Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION:

Electron Transport Investigation of Redox-Switching Azulenequinones/Hydroquinones via First-Principles Studies

El-Abed Haidar,[1] Sherif A. Tawfik,[2] Catherine Stampfl,[1] Kimihiko Hirao,[3] Kazunari Yoshizawa,[4] Safinaz H. El-Demerdash,[5] Takahito Nakajima,[3] and Ahmed M. El-Nahas[3,5]

[1]School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia

[2]School of Science, RMIT University, GPO Box 2476 Melbourne, Victoria 3001 Australia.

[3]RIKEN, Advanced Institute for Computational Science, 7-1-26 Minatojima-minami, Chuo, Kobe 650-0047, Japan.

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

[5]Chemistry Department, Faculty of Science, Menoufia University, Shebin El-Kom 32512, Egypt

Fig. S1. The frontier orbitals (FO) for the 4 molecules and their corresponding HOMO-LUMO energy gap calculated using SIESTA LDA:

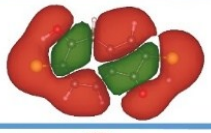
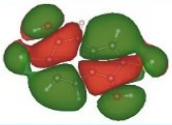
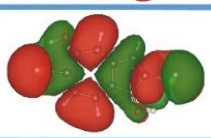
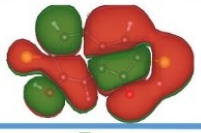
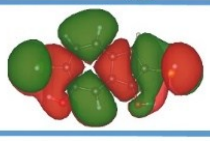
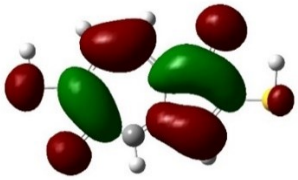
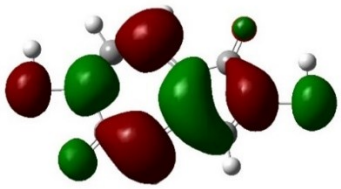
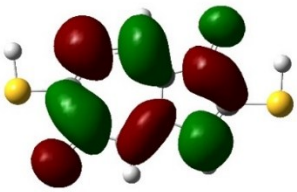
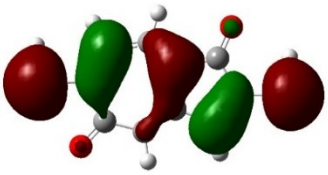
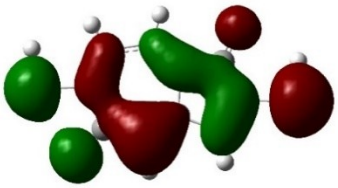
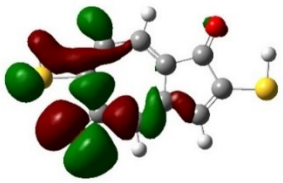
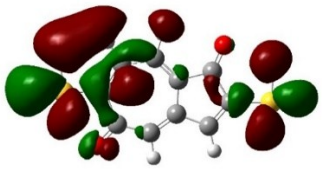
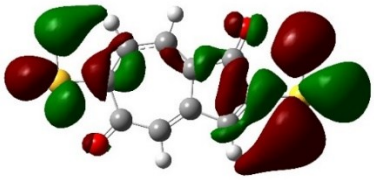
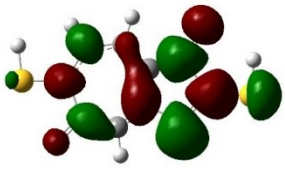
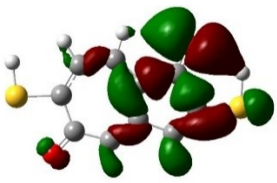
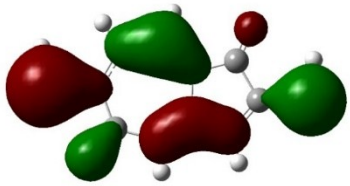
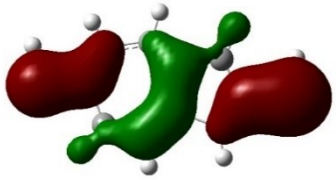
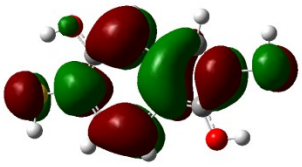
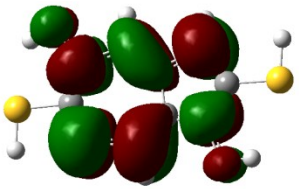
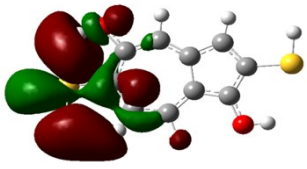
FO	HOMO(H)	LUMO (L)	$E_{gap} = E_L - E_H$
15Q			1.06 eV
15OH			1.16 eV
17Q			0.72 eV
17OH			1.14 eV

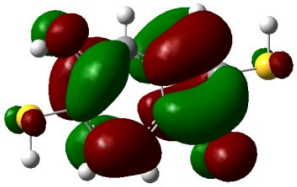
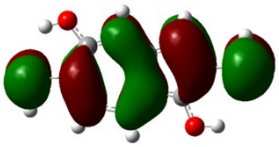
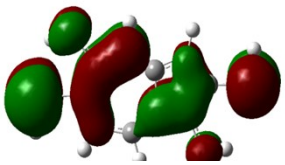
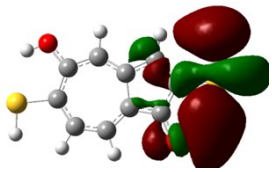
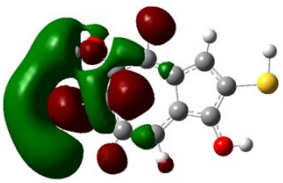
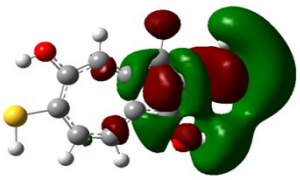
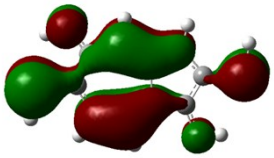
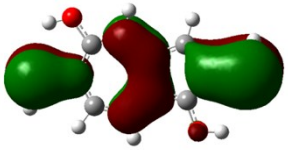
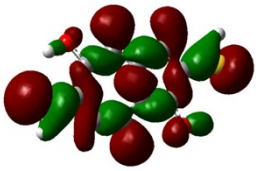
Fig. S2. The Frontier (as well as other) orbitals for the four free molecules, their associated energy levels (in eV) and calculated HOMO-LUMO energy gap at B3LYP/6-31G(d,p) level:

