Electronic Supplementary Information for:

Conducting neutral gold bisdithiolene complex $[Au(dspdt)_2]^{\bullet}$

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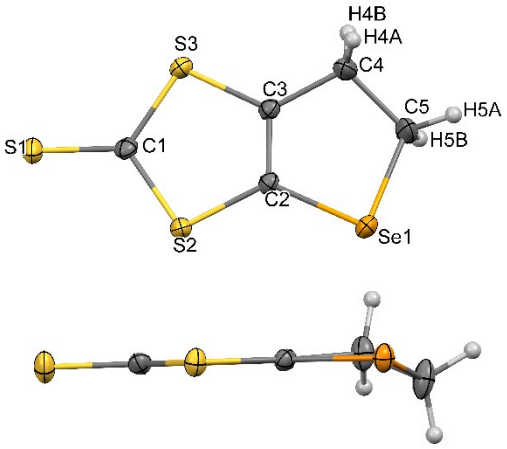


Fig. S1**.** ORTEP view and atomic numbering scheme of **1** with thermal ellipsoids at 50% probability level.

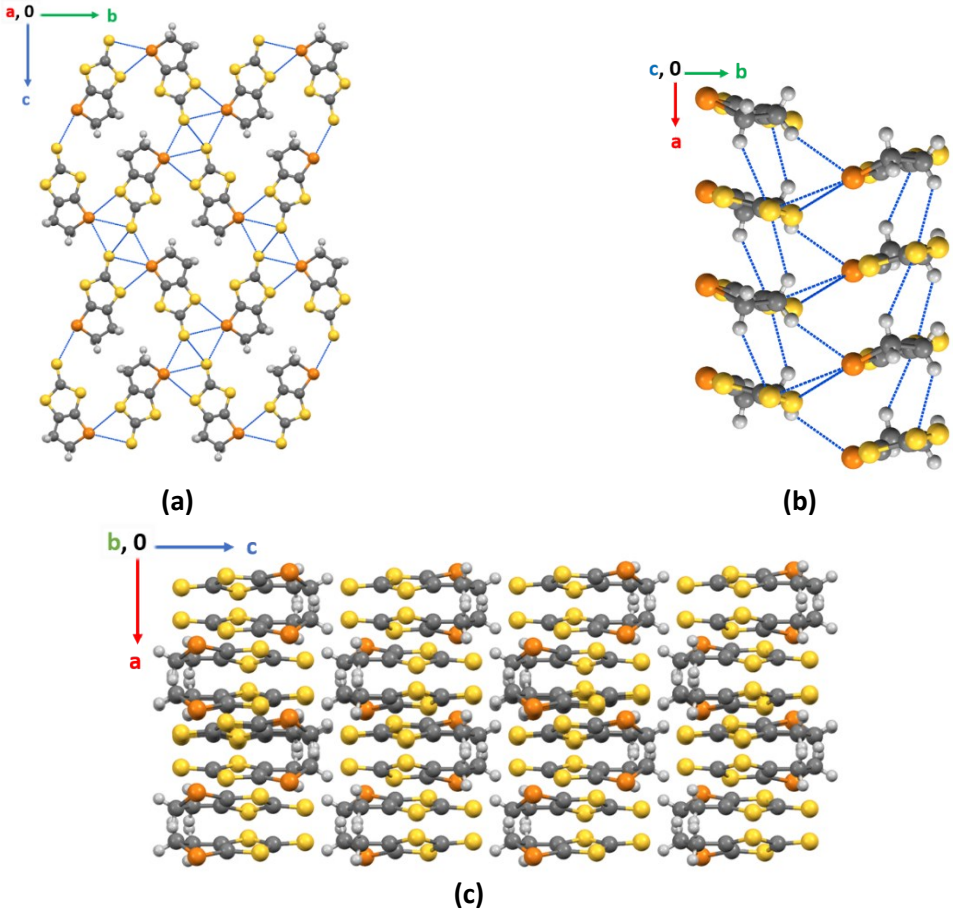


Fig. S2. Crystal structure of **1** viewed along *a*, *b*, and *c*.

Table S1. Bond lengths and angles for **1**.

Bond	Length (Å)	Angle	Amplitude (deg.)
Se(1)-C(2)	1.904(2)	C(2)-Se(1)-C(5)	85.25(9)
Se(1)-C(5)	1.984(2)	C(2)-S(2)-C(1)	96.28(10)
S(1)-C(1)	1.646(2)	C(3)-S(3)-C(1)	97.10(10)
S(2)-C(2)	1.729(2)	S(1)-C(1)-S(3)	124.17(14)
S(2)-C(1)	1.747(2)	S(1)-C(1)-S(2)	122.91(13)
S(3)-C(3)	1.735(2)	S(3)-C(1)-S(2)	112.91(11)
S(3)-C(1)	1.736(2)	C(3)-C(2)-S(2)	117.70(16)
C(2)-C(3)	1.338(3)	C(3)-C(2)-Se(1)	114.61(15)
C(3)-C(4)	1.505(3)	S(2)-C(2)-Se(1)	127.67(13)
C(4)-C(5)	1.528(3)	C(2)-C(3)-C(4)	117.76(19)
C(4)-H(4A)	0.99	C(2)-C(3)-S(3)	116.01(15)
C(4)-H(4B)	0.99	C(4)-C(3)-S(3)	126.13(17)
C(5)-H(5A)	0.99	C(3)-C(4)-C(5)	106.86(19)
C(5)-H(5B)	0.99	C(3)-C(4)-H(4A)	110.4
		C(5)-C(4)-H(4A)	110.4
		C(3)-C(4)-H(4B)	110.4
		C(5)-C(4)-H(4B)	110.4
		H(4A)-C(4)-H(4B)	108.6
		C(4)-C(5)-Se(1)	108.48(14)
		C(4)-C(5)-H(5A)	110
		Se(1)-C(5)-H(5A)	110
		C(4)-C(5)-H(5B)	110
		Se(1)-C(5)-H(5B)	110
		H(5A)-C(5)-H(5B)	108.4

Table S2. Short contacts and hydrogen bonds in **1**.

