Supporting information

Exploring quantum interference in heteroatom-substituted graphene-like molecule s

Sara Sangtarash*, Hatef Sadeghi, and Colin J. Lambert*

Quantum Technology Centre, Physics Department, Lancaster University, Lancaster LA1 4YB, UK

*s.sangtarash@lancaster.ac.uk; *c.lambert@lancaster.ac.uk*

1- For a naphthalene parental core, this shows the Hamiltonian H^p and mid-gap (E=0) M-table M^p of the parent, along with the Hamiltonian H^d and E=0 M-table M^d of the corresponding daughter.

H^p	1	3	5	7	9	2	4	6	8	10
1	0	0	0	0	0	-1	0	0	0	-1
3	0	0	0	0	0	-1	-1	0	0	0
5	0	0	0	0	0	0	-1	-1	0	-1
7	0	0	0	0	0	0	0	-1	-1	0
9	0	0	0	0	0	0	0	0	-1	-1
2	-1	-1	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0
10	-1	0	-1	0	-1	0	0	0	0	0

M^p	1	3	5	7	9	2	4	6	8	10
1	0	0	0	0	0	-2	2	-1	1	-1
3	0	0	0	0	0	-1	-2	1	-1	1
5	0	0	0	0	0	1	-1	-1	1	-1
7	0	0	0	0	0	-1	1	-2	-1	1
9	0	0	0	0	0	1	-1	2	-2	-1
2	-2	-1	1	-1	1	0	0	0	0	0
4	2	-2	-1	1	-1	0	0	0	0	0
6	-1	1	-1	-2	2	0	0	0	0	0
8	1	-1	1	-1	-2	0	0	0	0	0
10	-1	1	-1	1	-1	0	0	0	0	0

H^d	1	3	5	7	9	2	4	6	8	10
1	-0.5	0	0	0	0	-1	0	0	0	-1
3	0	0	0	0	0	-1	-1	0	0	0
5	0	0	0	0	0	0	-1	-1	0	-1
7	0	0	0	0	0	0	0	-1	-1	0
9	0	0	0	0	0	0	0	0	-1	-1
2	-1	-1	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0
10	-1	0	-1	0	-1	0	0	0	0	0

M^d	1	3	5	7	9	2	4	6	8	10
1	0	0	0	0	0	-2	2	-1	1	-1
3	0	0	0	0	0	-1	-2	1	-1	1
5	0	0	0	0	0	1	-1	-1	1	-1
7	0	0	0	0	0	-1	1	-2	-1	1
9	0	0	0	0	0	1	-1	2	-2	-1
2	-2	-1	1	-1	1	0.67	-0.67	0.33	-0.33	0.33
4	2	-2	-1	1	-1	-0.67	0.67	-0.33	0.33	-0.33
6	-1	1	-1	-2	2	0.33	-0.33	0.17	-0.17	0.17
8	1	-1	1	-1	-2	-0.33	0.33	-0.17	0.17	-0.17
10	-1	1	-1	1	-1	0.33	-0.33	0.17	-0.17	0.17

2- For a anthracene parental core, this shows the Hamiltonian H^p and mid-gap (E=0) M-table M^p of the parent, along with the Hamiltonian H^d and E=0 M-table M^d of the corresponding daughter.

H^p	1	3	5	7	9	11	13	2	4	6	8	10	12	14
1	0	0	0	0	0	0	0	-1	0	0	0	0	0	-1
3	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0
5	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0
7	0	0	0	0	0	0	0	-1	0	-1	-1	0	0	0
9	0	0	0	0	0	0	0	0	0	0	-1	-1	0	-1
11	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0
13	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1
2	-1	-1	0	-1	0	0	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
10	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
12	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0
14	-1	0	0	0	-1	0	-1	0	0	0	0	0	0	0

M^p	1	3	5	7	9	11	13	2	4	6	8	10	12	14
1	0	0	0	0	0	0	0	-2	2	-2	4	-2	2	-2
3	0	0	0	0	0	0	0	-1	-3	3	-2	1	-1	1
5	0	0	0	0	0	0	0	1	-1	-3	2	-1	1	-1
7	0	0	0	0	0	0	0	-1	1	-1	-2	1	-1	1
9	0	0	0	0	0	0	0	1	-1	1	-2	-1	1	-1
11	0	0	0	0	0	0	0	-1	1	-1	2	-3	-1	1
13	0	0	0	0	0	0	0	1	-1	1	-2	3	-3	-1
2	-2	-1	1	-1	1	-1	1	0	0	0	0	0	0	0
4	2	-3	-1	1	-1	1	-1	0	0	0	0	0	0	0
6	-2	3	-3	-1	1	-1	1	0	0	0	0	0	0	0
8	4	-2	2	-2	-2	2	-2	0	0	0	0	0	0	0
10	-2	1	-1	1	-1	-3	3	0	0	0	0	0	0	0
12	2	-1	1	-1	1	-1	-3	0	0	0	0	0	0	0
14	-2	1	-1	1	-1	1	-1	0	0	0	0	0	0	0

H^d	1	3	5	7	9	11	13	2	4	6	8	10	12	14
1	-0.5	0	0	0	0	0	0	-1	0	0	0	0	0	-1
3	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0
5	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0
7	0	0	0	0	0	0	0	-1	0	-1	-1	0	0	0
9	0	0	0	0	0	0	0	0	0	0	-1	-1	0	-1
11	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0
13	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1
2	-1	-1	0	-1	0	0	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
10	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
12	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0
14	-1	0	0	0	-1	0	-1	0	0	0	0	0	0	0