(a) 1,5-azulenequinone 2,6- dithiolate (15Q), ΔE=3.2099 eV:

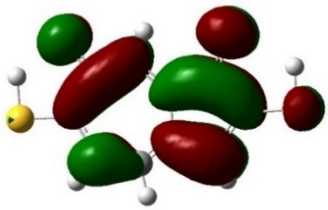
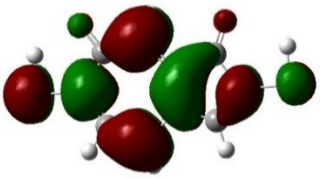
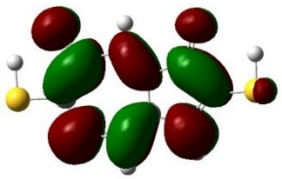
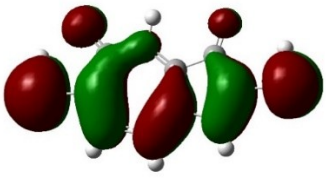
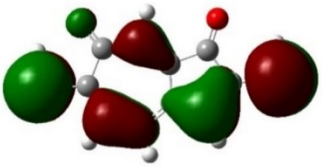
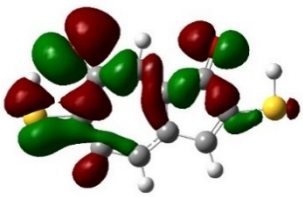
 LUMO E= -3.1740	 LUMO+1 E= -2.3771	 LUMO+2 E= -0.9742
 HOMO E= -6.3839	 HOMO-1 E= -6.5636	 HOMO-2 E= -7.2167
 LUMO+3 E= 0.2618	 LUMO+4 E= 0.3676	 LUMO+5 E= 1.5933
 HOMO-3 E= -7.7067	 HOMO-4 E= -7.8155	 HOMO-5 E= -8.9777

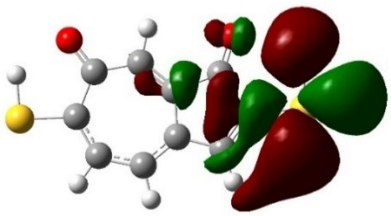
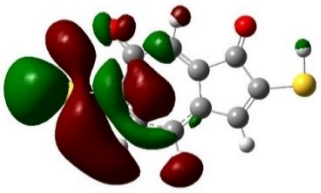
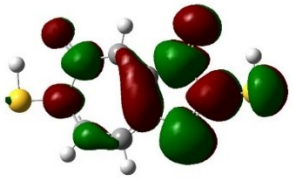
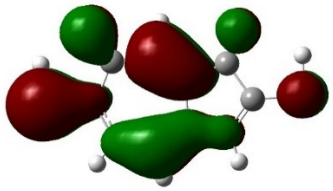
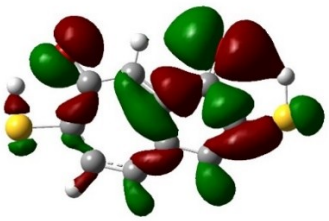
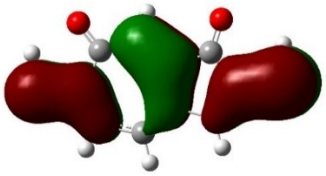
(b) 1,5-azulene hydroquinone 2,6- dithiolate (15OH), ΔE=2.83 eV:

 LUMO E=-1.8857	 LUMO+1 E= -0.8156	 LUMO+2 E= -0.2336

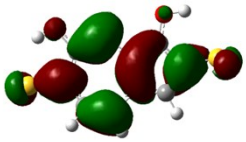
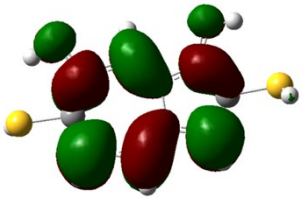
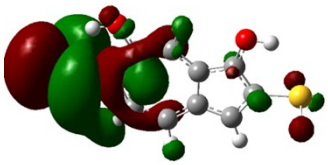
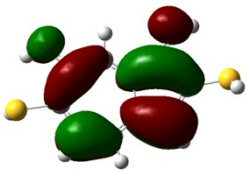
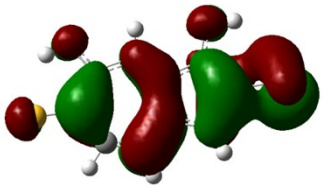
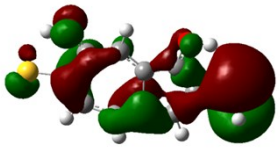
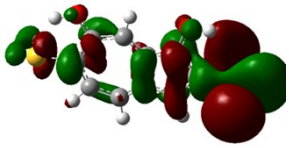
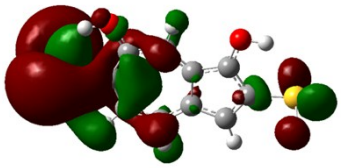
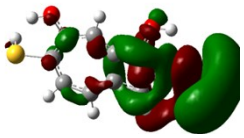
 HOMO E= -4.7131	 HOMO-1 E= -5.6340	 HOMO-2 E= -6.8811
 LUMO+3 E= 0.0242	 LUMO+4 E=1.0340	 LUMO+5 E= 1.5707
 HOMO-3 E= -7.6534	 HOMO-4 E= -8.3601	 HOMO-5 E= -9.1089

(c) 1,7-azulenequinone 2,6- dithiolate (17Q), ΔE=2.6691 eV:

