Supporting Information

Theoretical study on the conductance in polycyclic aromatic hydrocarbons with different molecular size and edge type structures

Xinqian Li, Aleksandar Staykov, and Kazunari Yoshizawa*

Institute for Materials Chemistry and Engineering, Kyushu University, Nishi-ku, Fukuoka 819-0395, Japan

*Author to whom correspondence should be addressed.

E-mail: kazunari@ms.ifoc.kyushu-u.ac.jp

Kyushu University

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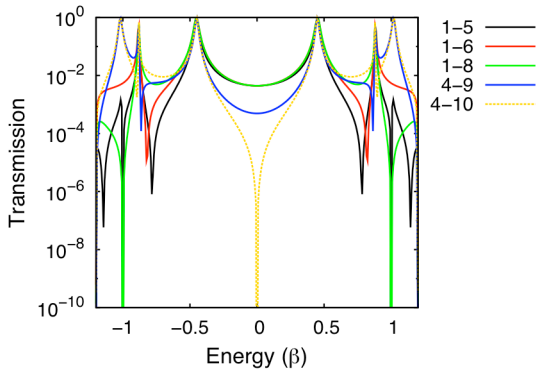

Figure S1. Computed transmission spectra for the predicted routes of pyrene at the Hückel level of theory.

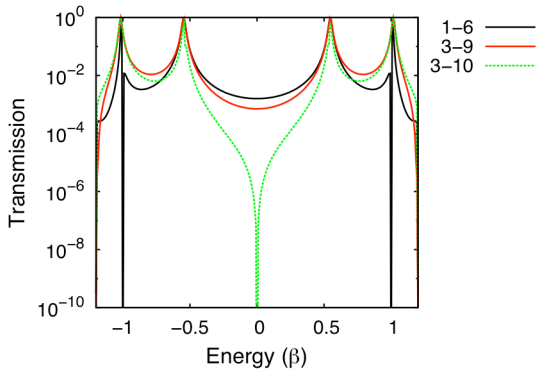

Figure S2. Computed transmission spectra for the predicted routes of coronene at the Hückel level of theory.

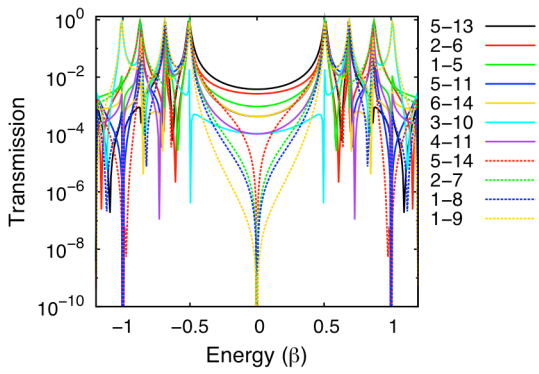

Figure S3. Computed transmission spectra for the predicted routes of picene at the Hückel level of theory.

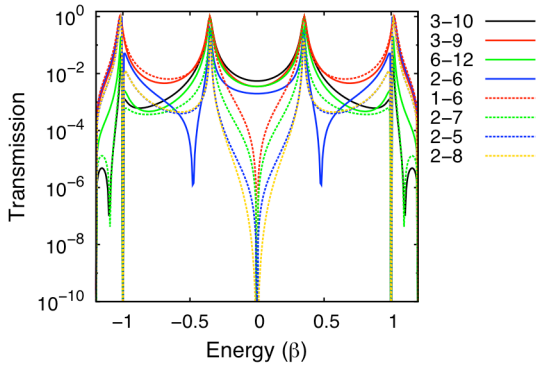

Figure S4. Computed transmission spectra for the predicted routes of perylene at the Hückel level of theory.

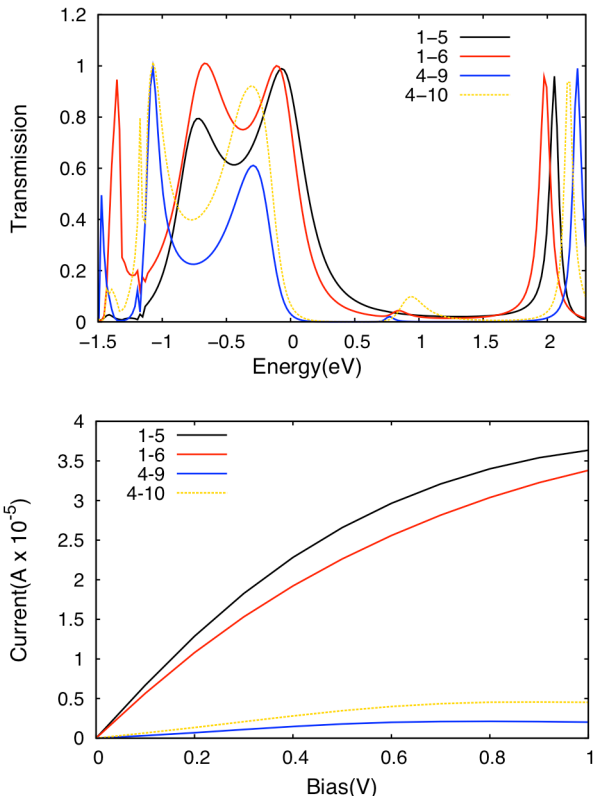

Figure S5. Calculated transmission spectra at the zero-bias and *I-V* curves for pyrene dithiolate junctions at the Perdew-Zunger LDA level of theory.

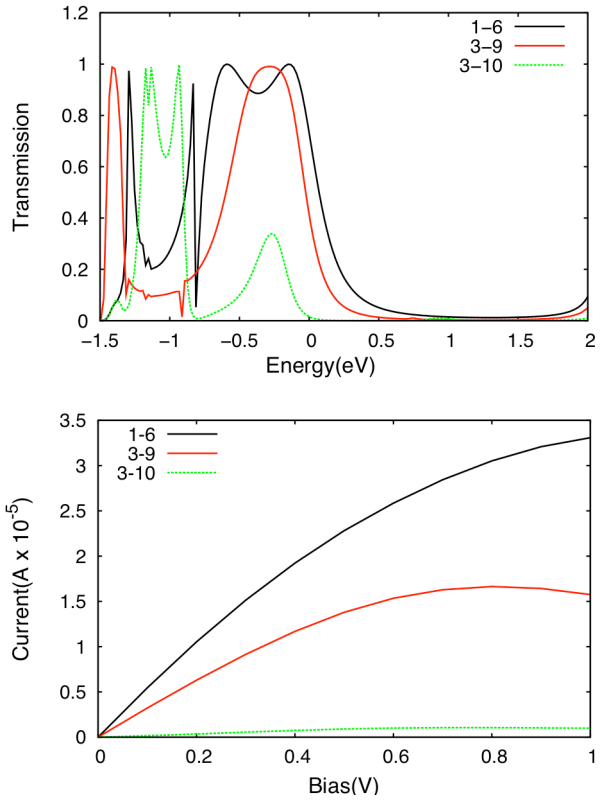

Figure S6. Calculated transmission spectra at the zero-bias and *I-V* curves for coronene dithiolate junctions at the Perdew-Zunger LDA level of theory.

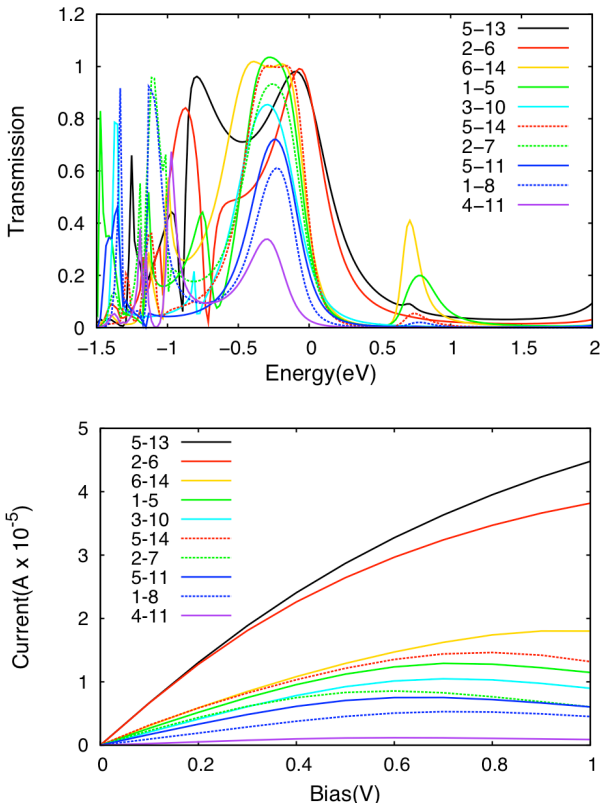

Figure S7. Calculated transmission spectra at the zero-bias and *I-V* curves for picene dithiolate junctions at the Perdew-Zunger LDA level of theory.