M^d	1	3	5	7	9	11	13	2	4	6	8	10	12	14
1	0	0	0	0	0	0	0	-2	2	-2	4	-2	2	-2
3	0	0	0	0	0	0	0	-1	-3	3	-2	1	-1	1
5	0	0	0	0	0	0	0	1	-1	-3	2	-1	1	-1
7	0	0	0	0	0	0	0	-1	1	-1	-2	1	-1	1
9	0	0	0	0	0	0	0	1	-1	1	-2	-1	1	-1
11	0	0	0	0	0	0	0	-1	1	-1	2	-3	-1	1
13	0	0	0	0	0	0	0	1	-1	1	-2	3	-3	-1
2	-2	-1	1	-1	1	-1	1	0.5	-0.5	0.5	-1	0.5	-0.5	0.5
4	2	-3	-1	1	-1	1	-1	-0.5	0.5	-0.5	1	-0.5	0.5	-0.5
6	-2	3	-3	-1	1	-1	1	0.5	-0.5	0.5	-1	0.5	-0.5	0.5
8	4	-2	2	-2	-2	2	-2	-1	1	-1	2	-1	1	-1
10	-2	1	-1	1	-1	-3	3	0.5	-0.5	0.5	-1	0.5	-0.5	0.5
12	2	-1	1	-1	1	-1	-3	-0.5	0.5	-0.5	1	-0.5	0.5	-0.5
14	-2	1	-1	1	-1	1	-1	0.5	-0.5	0.5	-1	0.5	-0.5	0.5

3- For a pyrene parental core, this shows the Hamiltonian H^p and mid-gap (E=0) M-table M^p of the parent, along with the Hamiltonian H^d and E=0 M-table M^d of the corresponding daughter.

H^p	1	3	5	7	9	11	13	15	2	4	6	8	10	12	14	16
1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	-1	0
3	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	-1
5	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	-1
9	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0
15	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	-1	-1
2	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	-1	-1	0	-1	0	0	0	0	0	0	0	0
12	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
14	-1	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
16	0	-1	0	-1	0	0	0	-1	0	0	0	0	0	0	0	0

M^p	1	3	5	7	9	11	13	15	2	4	6	8	10	12	14	16
1	0	0	0	0	0	0	0	0	-5	3	-3	1	-1	1	-1	2
3	0	0	0	0	0	0	0	0	-1	-3	3	-1	1	-1	1	-2
5	0	0	0	0	0	0	0	0	1	-3	-3	1	-1	1	-1	2
7	0	0	0	0	0	0	0	0	-1	3	-3	-1	1	-1	1	-2
9	0	0	0	0	0	0	0	0	1	-3	3	-5	-1	1	-1	2
11	0	0	0	0	0	0	0	0	-3	3	-3	3	-3	-3	3	0
13	0	0	0	0	0	0	0	0	3	-3	3	-3	3	-3	-3	0
15	0	0	0	0	0	0	0	0	2	0	0	2	-2	2	-2	-2
2	-5	-1	1	-1	1	-3	3	2	0	0	0	0	0	0	0	0
4	3	-3	-3	3	-3	3	-3	0	0	0	0	0	0	0	0	0
6	-3	3	-3	-3	3	-3	3	0	0	0	0	0	0	0	0	0
8	1	-1	1	-1	-5	3	-3	2	0	0	0	0	0	0	0	0
10	-1	1	-1	1	-1	-3	3	-2	0	0	0	0	0	0	0	0
12	1	-1	1	-1	1	-3	-3	2	0	0	0	0	0	0	0	0
14	-1	1	-1	1	-1	3	-3	-2	0	0	0	0	0	0	0	0
16	2	-2	2	-2	2	0	0	-2	0	0	0	0	0	0	0	0

H^d	1	3	5	7	9	11	13	15	2	4	6	8	10	12	14	16
1	-0.5	0	0	0	0	0	0	0	-1	0	0	0	0	0	-1	0
3	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	-1
5	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	-1
9	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0
15	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	-1	-1
2	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	-1	-1	0	-1	0	0	0	0	0	0	0	0
12	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
14	-1	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
16	0	-1	0	-1	0	0	0	-1	0	0	0	0	0	0	0	0

M^d	1	3	5	7	9	11	13	15	2	4	6	8	10	12	14	16
1	0	0	0	0	0	0	0	0	-5	3	-3	1	-1	1	-1	2
3	0	0	0	0	0	0	0	0	-1	-3	3	-1	1	-1	1	-2
5	0	0	0	0	0	0	0	0	1	-3	-3	1	-1	1	-1	2
7	0	0	0	0	0	0	0	0	-1	3	-3	-1	1	-1	1	-2
9	0	0	0	0	0	0	0	0	1	-3	3	-5	-1	1	-1	2
11	0	0	0	0	0	0	0	0	-3	3	-3	3	-3	-3	3	0
13	0	0	0	0	0	0	0	0	3	-3	3	-3	3	-3	-3	0
15	0	0	0	0	0	0	0	0	2	0	0	2	-2	2	-2	-2
2	-5	-1	1	-1	1	-3	3	2	2.08	-1.25	1.25	-0.42	0.42	-0.42	0.42	-0.83
4	3	-3	-3	3	-3	3	-3	0	-1.25	0.75	-0.75	0.25	-0.25	0.25	-0.25	0.50
6	-3	3	-3	-3	3	-3	3	0	1.25	-0.75	0.75	-0.25	0.25	-0.25	0.25	-0.50
8	1	-1	1	-1	-5	3	-3	2	-0.42	0.25	-0.25	0.08	-0.08	0.08	-0.08	0.17
10	-1	1	-1	1	-1	-3	3	-2	0.42	-0.25	0.25	-0.08	0.08	-0.08	0.08	-0.17
12	1	-1	1	-1	1	-3	-3	2	-0.42	0.25	-0.25	0.08	-0.08	0.08	-0.08	0.17
14	-1	1	-1	1	-1	3	-3	-2	0.42	-0.25	0.25	-0.08	0.08	-0.08	0.08	-0.17
16	2	-2	2	-2	2	0	0	-2	-0.83	0.50	-0.50	0.17	-0.17	0.17	-0.17	0.33

4- For a anthanthrene parental core, this shows the Hamiltonian H^p and mid-gap (E=0) M-table M^p of the parent, along with the Hamiltonian H^d and E=0 M-table M^d of the corresponding daughter.