Contact	Length	Symm. op.*
H4B···S1	2.957	x,y,z
H4B···Se1	3.067	x,y,z
Se1···S1	3.484	x,y,z
S1···H4A	2.925	x,y,z
H5B···S1	3.035	x,y,z
Se1···S3	3.551	1/2+x,1/2-y,1-z
S1···S1	3.508	1/2-x,1-y,1/2+z

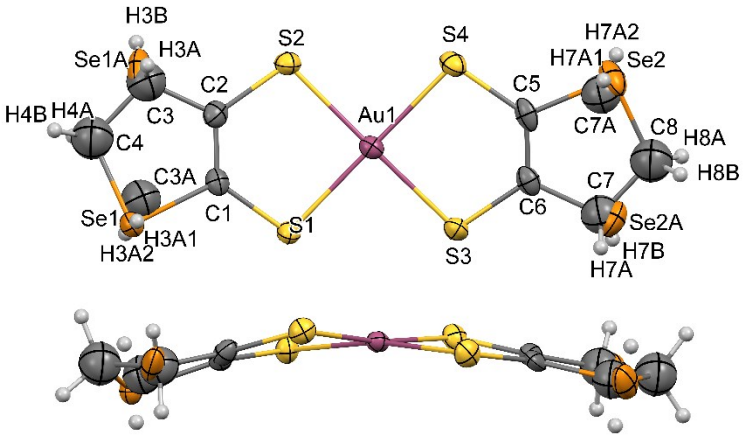


Fig. S3. ORTEP view and atomic numbering scheme of the anionic complex of **2a**, with thermal ellipsoids at 50% probability level.

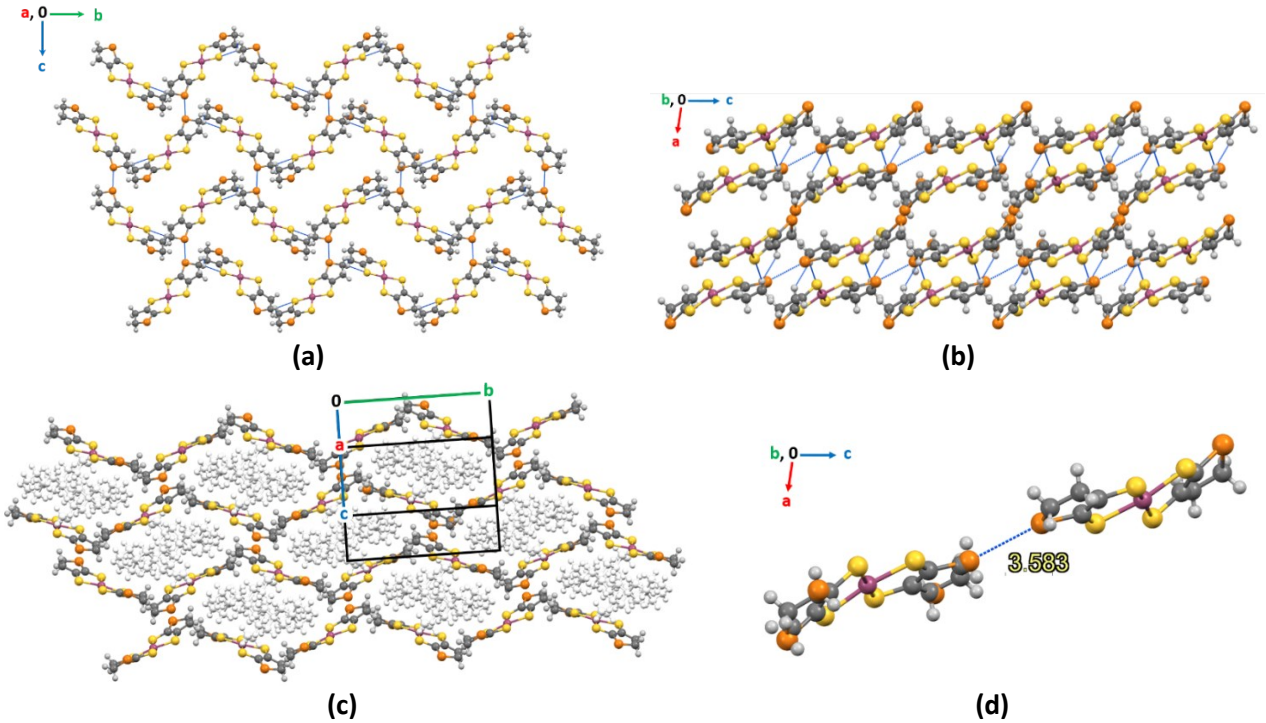


Fig. S4. Views of the crystal structure of **2a**. Partial views along *a*, and *b* with cations omitted for clarity in (a) and (b). (c) Detail showing the complex anions surrounding two cation molecules. (d) Detail of short Se···Se contacts between anions.

Table S3. Bond lengths for **2a**.