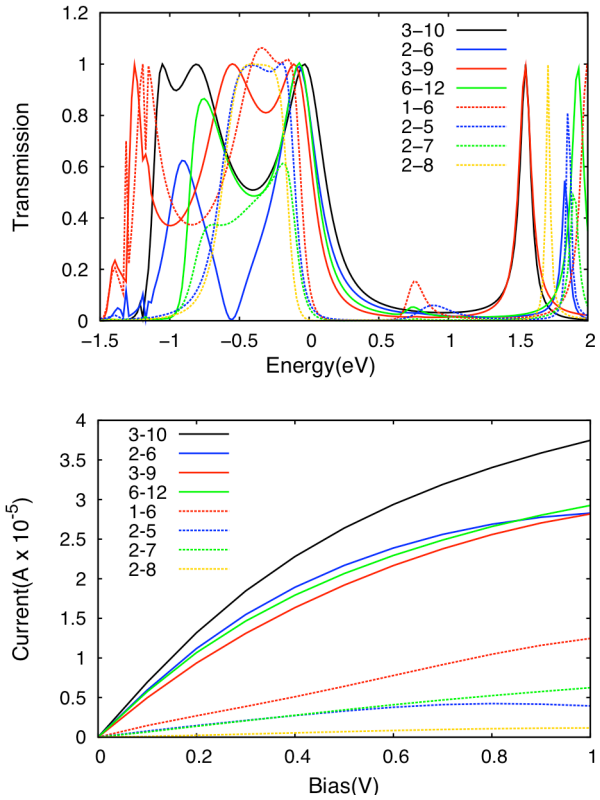

Figure S8. Calculated transmission spectra at the zero-bias and *I-V* curves for perylene dithiolate junctions at the Perdew-Zunger LDA level of theory.

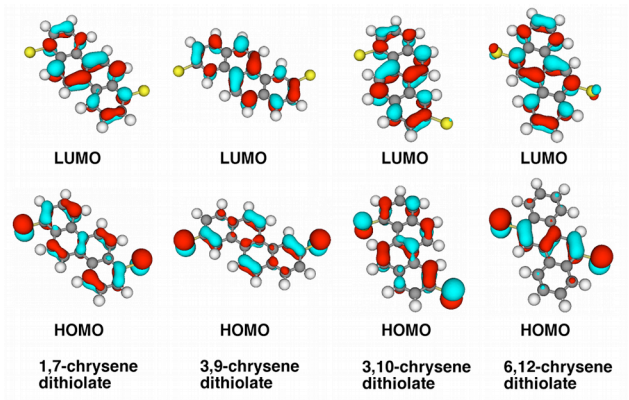

Figure S9. MPSH states of HOMO and LUMO for 1,7-, 3,9- 3,10-, and 6,12-chrysene dithiolates at zero bias.

Table S1. Geometrical parameters of Au_2(1,4-tetracene dithiolate). Units are Å. Energy = -1759.256269 Hartree.

atom	x	y	z
C	-0.01	0.00	0.00
C	-0.01	0.00	1.43
C	1.15	0.00	2.15
C	2.42	0.00	1.45
C	2.42	0.00	-0.01
C	1.15	0.00	-0.72
C	3.64	0.00	-0.68
C	4.88	0.00	-0.01
C	4.88	0.00	1.44
C	3.64	0.00	2.11
C	6.11	0.00	-0.69
C	7.33	0.00	-0.01
C	7.33	0.00	1.44
C	6.11	0.00	2.13
C	8.59	0.00	-0.69
C	9.77	0.00	0.01
C	9.77	0.00	1.44
C	8.59	0.00	2.13
H	10.72	0.00	-0.53
H	-0.97	0.00	-0.50
H	-0.97	0.00	1.93
S	1.24	0.00	3.94
H	3.66	0.00	3.20
H	8.59	0.00	3.22
H	8.59	0.00	-1.78
H	3.66	0.00	-1.77
S	1.25	0.00	-2.51
H	6.11	0.00	3.21
H	6.11	0.00	-1.78
H	10.71	0.00	1.97
Au	-0.93	0.00	-3.29
Au	-0.93	0.00	4.72

Table S2. Geometrical parameters of Au_2(1,5-tetracene dithiolate). Units are Å. Energy = -1759.243509 Hartree.

atom	x	y	z
C	-0.01	0.00	-0.02
C	-0.03	0.00	1.40
C	1.12	0.00	2.12
C	2.41	0.00	1.50
C	2.44	0.00	0.04
C	1.18	0.00	-0.70
C	3.65	0.00	-0.63
C	4.88	0.00	0.06
C	4.89	0.00	1.51
C	3.63	0.00	2.21
C	6.10	0.00	-0.66
C	7.33	0.00	-0.02
C	7.35	0.00	1.43
C	6.15	0.00	2.14
C	8.57	0.00	-0.73
C	9.77	0.00	-0.05
C	9.79	0.00	1.38
C	8.63	0.00	2.09
H	10.70	0.00	-0.60
H	-0.95	0.00	-0.56
H	-0.99	0.00	1.91
H	1.06	0.00	3.20
S	3.89	0.00	3.99
H	8.64	0.00	3.18
H	8.55	0.00	-1.81
H	3.68	0.00	-1.71
S	1.32	0.00	-2.49
H	6.22	0.00	3.22
H	6.06	0.00	-1.74
H	10.75	0.00	1.89
Au	-0.84	0.00	-3.33
Au	2.01	0.00	5.33

Table S3. Geometrical parameters of Au_2(1,6-tetracene dithiolate). Units are Å. Energy = -1759.244984 Hartree.

atom	x	y	z
C	0.00	0.00	-0.03
C	-0.07	0.00	1.41
C	1.21	0.00	2.11
C	2.43	0.00	1.35
C	2.43	0.00	-0.01
C	1.19	0.00	-0.71
C	-1.27	0.00	2.16
C	-1.21	0.00	3.60
C	0.08	0.00	4.26
C	1.25	0.00	3.49
C	-2.35	0.00	4.43
C	-2.28	0.00	5.83
C	-0.99	0.00	6.48
C	0.15	0.00	5.67
C	-0.95	0.00	7.93
C	-2.12	0.00	8.64
C	-3.39	0.00	7.98
C	-3.47	0.00	6.62
S	0.69	0.00	8.67
Au	0.38	0.00	10.96
H	3.36	0.00	-0.56
H	-2.10	0.00	9.73
H	-4.29	0.00	8.59
H	-4.43	0.00	6.12
H	-0.92	0.00	-0.60
H	3.36	0.00	1.91
H	1.13	0.00	6.12
S	-2.97	0.00	1.57
H	2.21	0.00	4.00
H	1.18	0.00	-1.79
Au	-3.26	0.00	-0.72
H	-3.34	0.00	3.99

Table S4. Geometrical parameters of Au_2(1,7-tetracene dithiolate). Units are Å. Energy = -1759.256880 Hartree.

atom	x	y	z
C	-0.07	0.00	0.00
C	0.00	0.00	1.45
C	1.22	0.00	2.08
C	2.44	0.00	1.33
C	2.42	0.00	-0.03
C	1.18	0.00	-0.74
S	-1.58	0.00	2.30
H	1.27	0.00	3.16
H	3.38	0.00	1.88
H	3.35	0.00	-0.60
C	1.15	0.00	-2.14
C	-0.06	0.00	-2.86
C	-1.30	0.00	-2.12
C	-1.27	0.00	-0.71
H	2.09	0.00	-2.68
H	-2.21	0.00	-0.18
C	-0.09	0.00	-4.27
C	-1.29	0.00	-4.98
C	-2.54	0.00	-4.24
C	-2.51	0.00	-2.85
H	0.86	0.00	-4.80
H	-3.45	0.00	-2.30
C	-1.35	0.00	-6.44
C	-2.58	0.00	-7.06
C	-3.79	0.00	-6.32
C	-3.78	0.00	-4.95
S	0.22	0.00	-7.28
H	-2.63	0.00	-8.15
H	-4.74	0.00	-6.86
H	-4.71	0.00	-4.38
Au	-0.24	0.00	-9.55
Au	-1.12	0.00	4.57

Table S5. Geometrical parameters of Au_2(2,9-tetracene dithiolate). Units are Å. Energy = -1759.262033 Hartree.

atom	x	y	z
C	0.00	0.00	0.06
C	0.00	0.00	1.50
C	1.17	0.00	2.20
C	2.44	0.00	1.53
C	2.44	0.00	0.08
C	1.19	0.00	-0.61
C	3.66	0.00	-0.59
C	4.90	0.00	0.10
C	4.89	0.00	1.55
C	3.65	0.00	2.22
C	6.14	0.00	-0.58
C	7.35	0.00	0.11
C	7.33	0.00	1.56
C	6.12	0.00	2.24
C	8.61	0.00	-0.57
C	9.79	0.00	0.13
C	9.78	0.00	1.56
C	8.59	0.00	2.24
S	11.28	0.00	-0.86
S	-1.48	0.00	-0.95
Au	-3.29	0.00	0.49
H	-0.95	0.00	2.03
H	1.16	0.00	3.28
H	3.64	0.00	3.31
H	8.59	0.00	3.33
H	8.60	0.00	-1.65
H	3.67	0.00	-1.68
H	1.21	0.00	-1.70
H	6.14	0.00	-1.67
H	6.11	0.00	3.32
Au	13.08	0.00	0.60
H	10.72	0.00	2.10

