Electronic Supplementary Information for:

"Ligand effect on isomer stability of $Au_{24}(SR)_{20}$ clusters"

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Exploration of the orientational isomers of $Au_{24}(SR)_{20}$ clusters: Chart S1 shows how many orientational configurations we explored for each isomer with different R- groups based on minimizing steric repulsion and maximizing symmetry from visual inspection. Each R- group can be oriented at left or right of the S-Au-S bond. We use the most stable structure as a reference to identify the orientations of all RS- groups. The coordinates of the most structures are provided below.

Chart S1. The numbers of orientational configurations explored for $Au_{24}(SR)_{20}$ clusters based on minimizing steric repulsion and maximizing symmetry from visual inspection

Isomer	P	J
R=CH_2CH_2Ph	17 configurations: Figure S1 and Table S1	16 configurations: Figure S2 and Table S2
R=CH_2Ph-^{t}Bu	12 configurations: Figure S3 and Table S3	16 configurations: Figure S4 and Table S4

In addition, 25 additional different orientational configurations for each of the four isomers are generated by classical molecular dynamics (MD) and then optimized by DFT-D3. When generating configurations from MD, we fixed the positions of the Au and S atoms, and then modified force field

parameters of ∠Au-S-C and improper dihedral angle for C-S-Au(staple)-Au(core) such that the –R group can adopt either the left or right positions regarding the Au(staple)-S-Au(core) plane. The MD trajectory was run at 1000K so that many left-right (or cis-trans) transitions took place in our simulation timeframe. Then 25 random snapshots were picked up from the trajectory and cooled down to 0 K. Consistent Valence Force Field (CVFF)[1] was utilized as the origin force field, and MD simulation and minimization based on force field were performed by LAMMPS code.[2-3] These 25 MD-generated configurations for each isomer were then fed into DFT-D3 optimization by VASP. The ten most stable energies from DFT-D3 out of the 25 configurations are listed in Table S5.

1. Dauber-Osguthorpe, P.; Roberts, V. A.; Osguthorpe, D. J.; Wolff, J.; Genest, M.; Hagler, A. T.. *Proteins: Struct., Funct., Genet.* 1988, 4, 31−47.

2. Plimpton, S. Fast Parallel Algorithms for Short-Range Molecular Dynamics, *J Comp Phys,* 1995, 117, 1-19.

3. http://lammps.sandia.gov.

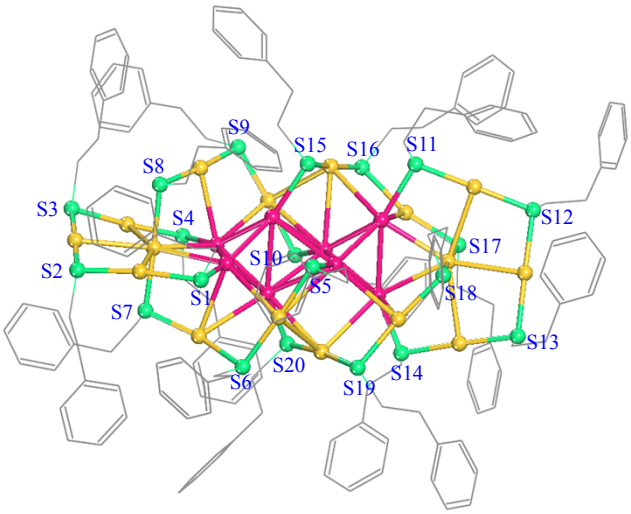

Figure S1. Geometry of the $Au_{24}(SCH_2CH_2Ph)_{20}$ P_1 isomer. S atoms are marked with numbers.

Table S1. The rotating modes and total energies of the $Au_{24}(SCH_2CH_2Ph)_{20}$ P isomer with different orientational configurations. The rotating modes are based on the $Au_{24}(SCH_2CH_2Ph)_{20}$ P_1 isomer (the most stable configuration; Figure S1). For each denoted S atom in Column 2, the S-C bond with the bonded tail group will be rotated from the initial cis- (or trans-) site to the trans- (or cis-) site relative to the orientation at the same S-atom site of the P1 isomer. Note the P2 isomer has the same configuration as the reported $Au_{24}(SePh)_{20}$ structure (ref. 25 in the main text).

