9	-5.56	LUMO	-2.74

10 KS orbital energy and composition of $Au_{29}(SCH_3)_{27}$ isomer 1.

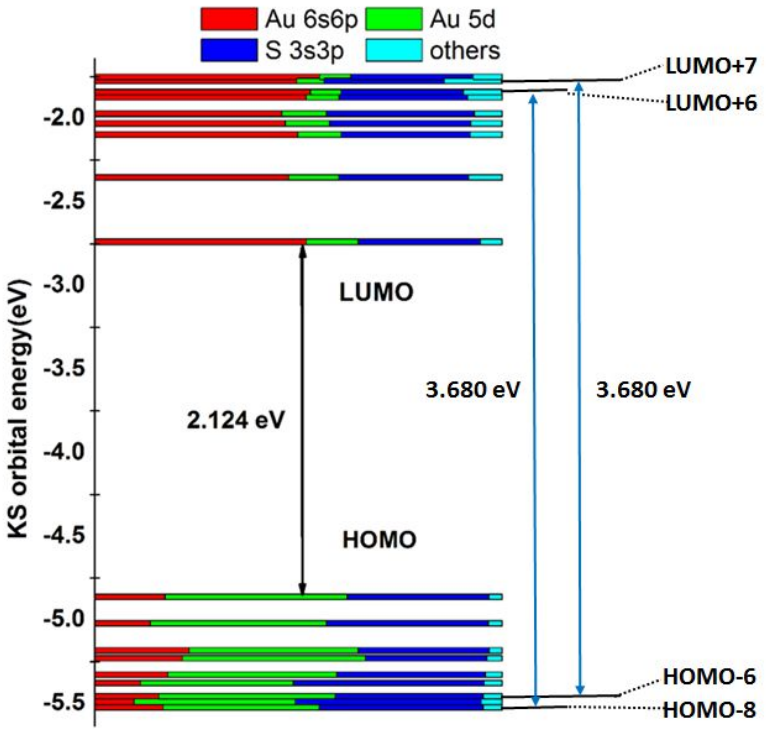

Figure S3. KS orbital energy and composition of $Au_{29}(SCH_3)_{27}$ isomer 1. The 337 nm peak (3.680 eV) stems from the electronic transition from Au5d in the Au core to Au6s6p in the staple motifs (HOMO-8 to LUMO+6) and the electronic transition from Au5d in the Au core to Au5d in the ring motifs (HOMO-6 to LUMO+7).