Table S6. Geometrical parameters of Au_2(3,9-tetracene dithiolate). Units are Å. Energy = -1759.262113 Hartree.

atom	x	y	z
C	-0.01	0.00	0.00
C	0.01	0.00	1.43
C	1.28	0.00	2.12
C	2.47	0.00	1.33
C	2.42	0.00	-0.04
C	1.16	0.00	-0.73
C	-1.17	0.00	2.18
C	-1.15	0.00	3.59
C	0.13	0.00	4.28
C	1.31	0.00	3.51
C	-2.33	0.00	4.36
C	-2.31	0.00	5.75
C	-1.03	0.00	6.44
C	0.14	0.00	5.69
C	-1.02	0.00	7.87
C	-2.19	0.00	8.60
C	-3.45	0.00	7.91
C	-3.50	0.00	6.55
S	-2.01	0.00	10.38
Au	-4.14	0.00	11.28
H	3.34	0.00	-0.62
H	-4.37	0.00	8.49
H	-4.46	0.00	6.04
H	-3.29	0.00	3.85
H	-0.97	0.00	-0.50
H	3.44	0.00	1.83
H	1.10	0.00	6.20
H	-0.06	0.00	8.38
H	2.27	0.00	4.03
H	-2.13	0.00	1.67
S	0.98	0.00	-2.51
Au	3.11	0.00	-3.41

Table S7. Geometrical parameters of Au_2(5,11-tetracene dithiolate). Units are Å. Energy = -1759.230736 Hartree.

atom	x	y	z
C	-0.07	0.00	0.03
C	0.04	0.00	1.46
C	1.24	0.00	2.11
C	2.47	0.00	1.38
C	2.43	0.00	0.02
H	-0.86	0.00	2.06
H	1.27	0.00	3.20
H	3.42	0.00	1.91
H	3.35	0.00	-0.56
C	-1.26	0.00	-0.71
C	-1.24	0.00	-2.16
C	0.04	0.00	-2.87
C	1.20	0.00	-2.09
C	1.19	0.00	-0.70
S	-2.95	0.00	-0.08
H	2.17	0.00	-2.57
C	-2.42	0.00	-2.92
C	-2.42	0.00	-4.30
C	-1.17	0.00	-5.03
C	0.05	0.00	-4.30
H	-3.38	0.00	-2.42
S	1.48	0.00	-5.40
C	-3.65	0.00	-5.03
C	-3.68	0.00	-6.39
C	-2.46	0.00	-7.12
C	-1.25	0.00	-6.47
H	-4.58	0.00	-4.45
H	-4.63	0.00	-6.93
H	-2.48	0.00	-8.21
H	-0.34	0.00	-7.06
Au	-3.20	0.00	2.22
Au	3.57	0.00	-4.42

Table S8. Geometrical parameters of Au_2(5,12-tetracene dithiolate). Units are Å. Energy = -1759.228294 Hartree.

atom	x	y	z
C	0.03	0.00	-0.01
C	0.03	0.00	1.41
C	1.21	0.00	2.09
C	2.49	0.00	1.43
C	2.49	0.00	-0.03
C	1.21	0.00	-0.69
C	3.71	0.00	-0.75
C	4.94	0.00	-0.04
C	4.94	0.00	1.43
C	3.71	0.00	2.14
C	6.20	0.00	-0.68
C	7.42	0.00	-0.02
C	7.42	0.00	1.42
C	6.20	0.00	2.08
C	8.68	0.00	-0.71
C	9.85	0.00	-0.02
C	9.85	0.00	1.42
C	8.68	0.00	2.11
S	3.45	0.00	3.93
Au	5.33	0.00	5.29
S	3.45	0.00	-2.53
Au	5.33	0.00	-3.89
H	-0.91	0.00	-0.56
H	-0.91	0.00	1.96
H	1.18	0.00	3.17
H	8.67	0.00	3.20
H	8.67	0.00	-1.80
H	1.18	0.00	-1.77
H	6.23	0.00	3.16
H	6.23	0.00	-1.76
H	10.80	0.00	1.95
H	10.80	0.00	-0.55

Table S9. Geometrical parameters of Au_2(1,5-pyrene dithiolate). Units are Å. Energy = -1681.865081 Hartree.

atom	x	y	z
C	0.01	0.00	0.00
C	-0.01	0.00	1.40
C	1.25	0.00	2.10
C	2.47	0.00	1.36
C	2.43	0.00	-0.04
C	1.21	0.00	-0.71
C	3.71	0.00	2.08
C	3.75	0.00	3.44
C	2.54	0.00	4.23
C	1.29	0.00	3.53
C	0.06	0.00	4.26
C	0.11	0.00	5.66
C	1.33	0.00	6.34
C	2.54	0.00	5.65
C	-1.24	0.00	2.18
C	-1.18	0.00	3.55
S	-2.76	0.00	1.23
Au	-4.49	0.00	2.76
H	4.71	0.00	3.94
H	1.19	0.00	-1.80
H	-0.92	0.00	-0.55
H	3.36	0.00	-0.60
H	-0.82	0.00	6.22
H	1.33	0.00	7.42
S	4.14	0.00	6.46
H	-2.09	0.00	4.13
H	4.63	0.00	1.51
Au	3.74	0.00	8.74

Table S10. Geometrical parameters of Au_2(1,6-pyrene dithiolate). Units are Å. Energy = -1681.865097 Hartree.

atom	x	y	z
C	0.00	0.00	-0.01
C	-0.03	0.00	1.39
C	1.19	0.00	2.12
C	2.43	0.00	1.40
C	2.43	0.00	-0.03
C	1.21	0.00	-0.70
C	3.68	0.00	2.11
C	3.68	0.00	3.54
C	2.43	0.00	4.23
C	1.24	0.00	3.56
C	3.69	0.00	-0.72
C	4.87	0.00	-0.05
C	4.92	0.00	1.39
C	4.91	0.00	4.21
C	6.11	0.00	3.52
C	6.14	0.00	2.12
H	5.80	0.00	-0.61
H	0.31	0.00	4.12
H	7.04	0.00	4.07
S	7.66	0.00	1.16
H	4.92	0.00	5.30
H	1.20	0.00	-1.79
H	-0.93	0.00	-0.56
S	-1.54	0.00	2.35
H	2.44	0.00	5.32
H	3.68	0.00	-1.81
Au	-3.30	0.00	0.83
Au	9.41	0.00	2.67

Table S11. Geometrical parameters of Au_2(4,9-pyrene dithiolate). Units are Å. Energy = -1681.865252 Hartree.

atom	x	y	z
C	0.02	0.00	0.02
C	0.04	0.00	1.42
C	1.26	0.00	-0.70
C	1.22	0.00	-2.12
C	2.45	0.00	-2.84
C	3.69	0.00	-2.11
C	3.74	0.00	-0.75
C	2.50	0.00	0.02
H	4.61	0.00	-2.69
C	-1.21	0.00	-0.71
C	-1.26	0.00	-2.08
C	-0.02	0.00	-2.84
H	-2.13	0.00	-0.14
C	2.44	0.00	-4.25
C	0.02	0.00	-4.25
C	1.23	0.00	-4.94
C	2.46	0.00	1.42
C	1.25	0.00	2.11
H	1.23	0.00	-6.02
H	3.38	0.00	-4.79
H	-0.91	0.00	-4.81
H	3.39	0.00	1.99
H	1.25	0.00	3.20
H	-0.90	0.00	1.97
S	5.24	0.00	0.22
S	-2.77	0.00	-3.04
Au	7.00	0.00	-1.29
Au	-4.52	0.00	-1.53

Table S12. Geometrical parameters of Au_2(4,10-pyrene dithiolate). Units are Å. Energy = -1681.864824 Hartree.

atom	x	y	z
C	0.01	0.00	-0.01
C	0.00	0.00	1.38
C	1.20	0.00	2.11
C	2.44	0.00	1.40
C	2.44	0.00	-0.03
C	1.21	0.00	-0.71
C	3.67	0.00	2.11
C	3.67	0.00	3.55
C	2.39	0.00	4.25
C	1.23	0.00	3.54
C	3.69	0.00	-0.72
C	4.89	0.00	-0.06
C	4.92	0.00	1.40
C	4.91	0.00	4.22
C	6.11	0.00	3.52
C	6.12	0.00	2.13
S	2.50	0.00	6.04
Au	0.33	0.00	6.83
S	6.49	0.00	-0.86
H	0.27	0.00	4.06
H	7.05	0.00	4.07
H	7.07	0.00	1.61
H	4.93	0.00	5.31
H	1.21	0.00	-1.80
H	-0.93	0.00	-0.56
H	-0.94	0.00	1.92
H	3.67	0.00	-1.80
Au	6.09	0.00	-3.14