Anionic Gold Complex		Tetrabutylammonium Cation			
Bond	**Length (Å)**	**Bond**	**Length (Å)**	**Bond**	**Length (Å)**
Au(1)-S(4)	2.3199(13)	**N(1)-C(9)**	1.507(6)	**C(16)-H(16C)**	0.98
Au(1)-S(2)	2.3224(12)	**N(1)-C(17)**	1.511(6)	**C(17)-C(18)**	1.512(7)
Au(1)-S(3)	2.3233(12)	**N(1)-C(13)**	1.519(6)	**C(17)-H(17A)**	0.99
Au(1)-S(1)	2.3266(13)	**N(1)-C(21)**	1.521(6)	**C(17)-H(17B)**	0.99
Se(1)-C(4)	1.888(7)	**C(9)-C(10)**	1.521(7)	**C(18)-C(19)**	1.530(7)
Se(1)-C(1)	1.941(5)	**C(9)-H(9A)**	0.99	**C(18)-H(18A)**	0.99
C(3)-C(4)	1.535(19)	**C(9)-H(9B)**	0.99	**C(18)-H(18B)**	0.99
C(3)-C(2)	1.546(17)	**C(10)-C(11)**	1.534(7)	**C(19)-C(20)**	1.503(8)
C(3)-H(3A)	0.99	**C(10)-H(10A)**	0.99	**C(19)-H(19A)**	0.99
C(3)-H(3B)	0.99	**C(10)-H(10B)**	0.99	**C(19)-H(19B)**	0.99
Se(1A)-C(4)	1.646(12)	**C(11)-H(11A)**	0.99	**C(20)-H(20A)**	0.98
Se(1A)-C(2)	1.785(10)	**C(11)-H(11B)**	0.99	**C(20)-H(20B)**	0.98
C(3A)-C(1)	1.56(5)	**C(12)-H(12A)**	0.98	**C(20)-H(20C)**	0.98
C(3A)-C(4)	1.535(19)	**C(12)-H(12B)**	0.98	**C(21)-C(22)**	1.522(6)
C(3A)-H(3A1)	0.99	**C(12)-H(12C)**	0.98	**C(21)-H(21A)**	0.99
C(3A)-H(3A2)	0.99	**C(13)-C(14)**	1.519(6)	**C(21)-H(21B)**	0.99
Se(2)-C(8)	1.816(7)	**C(13)-H(13A)**	0.99	**C(22)-C(23)**	1.527(7)
Se(2)-C(5)	1.894(5)	**C(13)-H(13B)**	0.99	**C(22)-H(22A)**	0.99
C(7)-C(8)	1.47(2)	**C(14)-C(15)**	1.532(7)	**C(22)-H(22B)**	0.99
C(7)-C(6)	1.568(19)	**C(14)-H(14A)**	0.99	**C(23)-C(24)**	1.508(7)
C(7)-H(7A)	0.99	**C(14)-H(14B)**	0.99	**C(23)-H(23A)**	0.99
C(7)-H(7B)	0.99	**C(15)-C(16)**	1.516(7)	**C(23)-H(23B)**	0.99
Se(2A)-C(8)	1.383(10)	**C(15)-H(15A)**	0.99	**C(11)-C(12)**	1.493(8)
Se(2A)-C(6)	1.819(9)	**C(15)-H(15B)**	0.99	**C(24)-H(24A)**	0.98
C(7A)-C(5)	1.568(19)	**C(16)-H(16A)**	0.98	**C(24)-H(24B)**	0.98
C(7A)-C(8)	1.656(19)	**C(16)-H(16B)**	0.98	**C(24)-H(24C)**	0.98
C(7A)-H(7A1)	0.99				
C(7A)-H(7A2)	0.99				
S(1)-C(1)	1.752(5)				
S(2)-C(2)	1.757(5)				
S(3)-C(6)	1.758(5)				
S(4)-C(5)	1.745(5)				
C(1)-C(2)	1.323(7)				
C(4)-H(4A)	0.99				
C(4)-H(4B)	0.99				
C(5)-C(6)	1.325(7)				
C(8)-H(8A)	0.99				
C(8)-H(8B)	0.99				

Table S4. Bond angles for the anionic gold complex in **2a**.

Anionic Gold Complex			
Angle	**Amplitude (deg.)**	**Angle**	**Amplitude (deg.)**
S(4)-Au(1)-S(2)	89.41(5)	**C(6)-S(3)-Au(1)**	99.97(18)
S(4)-Au(1)-S(3)	90.80(5)	**C(5)-S(4)-Au(1)**	99.74(18)
S(2)-Au(1)-S(3)	172.64(5)	**C(2)-C(1)-C(3A)**	101.2(12)
S(4)-Au(1)-S(1)	170.49(5)	**C(2)-C(1)-S(1)**	126.0(4)
S(2)-Au(1)-S(1)	90.75(4)	**C(3A)-C(1)-S(1)**	132.6(12)
S(3)-Au(1)-S(1)	90.25(4)	**C(2)-C(1)-Se(1)**	113.8(4)
C(4)-Se(1)-C(1)	85.8(3)	**S(1)-C(1)-Se(1)**	120.0(3)
C(4)-C(3)-C(2)	106.5(12)	**C(1)-C(2)-C(3)**	115.9(9)
C(4)-C(3)-H(3A)	110.4	**C(1)-C(2)-S(2)**	122.9(4)
C(2)-C(3)-H(3A)	110.4	**C(3)-C(2)-S(2)**	121.2(8)
C(4)-C(3)-H(3B)	110.4	**C(1)-C(2)-Se(1A)**	121.7(5)
C(2)-C(3)-H(3B)	110.4	**S(2)-C(2)-Se(1A)**	115.4(4)
H(3A)-C(3)-H(3B)	108.6	**C(3A)-C(4)-Se(1A)**	107(2)
C(4)-Se(1A)-C(2)	92.0(6)	**C(3)-C(4)-Se(1)**	109.9(8)
C(1)-C(3A)-C(4)	115(3)	**C(3)-C(4)-H(4A)**	109.7
C(1)-C(3A)-H(3A1)	108.6	**Se(1)-C(4)-H(4A)**	109.7
C(4)-C(3A)-H(3A1)	108.6	**C(3)-C(4)-H(4B)**	109.7
C(1)-C(3A)-H(3A2)	108.6	**Se(1)-C(4)-H(4B)**	109.7
C(4)-C(3A)-H(3A2)	108.6	**H(4A)-C(4)-H(4B)**	108.2
H(3A1)-C(3A)-H(3A2)	107.6	**C(6)-C(5)-C(7A)**	105.9(9)
C(8)-Se(2)-C(5)	89.6(3)	**C(6)-C(5)-S(4)**	125.3(4)
C(8)-C(7)-C(6)	109.3(13)	**C(7A)-C(5)-S(4)**	128.7(9)
C(8)-C(7)-H(7A)	109.8	**C(6)-C(5)-Se(2)**	113.0(4)
C(6)-C(7)-H(7A)	109.8	**S(4)-C(5)-Se(2)**	121.6(3)
C(8)-C(7)-H(7B)	109.8	**C(5)-C(6)-C(7)**	114.6(9)
C(6)-C(7)-H(7B)	109.8	**C(5)-C(6)-S(3)**	123.6(4)
H(7A)-C(7)-H(7B)	108.3	**C(7)-C(6)-S(3)**	121.8(9)
C(8)-Se(2A)-C(6)	100.4(5)	**C(5)-C(6)-Se(2A)**	113.8(4)
C(5)-C(7A)-C(8)	108.3(14)	**S(3)-C(6)-Se(2A)**	122.5(4)
C(5)-C(7A)-H(7A1)	110	**Se(2A)-C(8)-C(7A)**	110.0(10)
C(8)-C(7A)-H(7A1)	110	**C(7)-C(8)-Se(2)**	112.6(9)
C(5)-C(7A)-H(7A2)	110	**C(7)-C(8)-H(8A)**	109.1
C(8)-C(7A)-H(7A2)	110	**Se(2)-C(8)-H(8A)**	109.1
H(7A1)-C(7A)-H(7A2)	108.4	**C(7)-C(8)-H(8B)**	109.1
C(1)-S(1)-Au(1)	98.62(17)	**Se(2)-C(8)-H(8B)**	109.1
C(2)-S(2)-Au(1)	99.86(17)	**H(8A)-C(8)-H(8B)**	107.8

Table S5. Bond angles for the tetrabutylammonium cation in **2a**.

