

Supporting Information:

Chiral Au₂₂(SR)₁₇⁻: A New Ligand-Binding Strategy for Structural Prediction of Thiolate-Protected Gold Nanocluster

Wen Wu Xu,^{†,§*} Dongdong Lin,^{†,§} Jie Fu,^{†,§} Wenhui, Zhao,^{†,§} Xiangmei Duan,^{†,§} Xiao Cheng Zeng^{‡*}

[†]Department of Physics, School of Physical Science and Technology, Ningbo University, Ningbo, 315211, China

[§]Laboratory of Clean Energy Storage and Conversion, Ningbo University, Ningbo, 315211, China

[‡]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, United States

*Correspondence should be addressed to: **W. W. Xu* (xuwenwu@nbu.edu.cn); *X. C. Zeng*

(xzeng1@unl.edu)

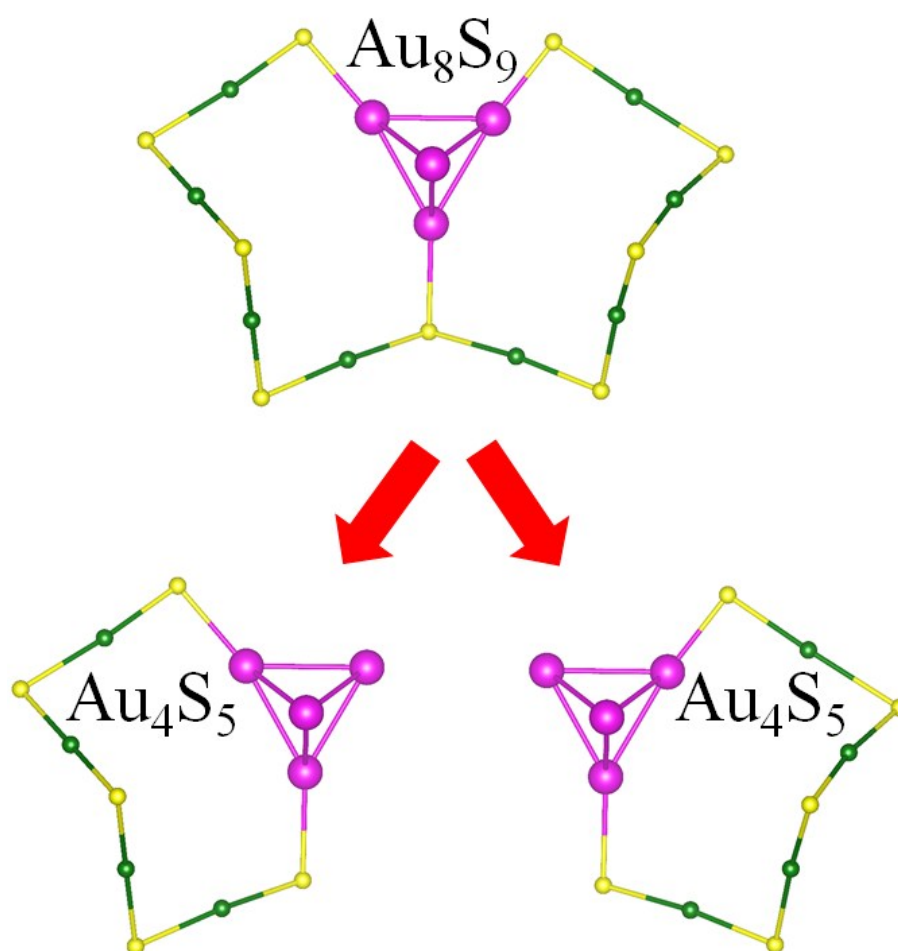


Figure S1. $\text{Au}_8(\text{SR})_9$ “staple” motif, binding with Au_4 unit in $\text{Au}_{21}(\text{SR})_{15}$, can be viewed as two $\text{Au}_4(\text{SR})_5$ “staple” motifs with sharing one SR ligand. Au atoms are presented in wine and dark green, respectively. S is presented in yellow. The R groups are omitted for clarity.

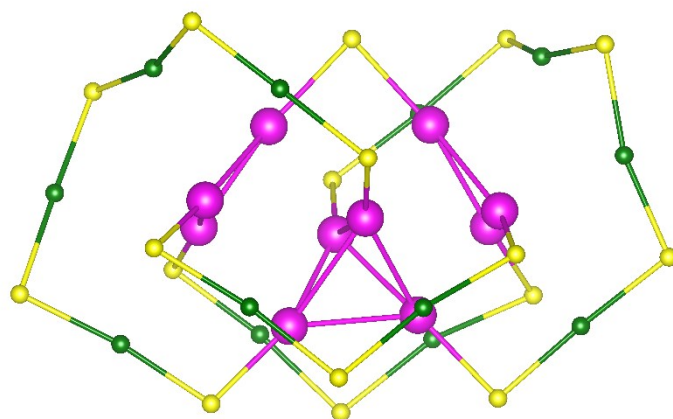


Figure S2. *Ab initio* molecular dynamics (AIMD) snapshots of the Au₂S monolayers after annealing at 355 K for 60 ps. Au atoms are presented in wine and dark green, respectively. S is presented in yellow. The R groups are omitted for clarity.