 LUMO E= -3.2219	 LUMO+1 E= -2.4705	 LUMO+2 E= -1.0530
 HOMO E= -5.8910	 HOMO-1 E= -7.1601	 HOMO-2 E= -7.3741

 LUMO+3 E= 0.2884	 LUMO+4 E= 0.4736	 LUMO+5 E= 1.6013
 HOMO-3 E= -7.6760	 HOMO-4 E= -7.8800	 HOMO-5 E= -9.0622

d) 1,7-azulene hydroquinone 2,6- dithiolate (17OH), ΔE=2.53 eV:

 LUMO E= -2.2983	 LUMO+1 E= -0.9472	 LUMO+2 E= 0.2902
 HOMO E= -4.8230	 HOMO-1 E= -6.2965	 HOMO-2 E= -7.2282
 LUMO+3 E= 0.6409	 LUMO+4 E=1.1124	 LUMO+5 E= 1.6770

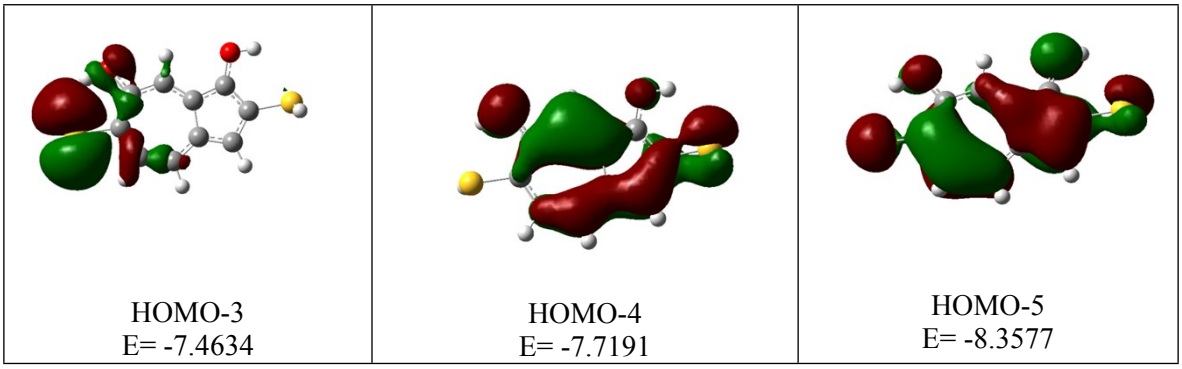
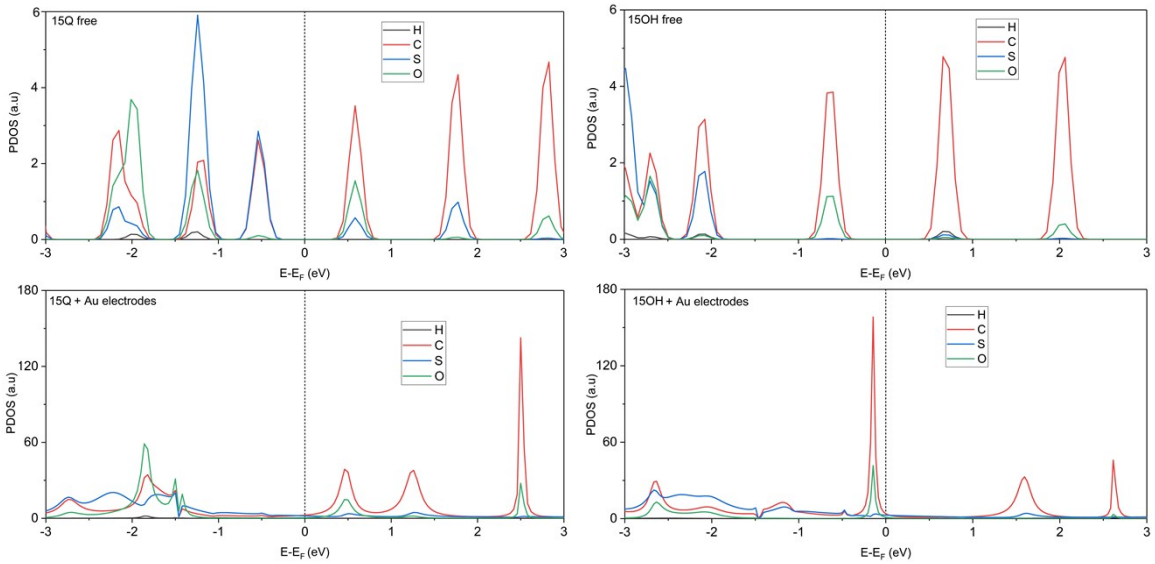


Fig S3**.** Projected Density of States **(**PDOS) of the free molecules and when connected to gold electrodes:

(a) 1,5-azulenequinone 2,6- dithiolate (15Q) (b) 1,5-azulene hydroquinone 2,6- dithiolate (15OH)



(c) 1,7-azulenequinone 2,6-dithiolate (17Q) (d)1,7-azulene hydroquinone 2,6- dithiolate (17OH)