Tetrabutylammonium Cation					
Angle	**Amplitude (deg.)**	**Angle**	**Amplitude (deg.)**	**Angle**	**Amplitude (deg.)**
C(9)-N(1)-C(17)	111.8(3)	**H(13A)-C(13)-H(13B)**	107.1	**C(20)-C(19)-H(19B)**	109
C(9)-N(1)-C(13)	112.4(4)	**C(13)-C(14)-C(15)**	107.9(4)	**C(18)-C(19)-H(19B)**	109
C(17)-N(1)-C(13)	104.7(3)	**C(13)-C(14)-H(14A)**	110.1	**H(19A)-C(19)-H(19B)**	107.8
C(9)-N(1)-C(21)	104.3(3)	**C(15)-C(14)-H(14A)**	110.1	**C(19)-C(20)-H(20A)**	109.5
C(17)-N(1)-C(21)	112.6(4)	**C(13)-C(14)-H(14B)**	110.1	**C(19)-C(20)-H(20B)**	109.5
C(13)-N(1)-C(21)	111.2(3)	**C(15)-C(14)-H(14B)**	110.1	**H(20A)-C(20)-H(20B)**	109.5
N(1)-C(9)-C(10)	115.5(4)	**H(14A)-C(14)-H(14B)**	108.4	**C(19)-C(20)-H(20C)**	109.5
N(1)-C(9)-H(9A)	108.4	**C(16)-C(15)-C(14)**	113.7(4)	**H(20A)-C(20)-H(20C)**	109.5
C(10)-C(9)-H(9A)	108.4	**C(16)-C(15)-H(15A)**	108.8	**H(20B)-C(20)-H(20C)**	109.5
N(1)-C(9)-H(9B)	108.4	**C(14)-C(15)-H(15A)**	108.8	**C(22)-C(21)-N(1)**	117.4(4)
C(10)-C(9)-H(9B)	108.4	**C(16)-C(15)-H(15B)**	108.8	**C(22)-C(21)-H(21A)**	107.9
H(9A)-C(9)-H(9B)	107.5	**C(14)-C(15)-H(15B)**	108.8	**N(1)-C(21)-H(21A)**	107.9
C(9)-C(10)-C(11)	110.6(4)	**H(15A)-C(15)-H(15B)**	107.7	**C(22)-C(21)-H(21B)**	107.9
C(9)-C(10)-H(10A)	109.5	**C(15)-C(16)-H(16A)**	109.5	**N(1)-C(21)-H(21B)**	107.9
C(11)-C(10)-H(10A)	109.5	**C(15)-C(16)-H(16B)**	109.5	**H(21A)-C(21)-H(21B)**	107.2
C(9)-C(10)-H(10B)	109.5	**H(16A)-C(16)-H(16B)**	109.5	**C(21)-C(22)-C(23)**	109.9(4)
C(11)-C(10)-H(10B)	109.5	**C(15)-C(16)-H(16C)**	109.5	**C(21)-C(22)-H(22A)**	109.7
H(10A)-C(10)-H(10B)	108.1	**H(16A)-C(16)-H(16C)**	109.5	**C(23)-C(22)-H(22A)**	109.7
C(12)-C(11)-C(10)	113.3(5)	**H(16B)-C(16)-H(16C)**	109.5	**C(21)-C(22)-H(22B)**	109.7
C(12)-C(11)-H(11A)	108.9	**N(1)-C(17)-C(18)**	117.0(4)	**C(23)-C(22)-H(22B)**	109.7
C(10)-C(11)-H(11A)	108.9	**N(1)-C(17)-H(17A)**	108.1	**H(22A)-C(22)-H(22B)**	108.2
C(12)-C(11)-H(11B)	108.9	**C(18)-C(17)-H(17A)**	108.1	**C(24)-C(23)-C(22)**	112.2(4)
C(10)-C(11)-H(11B)	108.9	**N(1)-C(17)-H(17B)**	108.1	**C(24)-C(23)-H(23A)**	109.2
H(11A)-C(11)-H(11B)	107.7	**C(18)-C(17)-H(17B)**	108.1	**C(22)-C(23)-H(23A)**	109.2
C(11)-C(12)-H(12A)	109.5	**H(17A)-C(17)-H(17B)**	107.3	**C(24)-C(23)-H(23B)**	109.2
C(11)-C(12)-H(12B)	109.5	**C(17)-C(18)-C(19)**	109.2(4)	**C(22)-C(23)-H(23B)**	109.2
H(12A)-C(12)-H(12B)	109.5	**C(17)-C(18)-H(18A)**	109.8	**H(23A)-C(23)-H(23B)**	107.9
C(11)-C(12)-H(12C)	109.5	**C(19)-C(18)-H(18A)**	109.8	**C(23)-C(24)-H(24A)**	109.5
H(12A)-C(12)-H(12C)	109.5	**C(17)-C(18)-H(18B)**	109.8	**C(23)-C(24)-H(24B)**	109.5
H(12B)-C(12)-H(12C)	109.5	**C(19)-C(18)-H(18B)**	109.8	**H(24A)-C(24)-H(24B)**	109.5
N(1)-C(13)-C(14)	118.0(4)	**H(18A)-C(18)-H(18B)**	108.3	**C(23)-C(24)-H(24C)**	109.5
N(1)-C(13)-H(13A)	107.8	**C(20)-C(19)-C(18)**	112.8(5)	**H(24A)-C(24)-H(24C)**	109.5
C(14)-C(13)-H(13A)	107.8	**C(20)-C(19)-H(19A)**	109	**H(24B)-C(24)-H(24C)**	109.5
N(1)-C(13)-H(13B)	107.8	**C(18)-C(19)-H(19A)**	109		
C(14)-C(13)-H(13B)	107.8				

Table S6. Short contacts and hydrogen bonds in **2a** (M - metal complex and C - cation).