$Au_{24}(SCH_2CH_2Ph)_{20}$ P	Rotated S atom	Total energies (eV)
P1	-	-2286.306
P2	S2, S3, S7, S8, S12, S13, S14, S17, S18	-2285.132
P3	S1, S11	-2285.503
P4	S2, S12	-2285.745
P5	S3, S12	-2285.580
P6	S8, S18	-2285.753
P7	S9, S19	-2285.895
P8	S2, S3, S12, S13	-2285.084
P9	S1, S2, S13, S14	-2284.810
P10	S6, S9, S16, S19	-2285.077
P11	S7, S8, S17, S18	-2285.609
P12	S2, S9, S12, S19	-2285.524
P13	S1, S6, S11, S16	-2285.588
P14	S5, S9, S15, S19	-2285.889
P15	S1, S10, S11, S20	-2284.737
P16	S5, S10, S15, S20	-2284.886
P17	S5, S6, S9, S10, S15, S16, S19, S20	-2284.096

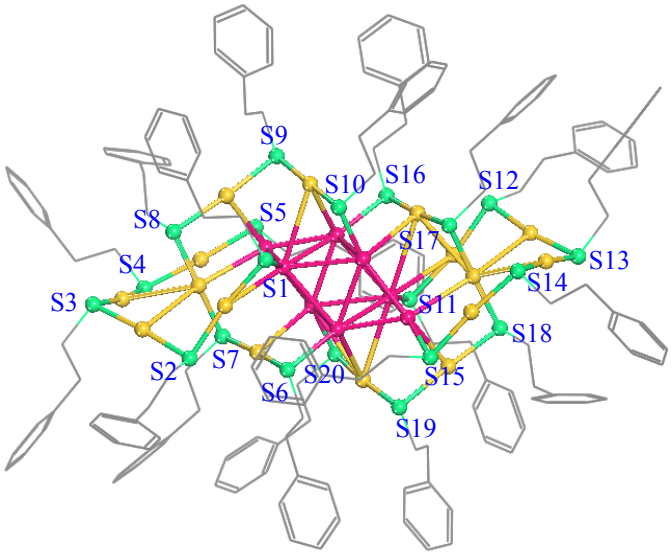

Figure S2. Geometry of the $Au_{24}(SCH_2CH_2Ph)_{20}$ J_1 isomer. S atoms are marked with numbers.

Table S2. The rotating modes and energies of the $Au_{24}(SCH_2CH_2Ph)_{20}$ J isomer with different orientational configurations. The rotating modes from J2 to J16 are based on the $Au_{24}(SCH_2CH_2Ph)_{20}$ J_1 isomer (the most stable one; Figure S2).

$Au_{24}(SCH_2CH_2Ph)_{20}$ J orientational isomers	Rotated S atom	Total energies (eV)
J1	-	-2285.941
J2	S1, S11	-2285.134
J3	S5, S15	-2285.511
J4	S7, S17	-2284.991
J5	S8, S18	-2285.424
J6	S6, S10, S16, S20	-2285.460
J7	S4, S5, S14, S15	-2285.613
J8	S7, S9, S17, S19	-2284.417
J9	S8, S9, S18, S19	-2285.095
J10	S7, S8, S17, S18	-2284.518
J11	S1, S7, S11, S17	-2284.579
J12	S1, S8, S11, S18	-2284.990
J13	S1, S9, S11, S19	-2285.457
J14	S5, S7, S15, S17	-2284.284
J15	S5, S8, S8, S18	-2284.997
J16	S5, S9, S15, S19	-2284.578

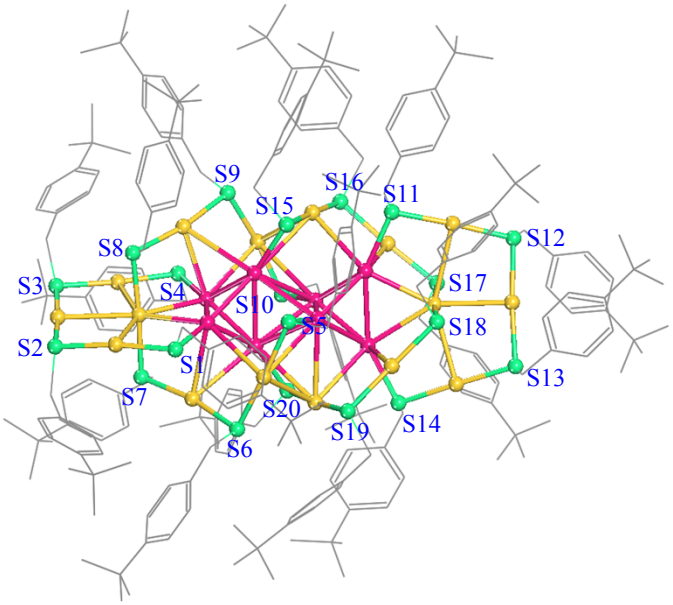

Figure S3. Geometry of the $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ P_1 isomer. S atoms are marked with numbers.

