Supplementary Information for

Structure and properties of heterobimetallic Au···Ag and Au···Cu interlocking thiolate [2]catenanes: a theoretical comparison study with homometallic Au···Au interlocking gold(I) thiolate [2]catenanes

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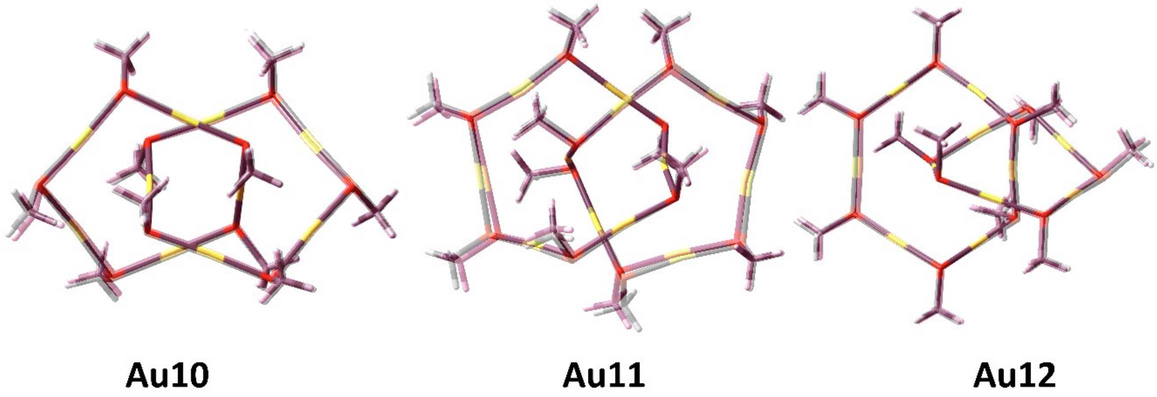


Fig. S1 Comparation of S_0 geometry optimization for **Au10-Au12** by ADF program (red) and Gaussian program (black).

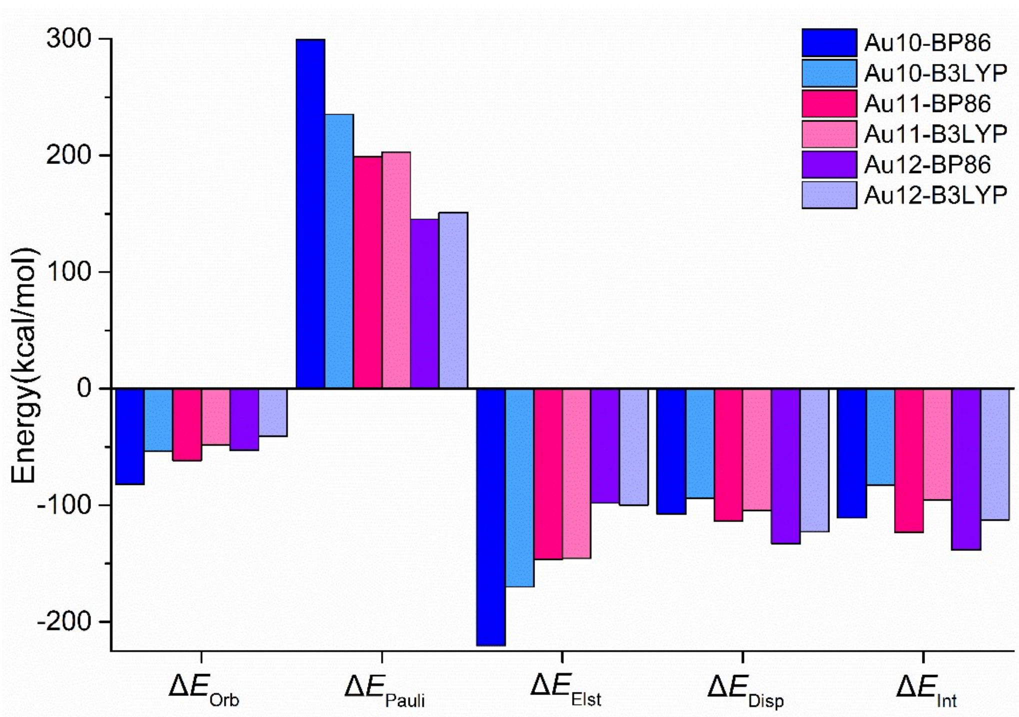


Fig. S2 Results of energy decomposition analysis for **Au10-Au12** calculated by the DFT/B3LYP and DFT/BP86 method.

Table S1 Results of energy decomposition analysis for **Au10-Au12** calculated by the DFT/BP86 method and for all complexes by the DFT/B3LYP method (kcal/mol).

Complex	Functional	ΔE_{Orb}	ΔE_{Pauli}	ΔE_{Elst}	ΔE_{Disp}	ΔE_{Steric}	ΔE_{Int}
Au10	BP86	-82.18	299.21	-220.34	-107.55	78.88	-110.86
Au11		-61.63	198.91	-146.59	-113.74	52.32	-123.05
Au12		-52.66	145.35	-98.13	-132.90	47.22	-138.34
Au10	B3LYP	-53.92	235.19	-169.99	-94.24	65.20	-82.96
Au11		-48.19	202.88	-145.43	-104.64	57.45	-95.37
Au12		-40.95	150.99	-99.87	-122.87	51.12	-112.70
Au5Ag5		-45.98	197.70	-147.26	-83.85	50.44	-79.39
Au5Ag6		-45.67	184.59	-134.88	-92.73	49.71	-88.69
Au6Ag5		-40.79	170.25	-125.25	-92.04	45.00	-87.83
Au6Ag6		-39.77	145.27	-102.68	-107.95	42.59	-105.13
Au5Cu5		-53.14	215.03	-158.98	-111.78	56.05	-108.87
Au5Cu6		-51.07	188.89	-134.40	-126.40	54.50	-122.98
Au6Cu5		-49.39	195.83	-141.26	-121.53	54.57	-116.34
Au6Cu6		-48.17	166.11	-115.88	-146.00	50.23	-143.93

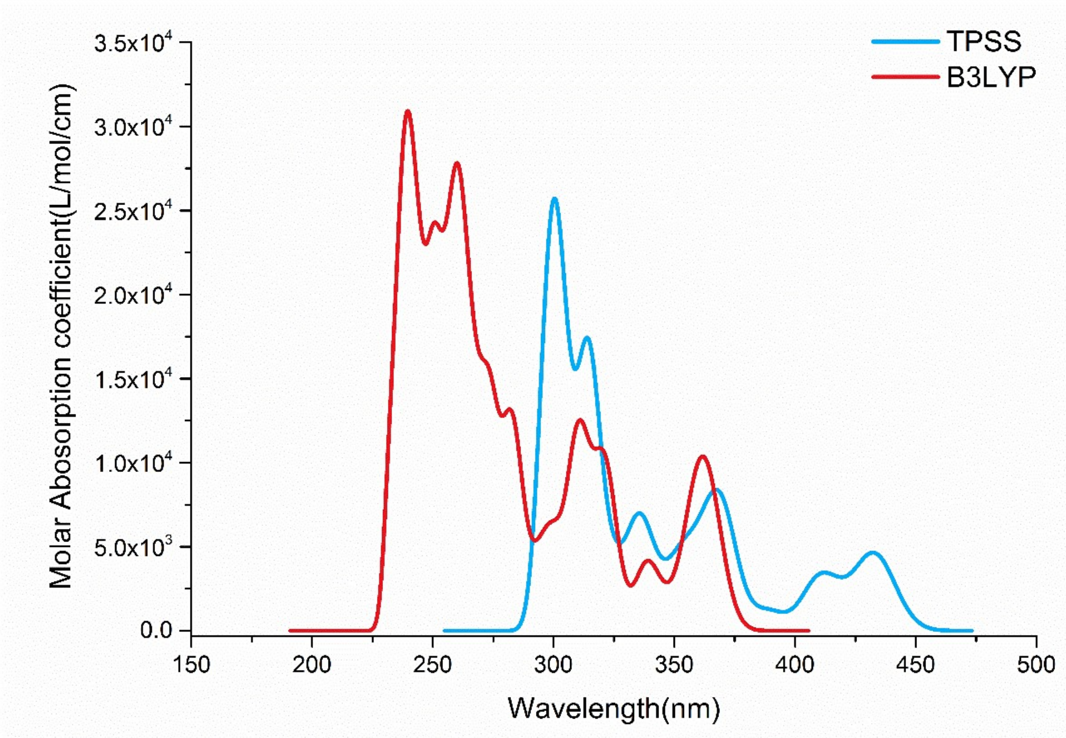


Fig. S3 Comparison for UV-Vis spectrums of **Au10** simulated in ADF program (red) by TD-DFT/B3LYP method and in Gaussian program (blue) by TD-DFT/TPSS method.