11 XYZ coordinates and Mulliken charges of Iso1 of $Au_{29}(SCH_3)_{27}$

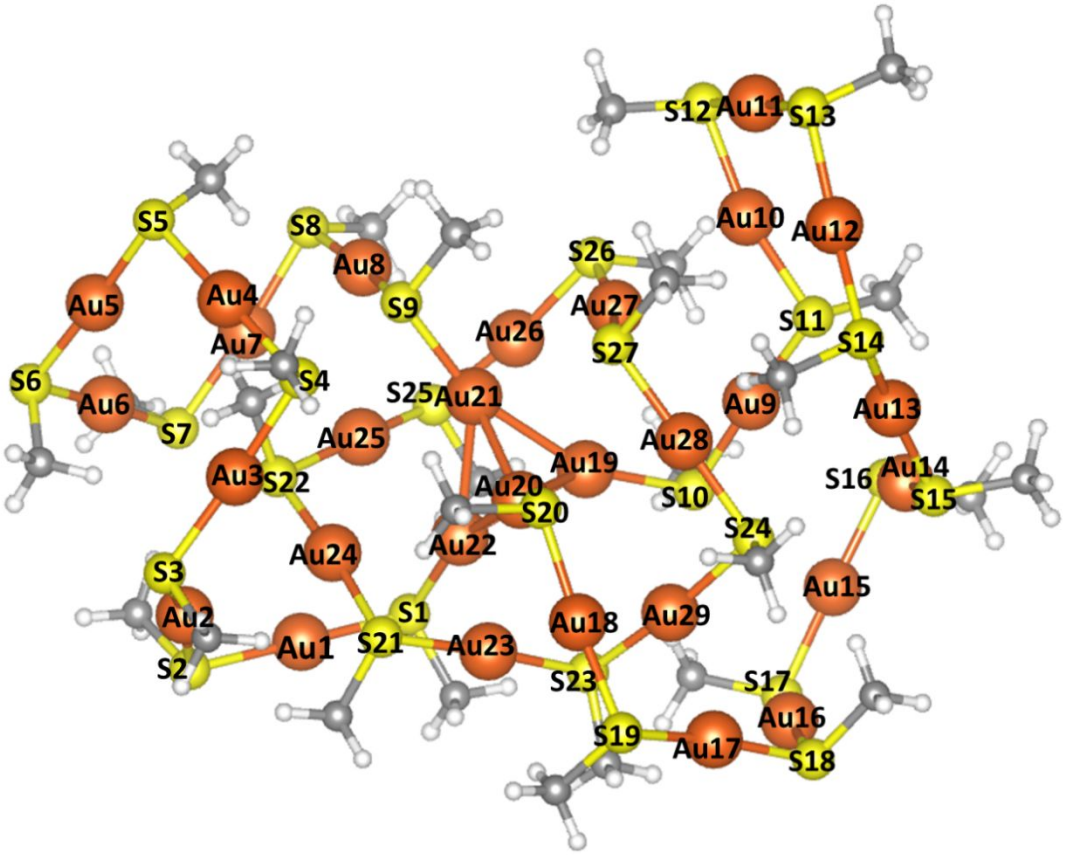

Figure S4. Structure diagram of isomer 1 with Au, S atom numbers.

Table S8. The atomic numbers of Au and S in the table correspond to Figure S4. The atom number of C connected to the S atom is the same as the S atom.

Atoms	X	Y	Z	Mulliken charges
Au1	−4.617669	−3.851714	−1.527998	−0.631091
Au2	−6.541596	−3.349843	1.599370	−0.565845
Au3	−5.295737	−0.590413	3.927544	−0.451550
Au4	−5.609614	2.905031	3.376591	−0.283075
Au5	−8.476170	2.759063	1.400173	−0.219630
Au6	−8.599752	0.745224	−1.600703	−0.325869
Au7	−6.070828	2.240849	−3.497158	−0.464542
Au8	−3.545434	3.541426	−1.595427	−0.681400
C1	−1.683484	−4.863736	−2.688701	−0.672539
H	−1.555148	−5.266634	−1.672641	0.257117
H	−0.693106	−4.665121	−3.126514	0.251243
H	−2.238584	−5.578582	−3.316377	0.232519
C2	−7.879743	−3.350692	−1.442221	−0.651513
H	−7.925691	−3.714387	−2.480314	0.234922
H	−7.557286	−2.299583	−1.430002	0.279922
H	−8.868610	−3.453860	−0.969014	0.222108
C3	−5.682159	−3.750895	4.782669	−0.657454