Table S3. The rotating modes and total energies of the $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ P isomer with different orientational configurations. The rotating modes from P2 to P12 are based on the $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ P_1 isomer (the most stable one; Figure S3). Note the P2 isomer has the same configuration as the reported $Au_{24}(SePh)_{20}$ structure (ref. 25 in the main text).

$Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ P orientational isomers	Rotated S atom	Total energies (eV)
P1	-	-3282.899
P2	S2, S3, S7, S8, S12, S13, S14, S17, S18	-3280.913
P3	S2, S12	-3282.184
P4	S2, S13	-3282.325
P5	S5, S15	-3281.008
P6	S6, S16	-3280.976
P7	S8, S18	-3281.130
P8	S2, S3, S12, S13	-3281.404
P9	S7, S8, S17, S18	-3279.421
P10	S2, S3, S9, S12, S13, S19	-3279.425
P11	S3, S7, S8, S12, S17, S18	-3279.639
P12	S2, S3, S7, S8, S12, S13, S17, S18	-3279.422

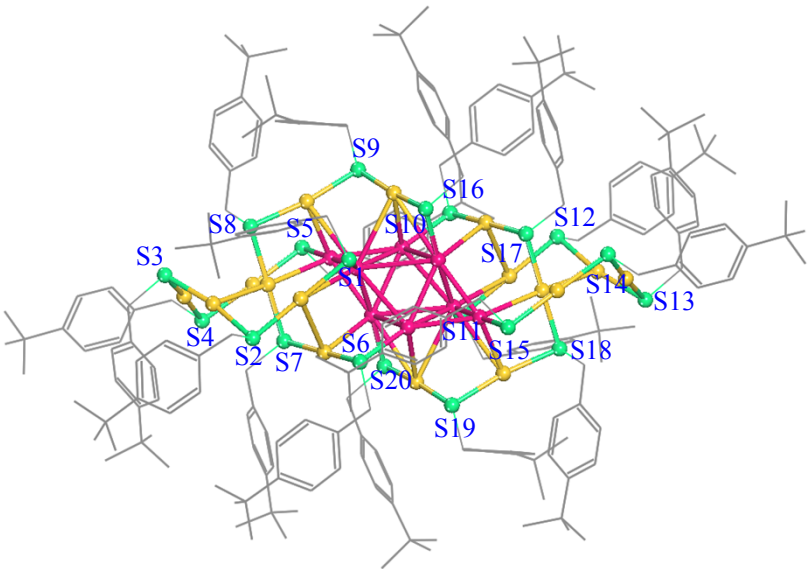

Figure S4. Geometry of the $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ J_1 isomer. S atoms are marked with numbers.

Table S4. The rotating modes and total energies of the $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ J isomer with different orientational configurations. The rotating modes from J2 to J16 are based on the $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ J_1 isomer (the most stable one; Figure S4).

$Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ J orientational isomers	Rotated S atom	Total energies (eV)
J1	-	-3283.721
J2	S1, S11	-3282.438
J3	S5, S15	-3282.636
J4	S7, S17	-3282.615
J5	S8, S18	-3282.854
J6	S6, S10, S16, S20	-3281.369
J7	S4, S5, S14, S15	-3282.739
J8	S7, S9, S17, S19	-3281.229
J9	S8, S9, S18, S19	-3280.808
J10	S7, S8, S17, S18	-3280.990
J11	S1, S7, S11, S17	-3282.137
J12	S1, S8, S11, S18	-3282.350
J13	S1, S9, S11, S19	-3281.364
J14	S5, S7, S15, S17	-3281.630
J15	S5, S8, S8, S18	-3281.953
J16	S5, S9, S15, S19	-3281.405

Table S5. Energies of the ten most stable configurations out of the 25 MD-generated initial configurations for each isomer. For comparison, the bottom row lists the energies of the most stable configurations among all explored (which are discussed in the main text).

	$Au_{24}(SCH_2CH_2Ph)_{20}$ P (eV)	$Au_{24}(SCH_2CH_2Ph)_{20}$ J (eV)	$Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ P (eV)	$Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ J (eV)
MD-1	-2284.459	-2284.363	-3279.427	-3279.979
MD-2	-2284.323	-2284.358	-3279.009	-3279.461
MD-3	-2284.044	-2284.268	-3278.408	-3279.290
MD-4	-2283.754	-2284.207	-3278.364	-3279.278
MD-5	-2283.691	-2284.129	-3278.343	-3279.235
MD-6	-2283.680	-2283.918	-3278.316	-3279.168
MD-7	-2283.674	-2283.744	-3278.136	-3279.146
MD-8	-2283.522	-2283.549	-3278.110	-3279.062
MD-9	-2283.514	-2283.483	-3278.040	-3278.801
MD-10	-2283.430	-2283.435	-3277.740	-3278.707
Putative global minimum	-2286.306	-2285.941	-3282.899	-3283.721

After structure sampling, the energetically favorable $Au_{24}(SR)_{20}$ P and J isomers were chosen for further optimizations using Turbomole. The atomic coordinates of lowest-energy $Au_{24}(SR)_{20}$ P and J isomers are shown below.