H^p	1	3	5	7	9	11	13	15	17	19	21	2	4	6	8	10	12	14	16	18	20	22
1	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	-1
3	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	-1	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	-1	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	-1
19	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	-1	-1	0
21	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	-1	0	0	0	0	0	-1	0
2	-1	-1	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
4	0	-1	-1	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
6	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	-1	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	-1	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0
22	-1	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0

M^p	1	3	5	7	9	11	13	15	17	19	21	2	4	6	8	10	12	14	16	18	20	22
1	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	3	-6	6	3	-2	-9
3	0	0	0	0	0	0	0	0	0	0	0	-7	-3	3	-3	3	-9	8	-8	1	6	7
5	0	0	0	0	0	0	0	0	0	0	0	4	-4	-6	6	-6	8	-6	6	-2	-2	-4
7	0	0	0	0	0	0	0	0	0	0	0	-4	4	-4	-6	6	-8	6	-6	2	2	4
9	0	0	0	0	0	0	0	0	0	0	0	1	-1	1	-1	-9	7	-4	4	-3	2	-1
11	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	-7	4	-4	3	-2	1
13	0	0	0	0	0	0	0	0	0	0	0	1	-1	1	-1	1	-3	-4	4	-3	2	-1
15	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	3	-6	-4	3	-2	1
17	0	0	0	0	0	0	0	0	0	0	0	1	-1	1	-1	1	-3	6	-6	-3	2	-1
19	0	0	0	0	0	0	0	0	0	0	0	-2	2	-2	2	-2	6	-2	2	-4	-4	2
21	0	0	0	0	0	0	0	0	0	0	0	3	-3	3	-3	3	1	-2	2	1	-4	-3
2	-1	-7	4	-4	1	-1	1	-1	1	-2	3	0	0	0	0	0	0	0	0	0	0	0
4	1	-3	-4	4	-1	1	-1	1	-1	2	-3	0	0	0	0	0	0	0	0	0	0	0
6	-1	3	-6	-4	1	-1	1	-1	1	-2	3	0	0	0	0	0	0	0	0	0	0	0
8	1	-3	6	-6	-1	1	-1	1	-1	2	-3	0	0	0	0	0	0	0	0	0	0	0
10	-1	3	-6	6	-9	-1	1	-1	1	-2	3	0	0	0	0	0	0	0	0	0	0	0
12	3	-9	8	-8	7	-7	-3	3	-3	6	1	0	0	0	0	0	0	0	0	0	0	0
14	-6	8	-6	6	-4	4	-4	-6	6	-2	-2	0	0	0	0	0	0	0	0	0	0	0
16	6	-8	6	-6	4	-4	4	-4	-6	2	2	0	0	0	0	0	0	0	0	0	0	0
18	3	1	-2	2	-3	3	-3	3	-3	-4	1	0	0	0	0	0	0	0	0	0	0	0
20	-2	6	-2	2	2	-2	2	-2	2	-4	-4	0	0	0	0	0	0	0	0	0	0	0
22	-9	7	-4	4	-1	1	-1	1	-1	2	-3	0	0	0	0	0	0	0	0	0	0	0

H^d	1	3	5	7	9	11	13	15	17	19	21	2	4	6	8	10	12	14	16	18	20	22
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3	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0	-1	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	-1	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	0	-1
19	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	-1	-1	0
21	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	-1	0	0	0	0	0	-1	0
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6	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	-1	-1	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	-1	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	-1	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0
22	-1	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0

M^d	1	3	5	7	9	11	13	15	17	19	21	2	4	6	8	10	12	14	16	18	20	22
1	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	3	-6	6	3	-2	-9
3	0	0	0	0	0	0	0	0	0	0	0	-7	-3	3	-3	3	-9	8	-8	1	6	7
5	0	0	0	0	0	0	0	0	0	0	0	4	-4	-6	6	-6	8	-6	6	-2	-2	-4
7	0	0	0	0	0	0	0	0	0	0	0	-4	4	-4	-6	6	-8	6	-6	2	2	4
9	0	0	0	0	0	0	0	0	0	0	0	1	-1	1	-1	-9	7	-4	4	-3	2	-1
11	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	-7	4	-4	3	-2	1
13	0	0	0	0	0	0	0	0	0	0	0	1	-1	1	-1	1	-3	-4	4	-3	2	-1
15	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	3	-6	-4	3	-2	1
17	0	0	0	0	0	0	0	0	0	0	0	1	-1	1	-1	1	-3	6	-6	-3	2	-1
19	0	0	0	0	0	0	0	0	0	0	0	-2	2	-2	2	-2	6	-2	2	-4	-4	2
21	0	0	0	0	0	0	0	0	0	0	0	3	-3	3	-3	3	1	-2	2	1	-4	-3
2	-1	-7	4	-4	1	-1	1	-1	1	-2	3	0.05	-0.05	0.05	-0.05	0.05	-0.15	0.3	-0.3	-0.15	0.1	0.45
4	1	-3	-4	4	-1	1	-1	1	-1	2	-3	-0.05	0.05	-0.05	0.05	-0.05	0.15	-0.3	0.3	0.15	-0.1	-0.45
6	-1	3	-6	-4	1	-1	1	-1	1	-2	3	0.05	-0.05	0.05	-0.05	0.05	-0.15	0.3	-0.3	-0.15	0.1	0.45
8	1	-3	6	-6	-1	1	-1	1	-1	2	-3	-0.05	0.05	-0.05	0.05	-0.05	0.15	-0.3	0.3	0.15	-0.1	-0.45
10	-1	3	-6	6	-9	-1	1	-1	1	-2	3	0.05	-0.05	0.05	-0.05	0.05	-0.15	0.3	-0.3	-0.15	0.1	0.45
12	3	-9	8	-8	7	-7	-3	3	-3	6	1	-0.15	0.15	-0.15	0.15	-0.15	0.45	-0.9	0.9	0.45	-0.3	-1.35
14	-6	8	-6	6	-4	4	-4	-6	6	-2	-2	0.3	-0.3	0.3	-0.3	0.3	-0.9	1.8	-1.8	-0.9	0.6	2.7
16	6	-8	6	-6	4	-4	4	-4	-6	2	2	-0.3	0.3	-0.3	0.3	-0.3	0.9	-1.8	1.8	0.9	-0.6	-2.7
18	3	1	-2	2	-3	3	-3	3	-3	-4	1	-0.15	0.15	-0.15	0.15	-0.15	0.45	-0.9	0.9	0.45	-0.3	-1.35
20	-2	6	-2	2	2	-2	2	-2	2	-4	-4	0.1	-0.1	0.1	-0.1	0.1	-0.3	0.6	-0.6	-0.3	0.2	0.9
22	-9	7	-4	4	-1	1	-1	1	-1	2	-3	0.45	-0.45	0.45	-0.45	0.45	-1.35	2.7	-2.7	-1.35	0.9	4.05

