

Crystal Structure of $\text{Au}_{25}(\text{SePh})_{18}$ Nanocluster and Insights into the Electronic, Optical and Catalytic Properties

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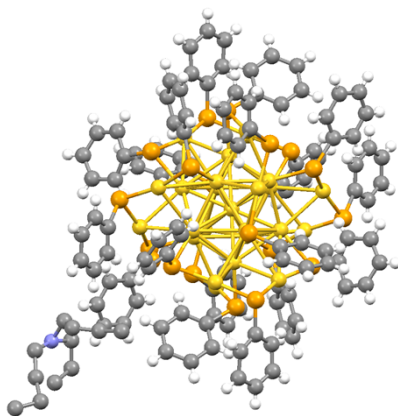


Figure S1 Crystal structure of a selenophenol-protected $[\text{Au}_{25}(\text{SeC}_6\text{H}_5)_{18}]^-\text{TOA}^+$ nanocluster.
(Color labels: yellow = Au, orange = Se, gray = C; white = H; blue = N.)

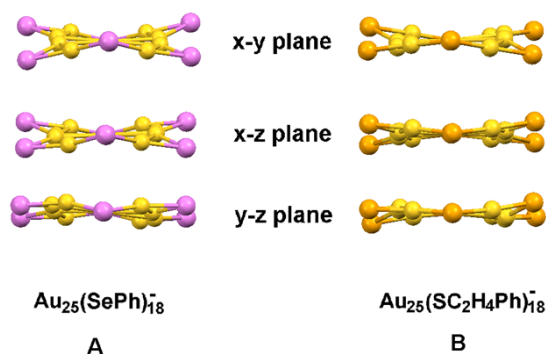


Figure S2 Comparison of the distortions of the Au_2Se_3 motifs (A) and the Au_2S_3 motifs (B) in the σ_h planes along x-y, x-z, y-z respectively (Color labels: yellow = Au, orange = Se, violet = S).



Figure S3 The currents of different residual oxygen content in the system. In the process of $a \rightarrow b \rightarrow c$, with the decrease of the oxygen content in the solution of Au_{25} by bubbling with high-purity nitrogen, the peak (*) becomes weaker and weaker, while in the process of $d \rightarrow e \rightarrow f$, when the solution of Au_{25} was exposed to air for 2, 3 and 4 minutes, the peak (*) is strengthened gradually.

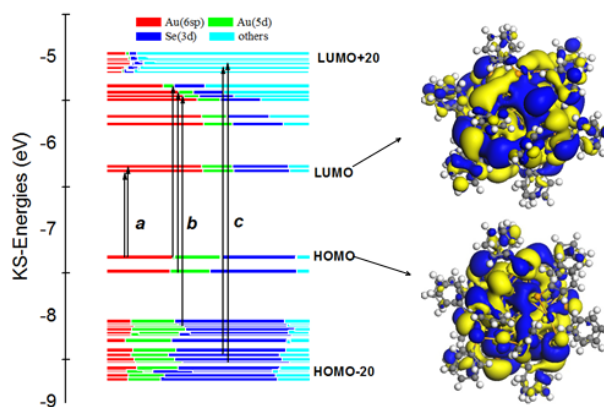


Figure S4 The electronic structure and the component of KS orbitals of $\text{Au}_{25}(\text{SePh})_{18}$.

Table S1. Crystal data and structure refinement for [Au₂₅(SePh)₁₈]⁻TOA⁺.

Identification code	Au ₂₅ (SePh) ₁₈
Empirical formula	C ₁₂₅ H ₉₅ Au ₂₅ N Se ₁₉
Formula weight	8037.35
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 16.751(5) Å α = 73.790(4)° b = 16.920(5) Å β = 77.398(4)° c = 17.211(5) Å γ = 62.104(3)°
Volume	4118(2) Å ³
Z, Calculated density	1, 3.141 Mg/m ³
Absorption coefficient	26.176 mm ⁻¹
F(000)	3353
Theta range for data collection	1.24 to 25.50°.
Limiting indices	-17<=h<=20, -20<=k<=20, -20<=l<=20
Reflections collected / unique	30485 / 15111 [R(int) = 0.0755]
Completeness to theta = 25.50°	98.6 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15111 / 0 / 750
Goodness-of-fit on F ²	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0656, wR2 = 0.1897
R indices (all data)	R1 = 0.1233, wR2 = 0.2208
Largest diff. peak and hole	4.885 and -5.022 e.Å ⁻³

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for Au₂₅(SePh)₁₈. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(62)	5000(900)	7600(800)	4100(700)	600(800)
Au(1)	0	10000	0	31(1)
Au(2)	-1391(1)	9762(1)	1129(1)	43(1)
Au(3)	599(1)	8703(1)	1433(1)	47(1)
Au(4)	-752(1)	7770(1)	2047(1)	72(1)
Au(5)	-38(1)	8325(1)	232(1)	41(1)
Au(6)	1573(1)	6737(1)	1137(1)	54(1)
Au(7)	1681(1)	8488(1)	-162(1)	41(1)
Au(8)	394(1)	9339(1)	-1423(1)	44(1)