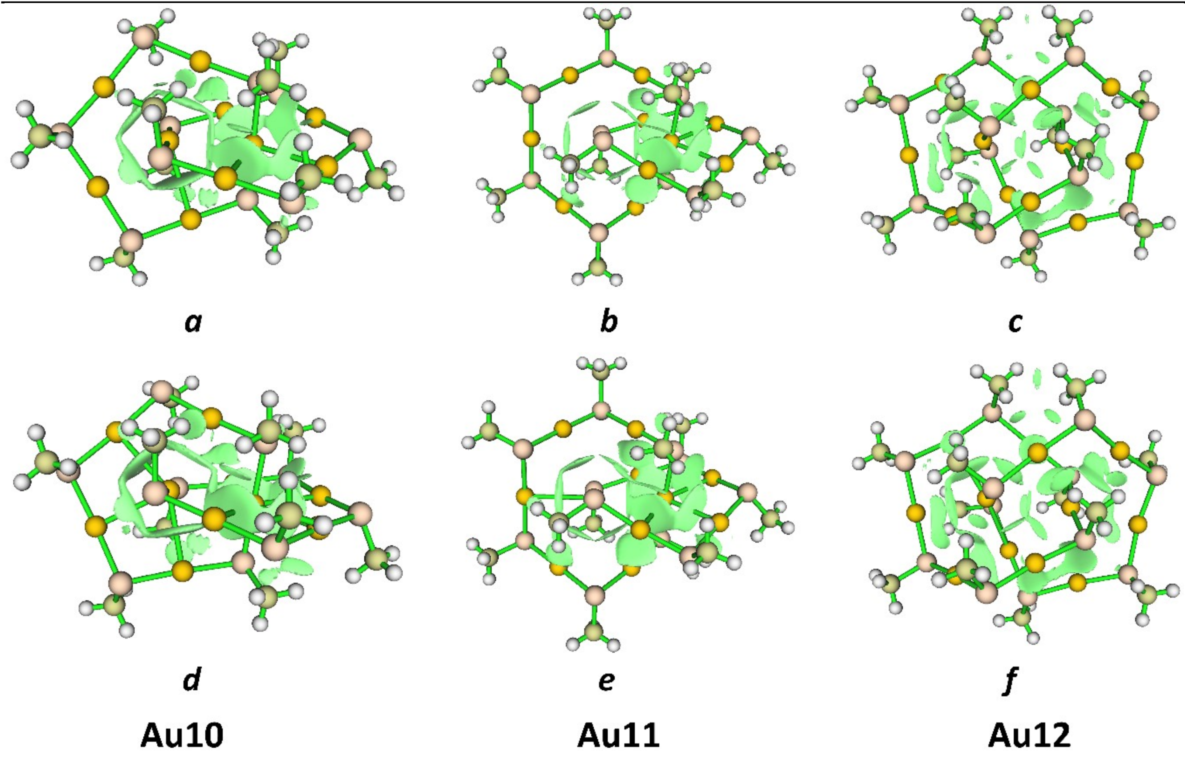
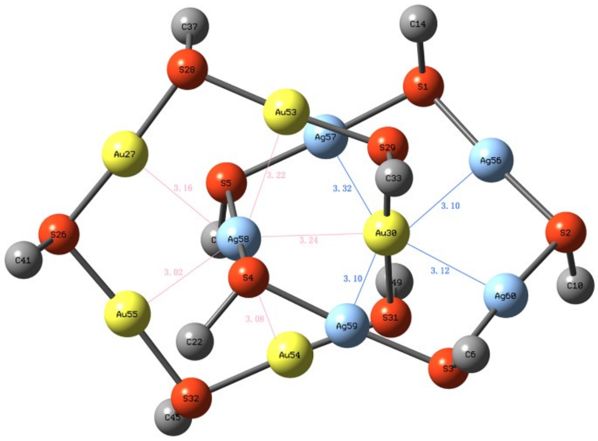
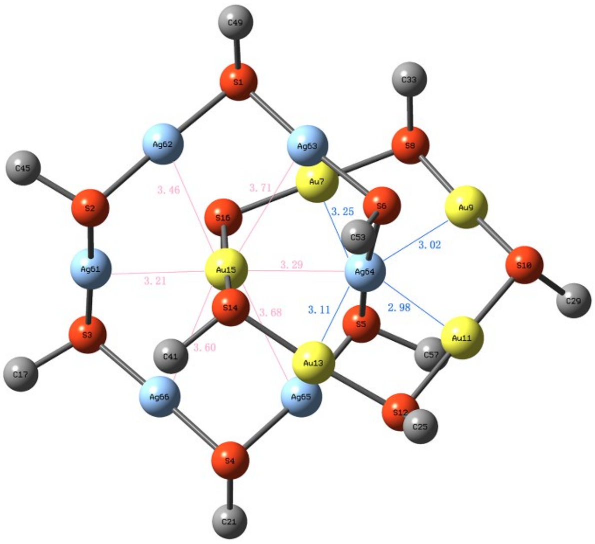


Fig. S4 (a-c) Results of IGMH analysis of **Au10-Au12** under B3LYP functional; (d-e) The results of IGMH analysis of **Au10-Au12** under BP86 functional. (color code： yellow (Au), pink (S), green (C), white (H), isoval.=0.009.)



Au5Ag5



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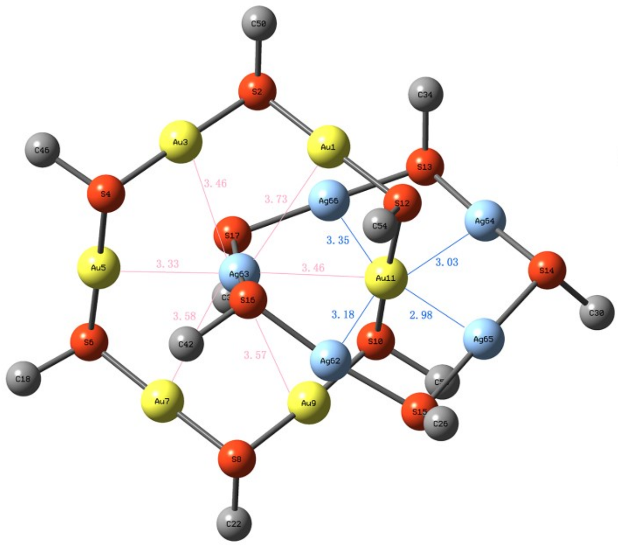
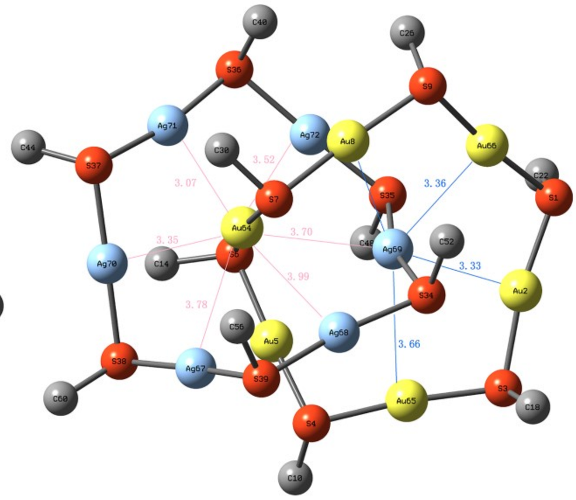
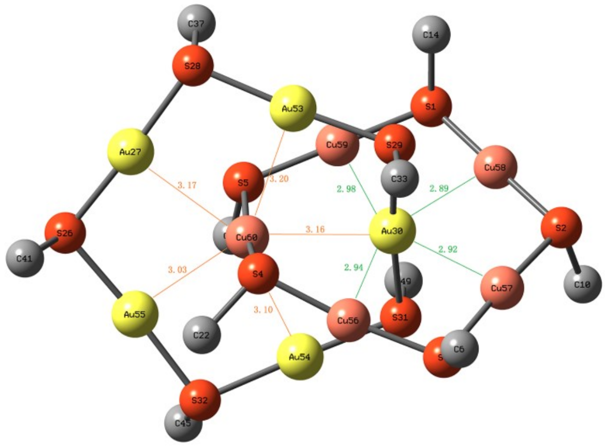


Au6Ag5

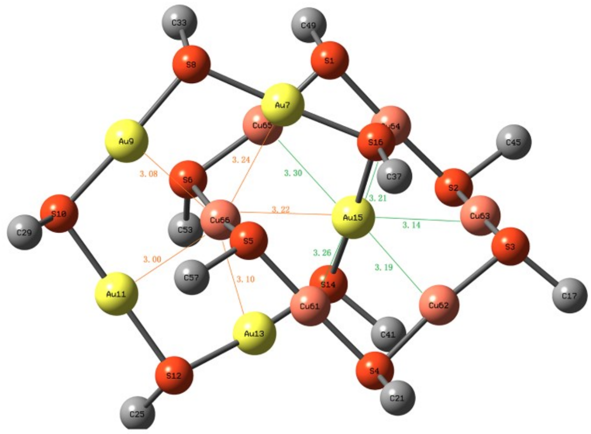


Au6Ag6

Fig S5 Optimized Au···Ag interlocking [2]catenanes. (Color code: yellow (Au), blue (Ag), red (S), gray (C). Hydrogen atoms are omitted for clarity.)



Au5Cu5



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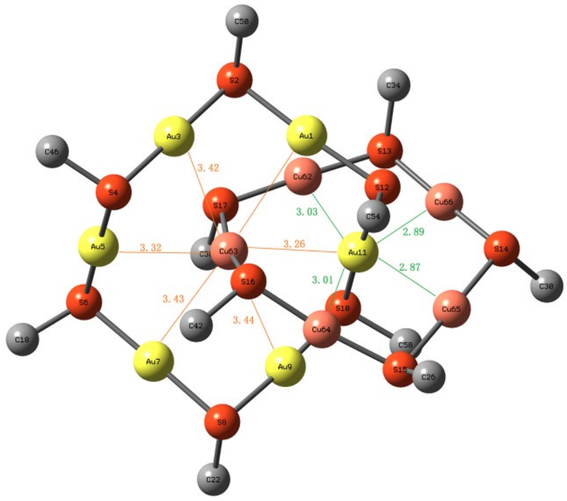
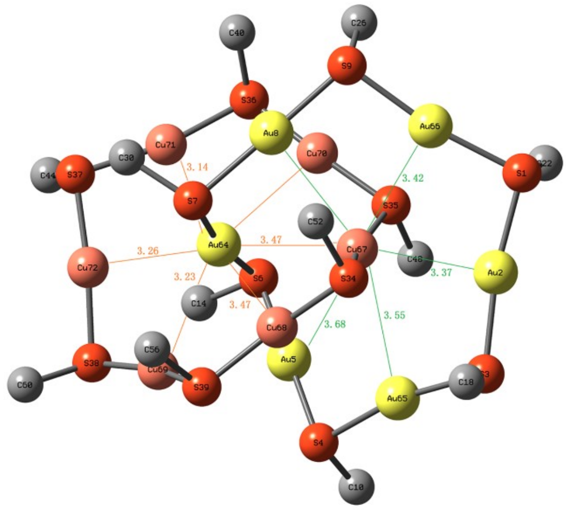


Au6Cu5



Au6Cu6

Fig S6 Optimized Au···Cu interlocking [2]catenanes. (Color code: yellow (Au), orange (Cu), red (S), gray (C). Hydrogen atoms are omitted for clarity.)

Table S2 Geometric parameters of Au···Ag interlocking [2]catenanes.