H	-6.179283	-4.729340	4.695532	0.229926
H	-5.679181	-3.432715	5.836624	0.234900
H	-4.649542	-3.809632	4.409190	0.263810
C4	-4.100848	1.644570	6.060265	-0.640397
H	-3.496405	0.864740	6.548874	0.230101
H	-5.137234	1.597092	6.420642	0.247380
H	-3.672005	2.634458	6.279510	0.232252
C5	-6.266615	5.240914	1.104805	-0.645171
H	-5.549915	5.946946	1.551812	0.227347
H	-6.995335	5.793093	0.492146	0.230183
H	-5.730774	4.509713	0.482763	0.274221
C6	-9.511759	-0.400111	1.376277	-0.641948
H	-10.057749	-1.235194	0.911044	0.229700
H	-9.893911	-0.230637	2.394231	0.232446
H	-8.438550	-0.634550	1.414863	0.258498
C7	-8.654201	0.706499	-4.913754	-0.642830
H	-8.136354	0.684748	-5.885003	0.234945
H	-9.097377	1.697591	-4.747453	0.245945
H	-9.439808	-0.064637	-4.897362	0.230020
C8	-3.804233	4.302011	-4.907478	-0.653676
H	-3.045845	5.088415	-4.772598	0.235771
H	-4.443246	4.547091	-5.770138	0.226652
H	-3.316229	3.330528	-5.061466	0.270475
C9	-1.389617	4.277527	0.886068	-0.673885
H	-0.760928	3.929887	1.720924	0.261522
H	-2.014591	5.124169	1.212330	0.229039
H	-0.751178	4.576564	0.043388	0.264645
S1	-2.622550	-3.278057	-2.657350	0.173768
S2	-6.691723	-4.426031	-0.519536	0.150982
S3	-6.670530	-2.516265	3.824255	0.148325
S4	-4.008670	1.380654	4.230466	0.101845
S5	-7.189931	4.426533	2.487660	0.113456
S6	-9.847747	1.121669	0.376906	0.117406
S7	-7.415484	0.290479	-3.601570	0.137809
S8	-4.880616	4.290780	-3.405301	0.140089
S9	-2.507474	2.891234	0.422418	0.140769
Au9	4.206349	1.062764	-1.771326	-0.436745
Au10	4.163651	4.699461	-0.814775	-0.474495
Au11	4.566456	6.951740	1.305607	-0.360142
Au12	6.449754	4.600166	3.376741	-0.307145
Au13	7.478760	1.007586	1.956442	-0.409706
Au14	7.312694	-0.479002	-1.737642	-0.446751
Au15	5.624151	-2.578498	-3.905163	-0.359501
Au16	5.110705	-5.205715	-1.609437	-0.479846
Au17	4.083464	-5.579453	2.042015	-0.594410

Au18	1.516264	-3.318254	3.453442	-0.668195
Au19	0.977513	-0.337171	-1.452759	0.751305
Au20	0.024189	-0.945639	1.134897	0.899138
Au21	-1.146026	1.060543	-0.415559	0.938942
Au22	-1.445867	-1.719308	-1.126827	1.079694
C20	-0.824458	-1.138278	4.442708	-0.691012
H	-0.541672	-1.265420	5.500002	0.226935
H	-1.481694	-1.960054	4.126970	0.269562
H	-1.342040	-0.175941	4.303901	0.265126
C19	1.115909	-6.631951	3.276741	-0.661446
H	1.549808	-7.633056	3.130554	0.229322
H	0.611888	-6.288076	2.360578	0.271029
H	0.387831	-6.663127	4.102408	0.231743
C18	7.123603	-4.656589	0.953169	-0.657538
H	7.982731	-4.791660	0.278265	0.227257
H	7.443064	-4.828292	1.992661	0.222558
H	6.723564	-3.639918	0.834579	0.277934
C17	2.845217	-4.385579	-4.003742	-0.660718
H	2.641604	-4.027851	-5.025343	0.222662
H	2.531759	-3.635008	-3.265507	0.291528
H	2.306179	-5.330763	-3.834577	0.217672
C16	8.199421	-0.744675	-4.948261	-0.642560
H	8.822598	0.160679	-4.882574	0.227680
H	7.934817	-0.935171	-5.999783	0.232033
H	8.743297	-1.606234	-4.538141	0.245588
C15	9.958055	-0.337294	0.248978	-0.644242
H	10.438232	-0.406080	1.237337	0.232277
H	10.116947	0.664237	-0.174022	0.240716
H	10.384105	-1.099537	-0.421718	0.229516
C14	5.617607	1.622061	4.628630	-0.656828
H	5.288526	2.274860	5.451429	0.229021
H	5.911979	0.642272	5.035490	0.229113
H	4.808103	1.490511	3.896099	0.270952
C13	7.455550	7.710857	2.752923	-0.629690
H	8.176810	7.599678	3.576877	0.230035
H	7.246964	8.778399	2.584855	0.229402
H	7.857586	7.257610	1.837004	0.238127
C12	1.525221	6.776128	-0.136014	-0.655024
H	1.424142	6.044462	0.676993	0.248126
H	0.924130	6.452449	-0.999698	0.259985
H	1.195036	7.769692	0.204323	0.226654
C11	6.808850	3.188286	-2.041836	-0.667547
H	7.474264	2.315188	-2.145563	0.267027
H	7.377029	4.053345	-1.665585	0.235000
H	6.353219	3.426447	-3.012841	0.253160