Au(9)	2526(1)	8513(1)	-1919(1)	62(1)
Au(10)	3334(1)	8931(1)	-448(1)	57(1)
Au(11)	1413(1)	9971(1)	636(1)	42(1)
Au(12)	-1125(1)	10344(1)	-2521(1)	66(1)
Au(13)	756(1)	11828(1)	1222(1)	58(1)
C(1)	4790(30)	7420(30)	-1690(30)	96(12)
C(2)	4630(30)	6710(30)	-1840(30)	97(13)
C(3)	5380(30)	5830(30)	-1830(30)	99(13)
C(4)	6200(30)	5670(30)	-1570(30)	100(13)
C(5)	6380(30)	6330(30)	-1380(30)	99(13)
C(6)	5660(30)	7230(30)	-1510(30)	98(13)
C(7)	3670(20)	6650(20)	600(20)	74(10)
C(8)	4570(20)	6160(20)	260(20)	76(10)
C(9)	5300(30)	5960(20)	690(20)	78(10)
C(10)	5150(30)	6300(20)	1400(20)	78(10)
C(11)	4250(20)	6820(20)	1700(20)	78(10)
C(12)	3500(30)	7000(20)	1310(20)	76(10)
C(13)	690(20)	6140(20)	-200(20)	69(9)
C(14)	810(20)	5240(20)	170(20)	70(9)
C(15)	1620(20)	4480(20)	-40(20)	71(9)
C(16)	2240(20)	4680(20)	-680(20)	71(9)
C(17)	2130(20)	5570(20)	-1090(20)	72(9)
C(18)	1330(20)	6310(20)	-840(20)	69(9)
C(19)	3290(9)	10414(10)	477(7)	99(13)
C(20)	4039(9)	10353(10)	758(8)	100(13)
C(21)	4292(10)	11066(11)	490(9)	102(13)
C(22)	3798(11)	11840(11)	-59(9)	102(13)
C(23)	3049(11)	11902(10)	-341(8)	101(13)
C(24)	2796(10)	11189(10)	-73(7)	100(13)
C(31)	-2691(8)	9244(9)	2940(11)	106(14)
C(32)	-3470(8)	9176(10)	3367(12)	106(14)
C(33)	-3726(8)	9309(10)	4161(12)	109(14)
C(34)	-3202(9)	9512(10)	4530(12)	112(15)
C(35)	-2423(8)	9580(9)	4103(10)	112(15)
C(36)	-2168(7)	9446(8)	3308(10)	110(14)
C(37)	2273(9)	10740(9)	2604(7)	105(14)
C(38)	2963(9)	9855(9)	2696(7)	108(14)
C(39)	3824(9)	9685(11)	2826(8)	110(14)
C(40)	3996(10)	10401(12)	2863(9)	111(15)
C(41)	3306(11)	11287(11)	2771(9)	108(14)
C(42)	2445(10)	11456(10)	2641(8)	105(14)
C(43)	1197(11)	4530(8)	2251(10)	103(13)
C(44)	478(10)	5393(8)	2240(9)	100(13)
C(45)	-394(11)	5535(9)	2174(9)	101(13)

C(46)	-547(12)	4813(10)	2119(10)	102(13)
C(47)	172(13)	3950(10)	2130(11)	104(14)
C(48)	1044(13)	3808(9)	2196(11)	104(14)
Se(1)	-2321(2)	8932(2)	1942(2)	70(1)
Se(2)	648(2)	6428(2)	2378(2)	62(1)
Se(3)	-427(2)	7116(2)	81(2)	50(1)
Se(4)	2727(2)	6814(2)	23(2)	52(1)
Se(5)	1395(2)	8284(2)	-2382(2)	64(1)
Se(6)	3885(2)	8614(2)	-1804(2)	62(1)
Se(7)	3035(2)	9413(2)	829(2)	59(1)
Se(8)	960(3)	11107(2)	2637(2)	70(1)
Se(9)	1005(8)	8180(5)	2877(5)	61(3)
C(49)	2251(18)	7510(20)	3245(11)	71(17)
C(50)	2590(20)	6580(20)	3264(11)	72(17)
C(51)	3420(20)	5974(19)	3570(12)	72(17)
C(52)	3900(20)	6290(20)	3857(12)	74(18)
C(53)	3560(20)	7220(20)	3837(12)	73(18)
C(54)	2740(20)	7830(20)	3531(12)	71(17)
C(25)	1480(30)	8780(30)	-3460(30)	90(12)
C(26)	2350(30)	8210(30)	-3810(30)	94(12)
C(27)	2496(17)	8579(18)	-4647(11)	97(12)
C(28)	1817(17)	9303(17)	-5093(11)	96(12)
C(29)	1007(17)	9843(16)	-4694(12)	93(12)
C(30)	875(15)	9660(16)	-3849(12)	91(12)
Se(9')	1557(9)	8087(5)	2612(6)	56(3)
C(49')	1230(40)	9030(30)	3200(30)	80(20)
C(50')	320(30)	9550(40)	3420(30)	80(20)
C(51')	70(30)	10210(30)	3870(30)	80(20)
C(52')	740(40)	10350(30)	4100(30)	80(20)
C(53')	1650(30)	9830(40)	3870(30)	80(20)
C(54')	1900(30)	9170(30)	3420(30)	80(20)
C(63)	5620(30)	7880(130)	3480(130)	600(600)
C(55)	6200(1100)	6900(1100)	4800(1000)	800(900)
N(1)	5400(800)	6700(800)	4700(500)	1000(1200)
C(57)	8200(900)	900(700)	4200(700)	600(700)
C(65)	5900(1000)	8200(900)	1700(500)	700(600)
C(58)	8800(700)	6000(700)	4700(600)	600(500)
C(59)	4900(200)	6300(300)	4450(180)	320(150)
C(60)	5600(300)	5300(300)	4560(180)	310(130)
C(56)	7200(1100)	6300(1500)	4600(1400)	1000(2000)
C(64)	5700(1000)	7900(900)	2600(500)	600(700)
C(61)	6500(300)	5300(200)	4710(180)	290(120)