Table S13. Geometrical parameters of Au_2(1,6-coronene dithiolate). Units are Å. Energy = -1987.969182 Hartree.

atom	x	y	z
C	0.01	0.00	0.01
C	0.01	0.00	1.43
C	1.25	0.00	2.12
C	2.47	0.00	1.38
C	2.44	0.00	-0.04
C	1.18	0.00	-0.70
C	1.26	0.00	3.55
C	0.04	0.00	4.29
C	-1.20	0.00	3.56
C	-1.19	0.00	2.18
C	2.53	0.00	4.22
C	2.57	0.00	5.64
C	1.35	0.00	6.36
C	0.14	0.00	5.71
C	3.75	0.00	3.48
C	3.73	0.00	2.05
C	4.96	0.00	1.30
C	4.89	0.00	-0.13
C	3.66	0.00	-0.76
C	4.99	0.00	4.17
C	6.19	0.00	3.42
C	6.17	0.00	2.05
C	5.00	0.00	5.60
C	3.83	0.00	6.31
H	-2.13	0.00	1.63
S	-2.91	0.00	4.15
H	3.60	0.00	-1.84
S	6.20	0.00	-1.37
H	3.84	0.00	7.39
H	5.96	0.00	6.11
H	7.12	0.00	1.52
H	7.14	0.00	3.95
H	1.38	0.00	7.45
H	1.16	0.00	-1.79
H	-0.95	0.00	-0.51
Au	8.36	0.00	-0.55
H	-0.77	0.00	6.31
Au	-3.17	0.00	6.45

Table S14. Geometrical parameters of Au_2(3,9-coronene dithiolate). Units are Å. Energy = -1987.969278 Hartree.

atom	x	y	z
C	0.01	0.00	-0.01
C	0.01	0.00	1.42
C	1.25	0.00	2.12
C	2.47	0.00	1.38
C	2.44	0.00	-0.04
C	1.18	0.00	-0.71
C	1.26	0.00	3.55
C	0.03	0.00	4.28
C	-1.18	0.00	3.54
C	-1.19	0.00	2.17
C	2.53	0.00	4.21
C	2.56	0.00	5.63
C	1.34	0.00	6.35
C	0.10	0.00	5.72
C	3.75	0.00	3.47
C	3.73	0.00	2.04
C	4.96	0.00	1.31
C	4.89	0.00	-0.13
C	3.66	0.00	-0.76
C	4.99	0.00	4.17
C	6.19	0.00	3.42
C	6.17	0.00	2.05
C	4.99	0.00	5.60
C	3.81	0.00	6.30
H	-2.14	0.00	1.64
H	-2.12	0.00	4.07
H	3.61	0.00	-1.84
S	6.20	0.00	-1.37
H	3.82	0.00	7.39
H	5.94	0.00	6.12
H	7.12	0.00	1.52
H	7.14	0.00	3.95
H	1.39	0.00	7.43
S	-1.21	0.00	6.96
H	1.17	0.00	-1.80
H	-0.94	0.00	-0.53
Au	8.36	0.00	-0.54
Au	-3.36	0.00	6.13

Table S15. Geometrical parameters of Au_2(3,10-coronene dithiolate). Units are Å. Energy = -1987.982905 Hartree.

atom	x	y	z
C	-0.05	0.00	0.03
C	-0.03	0.00	1.46
C	1.23	0.00	2.12
C	2.43	0.00	1.36
C	2.38	0.00	-0.05
C	1.11	0.00	-0.70
C	1.28	0.00	3.55
C	0.08	0.00	4.30
C	-1.17	0.00	3.61
C	-1.22	0.00	2.24
C	2.54	0.00	4.22
C	2.59	0.00	5.65
C	1.36	0.00	6.39
C	0.15	0.00	5.72
C	3.75	0.00	3.45
C	3.70	0.00	2.02
C	4.91	0.00	1.27
C	4.83	0.00	-0.17
C	3.59	0.00	-0.79
C	5.00	0.00	4.12
C	6.19	0.00	3.34
C	6.15	0.00	1.97
C	5.03	0.00	5.54
C	3.87	0.00	6.27
H	-2.18	0.00	1.73
H	3.53	0.00	-1.88
S	6.39	0.00	-1.05
H	3.94	0.00	7.36
H	5.99	0.00	6.04
H	7.08	0.00	1.41
H	7.15	0.00	3.85
S	1.51	0.00	8.17
H	1.07	0.00	-1.78
H	-1.01	0.00	-0.47
Au	5.89	0.00	-3.31
H	-0.78	0.00	6.28
H	-2.09	0.00	4.19
Au	-0.63	0.00	9.04

Table S16. Geometrical parameters of Au_2(1,6-chrysene dithiolate). Units are Å. Energy = -1759.271092 Hartree.

atom	x	y	z
C	-0.02	0.00	0.02
C	0.01	0.00	1.43
C	1.28	0.00	2.10
C	2.45	0.00	1.30
C	2.38	0.00	-0.08
C	1.14	0.00	-0.73
C	1.34	0.00	3.55
C	0.14	0.00	4.30
C	-1.10	0.00	3.60
C	-1.19	0.00	2.23
C	2.58	0.00	4.25
C	2.63	0.00	5.62
C	1.45	0.00	6.42
C	0.18	0.00	5.75
C	1.50	0.00	7.85
C	0.32	0.00	8.58
C	-0.92	0.00	7.92
C	-0.99	0.00	6.55
S	-2.74	0.00	1.33
Au	-4.44	0.00	2.90
H	-2.03	0.00	4.17
H	0.35	0.00	9.66
H	-1.97	0.00	6.08
H	3.51	0.00	3.71
H	3.42	0.00	1.77
H	1.08	0.00	-1.82
H	3.30	0.00	-0.66
H	-1.83	0.00	8.51
H	-0.98	0.00	-0.49
S	3.13	0.00	8.60
H	3.61	0.00	6.10
Au	2.82	0.00	10.89

Table S17. Geometrical parameters of Au_2(1,7-chrysene dithiolate). Units are Å. Energy = -1759.271019 Hartree.

atom	x	y	z
C	-0.05	0.00	0.04
C	-0.05	0.00	1.44
C	1.14	0.00	2.15
C	2.39	0.00	1.43
C	2.38	0.00	0.00
C	1.14	0.00	-0.67
C	3.65	0.00	-0.71
C	4.87	0.00	-0.01
C	4.83	0.00	1.42
C	3.65	0.00	2.11
C	3.70	0.00	-2.14
C	4.88	0.00	-2.83
C	6.14	0.00	-2.15
C	6.14	0.00	-0.72
C	7.38	0.00	-2.87
C	8.57	0.00	-2.16
C	8.57	0.00	-0.76
C	7.39	0.00	-0.05
H	5.75	0.00	1.99
H	3.67	0.00	3.19
S	7.28	0.00	-4.66
H	9.52	0.00	-2.69
H	7.43	0.00	1.03
H	4.85	0.00	-3.91
H	2.78	0.00	-2.71
H	1.10	0.00	-1.75
H	-1.00	0.00	1.97
S	1.24	0.00	3.94
H	-1.00	0.00	-0.50
H	9.52	0.00	-0.22
Au	-0.94	0.00	4.72
Au	9.46	0.00	-5.44

Table S18. Geometrical parameters of Au_2(2,8-chrysene dithiolate). Units are Å. Energy = -1759.278151 Hartree.

atom	x	y	z
C	0.01	0.00	0.01
C	-0.01	0.00	1.42
C	1.20	0.00	2.10
C	2.43	0.00	1.41
C	2.45	0.00	-0.01
C	1.20	0.00	-0.68
C	3.73	0.00	-0.71
C	4.94	0.00	0.04
C	4.86	0.00	1.47
C	3.66	0.00	2.13
C	3.81	0.00	-2.14
C	5.00	0.00	-2.79
C	6.24	0.00	-2.08
C	6.21	0.00	-0.65
C	7.47	0.00	-2.77
C	8.68	0.00	-2.09
C	8.66	0.00	-0.68
C	7.46	0.00	0.01
H	5.77	0.00	2.05
H	3.64	0.00	3.21
H	7.45	0.00	-3.86
H	7.51	0.00	1.10
H	5.03	0.00	-3.88
H	2.89	0.00	-2.72
H	1.16	0.00	-1.76
H	1.21	0.00	3.19
S	10.15	0.00	-3.11
S	-1.48	0.00	2.44
Au	-3.30	0.00	1.01
H	-0.93	0.00	-0.54
Au	11.96	0.00	-1.68
H	9.59	0.00	-0.13

Table S19. Geometrical parameters of Au_2(2,9-chrysene dithiolate). Units are Å. Energy = -1759.277965 Hartree.