The role of the anchor group.

M-theory is valid when the core of a PAH is weakly connected to the electrodes. The DFT results below show the effect of increasing the strength of the coupling to the electrodes by replacing the linker group of figure 1 (main text) with a direct carbon-gold bond.

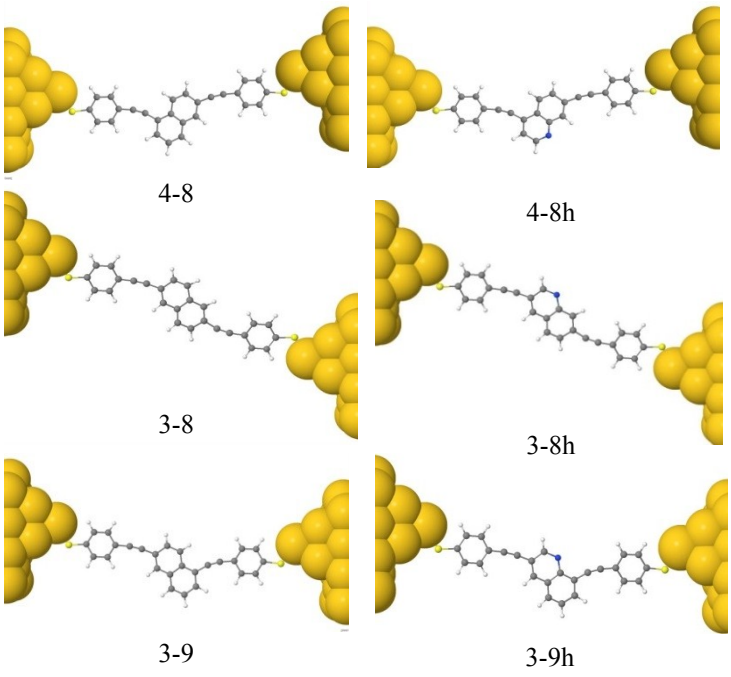

Figure SI.1. Relaxed structure for different connectivities of naphthalene with and without heteroatom connected to the electrode.

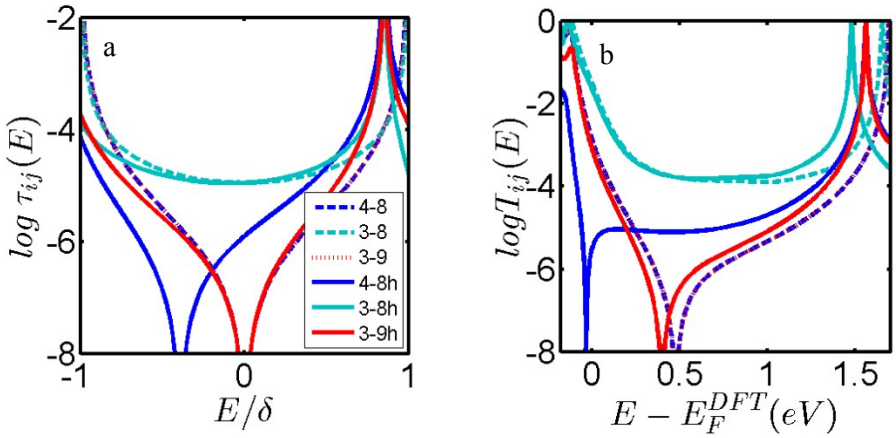

Figure SI.2. (a) Core transmission coefficients $\tau_{i,j}(E)$ of parents (dashed lines) and daughters (solid lines) plotted against E/δ, where δ is half of the HOMO-LUMO gap of the parental core; ie δ=0.62 (b) *DFT* results for the corresponding the transmission coefficients T_{ij}(E) of the naphthalene with the structures shown in figure SI.1.

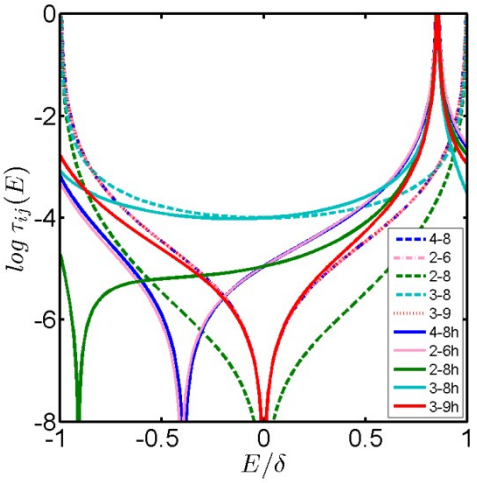

Figure SI.3. Core transmission coefficients $\tau_{i,j}(E)$ of naphthalene (dashed lines) and quinoline (solid lines).