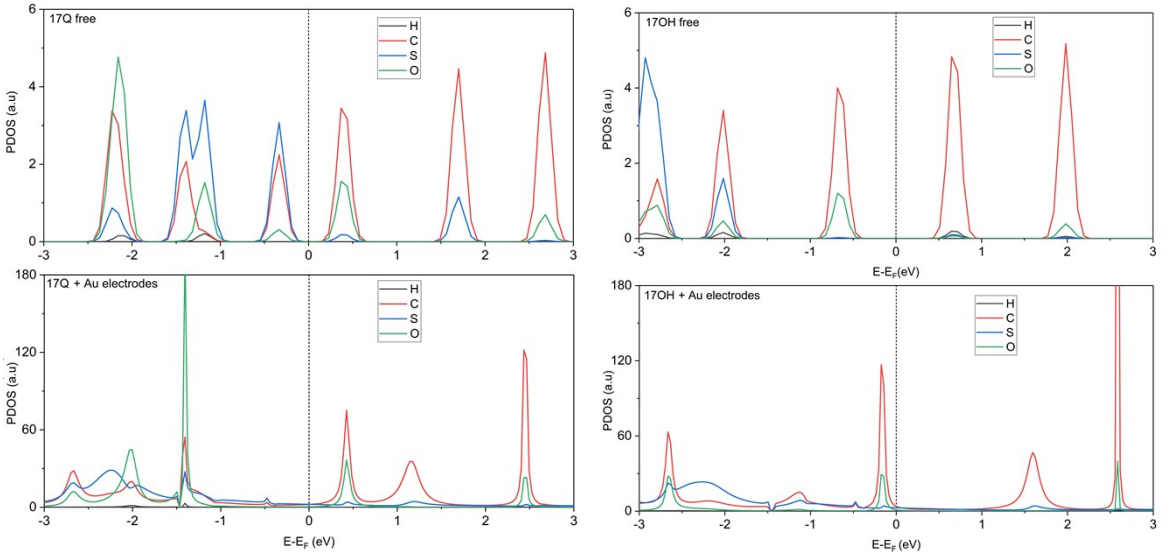
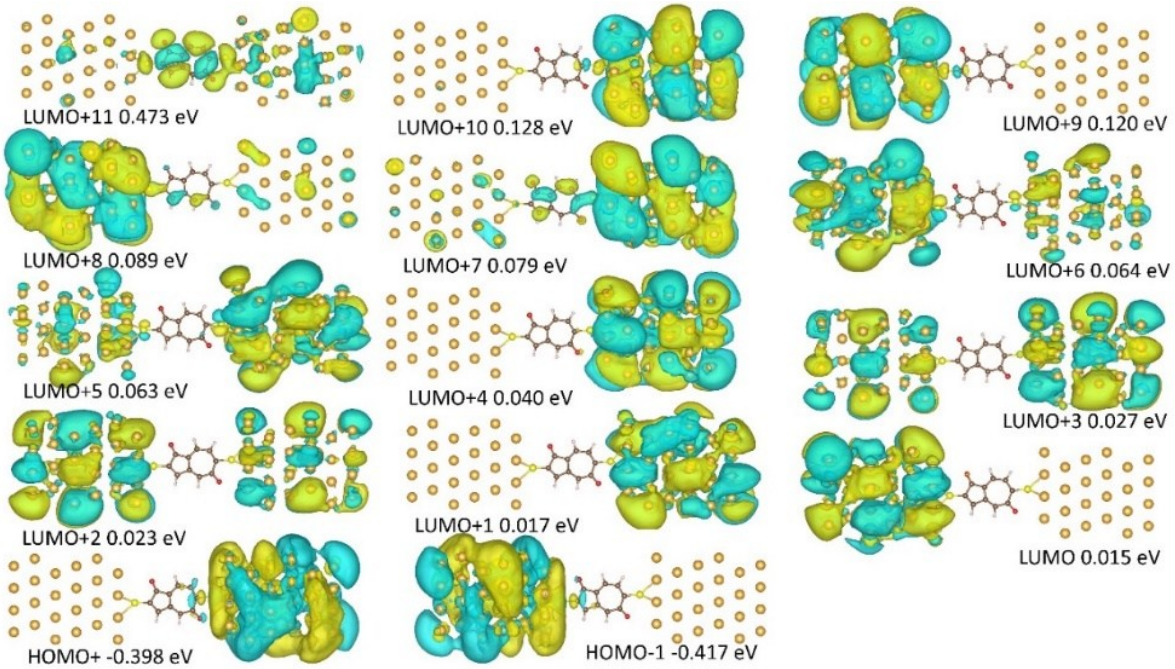
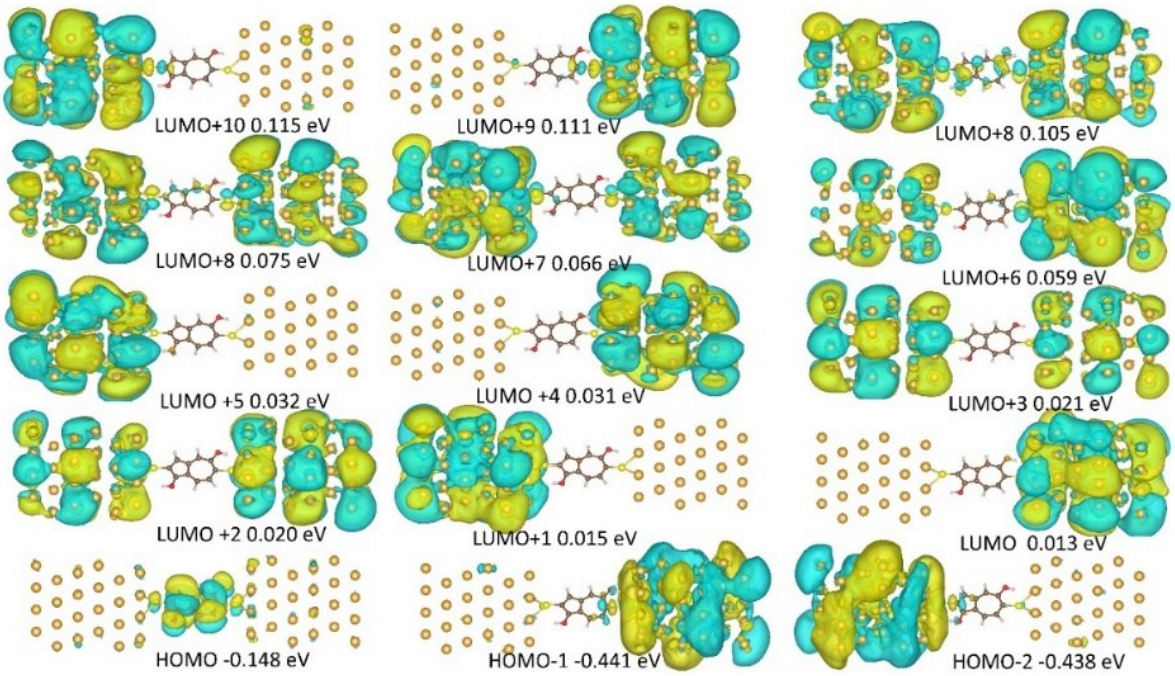


Fig. S4. Molecular Projected Self consistent Hamiltonian (MPSH) states at zero bias voltage for the four molecules.