atom	x	y	z
C	-0.01	0.00	0.01
C	-0.01	0.00	1.43
C	1.26	0.00	2.07
C	2.45	0.00	1.31
C	2.42	0.00	-0.08
C	1.16	0.00	-0.72
C	-1.22	0.00	2.23
C	-1.13	0.00	3.64
C	0.17	0.00	4.25
C	1.31	0.00	3.50
C	-2.51	0.00	1.62
C	-3.65	0.00	2.37
C	-3.61	0.00	3.79
C	-2.34	0.00	4.45
C	-2.32	0.00	5.86
C	-3.49	0.00	6.61
C	-4.74	0.00	5.95
C	-4.79	0.00	4.57
S	4.01	0.00	-0.90
Au	3.59	0.00	-3.17
H	-2.60	0.00	0.54
H	-4.63	0.00	1.88
H	3.41	0.00	1.84
H	-0.94	0.00	-0.54
H	2.29	0.00	3.99
H	0.26	0.00	5.33
H	-1.38	0.00	6.39
H	-5.75	0.00	4.06
S	-3.27	0.00	8.38
H	1.12	0.00	-1.81
H	-5.66	0.00	6.52
Au	-5.38	0.00	9.33

Table S20. Geometrical parameters of Au_2(3,9-chrysene dithiolate). Units are Å. Energy = -1759.277774 Hartree.

atom	x	y	z
C	0.01	0.00	0.03
C	0.00	0.00	1.48
C	1.23	0.00	-0.71
C	1.25	0.00	-2.08
C	0.04	0.00	-2.83
C	-1.21	0.00	-2.14
C	-1.22	0.00	-0.69
H	2.18	0.00	-0.18
H	2.19	0.00	-2.61
C	-1.25	0.00	2.17
C	-1.26	0.00	3.58
C	-0.09	0.00	4.31
C	1.15	0.00	3.64
C	1.18	0.00	2.26
H	-2.22	0.00	4.10
H	-0.13	0.00	5.40
H	2.15	0.00	1.76
C	-2.46	0.00	1.42
C	-2.45	0.00	0.05
C	0.05	0.00	-4.24
C	-1.12	0.00	-4.97
C	-2.40	0.00	-2.91
C	-2.37	0.00	-4.30
H	-3.41	0.00	1.95
H	-3.39	0.00	-0.47
H	-3.36	0.00	-2.42
H	-1.09	0.00	-6.06
H	1.01	0.00	-4.76
S	2.75	0.00	4.44
S	-3.97	0.00	-5.10
Au	-3.59	0.00	-7.38
Au	2.38	0.00	6.72

Table S21. Geometrical parameters of Au_2(3,10-chrysene dithiolate). Units are Å. Energy = -1759.261710 Hartree.

atom	x	y	z
C	-0.03	0.00	0.03
C	0.01	0.00	1.43
C	1.23	0.00	2.06
C	2.42	0.00	1.30
C	2.42	0.00	-0.14
C	1.12	0.00	-0.76
C	3.73	0.00	-0.80
C	4.94	0.00	-0.03
C	4.86	0.00	1.39
C	3.65	0.00	2.02
C	3.88	0.00	-2.23
C	5.10	0.00	-2.85
C	6.31	0.00	-2.11
C	6.24	0.00	-0.69
C	7.57	0.00	-2.75
C	8.74	0.00	-2.02
C	8.69	0.00	-0.61
C	7.46	0.00	0.03
S	10.11	0.00	0.48
Au	12.00	0.00	-0.86
H	-1.00	0.00	-0.45
H	5.76	0.00	1.99
H	3.61	0.00	3.11
H	7.61	0.00	-3.83
H	9.70	0.00	-2.53
H	7.45	0.00	1.12
H	5.14	0.00	-3.94
S	0.89	0.00	-2.55
H	-0.92	0.00	2.00
H	1.30	0.00	3.14
H	3.01	0.00	-2.86
Au	-1.38	0.00	-3.01

Table S22. Geometrical parameters of Au_2(3,11-chrysene dithiolate). Units are Å. Energy = -1759.260656 Hartree.

atom	x	y	z
C	-0.09	0.00	0.12
C	-0.05	0.00	1.52
C	1.18	0.00	2.14
C	2.39	0.00	1.40
C	2.37	0.00	-0.04
C	1.08	0.00	-0.62
C	3.64	0.00	-0.78
C	4.86	0.00	-0.02
C	4.80	0.00	1.40
C	3.63	0.00	2.09
C	3.77	0.00	-2.24
C	5.02	0.00	-2.81
C	6.22	0.00	-2.08
C	6.16	0.00	-0.66
C	7.48	0.00	-2.73
C	8.65	0.00	-2.02
C	8.61	0.00	-0.60
C	7.39	0.00	0.05
S	10.22	0.00	0.18
Au	9.87	0.00	2.47
H	-1.04	0.00	-0.40
H	5.72	0.00	1.97
H	3.62	0.00	3.18
H	7.50	0.00	-3.82
H	9.61	0.00	-2.53
H	7.39	0.00	1.14
H	5.10	0.00	-3.90
S	2.33	0.00	-3.34
H	0.97	0.00	-1.70
H	-0.96	0.00	2.10
H	1.26	0.00	3.23
Au	3.10	0.00	-5.53

Table S23. Geometrical parameters of Au_2(4,11-chrysene dithiolate). Units are Å. Energy = -1759.243062 Hartree.

atom	x	y	z
C	0.00	0.00	0.06
C	0.11	0.00	1.47
C	1.37	0.00	2.15
C	2.55	0.00	1.29
C	2.38	0.00	-0.09
C	1.13	0.00	-0.72
C	1.31	0.00	3.61
C	0.07	0.00	4.35
C	-1.17	0.00	3.58
C	-1.09	0.00	2.21
C	2.52	0.00	4.36
C	2.58	0.00	5.72
C	1.39	0.00	6.49
C	0.12	0.00	5.82
C	1.48	0.00	7.90
C	0.35	0.00	8.69
C	-0.91	0.00	8.06
C	-1.01	0.00	6.68
S	-2.81	0.00	4.32
H	0.42	0.00	9.77
H	-2.01	0.00	6.27
H	3.47	0.00	3.84
S	4.24	0.00	1.92
H	1.07	0.00	-1.80
H	3.27	0.00	-0.72
H	-1.82	0.00	8.65
H	-0.99	0.00	-0.39
H	2.47	0.00	8.35
H	3.54	0.00	6.23
Au	5.70	0.00	0.11
H	-2.01	0.00	1.63
Au	-4.39	0.00	2.62

Table S24. Geometrical parameters of Au_2(4,12-chrysene dithiolate). Units are Å. Energy = -1759.256494 Hartree.

atom	x	y	z
C	0.01	0.00	0.05
C	0.10	0.00	1.46
C	1.39	0.00	2.12
C	2.55	0.00	1.25
C	2.39	0.00	-0.13
C	1.13	0.00	-0.74
C	1.40	0.00	3.59
C	0.17	0.00	4.31
C	-1.06	0.00	3.60
C	-1.11	0.00	2.24
C	2.60	0.00	4.37
C	2.60	0.00	5.74
C	1.39	0.00	6.48
C	0.16	0.00	5.77
C	1.40	0.00	7.90
C	0.22	0.00	8.61
C	-1.01	0.00	7.92
C	-1.04	0.00	6.53
S	-2.66	0.00	1.32
Au	-4.37	0.00	2.88
H	-1.98	0.00	4.15
H	0.23	0.00	9.70
H	-2.00	0.00	6.05
H	3.56	0.00	3.88
S	4.25	0.00	1.88
H	1.06	0.00	-1.82
H	3.27	0.00	-0.76
H	-1.94	0.00	8.47
H	-0.97	0.00	-0.42
H	2.36	0.00	8.41
H	3.55	0.00	6.27
Au	5.70	0.00	0.08

Table S25. Geometrical parameters of Au_2(6,12-chrysene dithiolate). Units are Å. Energy = -1759.271124 Hartree.

atom	x	y	z
C	0.02	0.00	0.02
C	0.00	0.00	1.42
C	1.20	0.00	2.12
C	2.44	0.00	1.44
C	2.46	0.00	0.01
C	1.22	0.00	-0.66
C	3.73	0.00	-0.70
C	4.94	0.00	0.03
C	4.88	0.00	1.46
C	3.70	0.00	2.16
C	3.79	0.00	-2.12
C	4.96	0.00	-2.82
C	6.22	0.00	-2.11
C	6.20	0.00	-0.68
C	7.47	0.00	-2.78
C	8.66	0.00	-2.09
C	8.65	0.00	-0.69
C	7.45	0.00	0.00
H	5.81	0.00	2.02
H	7.49	0.00	-3.87
H	9.61	0.00	-2.63
H	7.48	0.00	1.08
S	5.07	0.00	-4.61
H	2.86	0.00	-2.69
H	1.19	0.00	-1.75
H	-0.94	0.00	1.96
H	1.18	0.00	3.20
S	3.60	0.00	3.95
H	9.59	0.00	-0.13
H	-0.92	0.00	-0.54
Au	2.90	0.00	-5.42
Au	5.76	0.00	4.76