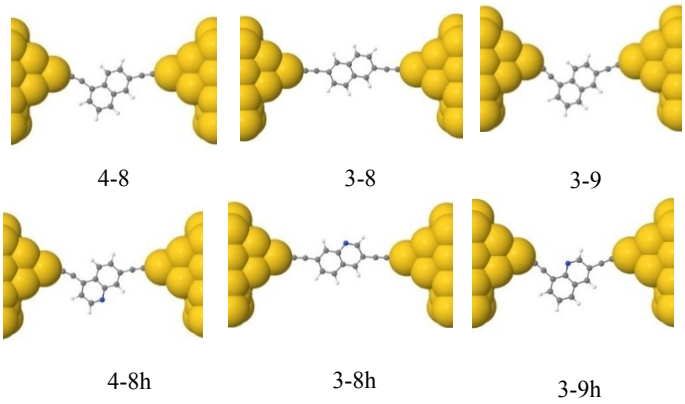

Figure SI.4. Relaxed structure for different connectivities of naphthalene with and without heteroatom connected to the electrode, with different anchor.

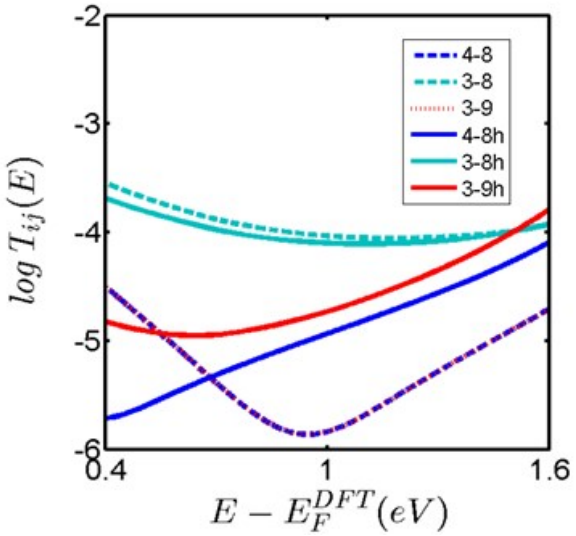

Figure SI.5. *DFT* results for the corresponding the transmission coefficients T_{ij}(E) of the naphthalene with the structures shown in figure SI4.

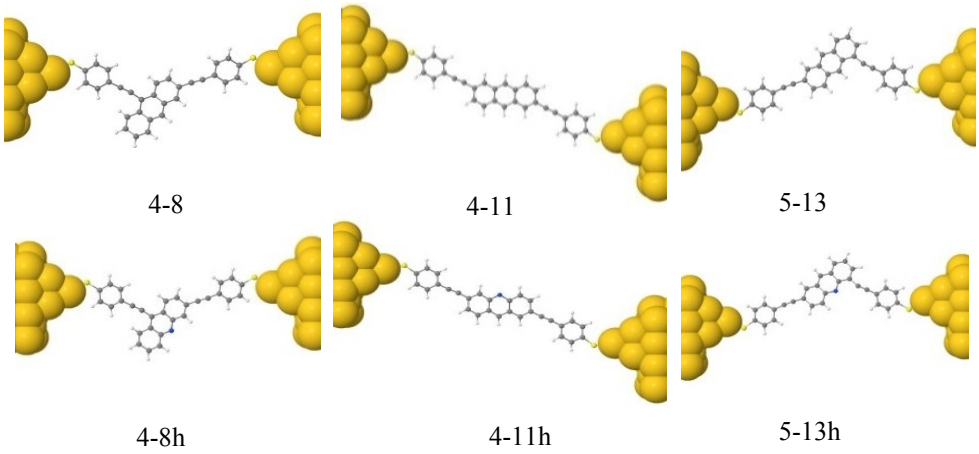

Figure SI.6. Relaxed structure for different connectivities of anthracene with and without heteroatom connected to the electrode

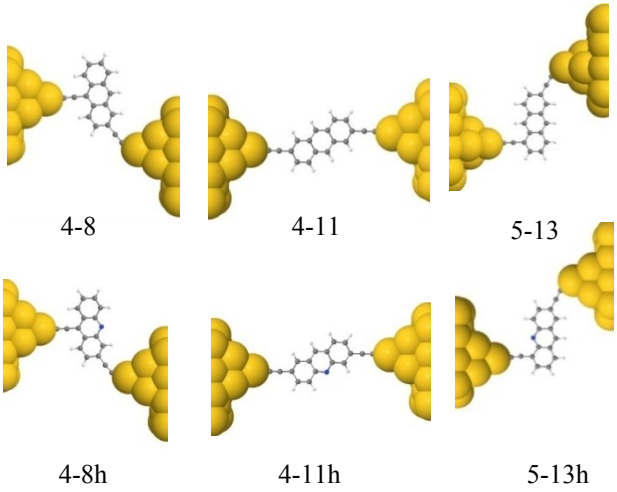

Figure SI.7. Relaxed structure for different connectivities of anthracene with and without heteroatom connected to the electrode, with different anchor