Au5Ag5		**Au5Ag6**		**Au6Ag5**		**Au6Ag6**	
			Au-S bond lengths (Å)				
Au(27)-S(26)	2.37	Au(7)-S(8)	2.37	Au(1)-S(2)	2.37	Au(2)-S(1)	2.37
Au(55)-S(26)	2.37	Au(9)-S(8)	2.37	Au(3)-S(2)	2.37	Au(2)-S(3)	2.37
Au(55)-S(32)	2.37	Au(9)-S(10)	2.38	Au(3)-S(4)	2.37	Au(65)-S(3)	2.36
Au(54)-S(32)	2.37	Au(11)-S(10)	2.38	Au(5)-S(4)	2.37	Au(65)-S(4)	2.37
Au(54)-S(31)	2.37	Au(11)-S(12)	2.38	Au(5)-S(6)	2.37	Au(5)-S(4)	2.36
Au(30)-S(31)	2.39	Au(13)-S(12)	2.38	Au(7)-S(6)	2.36	Au(5)-S(6)	2.37
Au(30)-S(29)	2.38	Au(13)-S(14)	2.37	Au(7)-S(8)	2.37	Au(64)-S(6)	2.39
Au(53)-S(29)	2.37	Au(15)-S(14)	2.37	Au(9)-S(8)	2.37	Au(64)-S(7)	2.36
Au(53)-S(28)	2.37	Au(15)-S(16)	2.37	Au(9)-S(10)	2.35	Au(8)-S(7)	2.38
Au(27)-S(28)	2.37	Au(7)-S(16)	2.38	Au(11)-S(10)	2.39	Au(8)-S(9)	2.36
				Au(11)-S(12)	2.39	Au(66)-S(9)	2.37
				Au(1)-S(12)	2.36	Au(66)-S(1)	2.36
			Ag-S bond lengths (Å)				
Ag(56)-S(1)	2.43	Ag(61)-S(2)	2.42	Ag(62)-S(16)	2.42	Ag(67)-S(39)	2.40
Ag(56)-S(2)	2.43	Ag(62)-S(2)	2.42	Ag(63)-S(16)	2.42	Ag(68)-S(39)	2.41
Ag(60)-S(2)	2.43	Ag(62)-S(1)	2.42	Ag(63)-S(17)	2.42	Ag(68)-S(34)	2.39
Ag(60)-S(3)	2.42	Ag(63)-S(1)	2.42	Ag(66)-S(17)	2.43	Ag(69)-S(34)	2.43
Ag(59)-S(3)	2.42	Ag(63)-S(6)	2.40	Ag(66)-S(13)	2.43	Ag(69)-S(35)	2.42
Ag(59)-S(4)	2.41	Ag(64)-S(6)	2.48	Ag(64)-S(13)	2.42	Ag(72)-S(35)	2.41
Ag(58)-S(4)	2.45	Ag(64)-S(5)	2.48	Ag(64)-S(14)	2.44	Ag(72)-S(36)	2.43
Ag(58)-S(5)	2.47	Ag(65)-S(5)	2.39	Ag(65)-S(14)	2.43	Ag(71)-S(36)	2.41
Ag(57)-S(5)	2.41	Ag(65)-S(4)	2.42	Ag(65)-S(15)	2.43	Ag(71)-S(37)	2.42
Ag(57)-S(1)	2.41	Ag(66)-S(4)	2.42	Ag(62)-S(15)	2.43	Ag(70)-S(37)	2.41
		Ag(66)-S(3)	2.42			Ag(70)-S(38)	2.42
		Ag(61)-S(3)	2.42			Ag(67)-S(38)	2.42
			Au···Ag contacts (Å) involving the Au atom at the center				
Au(30)-Ag(56)	3.10	Au(15)-Ag(61)	3.21	Au(11)-Ag(62)	3.18	Au(64)-Ag(67)	3.78
Au(30)-Ag(57)	3.32	Au(15)-Ag(62)	3.46	Au(11)-Ag(65)	2.98	Au(64)-Ag(68)	3.99
Au(30)-Ag(58)	3.24	Au(15)-Ag(63)	3.71	Au(11)-Ag(64)	3.03	Au(64)-Ag(69)	3.70
Au(30)-Ag(59)	3.10	Au(15)-Ag(64)	3.29	Au(11)-Ag(66)	3.35	Au(64)-Ag(70)	3.35
Au(30)-Ag(60)	3.12	Au(15)-Ag(65)	3.68	Au(11)-Ag(63)	3.46	Au(64)-Ag(71)	3.07
		Au(15)-Ag(66)	3.60			Au(64)-Ag(72)	3.52
			Au···Ag contacts (Å) involving the Ag atom at the center				
Ag(58)-Au(30)	3.24	Ag(64)-Au(7)	3.25	Au(11)-Ag(63)	3.46	Au(2)-Ag(69)	3.33
Ag(58)-Au(54)	3.08	Ag(64)-Au(9)	3.02	Au(9)-Ag(63)	3.57	Au(65)-Ag(69)	3.66
Ag(58)-Au(55)	3.02	Ag(64)-Au(11)	2.98	Au(7)-Ag(63)	3.58	Au(5)-Ag(69)	3.74
Ag(58)-Au(27)	3.16	Ag(64)-Au(13)	3.11	Au(5)-Ag(63)	3.33	Au(64)-Ag(69)	3.70
Ag(58)-Au(53)	3.22	Au(15)-Ag(64)	3.29	Au(3)-Ag(63)	3.46	Au(8)-Ag(69)	3.45
				Au(1)-Ag(63)	3.73	Au(66)-Ag(69)	3.36
			Au-S-Au bond angles (°)				
Au(27)-S(28)-Au(53)	103.64	Au(7)-S(8)-Au(9)	104.86	Au(1)-S(2)-Au(3)	95.12	Au(2)-S(3)-Au(65)	107.62
Au(53)-S(29)-Au(30)	101.07	Au(9)-S(10)-Au(11)	103.47	Au(3)-S(4)-Au(5)	98.56	Au(65)-S(4)-Au(5)	97.77
Au(30)-S(31)-Au(54)	100.10	Au(11)-S(12)-Au(13)	100.66	Au(5)-S(6)-Au(7)	97.90	Au(5)-S(6)-Au(64)	84.86

Au(54)-S(32)-Au(55)	103.98	Au(13)-S(14)-Au(15)	99.79	Au(7)-S(8)-Au(9)	93.88	Au(64)-S(7)-Au(8)	96.34
Au(55)-S262)-Au(27)	102.89	Au(15)-S(16)-Au(7)	99.59	Au(9)-S(10)-Au(11)	97.86	Au(8)-S(9)-Au(66)	104.70
				Au(11)-S(12)-Au(1)	92.95	Au(66)-S(1)-Au(2)	104.66
S-Au-S bond angles (°)							
S(28)-Au(53)-S(29)	175.74	S(8)-Au(9)-S(10)	176.88	S(2)-Au(3)-S(4)	178.33	S(1)-Au(2)-S(3)	170.59
S(29)-Au(30)-S(31)	176.81	S(10)-Au(11)-S(12)	178.45	S(4)-Au(5)-S(6)	178.45	S(3)-Au(65)-S(4)	174.01
S(31)-Au(54)-S(32)	176.40	S(12)-Au(13)-S(14)	175.74	S(6)-Au(7)-S(8)	179.07	S(4)-Au(5)-S(6)	175.14
S(32)-Au(55)-S(26)	176.39	S(14)-Au(15)-S(16)	170.86	S(8)-Au(9)-S(10)	175.58	S(6)-Au(64)-S(7)	165.16
S(26)-Au(27)-S(28)	176.21	S(16)-Au(7)-S(8)	176.20	S(10)-Au(11)-S(12)	169.98	S(7)-Au(8)-S(9)	171.18
				S(12)-Au(1)-S(2)	175.94	S(9)-Au(66)-S(1)	173.85
Ag-S-Ag bond angles (°)							
Ag(56)-S(1)-Ag(57)	101.93	Ag(61)-S(2)-Ag(62)	96.39	Ag(62)-S(15)-Ag(65)	101.58	Ag(67)-S(39)-Ag(68)	97.13
Ag(57)-S(5)-Ag(58)	98.15	Ag(62)-S(1)-Ag(63)	90.46	Ag(65)-S(14)-Ag(64)	102.70	Ag(68)-S(34)-Ag(69)	97.85
Ag(58)-S(4)-Ag(59)	100.03	Ag(63)-S(6)-Ag(64)	89.90	Ag(64)-S(13)-Ag(66)	105.90	Ag(69)-S(35)-Ag(72)	99.59
Ag(59)-S(3)-Ag(60)	100.86	Ag(64)-S(5)-Ag(65)	93.97	Ag(66)-S(17)-Ag(63)	98.56	Ag(72)-S(36)-Ag(71)	103.28
Ag(56)-S(2)-Ag(56)	102.65	Ag(65)-S(5)-Ag(66)	87.67	Ag(63)-S(16)-Ag(62)	98.38	Ag(71)-S(37)-Ag(70)	100.30
		Ag(66)-S(3)-Ag(61)	95.21			Ag(70)-S(38)-Ag(67)	90.19
S-Ag-S bond angles (°)							
S(1)-Ag(56)-S(2)	174.15	S(1)-Ag(62)-S(2)	177.14	S(13)-Ag(64)-S(14)	176.96	S(34)-Ag(69)-S(35)	163.10
S(2)-Ag(60)-S(3)	173.21	S(2)-Ag(61)-S(3)	175.72	S(14)-Ag(65)-S(15)	175.11	S(35)-Ag(72)-S(36)	176.32
S(3)-Ag(59)-S(4)	172.42	S(3)-Ag(66)-S(4)	178.53	S(15)-Ag(62)-S(16)	172.98	S(36)-Ag(71)-S(37)	169.53
S(4)-Ag(58)-S(5)	170.29	S(4)-Ag(65)-S(5)	172.03	S(16)-Ag(63)-S(17)	172.66	S(37)-Ag(70)-S(38)	176.96
S(5)-Ag(57)-S(1)	176.81	S(5)-Ag(64)-S(6)	168.27	S(17)-Ag(66)-S(13)	175.94	S(38)-Ag(67)-S(39)	171.60
		S(6)-Ag(63)-S(1)	174.90			S(39)-Ag(68)-S(34)	169.30
Au-S-S-Au dihedral angles (°)							
Au(27)-S(26)-S(32)-Au(54)	-13.60	Au(7)-S(8)-S(10)-Au(11)	5.41	Au(1)-S(2)-S(4)-Au(5)	-85.84	Au(2)-S(3)-S(4)-Au(5)	26.29
Au(55)-S(32)-S(31)-Au(30)	29.87	Au(9)-S(10)-S(12)-Au(13)	-34.07	Au(3)-S(4)-S(6)-Au(7)	83.05	Au(65)-S(4)-S(6)-Au(64)	-92.50
Au(54)-S(31)-S(29)-Au(53)	-33.14	Au(11)-S(12)-S(14)-Au(15)	56.65	Au(5)-S(6)-S(8)-Au(9)	-77.34	Au(5)-S(6)-S(7)-Au(8)	109.59
Au(30)-S(29)-S(28)-Au(27)	28.00	Au(13)-S(14)-S(15)-Au(16)	-51.65	Au(7)-S(8)-S(10)-Au(11)	88.96	Au(64)-S(7)-S(9)-Au(66)	-57.87
Au(53)-S(28)-S(26)-Au(55)	-10.38	Au(15)-S(16)-S(8)-Au(9)	23.66	Au(9)-S(10)-S(12)-Au(1)	-89.99	Au(8)-S(9)-S(1)-Au(2)	-10.72
				Au(11)-S(12)-S(2)-Au(3)	76.50	Au(66)-S(1)-S(3)-Au(65)	24.52
Ag-S-S-Ag dihedral angles (°)							
Ag(56)-S(2)-S(3)-Ag(59)	-1.46	Ag(61)-S(3)-S(4)-Ag(65)	-81.02	Ag(62)-S(15)-S(14)-Ag(64)	-35.48	Ag(67)-S(39)-S(34)-Ag(69)	11.39
Ag(60)-S(3)-S(4)-Ag(58)	39.70	Ag(66)-S(4)-S(5)-Ag(64)	91.97	Ag(65)-S(14)-S(13)-Ag(66)	6.01	Ag(68)-S(34)-S(35)-Ag(72)	50.47
Ag(59)-S(4)-S(5)-Ag(57)	-47.20	Ag(65)-S(5)-S(6)-Ag(63)	-96.56	Ag(64)-S(13)-S(17)-Ag(63)	23.91	Ag(69)-S(35)-S(36)-Ag(71)	-38.72
Ag(58)-S(5)-S(1)-Ag(56)	33.10	Ag(64)-S(6)-S(1)-Ag(62)	73.39	Ag(66)-S(17)-S(16)-Ag(62)	-53.44	Ag(72)-S(36)-S(37)-Ag(70)	-23.32
Ag(57)-S(1)-S(2)-Ag(60)	-24.66	Ag(63)-S(1)-S(2)-Ag(61)	-86.50	Ag(63)-S(16)-S(15)-Ag(65)	60.20	Ag(71)-S(37)-S(38)-Ag(67)	80.55
		Ag(62)-S(2)-S(3)-Ag(66)	88.90			Ag(70)-S(38)-S(39)-Ag(68)	-75.74