Table S26. Geometrical parameters of Au_2(1.5-picene dithiolate). Units are Å. Energy = -1912.897856 Hartree.

atom	x	y	z
C	-0.14	0.00	0.42
C	0.00	0.00	1.80
C	1.03	0.00	-0.43
C	2.30	0.00	0.25
C	2.38	0.00	1.66
C	1.24	0.00	2.43
C	3.53	0.00	-0.51
C	3.50	0.00	-1.88
C	1.04	0.00	-1.90
C	2.27	0.00	-2.61
C	2.31	0.00	-4.06
C	1.10	0.00	-4.80
C	-0.14	0.00	-2.70
C	-0.12	0.00	-4.07
C	3.54	0.00	-4.79
C	3.57	0.00	-6.16
C	1.12	0.00	-6.25
C	2.37	0.00	-6.93
C	2.41	0.00	-8.35
C	-0.06	0.00	-7.04
C	0.00	0.00	-8.43
C	1.25	0.00	-9.09
H	3.35	0.00	2.15
H	1.30	0.00	3.52
H	-0.89	0.00	2.42
S	-1.83	0.00	-0.24
S	5.07	0.00	0.43
H	4.43	0.00	-2.41
H	-1.11	0.00	-2.23
H	4.49	0.00	-4.27
H	4.53	0.00	-6.68
H	3.38	0.00	-8.84
H	1.29	0.00	-10.17
H	-1.03	0.00	-6.57
Au	6.80	0.00	-1.11
H	-1.07	0.00	-4.59
H	-0.92	0.00	-9.00
Au	-3.31	0.00	1.55

Table S27. Geometrical parameters of Au_2(1,8-picene dithiolate). Units are Å. Energy = -1912.899853 Hartree.

atom	x	y	z
C	-0.15	0.00	0.42
C	0.02	0.00	1.81
C	1.02	0.00	-0.44
C	2.29	0.00	0.23
C	2.40	0.00	1.64
C	1.27	0.00	2.42
C	3.50	0.00	-0.53
C	3.50	0.00	-1.88
C	1.04	0.00	-1.91
C	2.28	0.00	-2.62
C	2.30	0.00	-4.07
C	1.09	0.00	-4.81
C	-0.14	0.00	-2.71
C	-0.12	0.00	-4.08
C	3.53	0.00	-4.80
C	3.60	0.00	-6.17
C	1.13	0.00	-6.26
C	2.38	0.00	-6.95
C	2.39	0.00	-8.37
C	-0.06	0.00	-7.04
C	-0.02	0.00	-8.42
C	1.21	0.00	-9.09
H	3.39	0.00	2.08
H	1.34	0.00	3.51
H	-0.86	0.00	2.44
S	-1.83	0.00	-0.22
H	4.45	0.00	-2.40
H	-1.11	0.00	-2.24
S	5.13	0.00	-7.10
H	3.33	0.00	-8.89
H	1.24	0.00	-10.18
H	-1.02	0.00	-6.55
H	-1.07	0.00	-4.59
H	-0.95	0.00	-8.98
Au	-3.30	0.00	1.57
H	4.44	0.00	0.02
H	4.47	0.00	-4.26
Au	6.86	0.00	-5.57

Table S28. Geometrical parameters of Au_2(2,6-picene dithiolate). Units are Å. Energy = -1912.899840 Hartree.

atom	x	y	z
C	-0.10	0.00	0.28
C	-0.11	0.00	1.67
C	1.11	0.00	-0.45
C	2.33	0.00	0.30
C	2.29	0.00	1.71
C	1.10	0.00	2.39
C	3.56	0.00	-0.42
C	3.59	0.00	-1.78
C	1.16	0.00	-1.90
C	2.41	0.00	-2.60
C	2.45	0.00	-4.06
C	1.20	0.00	-4.77
C	-0.03	0.00	-2.66
C	-0.01	0.00	-4.02
C	3.67	0.00	-4.89
C	3.55	0.00	-6.26
C	1.11	0.00	-6.22
C	2.32	0.00	-6.96
C	2.28	0.00	-8.37
C	-0.10	0.00	-6.94
C	-0.13	0.00	-8.33
C	1.08	0.00	-9.05
H	3.24	0.00	2.25
H	1.08	0.00	3.48
H	-1.06	0.00	2.20
H	-1.06	0.00	-0.23
H	4.49	0.00	0.14
H	4.56	0.00	-2.24
H	-0.99	0.00	-2.16
H	-0.96	0.00	-4.54
S	5.33	0.00	-4.20
H	4.45	0.00	-6.87
H	3.22	0.00	-8.93
H	1.07	0.00	-10.14
S	-1.77	0.00	-9.06
H	-1.05	0.00	-6.41
Au	-1.47	0.00	-11.36
Au	6.86	0.00	-5.95

Table S29. Geometrical parameters of Au_2(2,7-picene dithiolate). Units are Å. Energy = -1912.899968 Hartree.

atom	x	y	z
C	-0.06	0.00	0.29
C	-0.08	0.00	1.68
C	1.15	0.00	-0.45
C	2.37	0.00	0.29
C	2.33	0.00	1.70
C	1.14	0.00	2.39
C	3.59	0.00	-0.43
C	3.62	0.00	-1.80
C	1.19	0.00	-1.90
C	2.43	0.00	-2.61
C	2.46	0.00	-4.07
C	1.21	0.00	-4.77
C	-0.01	0.00	-2.65
C	0.00	0.00	-4.01
C	3.67	0.00	-4.91
C	3.55	0.00	-6.28
C	1.11	0.00	-6.22
C	2.31	0.00	-6.97
C	2.27	0.00	-8.39
C	-0.11	0.00	-6.94
C	-0.13	0.00	-8.32
C	1.07	0.00	-9.05
H	3.28	0.00	2.25
H	1.14	0.00	3.48
S	-1.70	0.00	2.43
H	-1.01	0.00	-0.23
H	4.53	0.00	0.12
H	4.59	0.00	-2.26
H	-0.97	0.00	-2.15
H	-0.95	0.00	-4.53
S	5.35	0.00	-4.22
H	4.45	0.00	-6.89
H	3.21	0.00	-8.93
H	1.04	0.00	-10.14
H	-1.09	0.00	-8.84
H	-1.06	0.00	-6.41
Au	-1.39	0.00	4.72
Au	6.86	0.00	-5.99

Table S30. Geometrical parameters of Au_2(3,10-picene dithiolate). Units are Å. Energy = -1912.919808 Hartree.

atom	x	y	z
C	-0.06	0.00	0.33
C	-0.03	0.00	1.71
C	1.12	0.00	-0.45
C	2.36	0.00	0.25
C	2.38	0.00	1.67
C	1.21	0.00	2.40
C	3.58	0.00	-0.50
C	3.57	0.00	-1.86
C	1.12	0.00	-1.90
C	2.35	0.00	-2.61
C	2.35	0.00	-4.06
C	1.12	0.00	-4.77
C	-0.08	0.00	-2.65
C	-0.08	0.00	-4.02
C	3.57	0.00	-4.82
C	3.58	0.00	-6.18
C	1.12	0.00	-6.22
C	2.36	0.00	-6.93
C	2.38	0.00	-8.34
C	-0.06	0.00	-7.00
C	-0.03	0.00	-8.38
C	1.21	0.00	-9.08
H	3.34	0.00	2.17
S	1.06	0.00	4.18
H	-0.96	0.00	2.26
H	-1.03	0.00	-0.15
H	4.52	0.00	0.05
H	4.53	0.00	-2.37
H	-1.04	0.00	-2.14
H	-1.04	0.00	-4.54
H	4.53	0.00	-4.30
H	4.52	0.00	-6.72
H	3.34	0.00	-8.85
H	-0.96	0.00	-8.94
H	-1.03	0.00	-6.52
S	1.06	0.00	-10.86
Au	3.21	0.00	5.03
Au	3.21	0.00	-11.70

Table S31. Geometrical parameters of Au_2(4,11-picene dithiolate). Units are Å. Energy = -1912.915251 Hartree.

atom	x	y	z
C	0.00	0.00	0.05
C	0.00	0.00	1.51
C	1.21	0.00	-0.70
C	1.21	0.00	-2.07
C	0.01	0.00	-2.82
C	-1.22	0.00	-2.11
C	-1.23	0.00	-0.66
H	2.17	0.00	-0.19
H	2.17	0.00	-2.58
C	-1.24	0.00	2.20
C	-1.25	0.00	3.61
C	-0.08	0.00	4.34
C	1.17	0.00	3.66
C	1.19	0.00	2.27
H	-2.20	0.00	4.13
H	-0.11	0.00	5.42
H	2.15	0.00	1.78
C	-2.46	0.00	1.45
C	-2.45	0.00	0.09
C	0.02	0.00	-4.28
C	-1.23	0.00	-4.99
C	-2.44	0.00	-2.87
C	-2.44	0.00	-4.23
H	-3.40	0.00	1.99
H	-3.40	0.00	-0.43
H	-3.39	0.00	-2.36
C	1.22	0.00	-5.02
S	2.77	0.00	4.46
Au	2.39	0.00	6.74
C	1.20	0.00	-6.40
C	-0.02	0.00	-7.10
C	-1.22	0.00	-6.42
H	2.13	0.00	-6.96
H	-0.01	0.00	-8.19
H	2.18	0.00	-4.52
H	-3.39	0.00	-4.75
S	-2.83	0.00	-7.23
Au	-2.43	0.00	-9.51