Contacts	Length	Symm. op.*	Contact Type
Se1···C12*	3.575	x,y,z	M – C
Se1···H12A*	3.199	x,y,z	M – C
S3···H18B*	2.925	x,y,z	M – C
S3···H21B*	3.052	x,y,z	M – C
S3···H23B*	3.093	x,y,z	M – C
H3A···H17A*	2.381	1-x,-1/2+y,1.5-z	M – C
H3A···H22B*	2.331	1-x,-1/2+y,1.5-z	M – C
S1···H24C*	3.088	1-x,-1/2+y,1.5-z	M – C
S2···H13B*	2.961	1-x,-1/2+y,1.5-z	M – C
S2···H22A*	2.966	1-x,-1/2+y,1.5-z	M – C
S4···H15A*	3.085	1-x,-1/2+y,1.5-z	M – C
Se1···H14A*	3.18	1-x,1-y,1-z	M – C
Se1···H21A*	2.996	1-x,1-y,1-z	M – C
S1···H9A*	2.907	1-x,1-y,1-z	M – C
Se1··· H20B	3.056	x,1.5-y,-1/2+z	M – C
H4B··· C20	2.938	x,1.5-y,-1/2+z	M – C
H8A··· H3B	2.45	1-x,1/2+y,1.5-z	M – M
H8A··· S2	3.054	1-x,1/2+y,1.5-z	M – M
Se2··· Se2	3.583	1-x,1-y,2-z	M – M
S3··· H13A	3.097	x,y,z	M – C
S4··· H17B	3.037	x,y,z	M – C
C5··· H17B	2.854	x,y,z	M – C
C6··· H13A	2.937	x,y,z	M – C
H12B··· H15B	2.46	2-x,1-y,1-z	M – C

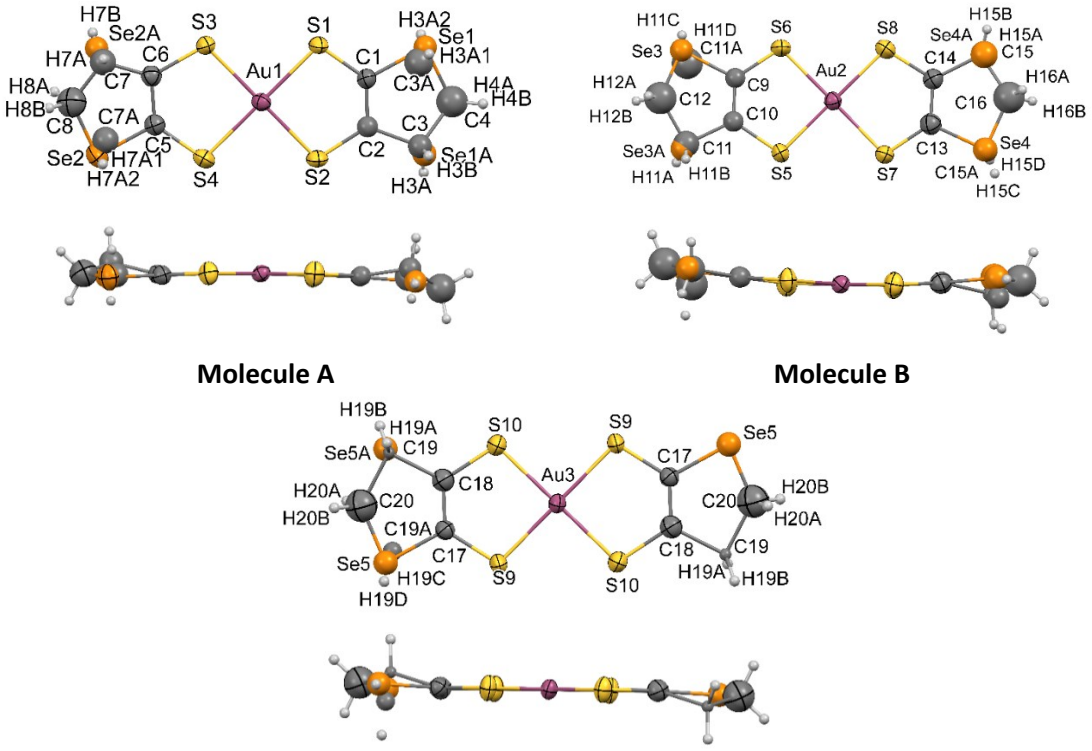


Fig. S5. ORTEP view and atomic numbering scheme of **3** with thermal ellipsoids at 50% probability level.

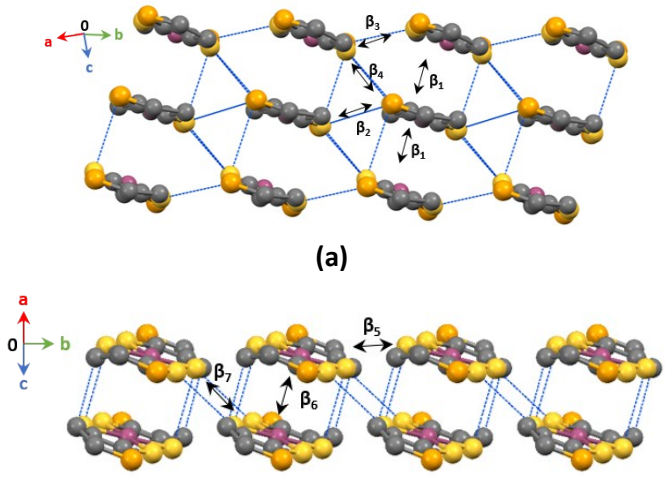


Fig. S6 Detail showing the propagation in **3** of trimers (a) and dimers (b) along the axis *b*.

Table S7. Bond lengths for **3**.