Atomic coordinates of $Au_{24}(SCH_2CH_2Ph)_{20}$ P_1:

Au -0.7023513 0.7220285 3.1382950
Au 1.2904807 -1.3981448 3.2570153
Au 2.1546439 -2.6216146 6.5328755
Au 0.1727946 -0.4323227 8.7313580
S -0.9761450 1.6435809 8.8128953
S 2.9937031 -2.8440162 4.3283115
S 1.2578272 -2.5615087 8.7515211
Au -1.5675681 1.9225533 6.5081756
S -2.0369657 2.4584957 4.2630080
Au 0.2499295 -0.3921632 5.7594832
Au 1.5326574 2.5694466 3.9057718
Au -0.5746122 -3.5424581 4.1026736
S 0.9027096 4.2606800 2.3309701
S -1.4644556 -2.0945580 5.7589550
S 0.2620959 -5.1653891 2.5593415
S 1.8655457 1.3800520 5.9104267
Au -0.8089150 3.0513760 1.1871218
S -2.5589345 1.8321758 0.1422622
Au -0.8114763 0.5231551 -0.9279855
Au 1.2284960 -1.4574107 -0.8058363
Au 1.7568048 -3.8501610 1.2656752
S 3.2536460 -2.4494591 0.0816683
Au -0.8337153 -1.5670616 -2.6798455
Au 1.2998242 0.3409313 -2.8129191
Au 1.6834407 2.0245097 -5.9189277
Au -0.6871390 0.2642424 -8.1064284
S -1.9134861 -1.7720121 -8.2852262
S 2.8328581 1.8951584 -3.8608029
S 0.5597202 2.2995878 -8.0036739
Au -2.1775708 -2.4392950 -6.0168824
S -2.2878919 -3.2173766 -3.7874585
Au -0.1485014 -0.3750612 -5.2763661
Au 1.2498828 -3.3687495 -3.8400908
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S 0.9763456 -5.0696398 -2.1627245
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S -2.4257589 -2.8120230 0.2762823

Au -0.8031227 -1.4014878 1.4241342
Au 1.3896451 0.5297277 1.3476801
Au 1.8102365 2.7274397 -0.7439760
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H 4.9938001 -3.7524001 -0.9329116
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C -4.0412661 -2.1977062 4.6035992
H -2.4595003 -0.8038181 3.9990665
H -3.1716672 -0.4347114 5.6003832
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H 3.5271304 -0.3069414 6.2955867
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C 3.5186312 8.2532081 -5.6714607
C 2.4838671 7.6419756 -4.9477401
H 2.6158216 4.5161450 -6.3262006
H 4.4451486 5.5988685 -7.6251128
H 5.0396733 8.0004891 -7.2041148
H 3.7703844 9.3043162 -5.4809703
H 1.9329341 8.2187974 -4.1925859
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H -7.4600338 4.2017388 2.8891510
H -6.8161589 2.8501592 0.9004066
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C -1.9710490 8.3024364 3.8884083
C -2.6313412 9.0725337 4.8592689
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Atomic coordinates of $Au_{24}(SCH_2CH_2Ph)_{20}$ J_1:

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Atomic coordinates of $Au_{24}(SCH_2Ph\text{-}^tBu)_{20}$ P_1:

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H -0.1190293 8.8938585 -6.7100643
C 1.2270072 9.9887193 -2.6482118
C 2.2653528 11.0649404 -3.0595249
H 1.8243475 12.0781983 -2.9672513
H 3.1698694 11.0262723 -2.4222878
H 2.5839425 10.9187939 -4.1098168
C 0.0001979 10.1236731 -3.5743117
H -0.4485288 11.1298522 -3.4584498
H 0.2773720 9.9992475 -4.6394385
H -0.7758981 9.3773158 -3.3230189
C 0.7646417 10.2420415 -1.1918978
H 0.2997372 11.2455853 -1.1072796
H 0.0215293 9.4855645 -0.8822021
H 1.6120335 10.2016015 -0.4801022