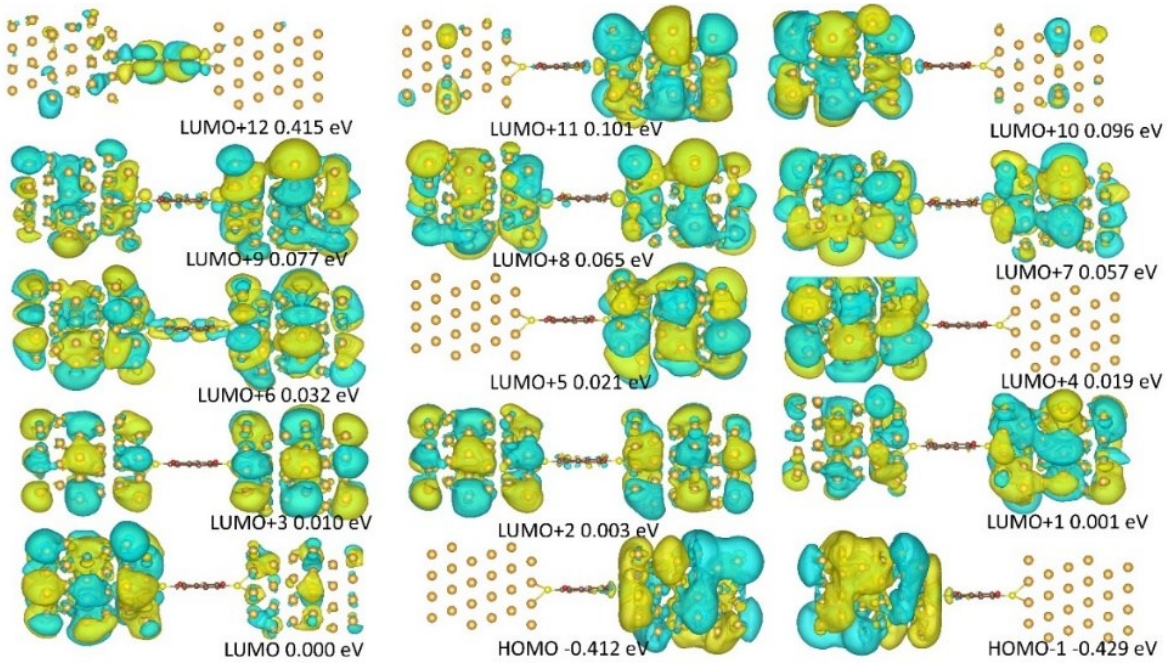
(a) 15Q



(b) 15OH



(c) 17Q


LUMO+12 0.415 eV
LUMO+11 0.101 eV
LUMO+10 0.096 eV
LUMO+9 0.077 eV
LUMO+8 0.065 eV
LUMO+7 0.057 eV
LUMO+6 0.032 eV
LUMO+5 0.021 eV
LUMO+4 0.019 eV
LUMO+3 0.010 eV
LUMO+2 0.003 eV
LUMO+1 0.001 eV
LUMO 0.000 eV
HOMO -0.412 eV
HOMO-1 -0.429 eV

(d) 17OH

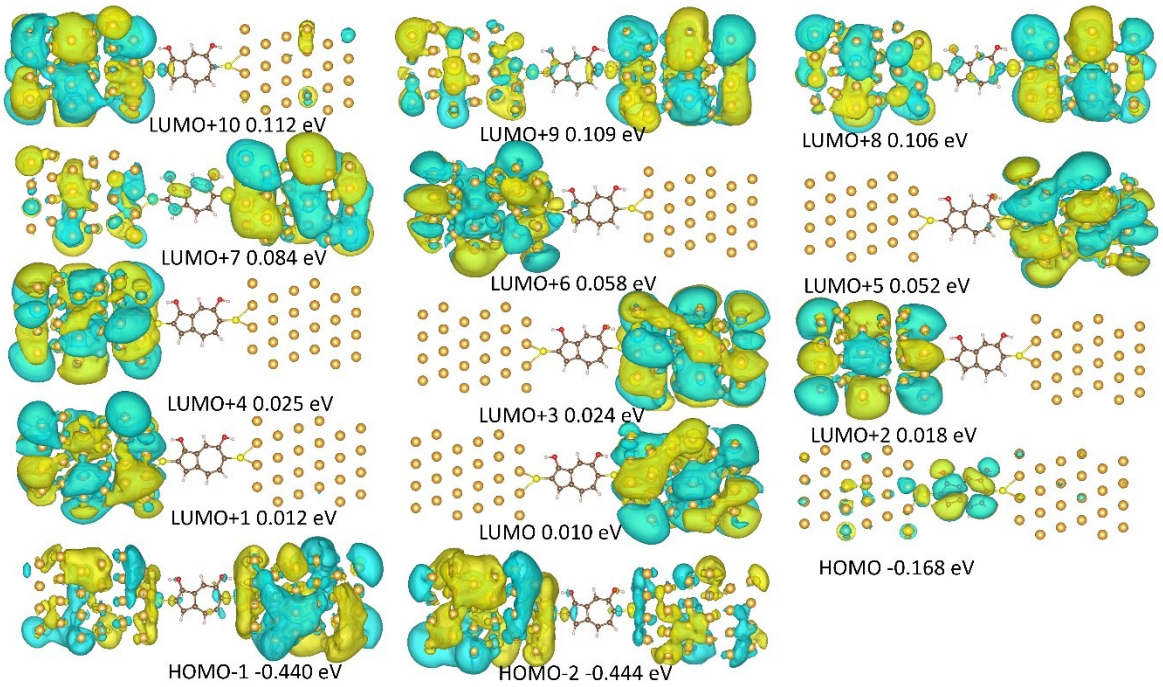
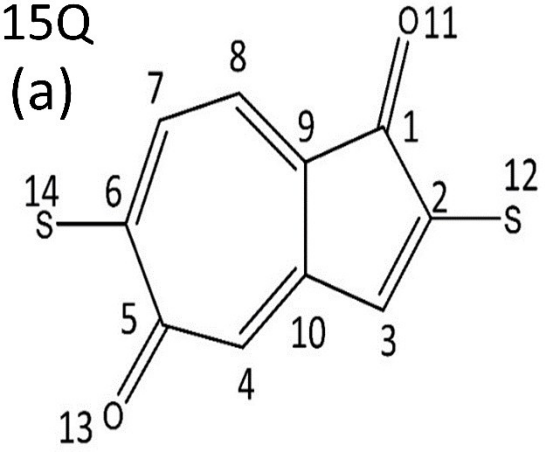