Table S3 Geometric parameters of Au···Cu interlocking [2]catenanes.

Au5Cu5		**Au5Cu6**		**Au6Cu5**		**Au6Cu6**	
Au-S bond length (Å)							
Au(27)-S(26)	2.37	Au(7)-S(8)	2.37	Au(1)-S(2)	2.37	Au(2)-S(1)	2.36
Au(27)-S(28)	2.37	Au(9)-S(8)	2.37	Au(3)-S(2)	2.37	Au(2)-S(3)	2.36
Au(53)-S(28)	2.37	Au(9)-S(10)	2.38	Au(3)-S(4)	2.37	Au(65)-S(3)	2.35
Au(53)-S(29)	2.36	Au(11)-S(10)	2.37	Au(5)-S(4)	2.37	Au(65)-S(4)	2.37
Au(30)-S(29)	2.39	Au(11)-S(12)	2.38	Au(5)-S(6)	2.37	Au(5)-S(4)	2.35
Au(30)-S(31)	2.40	Au(13)-S(12)	2.37	Au(7)-S(6)	2.37	Au(5)-S(6)	2.37
Au(54)-S(31)	2.36	Au(13)-S(14)	2.37	Au(7)-S(8)	2.38	Au(64)-S(6)	2.39
Au(54)-S(32)	2.37	Au(15)-S(14)	2.38	Au(9)-S(8)	2.37	Au(64)-S(7)	2.36
Au(55)-S(32)	2.37	Au(15)-S(16)	2.38	Au(9)-S(10)	2.34	Au(8)-S(7)	2.38
Au(55)-S(26)	2.37	Au(7)-S(16)	2.38	Au(11)-S(10)	2.41	Au(8)-S(9)	2.36
				Au(11)-S(12)	2.40	Au(66)-S(9)	2.36
				Au(1)-S(12)	2.35	Au(66)-S(1)	2.36
Cu-S bond length (Å)							
Cu(56)-S(3)	2.22	Cu(61)-S(4)	2.20	Cu(62)-S(17)	2.23	Cu(67)-S(34)	2.21
Cu(57)-S(3)	2.22	Cu(62)-S(4)	2.20	Cu(63)-S(17)	2.21	Cu(68)-S(34)	2.20
Cu(57)-S(2)	2.23	Cu(62)-S(3)	2.21	Cu(63)-S(16)	2.21	Cu(68)-S(39)	2.21
Cu(58)-S(2)	2.23	Cu(63)-S(3)	2.20	Cu(64)-S(16)	2.22	Cu(69)-S(39)	2.19
Cu(58)-S(1)	2.23	Cu(63)-S(2)	2.20	Cu(64)-S(15)	2.23	Cu(69)-S(38)	2.20
Cu(59)-S(1)	2.22	Cu(64)-S(2)	2.20	Cu(65)-S(15)	2.23	Cu(72)-S(38)	2.19
Cu(59)-S(5)	2.20	Cu(64)-S(1)	2.20	Cu(65)-S(14)	2.23	Cu(72)-S(37)	2.20
Cu(60)-S(5)	2.24	Cu(65)-S(1)	2.20	Cu(66)-S(14)	2.23	Cu(71)-S(37)	2.20
Cu(60)-S(4)	2.23	Cu(65)-S(6)	2.19	Cu(66)-S(13)	2.23	Cu(71)-S(36)	2.19
Cu(56)-S(4)	2.21	Cu(66)-S(6)	2.23	Cu(62)-S(13)	2.24	Cu(70)-S(36)	2.21
		Cu(66)-S(5)	2.23			Cu(70)-S(35)	2.20
		Cu(61)-S(5)	2.18			Cu(67)-S(35)	2.20
Au···Cu contacts (Å) involving the Au atom at the center							
Au(30)-Cu(56)	2.94	Au(15)-Cu(61)	3.26	Au(11)-Cu(62)	3.03	Au(64)-Cu(67)	3.47
Au(30)-Cu(57)	2.92	Au(15)-Cu(62)	3.19	Au(11)-Cu(63)	3.26	Au(64)-Cu(68)	3.47
Au(30)-Cu(58)	2.89	Au(15)-Cu(63)	3.14	Au(11)-Cu(64)	3.01	Au(64)-Cu(69)	3.23
Au(30)-Cu(59)	2.98	Au(15)-Cu(64)	3.21	Au(11)-Cu(65)	2.87	Au(64)-Cu(70)	3.28
Au(30)-Cu(60)	3.16	Au(15)-Cu(65)	3.30	Au(11)-Cu(66)	2.89	Au(64)-Cu(71)	3.14
		Au(15)-Cu(66)	3.22			Au(64)-Cu(72)	3.26
Au···Cu contacts (Å) involving the Cu atom at the center							
Cu(60)-Au(30)	3.16	Cu(66)-Au(7)	3.24	Au(11)-Cu(63)	3.26	Au(2)-Cu(67)	3.37
Cu(60)-Au(54)	3.10	Cu(66)-Au(9)	3.08	Au(9)-Cu(63)	3.44	Au(65)-Cu(67)	3.55
Cu(60)-Au(55)	3.03	Cu(66)-Au(11)	3.00	Au(7)-Cu(63)	3.43	Au(5)-Cu(67)	3.68
Cu(60)-Au(27)	3.17	Cu(66)-Au(13)	3.10	Au(5)-Cu(63)	3.32	Au(64)-Cu(67)	3.47
Cu(60)-Au(53)	3.20	Cu(66)-Au(15)	3.22	Au(3)-Cu(63)	3.42	Au(8)-Cu(67)	3.37
				Au(1)-Cu(63)	3.56	Au(66)-Cu(67)	3.42
Au-S-Au bond angle (°)							
Au(27)-S(28)-Au(53)	103.54	Au(7)-S(8)-Au(9)	104.94	Au(1)-S(2)-Au(3)	90.59	Au(2)-S(3)-Au(65)	105.67
Au(53)-S(29)-Au(30)	99.84	Au(9)-S(10)-Au(11)	103.69	Au(3)-S(4)-Au(5)	92.77	Au(65)-S(4)-Au(5)	96.75
Au(30)-S(31)-Au(54)	98.19	Au(11)-S(12)-Au(13)	101.12	Au(5)-S(6)-Au(7)	92.96	Au(5)-S(6)-Au(64)	83.63