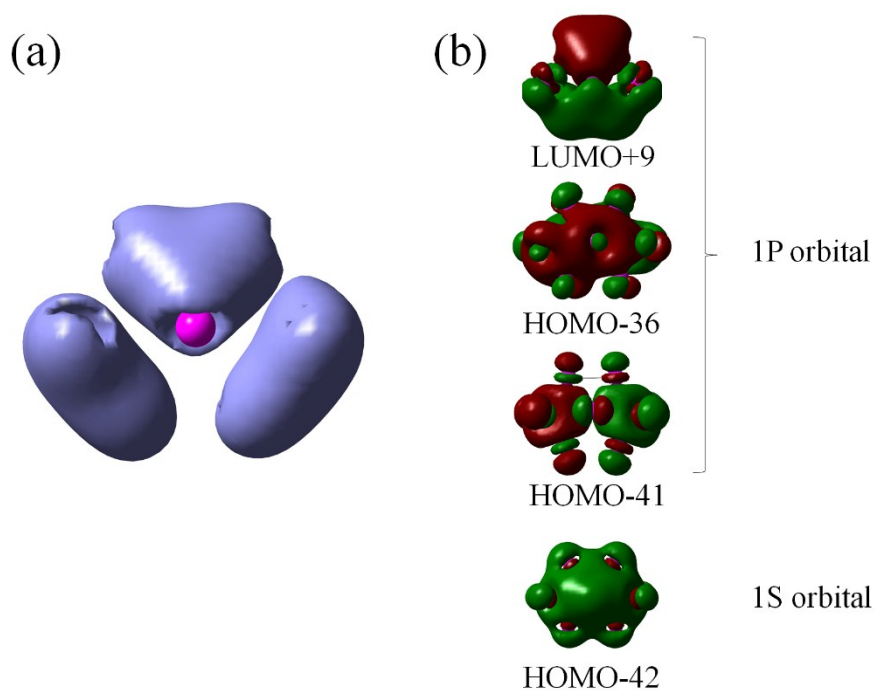


Figure S3. Visualization of the 6e valence electron distribution (a) and the superatomic orbitals (b) in the Au_{10}^{4+} of $\text{Au}_{22}(\text{SR})_{17}^-$. Au atoms are presented in wine.

The cartesian coordinates of Au₂₂(SH)₁₇⁻

Au	-1.404399991	-2.109800100	-0.077699997
Au	1.394199967	-2.093600035	0.246399999
Au	-2.856199980	-0.036400001	-1.649299979
Au	0.162100002	-0.226500005	-1.423400044
Au	3.266599894	0.049600001	-1.016399980
Au	-3.246599913	0.241099998	0.987500012
Au	-0.177000001	-0.066000000	1.360599995
Au	2.837300062	0.109399997	1.630900025
Au	1.164100051	-2.109699965	3.389800072
Au	-1.592100024	1.999899983	-0.237800002
Au	1.628700018	1.972200036	-0.035200000
Au	-1.254699945	-2.444700003	-3.213900089
Au	2.180099964	-2.457000017	-2.786799908
S	-4.186600208	-0.640999973	3.124700069
S	2.960099936	-0.653199971	3.984699965
S	-3.021899939	-1.004999995	-3.917399883
S	0.425799996	-4.077099800	-2.739900112
S	4.117300034	-1.072000027	-3.065200090
S	-3.091200113	-3.898699999	-0.324699998
S	-0.343100011	1.248499990	3.488600016
Au	-4.211800098	3.448400021	0.069100000
Au	-2.171099901	2.590899944	2.792599916
S	-3.948400021	4.125100136	2.341099977
S	-0.556900024	-3.737499952	3.062299967
Au	-2.277299881	-2.081500053	2.970499992
Au	-4.777100086	-2.221499920	-0.234999999
S	-6.732299805	-0.837599993	-0.145600006
S	0.375099987	0.875699997	-3.652800083
S	3.112699986	-3.825400114	0.661300004
Au	2.280100107	2.172300100	-3.101399899
Au	4.808499813	-2.154599905	0.626999974
S	4.181600094	3.592499971	-2.831500053
Au	5.586800098	1.194800019	1.278399944
S	6.774000168	-0.778900027	0.667400002
Au	4.264100075	3.340500116	-0.462700009
Au	-5.617700100	1.008299947	-1.163499951
S	4.623199940	3.305099964	1.918499947
S	-4.756100178	2.991699934	-2.227699995
S	0.044599999	3.845400095	-0.281100005
H	4.963600159	-1.928400040	-2.438100100
H	0.587499976	-4.535999775	-4.008299828
H	-2.212599993	-0.066000000	-4.471000195
H	1.057299972	-0.142100006	-4.237400055
H	5.098000050	2.631599903	-3.107000113
H	5.766600132	4.038199902	1.933400035
H	6.796400070	-0.511099994	-0.661800027
H	3.243799925	-4.188899994	-0.639999986
H	2.168600082	0.348899990	4.445799828
H	-0.727199972	-4.081500053	4.365600109
H	-3.638299942	0.313600004	3.920099974
H	-0.066299997	4.120299816	1.042500019

H	-1.069100022	0.309300005	4.147399902
H	-4.938700199	3.344000101	2.838500023
H	-5.912199974	3.703500032	-2.271899939
H	-6.539400101	-0.423599988	1.131899953
H	-3.145600080	-4.223700047	0.992100000