Molecule A		Molecule B		Molecule C	
Bond	**Length (Å)**	**Bond**	**Length (Å)**	**Bond**	**Length (Å)**
Au(1)-S(2)	2.300(12)	**Au(2)-S(7)**	2.288(12)	**Au(3)-S(10)#1**	2.311(12)
Au(1)-S(1)	2.314(12)	**Au(2)-S(6)**	2.291(13)	**Au(3)-S(10)**	2.311(12)
Au(1)-S(4)	2.323(12)	**Au(2)-S(5)**	2.303(13)	**Au(3)-S(9)#1**	2.318(11)
Au(1)-S(3)	2.340(12)	**Au(2)-S(8)**	2.308(13)	**Au(3)-S(9)**	2.318(11)
Se(1)-C(1)	1.84(4)	**Se(3)-C(9)**	1.95(5)	**Se(5)-C(20)**	1.65(9)
Se(1)-C(4)	1.89(2)	**Se(3)-C(12)**	2.09(10)	**Se(5)-C(17)**	1.68(8)
Se(2)-C(8)	1.63(6)	**Se(4)-C(13)**	1.85(6)	**S(9)-C(17)**	1.97(9)
Se(2)-C(5)	1.84(4)	**Se(4)-C(16)**	1.88(2)	**S(10)-C(18)**	1.83(4)
S(1)-C(1)	1.71(4)	**S(5)-C(10)**	1.72(5)	**C(17)-C(18)**	1.29(7)
S(2)-C(2)	1.73(4)	**S(6)-C(9)**	1.64(5)	**C(18)-C(19)**	1.79(7)
S(3)-C(6)	1.69(4)	**S(7)-C(13)**	1.68(6)	**C(19)-C(20)**	1.79(8)
S(4)-C(5)	1.62(8)	**S(8)-C(14)**	1.75(4)	**C(19)-H(19A)**	0.97
C(1)-C(2)	1.45(7)	**C(10)-C(9)**	1.33(7)	**C(19)-H(19B)**	0.97
C(3)-C(4)	1.72(2)	**C(10)-C(11)**	1.94(8)	**C(20)-H(20A)**	0.97
C(3)-C(2)	1.79(7)	**C(11)-C(12)**	1.80(10)	**C(20)-H(20B)**	0.97
C(3)-H(3A)	0.97	**C(11)-H(11A)**	0.97		
C(3)-H(3B)	0.97	**C(11)-H(11B)**	0.97		
C(4)-H(4A)	0.97	**C(12)-H(12A)**	0.97		
C(4)-H(4B)	0.97	**C(12)-H(12B)**	0.97		
C(5)-C(6)	1.44(9)	**C(13)-C(14)**	1.41(8)		
C(6)-C(7)	1.87(7)	**C(14)-C(15)**	1.90(7)		
C(7)-C(8)	1.84(8)	**C(15)-C(16)**	1.47(9)		
C(7)-H(7A)	0.97	**C(15)-H(15A)**	0.97		
C(7)-H(7B)	0.97	**C(15)-H(15B)**	0.97		
C(8)-H(8A)	0.97	**C(16)-H(16A)**	0.97		
C(8)-H(8B)	0.97	**C(16)-H(16B)**	0.97		

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z+1

Table S8. Angles for **3**.

Molecule A		Molecule B		Molecule C	
Angle	**Amplitude (deg.)**	**Angle**	**Amplitude (deg.)**	**Angle**	**Amplitude (deg.)**
S(2)-Au(1)-S(1)	90.6(4)	**S(7)-Au(2)-S(6)**	179.2(5)	**S(10)#1-Au(3)-S(10)**	180.0(4)
S(2)-Au(1)-S(4)	89.7(5)	**S(7)-Au(2)-S(5)**	89.8(5)	**S(10)#1-Au(3)-S(9)#1**	90.2(4)
S(1)-Au(1)-S(4)	179.1(5)	**S(6)-Au(2)-S(5)**	90.7(5)	**S(10)-Au(3)-S(9)#1**	89.8(4)
S(2)-Au(1)-S(3)	179.6(5)	**S(7)-Au(2)-S(8)**	91.1(5)	**S(10)#1-Au(3)-S(9)**	89.8(4)
S(1)-Au(1)-S(3)	89.4(4)	**S(6)-Au(2)-S(8)**	88.4(5)	**S(10)-Au(3)-S(9)**	90.2(4)
S(4)-Au(1)-S(3)	90.4(5)	**S(5)-Au(2)-S(8)**	178.3(5)	**S(9)#1-Au(3)-S(9)**	180.0(9)
C(1)-Se(1)-C(4)	94.3(15)	**C(9)-Se(3)-C(12)**	101(3)	**C(20)-Se(5)-C(17)**	83(4)
C(8)-Se(2)-C(5)	96(4)	**C(13)-Se(4)-C(16)**	86(4)	**C(17)-S(9)-Au(3)**	104(2)
C(1)-S(1)-Au(1)	101.8(17)	**C(10)-S(5)-Au(2)**	98(2)	**C(18)-S(10)-Au(3)**	101.4(15)
C(2)-S(2)-Au(1)	103.1(17)	**C(9)-S(6)-Au(2)**	100.4(19)	**C(18)-C(17)-Se(5)**	129(6)
C(6)-S(3)-Au(1)	100.6(16)	**C(13)-S(7)-Au(2)**	104(2)	**C(18)-C(17)-S(9)**	112(6)
C(5)-S(4)-Au(1)	100(2)	**C(14)-S(8)-Au(2)**	98.5(14)	**Se(5)-C(17)-S(9)**	116(3)
C(2)-C(1)-S(1)	123(3)	**C(9)-C(10)-S(5)**	125(5)	**C(17)-C(18)-C(19)**	113(5)
C(2)-C(1)-Se(1)	114.2(16)	**C(9)-C(10)-C(11)**	120(4)	**C(17)-C(18)-S(10)**	130(5)
S(1)-C(1)-Se(1)	120(3)	**S(5)-C(10)-C(11)**	114(3)	**C(19)-C(18)-S(10)**	115(3)
C(4)-C(3)-C(2)	98(3)	**C(12)-C(11)-C(10)**	104(4)	**C(18)-C(19)-C(20)**	84(4)
C(4)-C(3)-H(3A)	108.8	**C(12)-C(11)-H(11A)**	110.6	**C(18)-C(19)-H(19A)**	114.2
C(2)-C(3)-H(3A)	111.4	**C(10)-C(11)-H(11A)**	111.5	**C(20)-C(19)-H(19A)**	113.8
C(4)-C(3)-H(3B)	115.8	**C(12)-C(11)-H(11B)**	110.6	**C(18)-C(19)-H(19B)**	115.5
C(2)-C(3)-H(3B)	112.6	**C(10)-C(11)-H(11B)**	110.8	**C(20)-C(19)-H(19B)**	115.3
H(3A)-C(3)-H(3B)	110	**H(11A)-C(11)-H(11B)**	109.2	**H(19A)-C(19)-H(19B)**	111.9
C(3)-C(4)-Se(1)	114(3)	**C(11)-C(12)-Se(3)**	102(5)	**Se(5)-C(20)-C(19)**	129(6)
C(3)-C(4)-H(4A)	105.6	**C(11)-C(12)-H(12A)**	111.9	**Se(5)-C(20)-H(20A)**	104.4
Se(1)-C(4)-H(4A)	106.2	**Se(3)-C(12)-H(12A)**	110.8	**C(19)-C(20)-H(20A)**	104.6
C(3)-C(4)-H(4B)	112	**C(11)-C(12)-H(12B)**	111.6	**Se(5)-C(20)-H(20B)**	105.2
Se(1)-C(4)-H(4B)	110.6	**Se(3)-C(12)-H(12B)**	111.2	**C(19)-C(20)-H(20B)**	105.8
H(4A)-C(4)-H(4B)	108.1	**H(12A)-C(12)-H(12B)**	109.1	**H(20A)-C(20)-H(20B)**	105.8
C(6)-C(5)-S(4)	128(3)	**C(14)-C(13)-S(7)**	119(4)		
C(6)-C(5)-Se(2)	112(5)	**C(14)-C(13)-Se(4)**	115(4)		
S(4)-C(5)-Se(2)	120(5)	**S(7)-C(13)-Se(4)**	126(4)		
C(5)-C(6)-S(3)	121(3)	**C(13)-C(14)-S(8)**	126(3)		
C(5)-C(6)-C(7)	119(4)	**C(13)-C(14)-C(15)**	115(4)		
S(3)-C(6)-C(7)	119(3)	**S(8)-C(14)-C(15)**	117(3)		
C(8)-C(7)-C(6)	88(3)	**C(16)-C(15)-C(14)**	91(4)		
C(8)-C(7)-H(7A)	114.2	**C(16)-C(15)-H(15A)**	112		
C(6)-C(7)-H(7A)	114.5	**C(14)-C(15)-H(15A)**	113		
C(8)-C(7)-H(7B)	113.8	**C(16)-C(15)-H(15B)**	116		
C(6)-C(7)-H(7B)	113.6	**C(14)-C(15)-H(15B)**	112.7		
H(7A)-C(7)-H(7B)	111.2	**H(15A)-C(15)-H(15B)**	110.5		
Se(2)-C(8)-C(7)	123(4)	**C(15)-C(16)-Se(4)**	128(6)		
Se(2)-C(8)-H(8A)	106.8	**C(15)-C(16)-H(16A)**	103.7		
C(7)-C(8)-H(8A)	106.3	**Se(4)-C(16)-H(16A)**	105.1		
Se(2)-C(8)-H(8B)	106.2	**C(15)-C(16)-H(16B)**	105.8		
C(7)-C(8)-H(8B)	106.7	**Se(4)-C(16)-H(16B)**	106.7		
H(8A)-C(8)-H(8B)	106.5	**H(16A)-C(16)-H(16B)**	106.4		
C(1)-C(2)-S(2)	120(3)	**C(10)-C(9)-S(6)**	126(5)		
C(1)-C(2)-C(3)	117(2)	**C(10)-C(9)-Se(3)**	112(4)		
S(2)-C(2)-C(3)	123(3)	**S(6)-C(9)-Se(3)**	122(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z+1