Au(54)-S(32)-Au(55)	104.17	Au(13)-S(14)-Au(15)	99.44	Au(7)-S(8)-Au(9)	89.46	Au(64)-S(7)-Au(8)	93.12
Au(55)-S262)-Au(27)	103.09	Au(15)-S(16)-Au(7)	98.69	Au(9)-S(10)-Au(11)	94.35	Au(8)-S(9)-Au(66)	102.17
				Au(11)-S(12)-Au(1)	90.93	Au(66)-S(1)-Au(2)	102.29
S-Au-S bond angle (°)							
S(28)-Au(53)-S(29)	176.09	S(8)-Au(9)-S(10)	174.26	S(2)-Au(3)-S(4)	179.58	S(1)-Au(2)-S(3)	170.44
S(29)-Au(30)-S(31)	174.54	S(10)-Au(11)-S(12)	177.10	S(4)-Au(5)-S(6)	178.75	S(3)-Au(65)-S(4)	167.87
S(31)-Au(54)-S(32)	176.62	S(12)-Au(13)-S(14)	174.35	S(6)-Au(7)-S(8)	178.99	S(4)-Au(5)-S(6)	176.87
S(32)-Au(55)-S(26)	176.12	S(14)-Au(15)-S(16)	173.40	S(8)-Au(9)-S(10)	176.05	S(6)-Au(64)-S(7)	170.43
S(26)-Au(27)-S(28)	175.37	S(16)-Au(7)-S(8)	177.57	S(10)-Au(11)-S(12)	169.93	S(7)-Au(8)-S(9)	168.24
				S(12)-Au(1)-S(2)	175.66	S(9)-Au(66)-S(1)	171.24
Cu-S-Cu bond angle (°)							
Cu(56)-S(3)-Cu(57)	104.24	Cu(61)-S(4)-Cu(62)	92.00	Cu(62)-S(13)-Cu(66)	108.58	Cu(67)-S(34)-Cu(68)	79.85
Cu(57)-S(2)-Cu(58)	104.79	Cu(62)-S(3)-Cu(63)	97.11	Cu(66)-S(14)-Cu(67)	104.86	Cu(68)-S(39)-Cu(69)	106.52
Cu(58)-S(1)-Cu(59)	105.94	Cu(63)-S(2)-Cu(64)	94.05	Cu(65)-S(15)-Cu(64)	104.99	Cu(69)-S(38)-Cu(72)	97.85
Cu(59)-S(5)-Cu(60)	102.22	Cu(64)-S(1)-Cu(65)	91.03	Cu(64)-S(16)-Cu(63)	103.93	Cu(72)-S(37)-Cu(71)	101.20
Cu(56)-S(4)-Cu(56)	102.39	Cu(65)-S(6)-Cu(66)	93.86	Cu(63)-S(17)-Cu(62)	104.34	Cu(71)-S(36)-Cu(70)	106.68
		Cu(66)-S(5)-Cu(61)	96.11			Cu(70)-S(38)-Cu(67)	104.40
S-Cu-S bond angle (°)							
S(3)-Cu(56)-S(4)	169.96	S(3)-Cu(62)-S(4)	173.80	S(13)-Cu(66)-S(14)	174.71	S(34)-Cu(67)-S(35)	160.78
S(4)-Cu(60)-S(5)	168.22	S(4)-Cu(61)-S(5)	176.62	S(14)-Cu(65)-S(15)	178.54	S(35)-Cu(70)-S(36)	172.68
S(5)-Cu(59)-S(1)	173.99	S(5)-Cu(66)-S(6)	167.00	S(15)-Cu(64)-S(16)	173.79	S(36)-Cu(71)-S(37)	169.25
S(1)-Cu(58)-S(2)	178.82	S(6)-Cu(65)-S(1)	172.09	S(16)-Cu(63)-S(17)	167.21	S(37)-Cu(72)-S(38)	170.55
S(2)-Cu(57)-S(3)	172.10	S(1)-Cu(64)-S(2)	175.83	S(17)-Cu(62)-S(13)	175.06	S(38)-Cu(69)-S(39)	162.60
		S(2)-Cu(63)-S(3)	176.94			S(39)-Cu(68)-S(34)	157.63
Au-S-S-Au dihedral angles (°)							
Au(27)-S(26)-S(32)-Au(54)	-16.59	Au(7)-S(8)-S(10)-Au(11)	1.55	Au(1)-S(2)-S(4)-Au(5)	-90.06	Au(2)-S(3)-S(4)-Au(5)	7.50
Au(55)-S(32)-S(31)-Au(30)	32.20	Au(9)-S(10)-S(12)-Au(13)	-34.67	Au(3)-S(4)-S(6)-Au(7)	91.41	Au(65)-S(4)-S(6)-Au(64)	-75.09
Au(54)-S(31)-S(29)-Au(53)	-36.54	Au(11)-S(12)-S(14)-Au(15)	56.57	Au(5)-S(6)-S(8)-Au(9)	-85.15	Au(5)-S(6)-S(7)-Au(8)	108.07
Au(30)-S(29)-S(28)-Au(27)	28.89	Au(13)-S(14)-S(16)-Au(7)	-52.74	Au(7)-S(8)-S(10)-Au(11)	87.37	Au(64)-S(7)-S(9)-Au(66)	-59.17
Au(53)-S(28)-S(26)-Au(55)	-8.39	Au(15)-S(16)-S(8)-Au(9)	28.56	Au(9)-S(10)-S(12)-Au(1)	-86.89	Au(8)-S(9)-S(1)-Au(2)	-13.13
				Au(11)-S(12)-S(2)-Au(3)	76.52	Au(66)-S(1)-S(3)-Au(65)	34.64
Cu-S-S-Cu dihedral angles (°)							
Cu(56)-S(4)-S(5)-Cu(59)	-44.72	Cu(61)-S(4)-S(3)-Cu(63)	-73.88	Cu(62)-S(17)-S(16)-Cu(64)	-46.34	Cu(67)-S(34)-S(39)-Cu(69)	-17.21
Cu(60)-S(5)-S(1)-Cu(58)	24.02	Cu(62)-S(3)-S(2)-Cu(64)	79.63	Cu(63)-S(16)-S(15)-Cu(65)	52.66	Cu(68)-S(39)-S(38)-Cu(72)	-41.85
Cu(59)-S(1)-S(2)-Cu(57)	-10.49	Cu(63)-S(2)-S(1)-Cu(65)	-83.06	Cu(64)-S(15)-S(14)-Cu(66)	-30.86	Cu(69)-S(38)-S(37)-Cu(71)	49.14
Cu(58)-S(2)-S(3)-Cu(56)	-9.88	Cu(64)-S(1)-S(5)-Cu(66)	73.54	Cu(65)-S(14)-S(13)-Cu(62)	7.11	Cu(72)-S(37)-S(36)-Cu(70)	-22.41
Cu(57)-S(3)-S(4)-Cu(60)	44.25	Cu(65)-S(6)-S(5)-Cu(61)	-80.81	Cu(66)-S(13)-S(17)-Cu(63)	20.08	Cu(71)-S(36)-S(35)-Cu(67)	-33.68
		Cu(62)-S(5)-S(4)-Cu(62)	81.60			Cu(70)-S(35)-S(34)-Cu(68)	62.49

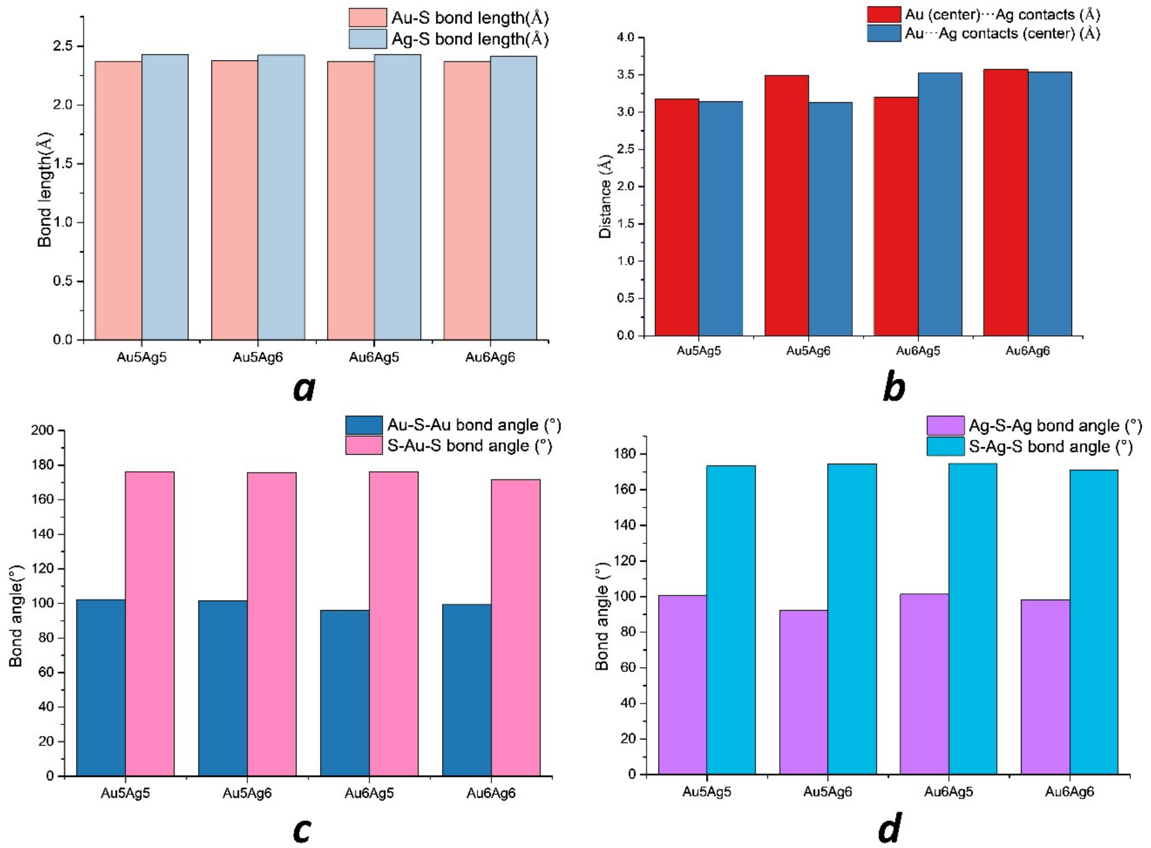


Fig S7 Comparison for the average geometric parameters of Au···Ag interlocking [2]catenanes: (a)Au-S and Ag-S bond length (Å); (b)Au···Ag contacts (Å) involving the Au atom at the center and Au···Ag contacts (Å) involving the Ag atom at the center; (c)Au-S-Au and S-Au-S bond angle (°); (d)Ag-S-Ag and S-Ag-S bond angle (°).