LUMO+10 0.112 eV
LUMO+9 0.109 eV
LUMO+8 0.106 eV
LUMO+7 0.084 eV
LUMO+6 0.058 eV
LUMO+5 0.052 eV
LUMO+4 0.025 eV
LUMO+3 0.024 eV
LUMO+2 0.018 eV
LUMO+1 0.012 eV
LUMO 0.010 eV
HOMO -0.168 eV
HOMO-1 -0.440 eV
HOMO-2 -0.444 eV

Fig. S5. Schematic diagrams of the other three molecules (with IUPAC numbering) (a), the corresponding matrix A from graph theory (from Eqs (3), (4) and (5)) (b), and the Green function $G(E_F)$. Note that $G(E_F)= -A^{-1}$ with A^{-1} the inverse of A.

15Q

(a)



(b)

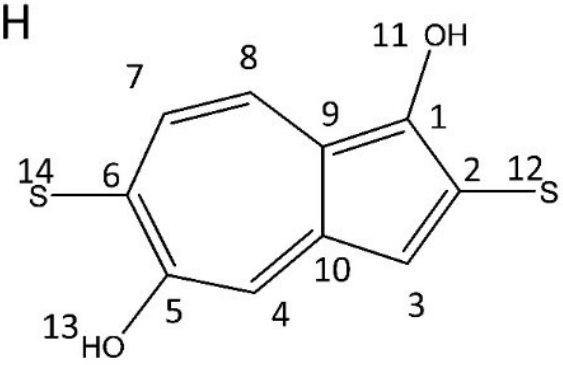
$$A=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\\11\\12\\13\\14 \end{array}\begin{array}{c}\begin{array}{cccccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \end{array}\\ \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{3}{8} & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{8} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{8} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{8} \end{bmatrix}\end{array}$$

(c)

$$G(E_F)=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\\11\\12\\13\\14 \end{array}\begin{array}{c}\begin{array}{cccccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \end{array}\\ \begin{bmatrix} -1.17 & -0.86 & 0.97 & -0.18 & -0.86 & -0.31 & 0.79 & 0.31 & -0.79 & 0.86 & 1.75 & 0.520 & 1.29 & 0.18 \\ -0.86 & -0.31 & -0.21 & 0.39 & -0.31 & -0.56 & 0.18 & 0.56 & -0.18 & 0.31 & 1.29 & 0.18 & 0.46 & 0.33 \\ 0.97 & -0.21 & -1.02 & 0.27 & 0.79 & 0.18 & -0.75 & -0.18 & 0.75 & -0.79 & -1.46 & 0.12 & -1.19 & -0.11 \\ -0.18 & 0.39 & 0.27 & 0.22 & -0.61 & -0.57 & 0.49 & 0.57 & -0.49 & -0.39 & 0.27 & -0.23 & 0.92 & 0.34 \\ -0.86 & -0.31 & 0.79 & -0.61 & -0.31 & -0.56 & 0.18 & 0.56 & -0.18 & 0.31 & 1.29 & 0.18 & 0.46 & 0.33 \\ -0.31 & -0.56 & 0.18 & -0.57 & -0.56 & 0.25 & -0.39 & -0.25 & 0.39 & 0.56 & 0.46 & 0.33 & 0.84 & -0.15 \\ 0.79 & 0.18 & -0.75 & 0.49 & 0.18 & -0.39 & -0.27 & -0.61 & 0.27 & -0.18 & -1.19 & -0.11 & -0.27 & 0.23 \\ 0.31 & 0.56 & -0.18 & 0.57 & 0.56 & -0.25 & -0.61 & 0.25 & -0.39 & -0.56 & -0.46 & -0.33 & -0.84 & 0.15 \\ -0.79 & -0.18 & 0.75 & -0.49 & -0.18 & 0.39 & 0.27 & -0.39 & -0.27 & 0.18 & 1.19 & 0.11 & 0.27 & -0.23 \\ 0.86 & 0.31 & -0.79 & -0.39 & 0.31 & 0.56 & -0.18 & -0.56 & 0.18 & -0.31 & -1.29 & -0.18 & -0.46 & -0.33 \\ 1.75 & 1.29 & -1.46 & 0.27 & 1.29 & 0.46 & -1.19 & -0.46 & 1.19 & -1.29 & -6.63 & -0.78 & -1.94 & -0.27 \\ 0.52 & 0.18 & 0.12 & -0.23 & 0.18 & 0.33 & -0.11 & -0.33 & 0.11 & -0.18 & -0.78 & -1.71 & -0.27 & -0.2 \\ 1.29 & 0.46 & -1.19 & 0.92 & 0.46 & 0.84 & -0.27 & -0.84 & 0.27 & -0.46 & -1.94 & -0.27 & -4.69 & -0.5 \\ 0.18 & 0.33 & -0.11 & 0.34 & 0.33 & -0.15 & 0.23 & 0.15 & -0.23 & -0.33 & -0.27 & -0.2 & -0.5 & -1.51 \end{bmatrix}\end{array}$$

15OH

(a)



(b)