Table S32. Geometrical parameters of Au_2(5,11-picene dithiolate). Units are Å. Energy = -1912.908130 Hartree.

atom	x	y	z
C	0.01	0.00	0.04
C	-0.01	0.00	1.49
C	1.23	0.00	-0.70
C	1.25	0.00	-2.06
C	0.05	0.00	-2.83
C	-1.18	0.00	-2.14
C	-1.21	0.00	-0.69
H	2.18	0.00	-0.17
H	2.21	0.00	-2.56
C	-1.26	0.00	2.17
C	-1.28	0.00	3.58
C	-0.12	0.00	4.33
C	1.13	0.00	3.67
C	1.17	0.00	2.28
H	-2.25	0.00	4.09
H	-0.16	0.00	5.41
H	2.14	0.00	1.79
C	-2.47	0.00	1.41
C	-2.44	0.00	0.04
C	0.06	0.00	-4.28
C	-1.17	0.00	-5.02
C	-2.38	0.00	-2.90
C	-2.41	0.00	-4.28
H	-3.42	0.00	1.94
H	-3.39	0.00	-0.49
H	-3.33	0.00	-2.38
C	1.27	0.00	-5.01
S	2.72	0.00	4.48
Au	2.33	0.00	6.76
C	1.30	0.00	-6.39
C	0.10	0.00	-7.11
C	-1.11	0.00	-6.44
H	2.25	0.00	-6.92
H	0.10	0.00	-8.20
H	2.22	0.00	-4.48
H	-2.02	0.00	-7.01
S	-4.12	0.00	-4.85
Au	-4.42	0.00	-7.14

Table S33. Geometrical parameters of Au_2(5,13-picene dithiolate). Units are Å. Energy = -1912.891235 Hartree.

atom	x	y	z
C	-0.06	0.00	-0.02
C	-0.02	0.00	1.40
C	1.26	0.00	2.04
C	2.42	0.00	1.23
C	2.35	0.00	-0.15
C	1.09	0.00	-0.78
C	-1.20	0.00	2.23
C	-1.07	0.00	3.60
C	0.19	0.00	4.28
C	1.36	0.00	3.49
C	0.29	0.00	5.72
C	1.56	0.00	6.39
C	2.74	0.00	5.54
C	2.60	0.00	4.17
C	-0.91	0.00	6.50
C	-0.90	0.00	7.85
C	0.32	0.00	8.58
C	1.57	0.00	7.86
C	0.29	0.00	9.99
C	1.45	0.00	10.74
C	2.68	0.00	10.06
C	2.73	0.00	8.68
S	-2.95	0.00	1.79
Au	-3.41	0.00	-0.47
S	4.42	0.00	6.21
H	3.50	0.00	3.58
H	-0.68	0.00	10.48
H	1.41	0.00	11.82
H	3.71	0.00	8.23
H	-1.84	0.00	8.41
H	-1.87	0.00	6.00
H	-1.98	0.00	4.18
H	3.26	0.00	-0.74
H	1.02	0.00	-1.87
H	3.40	0.00	1.68
H	-1.02	0.00	-0.52
H	3.61	0.00	10.62
Au	5.91	0.00	4.43

Table S34. Geometrical parameters of Au_2(5,14-picene dithiolate). Units are Å. Energy = -1912.898203 Hartree.

atom	x	y	z
C	-0.06	0.00	0.38
C	0.00	0.00	1.76
C	1.11	0.00	-0.41
C	2.36	0.00	0.26
C	2.40	0.00	1.68
C	1.24	0.00	2.42
C	3.56	0.00	-0.51
C	3.54	0.00	-1.88
C	1.09	0.00	-1.87
C	2.30	0.00	-2.61
C	2.24	0.00	-4.05
C	1.00	0.00	-4.77
C	-0.12	0.00	-2.59
C	-0.21	0.00	-3.97
C	3.47	0.00	-4.78
C	3.56	0.00	-6.14
C	1.08	0.00	-6.24
C	2.34	0.00	-6.91
C	2.40	0.00	-8.33
C	-0.06	0.00	-7.08
C	0.01	0.00	-8.46
C	1.26	0.00	-9.10
H	3.37	0.00	2.17
H	1.28	0.00	3.50
H	-0.92	0.00	2.34
H	-1.04	0.00	-0.09
H	4.52	0.00	0.01
H	4.48	0.00	-2.40
H	-1.04	0.00	-2.03
S	-1.86	0.00	-4.70
H	4.40	0.00	-4.22
S	5.10	0.00	-7.05
H	3.37	0.00	-8.82
H	1.33	0.00	-10.19
H	-0.91	0.00	-9.04
H	-1.05	0.00	-6.65
Au	6.81	0.00	-5.48
Au	-3.42	0.00	-2.98

Table S35. Geometrical parameters of Au_2(6,14-picene dithiolate). Units are Å. Energy = -1912.877456 Hartree.

atom	x	y	z
C	-0.09	0.00	0.33
C	-0.08	0.00	1.72
C	1.11	0.00	-0.42
C	2.33	0.00	0.31
C	2.33	0.00	1.72
C	1.14	0.00	2.42
C	3.55	0.00	-0.43
C	3.56	0.00	-1.79
C	1.15	0.00	-1.88
C	2.38	0.00	-2.60
C	2.36	0.00	-4.06
C	1.10	0.00	-4.78
C	-0.05	0.00	-2.60
C	-0.12	0.00	-3.97
C	3.60	0.00	-4.86
C	3.52	0.00	-6.23
C	1.07	0.00	-6.24
C	2.31	0.00	-6.95
C	2.36	0.00	-8.36
C	-0.08	0.00	-7.07
C	-0.03	0.00	-8.45
C	1.21	0.00	-9.12
H	3.28	0.00	2.25
H	1.14	0.00	3.51
H	-1.02	0.00	2.26
H	-1.05	0.00	-0.17
H	4.49	0.00	0.11
H	4.54	0.00	-2.25
H	-0.98	0.00	-2.05
S	-1.79	0.00	-4.68
S	5.27	0.00	-4.16
H	4.43	0.00	-6.81
H	3.34	0.00	-8.84
H	1.25	0.00	-10.20
H	-0.95	0.00	-9.01
H	-1.07	0.00	-6.63
Au	6.81	0.00	-5.91
Au	-3.34	0.00	-2.95

Table S36. Geometrical parameters of Au_2(1,6-perylene dithiolate). Units are Å. Energy = -1835.466283 Hartree.

atom	x	y	z
C	0.02	0.00	0.00
C	-0.04	0.00	1.41
C	1.15	0.00	2.19
C	2.43	0.00	1.49
C	2.42	0.00	0.06
C	1.21	0.00	-0.66
C	3.71	0.00	2.18
C	3.69	0.00	3.66
C	2.44	0.00	4.36
C	1.18	0.00	3.67
C	4.85	0.00	4.44
C	4.85	0.00	5.85
C	3.66	0.00	6.52
C	2.44	0.00	5.80
C	0.03	0.00	4.46
C	0.03	0.00	5.86
C	1.23	0.00	6.53
C	3.63	0.00	-0.67
C	4.82	0.00	-0.02
C	4.90	0.00	1.39
S	-1.71	0.00	2.10
S	6.57	0.00	2.07
H	1.27	0.00	7.62
H	-0.91	0.00	6.40
H	-0.90	0.00	-0.57
H	1.24	0.00	-1.75
H	5.74	0.00	-0.60
H	3.59	0.00	-1.76
H	5.80	0.00	6.37
H	3.63	0.00	7.61
H	-0.95	0.00	4.00
H	5.82	0.00	3.98
Au	8.10	0.00	0.32
Au	-3.25	0.00	0.36

Table S37. Geometrical parameters of Au_2(2,5-perylene dithiolate). Units are Å. Energy = -1835.499454 Hartree.