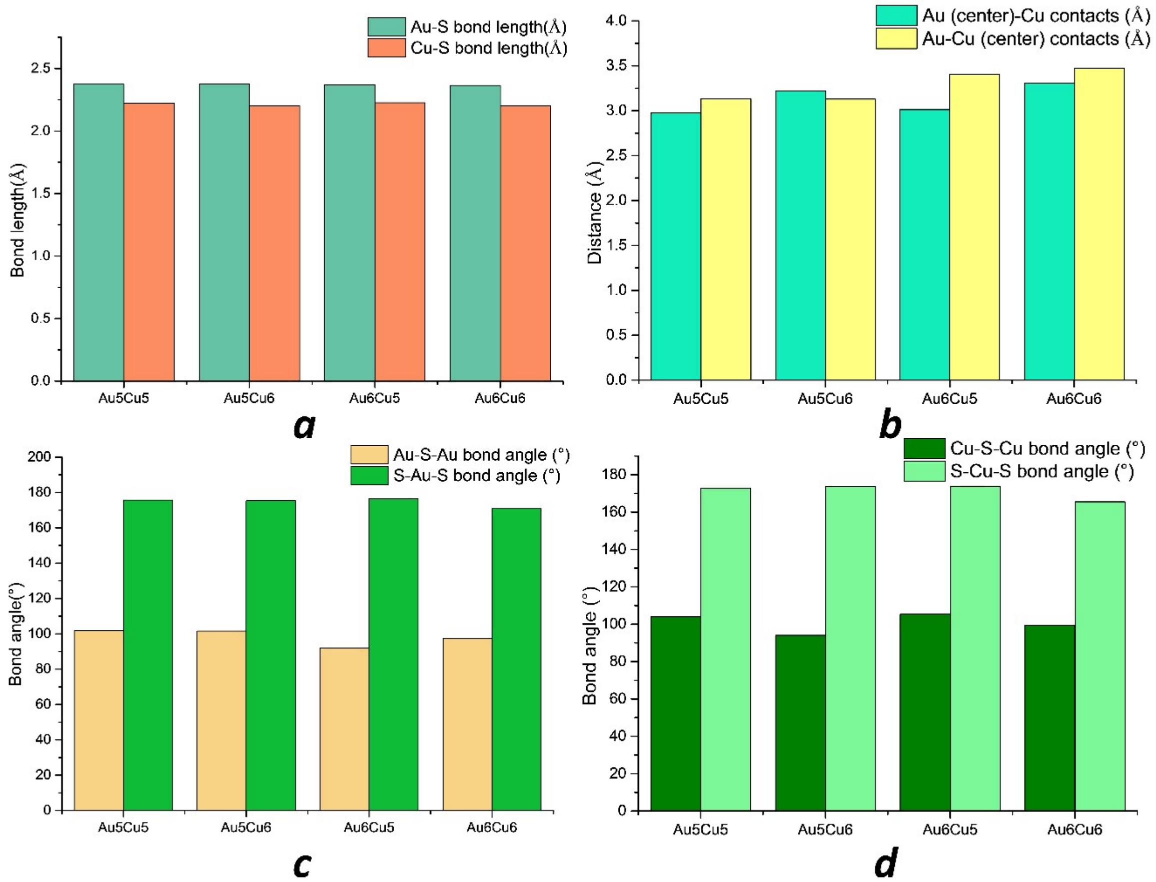


Fig S8 Comparison of the average geometric parameters of Au···Cu interlocking [2]catenanes: (a) Au-S and Cu-S bond length (Å); (b) Au···Cu contacts (Å) involving the Au atom at the center and Au···Cu contacts (Å) involving the Cu atom at the center; (c) Au-S-Au and S-Au-S bond angle (°); (d)Cu-S-Cu and S-Cu-S bond angle (°).

Table S4 Calculated stabilization energies (kcal/mol) of (MeSAu) and (MeSAg) units in Au···Ag interlocking [2]catenanes.

	Au5Ag5	**Au5Ag6**	**Au6Ag5**	**Au6Ag6**
$E(MeSAu)_{Stable}$	-39.84	-39.92	-39.85	-39.16
$E(MeSAg)_{Stable}$	-35.88	-35.99	-36.08	-35.72

Table S5 Calculated stabilization energies (kcal/mol) of (MeSAu) and (MeSCu) units in Au···Cu interlocking [2]catenanes.

	Au5Cu5	**Au5Cu6**	**Au6Cu5**	**Au6Cu6**
$E(MeSAu)_{Stable}$	-39.75	-39.88	-39.62	-39.10
$E(MeSCu)_{Stable}$	-41.35	-41.92	-41.40	-40.59

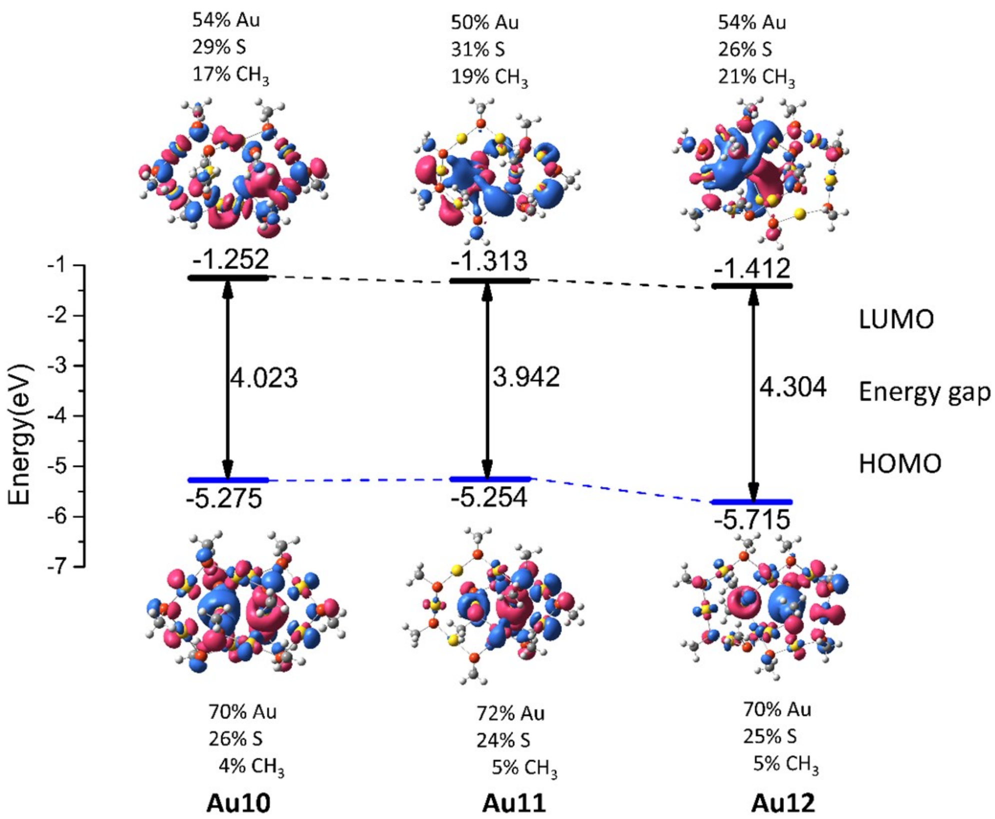


Fig S9 Calculated frontier molecular orbitals of Au···Au interlocking [2]catenanes at their S_0 geometries. (color code: yellow (Au), red (S), gray (C), isoval. =0.020.)

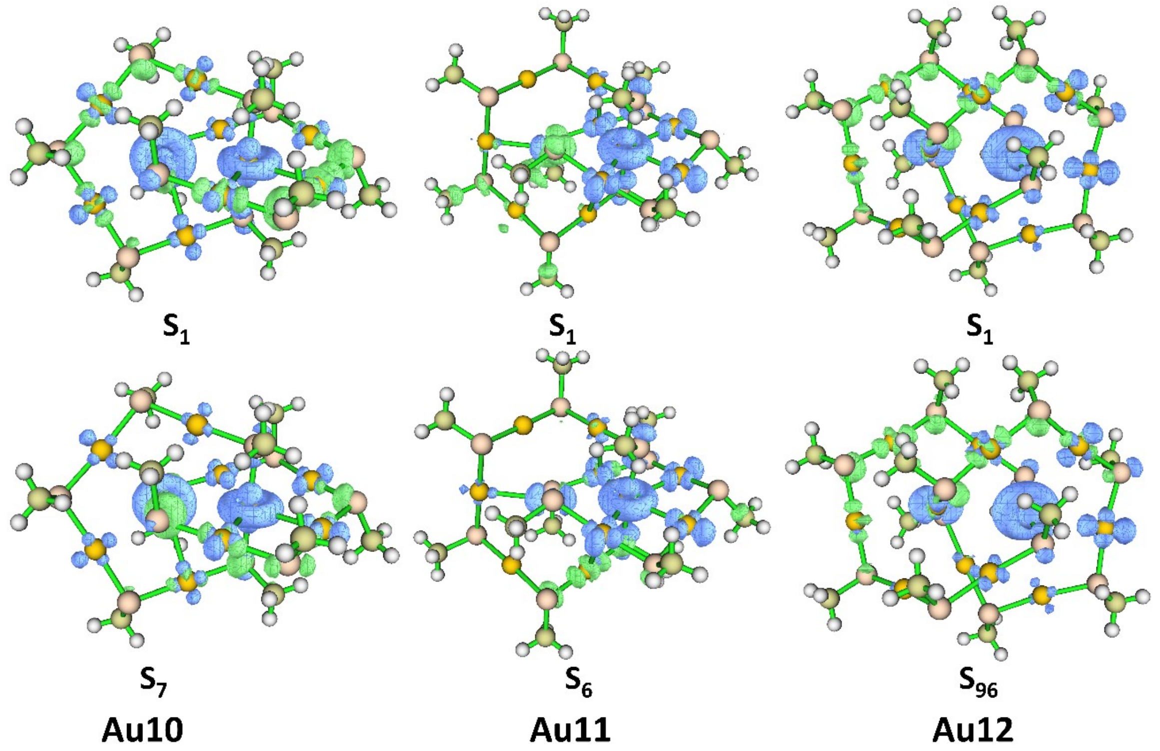


Fig S10 The holes (blue) and electrons (green) of Au···Au interlocking [2]catenanes calculated by TD-DFT/TPSS method. (color code：yellow (Au), pink (S), green (C), white (H), isoval.= 0.002.)

Table S6 H index (Å), t index (Å), D index (Å), S_r index (a.u.), Δσ index (Å) and E_c (eV) obtained by hole-electron analysis of all complexes.