Table S9. Short contacts and hydrogen bonds in **3**.

Contact	Length	Symm. op.*	Contact Type
S9···S9*	3.675	1/2-x,2.5-y,1-z	Chains of C
Se5···S10*	3.697	x,1+y,z	Chains of C
Se5···C19*	3.663	x,1+y,z	Chains of C
Se5···H19A*	3.129	x,1+y,z	Chains of C
H20B···S2*	3.014	1/2-x,2.5-y,1-z	C – A
S9···S7*	3.598	x,y,z	Stacks of B - C
S10···S8*	3.665	x,y,z	Stacks of B - C
H19B···H15A*	2.4	x,y,z	Stacks of B - C
S9···S6*	3.638	x,y,z	Stacks of B - C
S10···S5*	3.643	x,y,z	Stacks of B - C
Se5···Se3*	3.872	x,y,z	Stacks of B - C
C19···H11A*	2.721	x,y,z	Stacks of B - C
H19A···C11*	2.62	x,y,z	Stacks of B - C
H19A···H11A*	1.777	x,y,z	Stacks of B - C
S9···S5*	3.571	1/2-x,2.5-y,1-z	Chains of B
Se5···S5*	3.613	1/2-x,2.5-y,1-z	Chains of B
S10···S7*	3.554	1/2-x,2.5-y,1-z	Chains of B
S2···S3*	3.676	x,1+y,z	Stacks of A
S1···S3*	3.52	1-x,1-y,1-z	Chains of A
S3···S3*	3.654	1-x,1-y,1-z	Chains of A
C7···C3*	3.083	1-x,2-y,1-z	Stacks of A
C7···H3B*	2.158	1-x,2-y,1-z	Stacks of A
H7A···C3*	2.143	1-x,2-y,1-z	Stacks of A
H7A···H3B*	1.2	1-x,2-y,1-z	Stacks of A
S1···S4*	3.616	1-x,2-y,1-z	Stacks of A
H3B···C6*	2.944	1-x,2-y,1-z	Stacks of A
Se1···S6*	3.559	1-x,y,1.5-z	A – B
Se1···C10*	3.681	1-x,y,1.5-z	A – B
Se1···C9*	3.371	1-x,y,1.5-z	A – B
H4B···S5*	2.92	1-x,y,1.5-z	A – B
C4···Se3*	3.565	1-x,1+y,1.5-z	A – B
H4B···Se3*	3.071	1-x,1+y,1.5-z	A – B
Se2···S8*	3.597	x,2-y,-1/2+z	A – B
Se2···C14*	3.64	x,2-y,-1/2+z	A – B
S7···S6*	3.657	x,1+y,z	Chains of B
H11B···Se3*	3.145	x,1+y,z	Chains of B
Se4···S8*	3.576	x,1+y,z	Chains of B
Se4···C15*	3.667	x,1+y,z	Chains of B
Se4···H15A*	3.189	x,1+y,z	Chains of B