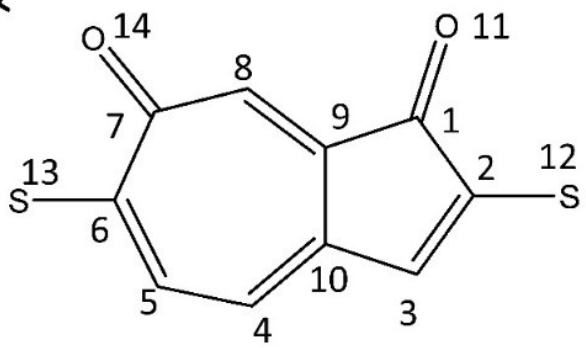
$$A=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\\11\\12\\13\\14 \end{array}\begin{array}{c}\begin{array}{cccccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \end{array}\\ \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{3}{4} & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{4} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{8} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{8} \end{bmatrix}\end{array}$$

(c)

$$G(E_F)=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\\11\\12\\13\\14 \end{array}\begin{array}{c}\begin{array}{cccccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \end{array}\\ \begin{bmatrix} 0.70 & 0.33 & -0.63 & 0.38 & 0.33 & 0.37 & -0.25 & -0.37 & 0.25 & -0.33 & -2.11 & -0.20 & -1.00 & -0.22 \\ 0.33 & 0.37 & -1.25 & 0.87 & 0.37 & -0.04 & -0.38 & 0.04 & 0.38 & -0.37 & -1.00 & -0.22 & -1.11 & 0.02 \\ -0.63 & -1.25 & 0.35 & -0.18 & -0.25 & -0.38 & 0.16 & 0.38 & -0.16 & 0.25 & 1.89 & 0.75 & 0.75 & 0.23 \\ 0.38 & 0.87 & -0.18 & 0.20 & -0.13 & -0.49 & 0.02 & 0.49 & -0.02 & -0.87 & -1.14 & -0.52 & 0.39 & 0.30 \\ 0.33 & 0.37 & -0.25 & -0.13 & 0.37 & -0.04 & -0.38 & 0.04 & 0.38 & -0.37 & -1. & -0.22 & -1.11 & 0.02 \\ 0.37 & -0.04 & -0.38 & -0.49 & -0.04 & 0.41 & -0.87 & -0.41 & 0.87 & 0.04 & -1.11 & 0.02 & 0.11 & -0.24 \\ -0.25 & -0.38 & 0.16 & 0.02 & -0.38 & -0.87 & 0.18 & -0.13 & -0.18 & 0.38 & 0.75 & 0.23 & 1.14 & 0.52 \\ -0.37 & 0.04 & 0.38 & 0.49 & 0.04 & -0.41 & -0.13 & 0.41 & -0.87 & -0.04 & 1.11 & -0.02 & -0.11 & 0.24 \\ 0.25 & 0.38 & -0.16 & -0.02 & 0.38 & 0.87 & -0.18 & -0.87 & 0.18 & -0.38 & -0.75 & -0.23 & -1.14 & -0.52 \\ -0.33 & -0.37 & 0.25 & -0.87 & -0.37 & 0.04 & 0.38 & -0.04 & -0.38 & 0.37 & 1. & 0.22 & 1.11 & -0.02 \\ -2.11 & -1. & 1.89 & -1.14 & -1. & -1.11 & 0.75 & 1.11 & -0.75 & 1. & 2.33 & 0.6 & 3.00 & 0.67 \\ -0.2 & -0.22 & 0.75 & -0.52 & -0.22 & 0.02 & 0.23 & -0.02 & -0.23 & 0.22 & 0.6 & -1.47 & 0.67 & -0.01 \\ -1. & -1.11 & 0.75 & 0.39 & -1.11 & 0.11 & 1.14 & -0.11 & -1.14 & 1.11 & 3. & 0.67 & -0.67 & -0.07 \\ -0.22 & 0.02 & 0.23 & 0.3 & 0.02 & -0.24 & 0.52 & 0.24 & -0.52 & -0.02 & 0.67 & -0.01 & -0.07 & -1.45 \end{bmatrix}\end{array}$$

17Q

(a)



(b)

$$A=$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0	1	0	0	0	0	0	0	1	0	$\frac{3}{8}$	0	0	0
2	1	0	1	0	0	0	0	0	0	0	0	$\frac{3}{8}$	0	0
3	0	1	0	0	0	0	0	0	0	1	0	0	0	0
4	0	0	0	0	1	0	0	0	0	1	0	0	0	0
5	0	0	0	1	0	1	0	0	0	0	0	0	$\frac{3}{8}$	0
6	0	0	0	0	1	0	1	0	0	0	0	0	0	$\frac{3}{8}$
7	0	0	0	0	0	1	0	1	0	0	0	0	0	0
8	0	0	0	0	0	0	1	0	1	0	0	0	0	0
9	1	0	0	0	0	0	0	1	0	1	0	0	0	0
10	0	0	1	1	0	0	0	0	1	0	0	0	0	0
11	$\frac{3}{8}$	0	0	0	0	0	0	0	0	0	$\frac{1}{4}$	0	0	0
12	0	$\frac{3}{8}$	0	0	0	0	0	0	0	0	0	$\frac{5}{8}$	0	0
13	0	0	0	0	0	$\frac{3}{8}$	0	0	0	0	0	0	$\frac{5}{8}$	0
14	0	0	0	0	0	0	$\frac{3}{8}$	0	0	0	0	0	0	$\frac{1}{4}$