		H^a	t^b	D^c	S_r^d	$\Delta\sigma^e$	E_c^f
Au5Ag5	$S_0 \rightarrow S_1$	3.936	-0.722	1.058	0.55	0.901	3.55
	$S_0 \rightarrow S_{16}$	4.197	-1.370	1.112	0.72	0.377	3.35
Au5Ag6	$S_0 \rightarrow S_1$	3.700	0.297	2.764	0.52	1.010	3.40
	$S_0 \rightarrow S_{12}$	4.184	-0.606	2.068	0.62	1.427	3.19
Au6Ag5	$S_0 \rightarrow S_1$	4.164	1.534	4.276	0.41	1.250	2.76
	$S_0 \rightarrow S_{21}$	4.517	-1.019	1.088	0.60	1.507	3.09
Au6Ag6	$S_0 \rightarrow S_1$	3.576	1.784	4.165	0.45	0.535	3.05
	$S_0 \rightarrow S_{34}$	4.450	-1.859	0.956	0.68	0.795	3.17
Au5Cu5	$S_0 \rightarrow S_1$	3.752	0.850	3.447	0.43	1.027	3.30
	$S_0 \rightarrow S_{27}$	3.989	-1.244	1.545	0.64	0.918	3.44
Au5Cu6	$S_0 \rightarrow S_1$	3.889	-1.354	1.091	0.52	1.454	3.50
	$S_0 \rightarrow S_7$	4.048	-2.054	0.955	0.63	1.347	3.46
Au6Cu5	$S_0 \rightarrow S_1$	3.783	2.242	4.685	0.37	1.237	2.79
	$S_0 \rightarrow S_7$	3.951	0.327	2.861	0.53	1.417	3.19
Au6Cu6	$S_0 \rightarrow S_1$	3.357	-0.682	1.355	0.48	0.875	4.08
	$S_0 \rightarrow S_{36}$	4.097	-1.842	0.383	0.62	0.664	3.51
Au10	$S_0 \rightarrow S_1$	4.065	-1.401	1.067	0.60	1.230	3.50
	$S_0 \rightarrow S_7$	3.811	-1.451	0.675	0.72	0.588	3.74
Au11	$S_0 \rightarrow S_1$	3.846	0.574	3.181	0.55	0.945	3.21
	$S_0 \rightarrow S_6$	4.012	-1.887	0.694	0.59	1.146	3.50
Au12	$S_0 \rightarrow S_1$	4.065	-0.004	2.844	0.55	0.773	3.24
	$S_0 \rightarrow S_{96}$	4.555	-2.131	0.459	0.71	1.352	3.12

[a] H index is the RMSD of the hole and electron distribution.
[b] t index represents the separation degree between holes and electrons, t > 0 indicates that the holes and electrons are separated sufficient due to CT, and t < 0 indicates the opposite.
[c] D index is the distance between centroid of hole and centroid of hole
[d] S_r index is the integral of S_r function. It can be used to measure the overlap degree between holes and electrons with the range of [0,1], where 1 represents complete coincidence of holes and electrons, and 0 represents no overlap.
[e] Δσ index is the difference between RMSD of holes and electrons.
[f] E_c is the coulomb attractive energy between electrons and holes, namely the exciton binding energy caused by the opposite electrical properties.

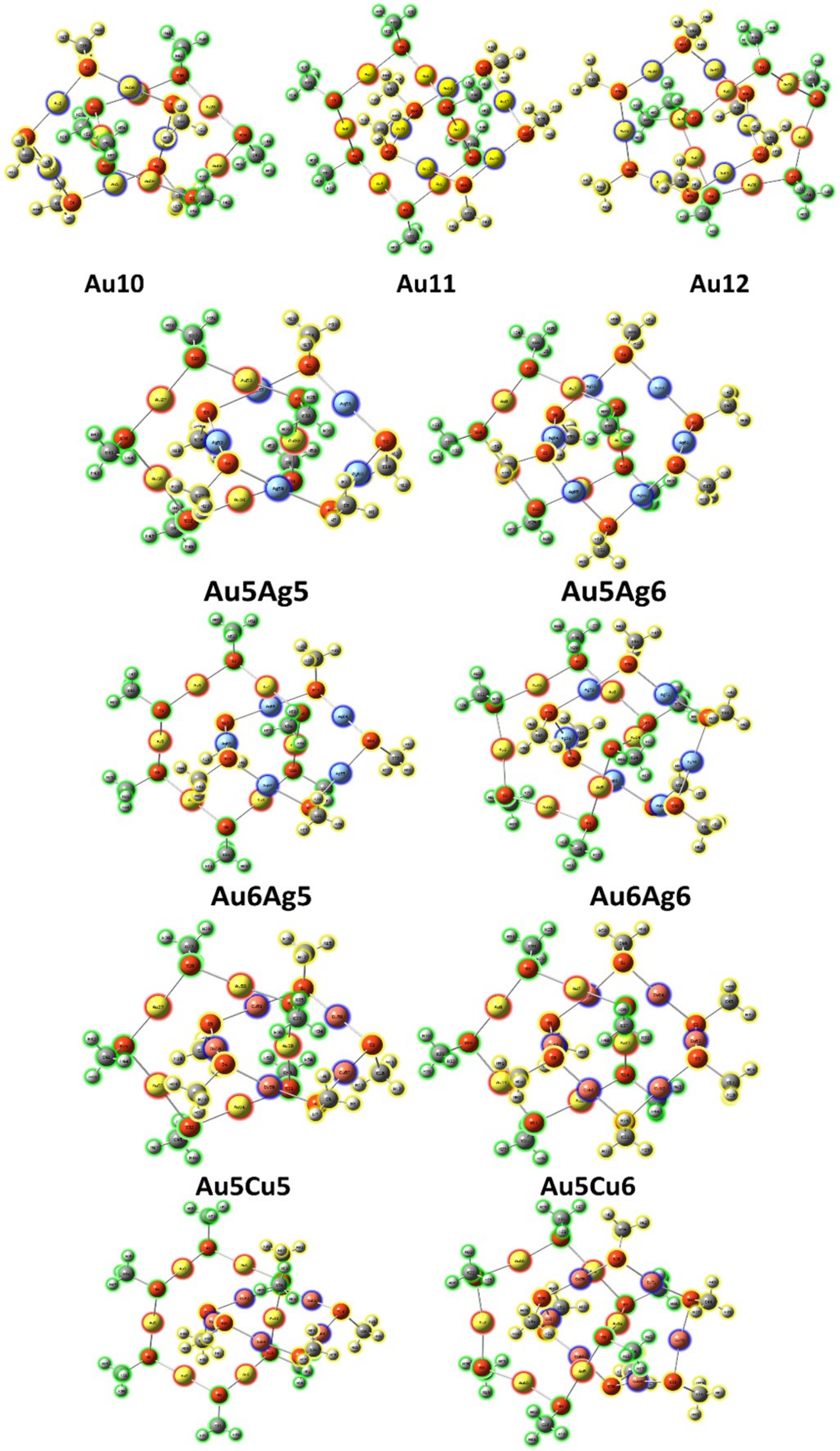


Fig S11 The atoms contained in the four fragments in the molecule during IFCT analysis (Partition color code: red (fragment 1)，green (fragment 2)，blue (fragment 3)，yellow (fragment 4).

Table S7 Information of the orbitals contributing more than 1% to the hole or electron in the main transition process of the complex. ("2" means occupied orbital with two electrons, ("0" means unoccupied orbital with no electron.)

complexes	excitation process	molecular orbital	occupancy	hole	electron
Au10	$S_0 \rightarrow S_1$	220	2	98.94%	0.00%
		221	0	0.00%	96.72%
		222	0	0.00%	2.33%
	$S_0 \rightarrow S_7$	219	2	15.78%	0.00%
		220	2	82.06%	0.00%
		222	0	0.00%	13.99%
		223	0	0.00%	1.22%
		224	0	0.00%	1.10%
		225	0	0.00%	1.02%
		226	0	0.00%	71.74%
		227	0	0.00%	4.29%
		228	0	0.00%	4.92%
Au11	$S_0 \rightarrow S_1$	242	2	98.89%	0.00%
		243	0	0.00%	91.49%
		244	0	0.00%	6.79%
	$S_0 \rightarrow S_6$	241	2	1.10%	0.00%
		242	2	97.83%	0.00%
		244	0	0.00%	1.40%
		245	0	0.00%	1.53%
		247	0	0.00%	9.24%
		248	0	0.00%	1.20%
		249	0	0.00%	84.75%
Au12	$S_0 \rightarrow S_1$	263	2	1.66%	0.00%
		264	2	97.48%	0.00%
		265	0	0.00%	83.13%
		266	0	0.00%	15.72%
	$S_0 \rightarrow S_{96}$	248	2	3.77%	0.00%
		249	2	2.42%	0.00%
		251	2	1.33%	0.00%
		256	2	8.64%	0.00%
		257	2	1.70%	0.00%
		258	2	8.72%	0.00%
		259	2	4.13%	0.00%
		261	2	3.28%	0.00%
		262	2	50.47%	0.00%
		263	2	6.13%	0.00%
		264	2	5.22%	0.00%
		265	0	0.00%	3.48%
		266	0	0.00%	4.36%
		267	0	0.00%	1.15%
		269	0	0.00%	2.49%
		270	0	0.00%	8.74%

		271	0	0.00%	12.43%
		272	0	0.00%	1.14%
		273	0	0.00%	50.53%
		274	0	0.00%	3.14%
		275	0	0.00%	5.75%
		279	0	0.00%	4.29%
Au5Ag5	$S_0 \rightarrow S_1$	219	2	1.17%	0.00%
		220	2	98.20%	0.00%
		221	0	0.00%	98.42%
	$S_0 \rightarrow S_{16}$	215	2	1.81%	0.00%
		217	2	16.57%	0.00%
		218	2	42.97%	0.00%
		219	2	20.62%	0.00%
		220	2	15.75%	0.00%
		221	0	0.00%	16.72%
		222	0	0.00%	43.77%
		224	0	0.00%	3.08%
		225	0	0.00%	1.95%
		226	0	0.00%	20.00%
		227	0	0.00%	7.96%
		228	0	0.00%	4.09%
Au5Ag6	$S_0 \rightarrow S_1$	242	2	99.15%	0.00%
		243	0	0.00%	97.23%
		245	0	0.00%	1.58%
	$S_0 \rightarrow S_{12}$	239	2	1.02%	0.00%
		240	2	22.89%	0.00%
		242	2	74.20%	0.00%
		243	0	0.00%	2.28%
		244	0	0.00%	21.96%
		249	0	0.00%	4.62%
		250	0	0.00%	57.64%
		251	0	0.00%	9.96%
Au6Ag5	$S_0 \rightarrow S_1$	242	2	98.86%	0.00%
		243	0	0.00%	97.50%
	$S_0 \rightarrow S_{21}$	238	2	1.75%	0.00%
		239	2	1.06%	0.00%
		240	2	9.80%	0.00%
		241	2	49.36%	0.00%
		242	2	37.24%	0.00%
		243	0	0.00%	2.32%
		245	0	0.00%	2.79%
		246	0	0.00%	3.82%
		247	0	0.00%	5.56%
		248	0	0.00%	47.23%
		250	0	0.00%	1.19%
		251	0	0.00%	36.11%
Au6Ag6	$S_0 \rightarrow S_1$	263	2	2.13%	0.00%
		264	2	96.03%	0.00%

