SUPPORTING INFORMATION FILE

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How important is the position of the molecule between the electrodes in tuning negative differential resistance behavior?

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Atomic co-ordinates of the two-probe system of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface: Arrangement 1(a)

ATOM	X (Å)	Y (Å)	Z (Å)
Au	1.44186	0.83246	1.17728
Au	4.32558	0.83246	1.17728
Au	7.20930	0.83246	1.17728
Au	-0.00000	3.32983	1.17728
Au	2.88372	3.32983	1.17728
Au	5.76744	3.32983	1.17728
Au	-1.44186	5.82721	1.17728
Au	1.44186	5.82721	1.17728
Au	4.32558	5.82721	1.17728
Au	0.00000	0.00000	3.53184
Au	2.88372	0.00000	3.53184
Au	5.76744	0.00000	3.53184
Au	-1.44186	2.49737	3.53184
Au	1.44186	2.49737	3.53184
Au	4.32558	2.49737	3.53184
Au	-2.88372	4.99475	3.53184
Au	0.00000	4.99475	3.53184
Au	2.88372	4.99475	3.53184
Au	0.00000	1.66492	5.88639
Au	2.88372	1.66492	5.88639
Au	5.76744	1.66492	5.88639
Au	-1.44186	4.16229	5.88639
Au	1.44186	4.16229	5.88639
Au	4.32558	4.16229	5.88639
Au	-2.88372	6.65966	5.88639
Au	0.00000	6.65966	5.88639
Au	2.88372	6.65966	5.88639
Au	1.44186	0.83246	8.24095
Au	-0.00000	-0.00000	10.59550
Au	4.32558	0.83246	8.24095
Au	2.88372	-0.00000	10.59550
Au	7.20931	0.83246	8.24095
Au	5.76745	-0.00000	10.59550
Au	-0.00000	3.32984	8.24095
Au	-1.44186	2.49738	10.59550
Au	2.88372	3.32984	8.24095
Au	1.44186	2.49738	10.59550
Au	5.76745	3.32984	8.24095
Au	4.32558	2.49738	10.59550
Au	-1.44186	5.82721	8.24095
Au	-2.88372	4.99475	10.59550
Au	1.44186	5.82721	8.24095
Au	-0.00000	4.99475	10.59550
Au	4.32558	5.82721	8.24095
Au	2.88372	4.99475	10.59550
C	1.61258	2.62248	22.39669
C	1.51407	3.69405	21.57998
C	1.48928	3.69013	20.12545
C	1.55995	2.61214	19.29897
C	1.53529	2.60755	17.84880
C	1.43646	3.68025	17.01830

C	1.41179	3.67486	15.56377
C	1.48260	2.59797	14.75116
H	1.68562	1.61078	22.01060
H	1.44442	4.67896	22.04025
H	1.40370	4.67853	19.67814
H	1.64553	1.62458	19.75002
H	1.60560	1.61711	17.40142
H	1.36602	4.67152	17.46190
H	1.32642	4.65683	15.09984
H	1.56883	1.58885	15.14129
S	1.44186	2.49738	12.98550
S	1.63183	2.76462	24.16177
Au	-0.00000	-0.00000	26.55177
Au	-0.00000	1.66492	28.90632
Au	2.88372	-0.00000	26.55177
Au	2.88372	1.66492	28.90632
Au	5.76745	-0.00000	26.55177
Au	5.76745	1.66492	28.90632
Au	-1.44186	2.49738	26.55177
Au	-1.44186	4.16230	28.90632
Au	1.44186	2.49738	26.55177
Au	1.44186	4.16230	28.90632
Au	4.32558	2.49738	26.55177
Au	4.32558	4.16230	28.90632
Au	-2.88372	4.99475	26.55177
Au	-2.88372	6.65967	28.90632
Au	-0.00000	4.99475	26.55177
Au	-0.00000	6.65967	28.90632
Au	2.88372	4.99475	26.55177
Au	2.88372	6.65967	28.90632
Au	4.32558	5.82721	31.26088
Au	7.20930	5.82721	31.26088
Au	10.09302	5.82721	31.26088
Au	2.88372	8.32458	31.26088
Au	5.76744	8.32458	31.26088
Au	8.65116	8.32458	31.26088
Au	1.44186	10.82196	31.26088
Au	4.32558	10.82196	31.26088
Au	7.20930	10.82196	31.26088
Au	2.88372	4.99475	33.61543
Au	5.76744	4.99475	33.61543
Au	8.65116	4.99475	33.61543
Au	1.44186	7.49213	33.61543
Au	4.32558	7.49213	33.61543
Au	7.20930	7.49213	33.61543
Au	-0.00000	9.98950	33.61543
Au	2.88372	9.98950	33.61543
Au	5.76744	9.98950	33.61543
Au	2.88372	6.65967	35.96999
Au	5.76744	6.65967	35.96999
Au	8.65116	6.65967	35.96999
Au	1.44186	9.15704	35.96999
Au	4.32558	9.15704	35.96999
Au	7.20930	9.15704	35.96999
Au	-0.00000	11.65442	35.96999
Au	2.88372	11.65442	35.96999
Au	5.76744	11.65442	35.96999

Atomic co-ordinates of the two-probe system of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface: Arrangement 1(b)