atom	x	y	z
C	-0.01	0.00	0.00
C	0.00	0.00	1.41
C	1.18	0.00	2.14
C	2.43	0.00	1.45
C	2.42	0.00	0.02
C	1.19	0.00	-0.69
C	3.68	0.00	2.14
C	3.69	0.00	3.61
C	2.44	0.00	4.32
C	1.18	0.00	3.62
C	4.87	0.00	4.35
C	4.87	0.00	5.76
C	3.68	0.00	6.45
C	2.44	0.00	5.75
C	0.01	0.00	4.37
C	0.02	0.00	5.77
C	1.21	0.00	6.46
C	3.65	0.00	-0.70
C	4.85	0.00	-0.02
C	4.86	0.00	1.40
H	-0.96	0.00	1.92
H	5.82	0.00	1.90
H	1.23	0.00	7.55
H	-0.92	0.00	6.31
S	-1.48	0.00	-1.02
H	1.21	0.00	-1.77
S	6.32	0.00	-1.05
H	3.62	0.00	-1.78
H	5.81	0.00	6.29
H	3.67	0.00	7.54
H	-0.95	0.00	3.87
H	5.83	0.00	3.85
Au	-3.30	0.00	0.40
Au	8.15	0.00	0.36

Table S38. Geometrical parameters of Au_2(2,6-perylene dithiolate). Units are Å. Energy = -1835.484828 Hartree.

atom	x	y	z
C	0.06	0.00	-0.11
C	0.02	0.00	1.30
C	1.16	0.00	2.10
C	2.43	0.00	1.42
C	2.47	0.00	-0.02
C	1.26	0.00	-0.77
C	3.67	0.00	2.13
C	3.64	0.00	3.60
C	2.38	0.00	4.29
C	1.11	0.00	3.59
C	4.82	0.00	4.33
C	4.86	0.00	5.73
C	3.66	0.00	6.42
C	2.43	0.00	5.72
C	-0.07	0.00	4.38
C	0.03	0.00	5.80
C	1.22	0.00	6.45
C	3.71	0.00	-0.70
C	4.89	0.00	0.01
C	4.86	0.00	1.41
H	-0.96	0.00	1.74
H	5.81	0.00	1.93
H	1.25	0.00	7.54
H	-0.89	0.00	6.38
H	-0.88	0.00	-0.66
H	1.31	0.00	-1.85
H	5.85	0.00	-0.51
H	3.71	0.00	-1.79
S	6.34	0.00	6.74
H	3.63	0.00	7.51
S	-1.73	0.00	3.69
H	5.77	0.00	3.81
Au	8.14	0.00	5.29
Au	-3.26	0.00	5.44

Table S39. Geometrical parameters of Au_2(2,7-perylene dithiolate). Units are Å. Energy = -1835.485243 Hartree.

atom	x	y	z
C	0.00	0.00	-0.03
C	-0.08	0.00	1.39
C	1.10	0.00	2.18
C	2.37	0.00	1.47
C	2.41	0.00	0.04
C	1.20	0.00	-0.68
C	3.63	0.00	2.16
C	3.66	0.00	3.63
C	2.42	0.00	4.35
C	1.15	0.00	3.67
C	4.86	0.00	4.34
C	4.90	0.00	5.75
C	3.72	0.00	6.46
C	2.47	0.00	5.78
C	0.02	0.00	4.48
C	0.06	0.00	5.88
C	1.27	0.00	6.53
C	3.64	0.00	-0.66
C	4.83	0.00	0.02
C	4.81	0.00	1.42
S	-1.74	0.00	2.09
H	5.77	0.00	1.93
H	1.33	0.00	7.62
H	-0.87	0.00	6.44
H	-0.92	0.00	-0.60
H	1.22	0.00	-1.77
H	5.78	0.00	-0.50
H	3.62	0.00	-1.75
S	6.55	0.00	6.44
H	3.72	0.00	7.54
H	-0.97	0.00	4.04
H	5.80	0.00	3.81
Au	6.30	0.00	8.74
Au	-3.28	0.00	0.35

Table S40. Geometrical parameters of Au_2(2,8-perylene dithiolate). Units are Å. Energy = -1835.500622 Hartree.

atom	x	y	z
C	-0.01	0.00	-0.01
C	0.00	0.00	1.41
C	1.18	0.00	2.14
C	2.43	0.00	1.44
C	2.42	0.00	0.01
C	1.19	0.00	-0.69
C	3.68	0.00	2.14
C	3.68	0.00	3.62
C	2.43	0.00	4.31
C	1.18	0.00	3.62
C	4.86	0.00	4.35
C	4.87	0.00	5.77
C	3.67	0.00	6.45
C	2.44	0.00	5.75
C	0.01	0.00	4.36
C	0.02	0.00	5.77
C	1.21	0.00	6.45
C	3.65	0.00	-0.70
C	4.85	0.00	-0.01
C	4.86	0.00	1.39
H	-0.95	0.00	1.92
H	5.82	0.00	1.89
H	1.23	0.00	7.54
H	-0.92	0.00	6.31
S	-1.64	0.00	-0.73
H	1.21	0.00	-1.78
H	5.79	0.00	-0.55
H	3.63	0.00	-1.79
S	6.51	0.00	6.49
H	3.66	0.00	7.54
H	-0.96	0.00	3.87
H	5.82	0.00	3.84
Au	-1.35	0.00	-3.03
Au	6.21	0.00	8.78

Table S41. Geometrical parameters of Au_2(3,9-perylene dithiolate). Units are Å. Energy = -1835.495206 Hartree.

atom	x	y	z
C	0.01	0.00	0.00
C	0.02	0.00	1.40
C	1.19	0.00	2.14
C	2.43	0.00	1.43
C	2.44	0.00	-0.01
C	1.19	0.00	-0.72
C	3.68	0.00	2.14
C	3.67	0.00	3.61
C	2.43	0.00	4.33
C	1.19	0.00	3.62
C	4.85	0.00	4.36
C	4.85	0.00	5.76
C	3.67	0.00	6.48
C	2.42	0.00	5.77
C	0.00	0.00	4.34
C	-0.01	0.00	5.74
C	1.18	0.00	6.45
C	3.69	0.00	-0.69
C	4.87	0.00	0.01
C	4.87	0.00	1.41
H	-0.95	0.00	1.89
H	5.82	0.00	1.92
H	1.16	0.00	7.53
H	-0.95	0.00	6.28
H	-0.94	0.00	-0.52
S	1.28	0.00	-2.51
H	5.82	0.00	-0.52
H	3.71	0.00	-1.78
H	5.81	0.00	6.28
S	3.58	0.00	8.27
H	-0.96	0.00	3.83
H	5.81	0.00	3.86
Au	5.76	0.00	9.05
Au	-0.89	0.00	-3.30

Table S42. Geometrical parameters of Au_2(3.10-perylene dithiolate). Units are Å. Energy = -1835.495092 Hartree.

atom	x	y	z
C	-0.01	0.00	0.01
C	0.00	0.00	1.42
C	1.19	0.00	2.14
C	2.43	0.00	1.43
C	2.42	0.00	-0.01
C	1.17	0.00	-0.69
C	3.67	0.00	2.14
C	3.68	0.00	3.61
C	2.44	0.00	4.33
C	1.19	0.00	3.62
C	4.86	0.00	4.34
C	4.87	0.00	5.75
C	3.69	0.00	6.47
C	2.44	0.00	5.77
C	0.01	0.00	4.35
C	0.01	0.00	5.76
C	1.20	0.00	6.45
C	3.67	0.00	-0.73
C	4.85	0.00	-0.01
C	4.85	0.00	1.39
H	-0.96	0.00	1.93
H	5.81	0.00	1.89
H	1.18	0.00	7.54
H	-0.93	0.00	6.29
H	-0.96	0.00	-0.51
H	5.80	0.00	-0.53
S	3.57	0.00	-2.52
H	5.82	0.00	6.26
S	3.61	0.00	8.26
H	-0.95	0.00	3.85
H	5.82	0.00	3.84
Au	5.79	0.00	9.03
H	1.15	0.00	-1.77
Au	5.75	0.00	-3.30

Table S43. Geometrical parameters of Au_2(6,12-perylene dithiolate). Units are Å. Energy = -1835.467830 Hartree.

atom	x	y	z
C	0.08	0.00	-0.09
C	0.07	0.00	1.31
C	1.21	0.00	2.12
C	2.49	0.00	1.44
C	2.48	0.00	0.00
C	1.28	0.00	-0.74
C	3.74	0.00	2.16
C	3.66	0.00	3.64
C	2.38	0.00	4.31
C	1.12	0.00	3.59
C	4.80	0.00	4.44
C	4.79	0.00	5.84
C	3.58	0.00	6.50
C	2.38	0.00	5.75
C	-0.08	0.00	4.36
C	-0.03	0.00	5.77
C	1.16	0.00	6.45
C	3.71	0.00	-0.69
C	4.89	0.00	-0.02
C	4.95	0.00	1.40
H	-0.91	0.00	1.77
S	6.60	0.00	2.11
H	1.17	0.00	7.54
H	-0.95	0.00	6.33
H	-0.86	0.00	-0.63
H	1.34	0.00	-1.83
H	5.82	0.00	-0.58
H	3.70	0.00	-1.78
H	5.73	0.00	6.38
H	3.53	0.00	7.58
S	-1.74	0.00	3.65
H	5.78	0.00	3.98
Au	8.17	0.00	0.39
Au	-3.30	0.00	5.36