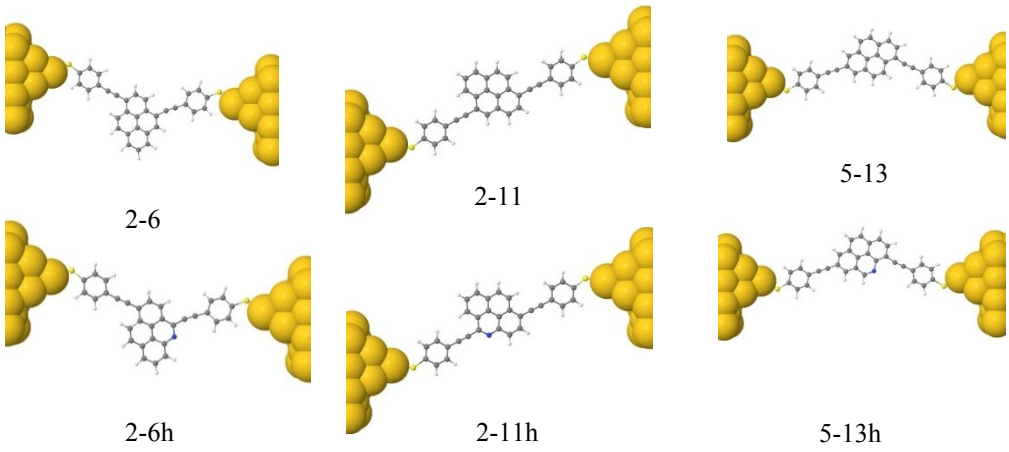

Figure SI.8. Relaxed structure for different connectivities of pyrene with and without heteroatom connected to the electrode

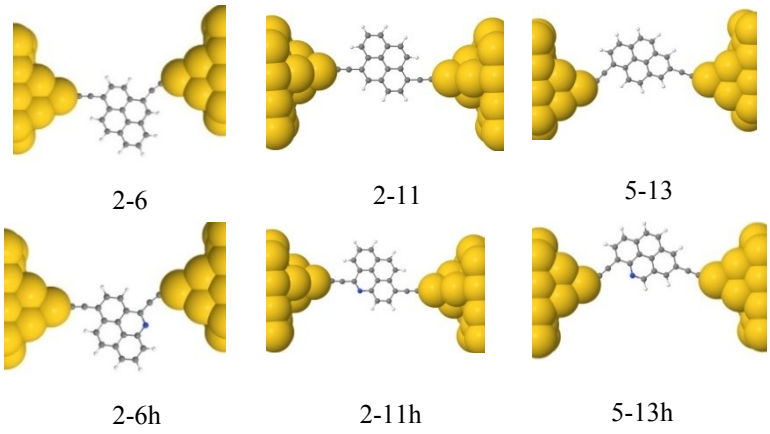

Figure SI.9. Relaxed structure for different connectivities of pyrene with and without heteroatom connected to the electrode, with different anchor

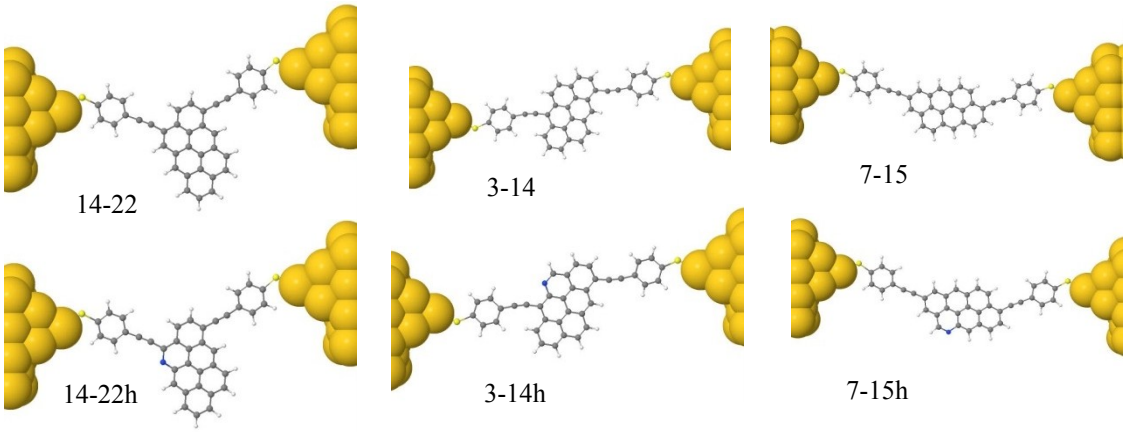

Figure SI.10. Relaxed structure for different connectivities of anthanthrene with and without heteroatom connected to the electrode

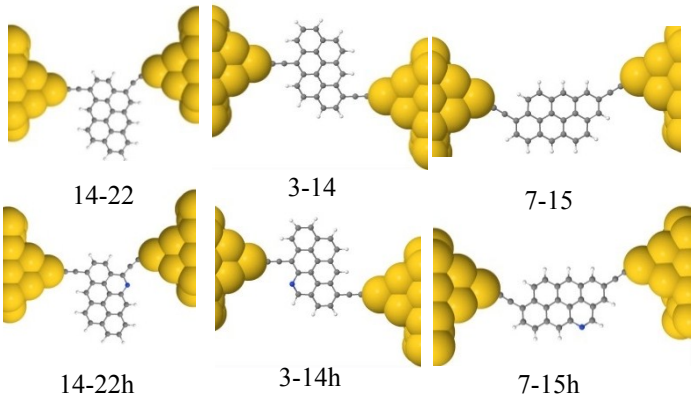

Figure SI.11. Relaxed structure for different connectivities of anthanthrene with and without heteroatom connected to the electrode, with different anchor