C10	2.542919	-0.142259	-4.465683	-0.682744
H	2.027048	-0.978108	-4.965102	0.241399
H	3.475963	0.085976	-5.004134	0.257488
H	1.878657	0.734362	-4.444456	0.267892
S10	2.971934	-0.705283	-2.758936	0.124290
S11	5.530015	2.761976	-0.779119	0.188485
S12	3.278133	6.920422	-0.699411	0.177918
S13	5.875103	6.901080	3.271164	0.106591
S14	7.117699	2.378550	3.856039	0.150977
S15	8.157316	-0.706688	0.462893	0.156164
S16	6.631269	-0.434436	-4.013342	0.127338
S17	4.655336	-4.734038	-3.886015	0.122368
S18	5.869227	-5.941322	0.513716	0.158306
S19	2.462772	-5.471822	3.780510	0.154263
S20	0.727824	-1.086898	3.442317	0.185153
Au23	-0.587932	-3.944959	0.861117	-1.033611
Au24	-3.720826	-2.068493	0.883987	0.344034
Au25	-3.598895	0.200779	-2.234381	-0.129273
Au26	-0.705730	2.195269	-3.307968	-0.763171
Au27	1.603679	2.842191	-0.612596	-0.184738
Au28	3.272691	0.271785	1.294204	-0.520922
Au29	2.960736	-3.114946	0.411904	0.485510
C27	2.976833	3.425527	2.425247	-0.679296
H	3.090905	3.163948	3.489323	0.236600
H	2.488682	4.409929	2.346835	0.241702
H	3.962038	3.467290	1.939605	0.280445
C24	5.012429	-2.047469	2.894005	-0.678473
H	5.403333	-3.077324	2.936176	0.250546
H	4.099660	-1.977099	3.503460	0.279679
H	5.779182	-1.342973	3.255449	0.246762
C23	1.618867	-6.118884	-0.533417	-0.676951
H	0.735252	-6.696603	-0.849259	0.230137
H	1.920801	-6.405039	0.485142	0.262499
H	2.460497	-6.314209	-1.219403	0.260938
C21	-3.439304	-5.267238	1.842961	-0.668532
H	-3.558958	-5.408935	0.757939	0.273913
H	-4.436039	-5.216852	2.311699	0.252316
H	-2.861765	-6.099160	2.276000	0.236601
C22	-5.439614	0.870236	0.527878	-0.687552
H	-4.544087	1.311978	0.984447	0.275639
H	-6.135086	0.538803	1.315428	0.248057
H	-5.940532	1.610090	-0.117002	0.256054
C25	-1.545436	-0.650856	-4.841253	-0.673581
H	-0.954914	-0.347255	-5.720204	0.224195
H	-2.299286	-1.397938	-5.130752	0.258216

H	-0.892589	-1.068527	-4.061052	0.292855
C26	2.292930	3.691678	-3.858639	-0.677630
H	3.003623	4.497435	-3.612548	0.258906
H	1.896815	3.835408	-4.875943	0.236783
H	2.804977	2.722282	-3.770750	0.272603
S21	-2.542161	-3.694158	2.208082	0.144622
S22	-5.026828	-0.595287	-0.495975	0.244423
S23	1.210785	-4.325552	-0.649578	0.181541
S34	4.675877	-1.629874	1.125880	0.118213
S25	-2.427840	0.843444	-4.221105	0.193571
S26	0.894400	3.822039	-2.664528	0.169179
S27	1.878108	2.157031	1.652856	0.248382