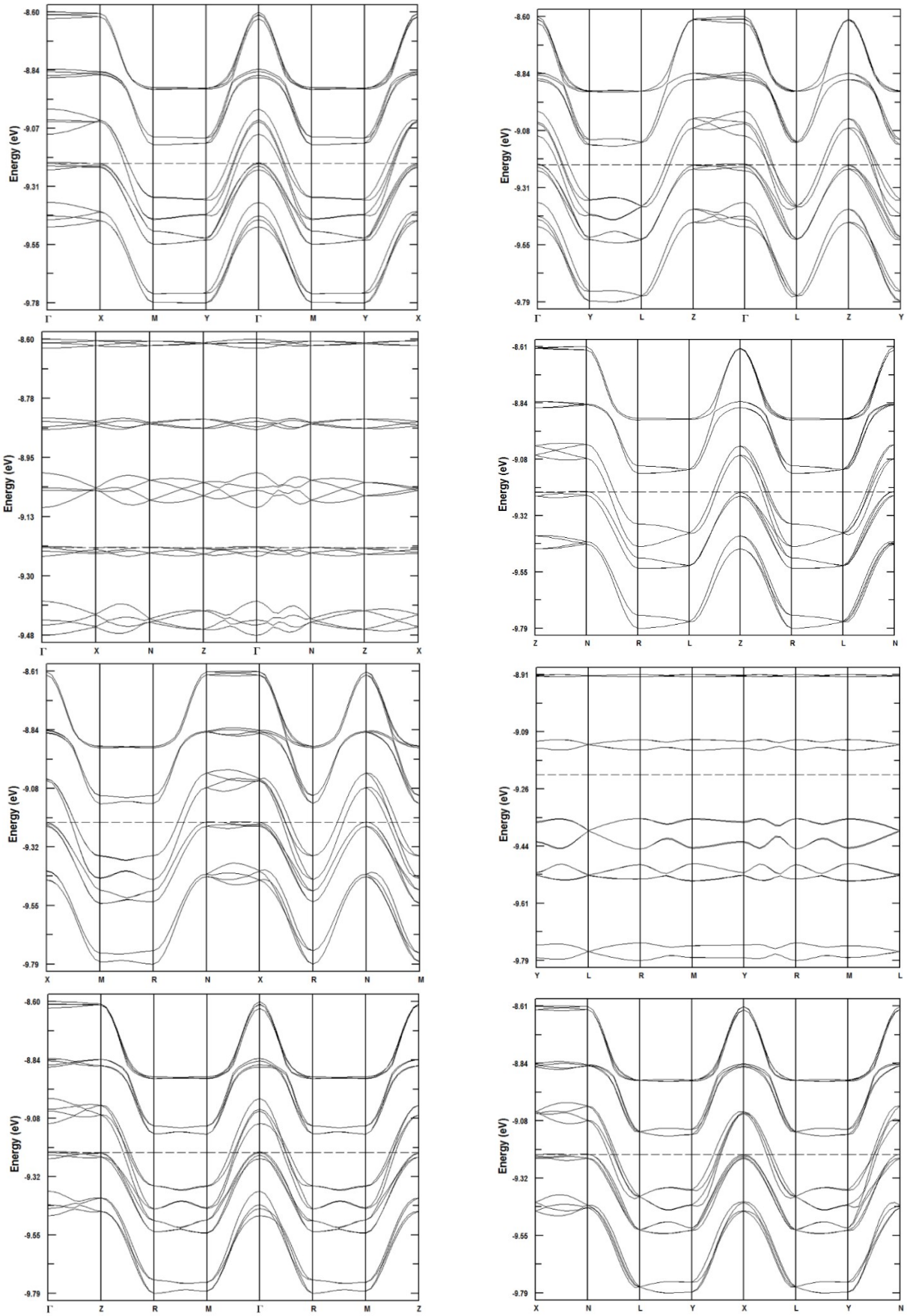
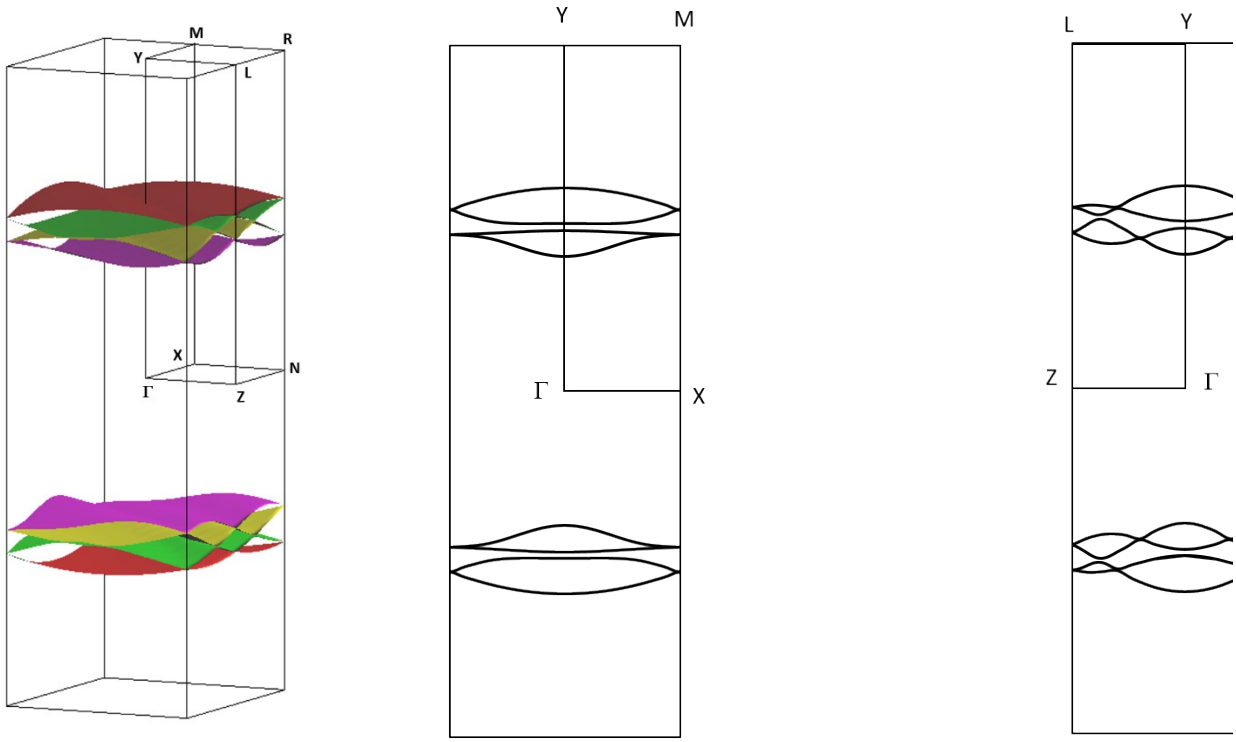


Fig. S7. Calculated band structure of **3**, showing 20 SOMO bands near the Fermi level (dashed line). The. Γ, X, Y, Z, M, L, N and R and refer to the (0, 0, 0), (½, 0, 0), (0, ½, 0), (0, 0, ½), (½, ½, 0), (0, ½, ½), (½, 0, ½), (½, ½, ½) points in k-space, respectively.



(a) **(b)** **(c)**

Fig. S8**.** Fermi Surface *of* **3**: (a) Three dimensional representation; (b) intersection in the plane *a*,b** and (c) intersection in *b*,c**.