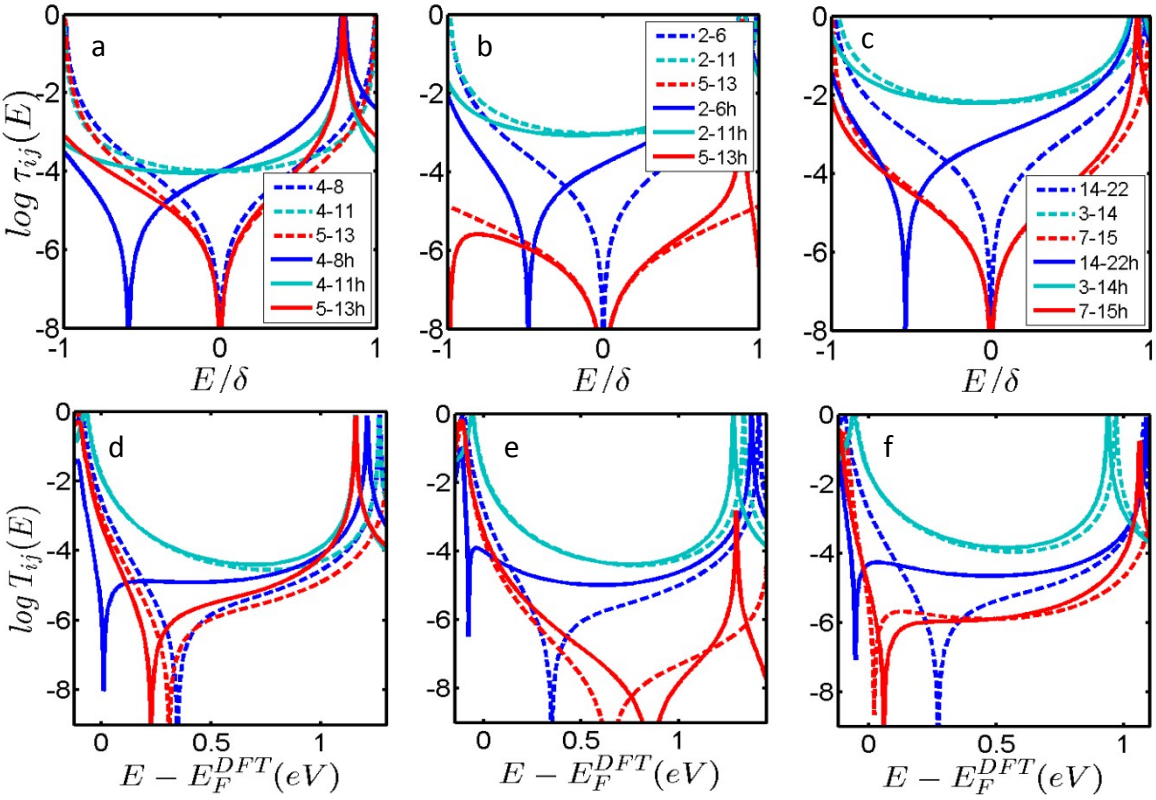

Figure SI.12. (a-c): Core transmissions of parents (dashed lines) and of daughters (solid lines), of (a) anthracene, (b) pyrene and (c) anthanthrene. (d-f): DFT-NEGF results for the zero-bias electrical conductances of daughters (solid lines) and parents (dashed Lines) of (d) anthracene, (e) pyrene and (f) anthanthrene.,for structures shown in fig SI.6., SI.8, SI.10.

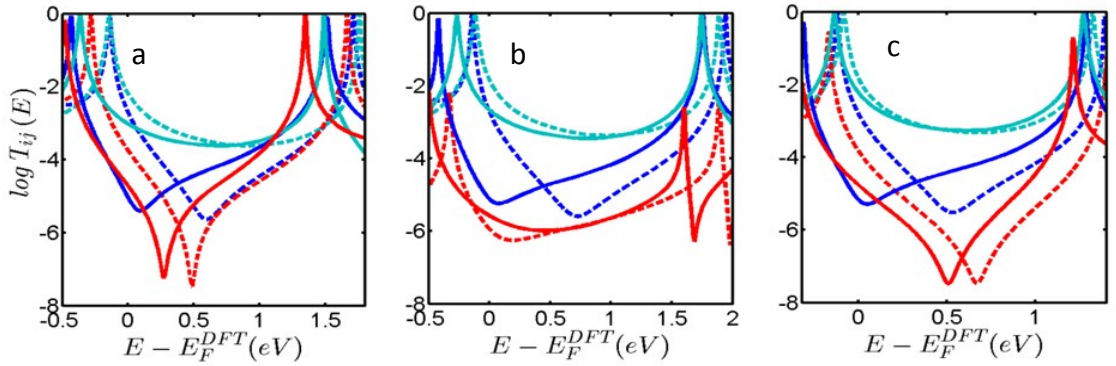

Figure SI.13. (a-c): DFT-NEGF results for the zero-bias electrical conductances of daughters (solid lines) and parents (dashed Lines) of (a) anthracene, (b) pyrene and (c) anthanthrene. .,for structures shown in fig SI.7., SI.9, SI.11.

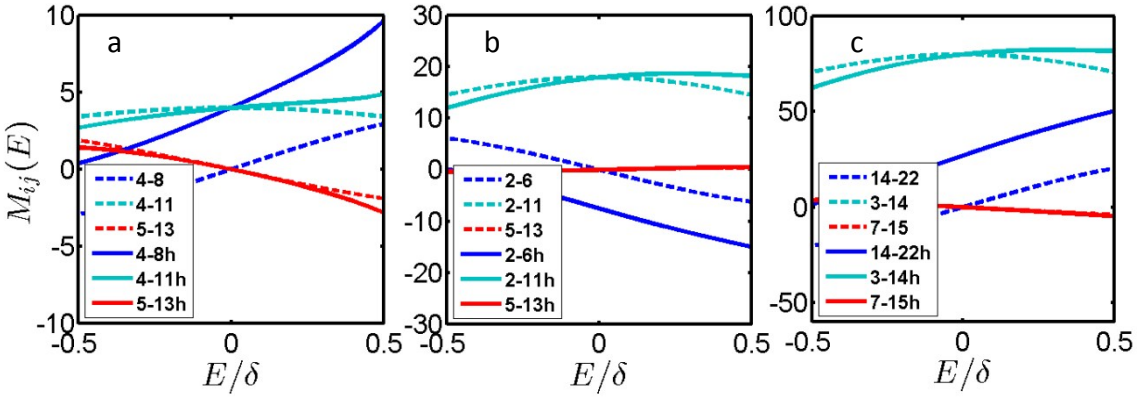

Figure SI.14. $M_{ij}(E)$ of the parent and daughter molecules of (a) anthracene, (b) pyrene and (c) anthanthrene