		265	0	0.00%	97.39%
		266	0	0.00%	1.70%
	$S_0 \rightarrow S_{34}$	253	2	2.91%	0.00%
		254	2	2.34%	0.00%
		258	2	2.78%	0.00%
		259	2	3.54%	0.00%
		260	2	6.02%	0.00%
		261	2	2.02%	0.00%
		262	2	21.83%	0.00%
		263	2	53.08%	0.00%
		264	2	3.02%	0.00%
		265	0	0.00%	6.36%
		266	0	0.00%	7.81%
		267	0	0.00%	5.84%
		269	0	0.00%	3.61%
		270	0	0.00%	29.85%
		271	0	0.00%	41.27%
		272	0	0.00%	3.46%
Au5Cu5	$S_0 \rightarrow S_1$	220	2	99.14%	0.00%
		221	0	0.00%	97.82%
	$S_0 \rightarrow S_{27}$	214	2	2.68%	0.00%
		215	2	1.08%	0.00%
		216	2	23.17%	0.00%
		217	2	30.94%	0.00%
		218	2	1.94%	0.00%
		219	2	26.73%	0.00%
		220	2	12.23%	0.00%
		221	0	0.00%	2.57%
		222	0	0.00%	25.61%
		223	0	0.00%	3.02%
		224	0	0.00%	28.85%
		225	0	0.00%	3.49%
		226	0	0.00%	15.46%
		227	0	0.00%	7.93%
		228	0	0.00%	1.61%
		229	0	0.00%	8.93%
		232	0	0.00%	1.15%
Au5Cu6	$S_0 \rightarrow S_1$	242	2	98.73%	0.00%
		243	0	0.00%	98.59%
	$S_0 \rightarrow S_7$	239	2	2.06%	0.00%
		240	2	4.95%	0.00%
		241	2	3.34%	0.00%
		242	2	86.45%	0.00%
		243	0	0.00%	3.93%
		244	0	0.00%	7.65%
		245	0	0.00%	2.98%
		246	0	0.00%	9.06%
		247	0	0.00%	71.87%

		250	0	0.00%	2.82%
Au6Cu5	$S_0 \rightarrow S_1$	242	2	99.36%	0.00%
		243	0	0.00%	97.84%
		244	0	0.00%	1.07%
	$S_0 \rightarrow S_7$	238	2	1.73%	0.00%
		240	2	79.65%	0.00%
		242	2	17.18%	0.00%
		243	0	0.00%	80.63%
		248	0	0.00%	15.98%
Au6Cu6	$S_0 \rightarrow S_1$	262	2	2.28%	0.00%
		264	2	96.41%	0.00%
		265	0	0.00%	99.02%
	$S_0 \rightarrow S_{36}$	250	2	2.94%	0.00%
		253	2	1.70%	0.00%
		254	2	9.33%	0.00%
		255	2	2.66%	0.00%
		258	2	2.70%	0.00%
		259	2	10.48%	0.00%
		260	2	42.40%	0.00%
		261	2	1.24%	0.00%
		262	2	7.58%	0.00%
		263	2	3.04%	0.00%
		264	2	13.61%	0.00%
		265	0	0.00%	18.12%
		266	0	0.00%	9.96%
		267	0	0.00%	1.98%
		268	0	0.00%	44.69%
		269	0	0.00%	8.56%
		270	0	0.00%	1.75%
		271	0	0.00%	6.65%
		272	0	0.00%	4.72%
		273	0	0.00%	3.03%

Table S8 The results of IFCT analysis of Au···Ag interlocking [2]catenanes.

complexes		Au5Ag5		Au5Ag6		Au6Ag5		Au6Ag6	
excitation process		$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{16}$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{12}$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{21}$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{34}$
intrafragment electron redistribution of fragment 1		0.090	0.044	0.095	0.060	0.088	0.056	0.066	0.039
intrafragment electron redistribution of fragment 2		0.038	0.018	0.019	0.009	0.017	0.012	0.024	0.021
intrafragment electron redistribution of fragment 3		0.043	0.077	0.063	0.097	0.029	0.075	0.094	0.094
intrafragment electron redistribution of fragment 4		0.049	0.096	0.048	0.087	0.035	0.070	0.064	0.099
transferred electrons between fragments	Net 1 -> 2	0.056	0.027	0.029	0.009	0.018	0.020	0.033	0.021
	Net 1 -> 3	-0.086	-0.059	-0.055	-0.008	-0.116	-0.076	-0.049	-0.049
	Net 1 -> 4	-0.065	-0.080	-0.045	0.006	-0.105	-0.059	-0.023	-0.044
	Net 2 -> 3	-0.108	-0.083	-0.051	-0.015	-0.067	-0.063	-0.074	-0.074
	Net 2 -> 4	-0.093	-0.105	-0.043	-0.008	-0.062	-0.053	-0.048	-0.071
	Net 3 -> 4	0.016	-0.017	0.002	0.018	0.010	0.015	0.021	0.009

Table S9 The results of IFCT analysis of Au···Cu interlocking [2]catenanes.

complexes		**Au5Cu5**		**Au5Cu6**		**Au6Cu5**		**Au6Cu6**	
excitation process		$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{27}$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_7$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_7$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{36}$
intrafragment electron redistribution of fragment 1		0.094	0.029	0.092	0.055	0.070	0.047	0.013	0.018
intrafragment electron redistribution of fragment 2		0.042	0.013	0.032	0.017	0.024	0.013	0.005	0.010
intrafragment electron redistribution of fragment 3		0.026	0.129	0.060	0.138	0.071	0.078	0.177	0.141
intrafragment electron redistribution of fragment 4		0.017	0.049	0.019	0.047	0.026	0.024	0.066	0.058
transferred electrons between fragments	Net 1 -> 2	0.048	0.021	0.044	0.019	0.029	0.024	0.004	0.008
	Net 1 -> 3	-0.205	-0.148	-0.188	-0.092	-0.159	-0.210	-0.168	-0.163
	Net 1 -> 4	-0.061	-0.033	-0.035	0.011	-0.048	-0.055	-0.072	-0.048
	Net 2 -> 3	-0.205	-0.181	-0.177	-0.087	-0.142	-0.184	-0.130	-0.168
	Net 2 -> 4	-0.069	-0.054	-0.044	-0.011	-0.050	-0.054	-0.057	-0.055
	Net 3 -> 4	0.036	0.100	0.048	0.107	0.038	0.053	0.065	0.101

Table S10 The results of IFCT analysis of Au···Au interlocking [2]catenanes.

		Au10		Au11		Au12	
excitation process		$S_0 \rightarrow S_1$	$S_0 \rightarrow S_7$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_6$	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_{96}$
intrafragment electron redistribution of fragment 1		0.085	0.109	0.086	0.088	0.092	0.059
intrafragment electron redistribution of fragment 2		0.037	0.050	0.011	0.011	0.036	0.051
intrafragment electron redistribution of fragment 3		0.085	0.061	0.094	0.087	0.084	0.079
intrafragment electron redistribution of fragment 4		0.038	0.024	0.035	0.033	0.032	0.055
transferred electrons between fragments	Net 1 -> 2	0.062	0.084	0.029	0.027	0.065	0.029
	Net 1 -> 3	-0.004	-0.046	-0.029	-0.034	-0.019	-0.036
	Net 1 -> 4	0.056	0.019	0.033	0.030	0.057	-0.002
	Net 2 -> 3	-0.064	-0.102	-0.043	-0.041	-0.077	-0.069
	Net 2 -> 4	-0.004	-0.025	-0.006	-0.006	-0.002	-0.029
	Net 3 -> 4	0.059	0.037	0.055	0.052	0.068	0.033

Table S11 The contribution percentage of four fragments to holes and electrons in each molecule.

		Au10		**Au11**		**Au12**		**Au5Ag5**		**Au5Ag6**		**Au6Ag5**		**Au6Ag6**		**Au5Cu5**		**Au5Cu6**		**Au6Cu5**		**Au6Cu6**	
		S_1	S_7	S_1	S_6	S_1	S_{96}	S_1	S_{16}	S_1	S_{12}	S_1	S_{21}	S_1	S_{34}	S_1	S_{27}	S_1	S_7	S_1	S_7	S_1	S_{36}
1	hole	35.38%	35.98%	31.87%	32.32%	35.93%	23.90%	25.57%	16.09%	28.31%	25.74%	22.68%	19.42%	23.76%	16.49%	21.57%	10.84%	22.73%	20.48%	19.29%	13.07%	4.74%	6.74%
	electron	23.97%	30.21%	26.88%	27.25%	25.60%	24.77%	35.07%	27.22%	33.56%	23.34%	38.68%	28.97%	27.62%	23.68%	43.41%	26.82%	40.63%	26.68%	36.06%	36.35%	28.36%	27.11%
2	hole	13.90%	14.18%	7.42%	7.29%	13.10%	17.10%	10.41%	6.56%	9.19%	8.13%	7.72%	6.00%	9.58%	8.33%	9.95%	4.48%	9.03%	8.26%	7.91%	4.15%	2.13%	3.86%
	electron	26.86%	35.36%	15.38%	14.61%	27.46%	29.77%	36.05%	28.10%	21.13%	10.84%	21.12%	19.15%	25.07%	24.95%	42.13%	30.00%	35.63%	20.02%	29.80%	30.28%	21.24%	26.95%
3	hole	36.11%	35.75%	39.27%	38.87%	38.32%	35.74%	33.66%	34.72%	32.54%	34.53%	34.93%	38.99%	38.62%	37.89%	49.88%	63.29%	52.64%	54.20%	51.36%	62.42%	63.99%	65.59%
	electron	23.46%	17.20%	24.00%	22.34%	21.94%	22.01%	12.72%	22.20%	19.26%	28.15%	8.23%	19.16%	24.33%	24.72%	5.22%	20.44%	11.31%	25.51%	13.77%	12.56%	27.63%	21.45%
4	hole	14.62%	14.09%	15.04%	14.93%	12.66%	23.26%	30.36%	42.63%	27.81%	29.62%	33.40%	34.16%	28.05%	37.30%	18.60%	21.39%	15.60%	17.06%	20.22%	19.55%	29.13%	23.81%
	electron	25.72%	17.23%	23.08%	21.95%	25.00%	23.45%	16.16%	22.47%	17.10%	29.29%	10.59%	20.63%	22.98%	26.66%	9.25%	22.73%	12.43%	27.80%	12.85%	12.41%	22.78%	24.49%