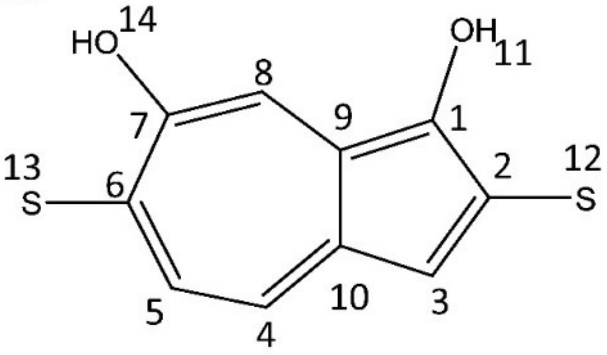
(c)

$$G(E_F)=$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	-1.15	-0.81	0.97	-0.13	-0.81	0.13	0.84	0.34	-0.84	0.81	1.73	0.49	-0.08	-1.26
2	-0.81	-0.28	-0.25	0.43	-0.28	-0.43	0.18	0.53	-0.18	0.28	1.21	0.17	0.26	-0.27
3	0.97	-0.25	-1.03	0.23	0.75	-0.23	-0.8	-0.22	0.8	-0.75	-1.45	0.15	0.14	1.2
4	-0.13	0.43	0.23	0.28	-0.57	-0.28	0.51	0.56	-0.51	-0.43	0.2	-0.26	0.17	-0.76
5	-0.81	-0.28	0.75	-0.57	-0.28	-0.43	0.18	0.53	-0.18	0.28	1.21	0.17	0.26	-0.27
6	0.13	-0.43	-0.23	-0.28	-0.43	0.28	-0.51	-0.56	0.51	0.43	-0.2	0.26	-0.17	0.76
7	0.84	0.18	-0.8	0.51	0.18	-0.51	-0.29	-0.66	0.29	-0.18	-1.26	-0.11	0.3	0.44
8	0.34	0.53	-0.22	0.56	0.53	-0.56	-0.66	0.19	-0.34	-0.53	-0.51	-0.32	0.34	0.99
9	-0.84	-0.18	0.8	-0.51	-0.18	0.51	0.29	-0.34	-0.29	0.18	1.26	0.11	-0.3	-0.44
10	0.81	0.28	-0.75	-0.43	0.28	0.43	-0.18	-0.53	0.18	-0.28	-1.21	-0.17	-0.26	0.27
11	1.73	1.21	-1.45	0.2	1.21	-0.2	-1.26	-0.51	1.26	-1.21	-6.59	-0.73	0.12	1.89
12	0.49	0.17	0.15	-0.26	0.17	0.26	-0.11	-0.32	0.11	-0.17	-0.73	-1.7	-0.16	0.16
13	-0.08	0.26	0.14	0.17	0.26	-0.17	0.3	0.34	-0.3	-0.26	0.12	-0.16	-1.5	-0.45
14	-1.26	-0.27	1.2	-0.76	-0.27	0.76	0.44	0.99	-0.44	0.27	1.89	0.16	-0.45	-4.66

17OH

(a)



(b)

$$A=$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0	1	0	0	0	0	0	0	1	0	$\frac{3}{4}$	0	0	0
2	1	0	1	0	0	0	0	0	0	0	0	$\frac{3}{8}$	0	0
3	0	1	0	0	0	0	0	0	0	1	0	0	0	0
4	0	0	0	0	1	0	0	0	0	1	0	0	0	0
5	0	0	0	1	0	1	0	0	0	0	0	0	$\frac{3}{8}$	0
6	0	0	0	0	1	0	1	0	0	0	0	0	0	$\frac{3}{4}$
7	0	0	0	0	0	1	0	1	0	0	0	0	0	0
8	0	0	0	0	0	0	1	0	1	0	0	0	0	0
9	1	0	0	0	0	0	0	1	0	1	0	0	0	0
10	0	0	1	1	0	0	0	0	1	0	0	0	0	0
11	$\frac{3}{4}$	0	0	0	0	0	0	0	0	0	$\frac{1}{4}$	0	0	0
12	0	$\frac{3}{8}$	0	0	0	0	0	0	0	0	0	$\frac{5}{8}$	0	0
13	0	0	0	0	0	$\frac{3}{8}$	0	0	0	0	0	0	$\frac{5}{8}$	0
14	0	0	0	0	0	0	$\frac{3}{4}$	0	0	0	0	0	0	$\frac{1}{4}$

(c)

$$G(E_F)=$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.71	0.27	-0.65	0.32	0.27	-0.32	-0.34	-0.45	0.34	-0.27	-2.14	-0.16	0.19	1.02
2	0.27	0.21	-1.22	0.83	0.21	-0.83	-0.39	-0.06	0.39	-0.21	-0.8	-0.12	0.5	1.18
3	0.65	-1.22	0.38	-0.13	-0.22	0.13	0.25	0.43	-0.25	0.22	1.96	0.73	-0.08	-0.75
4	0.32	0.83	-0.13	0.25	-0.17	-0.25	0.12	0.51	-0.12	-0.83	-0.95	-0.5	0.15	-0.35
5	0.27	0.21	-0.22	-0.17	0.21	-0.83	-0.39	-0.06	0.39	-0.21	-0.8	-0.12	0.5	1.18
6	0.32	-0.83	0.13	-0.25	-0.83	0.25	-0.12	-0.51	0.12	0.83	0.95	0.5	-0.15	0.35
7	0.34	-0.39	0.25	0.12	-0.39	-0.12	0.37	-0.06	-0.37	0.39	1.02	0.24	0.07	-1.1
8	0.45	-0.06	0.43	0.51	-0.06	-0.51	-0.06	0.39	-0.94	0.06	1.34	0.04	0.31	0.17
9	0.34	0.39	-0.25	-0.12	0.39	0.12	-0.37	-0.94	0.37	-0.39	-1.02	-0.24	-0.07	1.1
10	0.27	-0.21	0.22	-0.83	-0.21	0.83	0.39	0.06	-0.39	0.21	0.8	0.12	-0.5	-1.18
11	2.14	-0.8	1.96	-0.95	-0.8	0.95	1.02	1.34	-1.02	0.8	2.42	0.48	-0.57	-3.05
12	0.16	-0.12	0.73	-0.5	-0.12	0.5	0.24	0.04	-0.24	0.12	0.48	-1.53	-0.3	-0.71
13	0.19	0.5	-0.08	0.15	0.5	-0.15	0.07	0.31	-0.07	-0.5	-0.57	-0.3	-1.51	-0.21
14	1.02	1.18	-0.75	-0.35	1.18	0.35	-1.1	0.17	1.1	-1.18	-3.05	-0.71	-0.21	-0.69