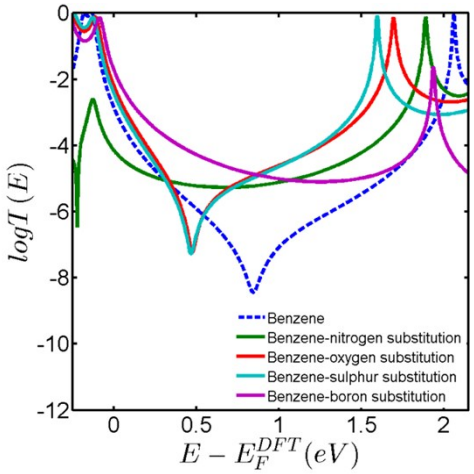

Figure SI.15. DFT-NEGF results for the zero-bias electrical conductances of daughters (solid lines) and parent (dashed Lines) of structures shown in figure 6) a-e.

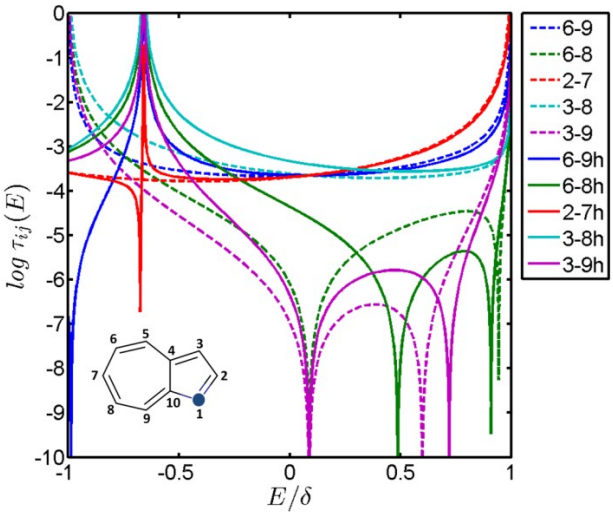

Figure SI.16. Core transmission coefficients $\tau_{i,j}(E)$ of azulene parents (dashed lines) and of daughters (solid lines) where the hetero atoms (ε = 0.5) is located on site 1. Results are plotted against E/δ, where δ is 0.439.

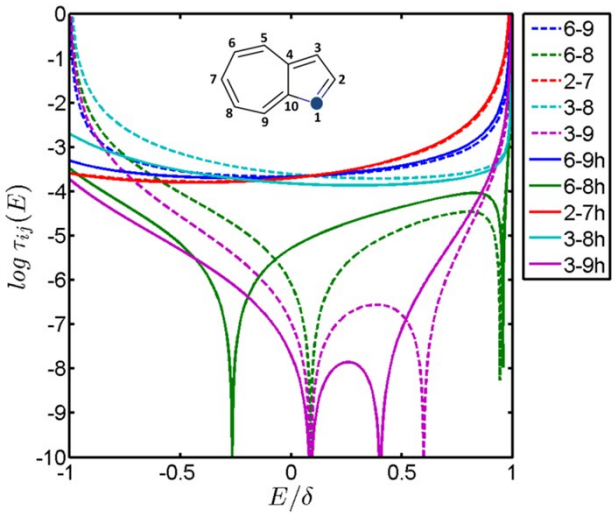

Figure SI.17. Core transmission coefficients $\tau_{i,j}(E)$ of azulene parents (dashed lines) and of daughters (solid lines) where the hetero atoms (ε = -0.5) located on site 1, plotted against E/δ, where δ is 0.439.

M-functions for parents and daughters with heteroatoms added to sites l=10 and l=11.

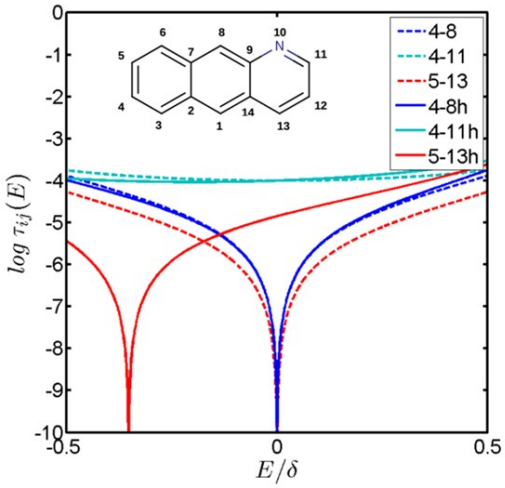

Figure SI.18. Core transmission coefficients $\tau_{i,j}(E)$ of anthracene parents (dashed lines) and of daughters (solid lines) where the hetero atoms (ε = 0.5) is located on site 10.

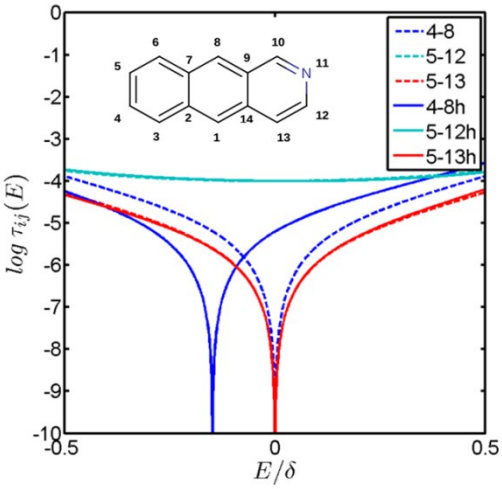

Figure SI.19. Core transmission coefficients $\tau_{i,j}(E)$ of anthracene parents (dashed lines) and of daughters (solid lines) where the hetero atoms (ε = 0.5) is located on site 11. Note that $\tau_{4,11}(E)$ (not shown) is identical to $\tau_{5,12}(E)$.