ATOM	X (Å)	Y (Å)	Z (Å)
Au	1.44186	0.83246	1.17728
Au	4.32558	0.83246	1.17728
Au	7.20930	0.83246	1.17728
Au	-0.00000	3.32983	1.17728
Au	2.88372	3.32983	1.17728
Au	5.76744	3.32983	1.17728
Au	-1.44186	5.82721	1.17728
Au	1.44186	5.82721	1.17728
Au	4.32558	5.82721	1.17728
Au	0.00000	0.00000	3.53184
Au	2.88372	0.00000	3.53184
Au	5.76744	0.00000	3.53184
Au	-1.44186	2.49737	3.53184
Au	1.44186	2.49737	3.53184
Au	4.32558	2.49737	3.53184
Au	-2.88372	4.99475	3.53184
Au	0.00000	4.99475	3.53184
Au	2.88372	4.99475	3.53184
Au	0.00000	1.66492	5.88639
Au	2.88372	1.66492	5.88639
Au	5.76744	1.66492	5.88639
Au	-1.44186	4.16229	5.88639
Au	1.44186	4.16229	5.88639
Au	4.32558	4.16229	5.88639
Au	-2.88372	6.65966	5.88639
Au	0.00000	6.65966	5.88639
Au	2.88372	6.65966	5.88639
Au	1.44186	0.83246	8.24095
Au	-0.00000	-0.00000	10.59550
Au	4.32558	0.83246	8.24095
Au	2.88372	-0.00000	10.59550
Au	7.20931	0.83246	8.24095
Au	5.76745	-0.00000	10.59550
Au	-0.00000	3.32984	8.24095
Au	-1.44186	2.49738	10.59550
Au	2.88372	3.32984	8.24095
Au	1.44186	2.49738	10.59550
Au	5.76745	3.32984	8.24095
Au	4.32558	2.49738	10.59550
Au	-1.44186	5.82721	8.24095
Au	-2.88372	4.99475	10.59550
Au	1.44186	5.82721	8.24095
Au	-0.00000	4.99475	10.59550
Au	4.32558	5.82721	8.24095
Au	2.88372	4.99475	10.59550
C	1.47813	1.35345	14.67763
C	1.57459	2.65159	15.03891
C	1.61241	3.18615	16.39135
C	1.55853	2.49006	17.55868
C	1.59619	3.02238	18.90732
C	1.69309	4.32667	19.28098
C	1.73080	4.85986	20.63397

C	1.67664	4.15966	21.78802
H	1.41736	0.55602	15.41135
H	1.63153	3.39669	14.24622
H	1.69336	4.27031	16.44035
H	1.47753	1.40529	17.50591
H	1.53852	2.26737	19.69009
H	1.75091	5.08384	18.50143
H	1.81174	5.94419	20.70079
H	1.59573	3.07740	21.79981
S	1.44186	0.83246	12.98550
S	1.73203	4.93428	23.37960
Au	-0.00000	-0.00000	25.76960
Au	-0.00000	1.66492	28.12415
Au	2.88372	-0.00000	25.76960
Au	2.88372	1.66492	28.12415
Au	5.76745	-0.00000	25.76960
Au	5.76745	1.66492	28.12415
Au	-1.44186	2.49738	25.76960
Au	-1.44186	4.16230	28.12415
Au	1.44186	2.49738	25.76960
Au	1.44186	4.16230	28.12415
Au	4.32558	2.49738	25.76960
Au	4.32558	4.16230	28.12415
Au	-2.88372	4.99475	25.76960
Au	-2.88372	6.65967	28.12415
Au	-0.00000	4.99475	25.76960
Au	-0.00000	6.65967	28.12415
Au	2.88372	4.99475	25.76960
Au	2.88372	6.65967	28.12415
Au	4.32558	5.82721	30.47870
Au	7.20930	5.82721	30.47870
Au	10.09302	5.82721	30.47870
Au	2.88372	8.32458	30.47870
Au	5.76744	8.32458	30.47870
Au	8.65116	8.32458	30.47870
Au	1.44186	10.82196	30.47870
Au	4.32558	10.82196	30.47870
Au	7.20930	10.82196	30.47870
Au	2.88372	4.99475	32.83326
Au	5.76744	4.99475	32.83326
Au	8.65116	4.99475	32.83326
Au	1.44186	7.49213	32.83326
Au	4.32558	7.49213	32.83326
Au	7.20930	7.49213	32.83326
Au	-0.00000	9.98950	32.83326
Au	2.88372	9.98950	32.83326
Au	5.76744	9.98950	32.83326
Au	2.88372	6.65967	35.18782
Au	5.76744	6.65967	35.18782
Au	8.65116	6.65967	35.18782
Au	1.44186	9.15704	35.18782
Au	4.32558	9.15704	35.18782
Au	7.20930	9.15704	35.18782
Au	-0.00000	11.65442	35.18782
Au	2.88372	11.65442	35.18782
Au	5.76744	11.65442	35.18782

Atomic co-ordinates of the two-probe system of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface: Arrangement 1(c)

ATOM	X (Å)	Y (Å)	Z (Å)
Au	1.44186	0.83246	1.17728
Au	4.32558	0.83246	1.17728
Au	7.20930	0.83246	1.17728
Au	-0.00000	3.32983	1.17728
Au	2.88372	3.32983	1.17728
Au	5.76744	3.32983	1.17728
Au	-1.44186	5.82721	1.17728
Au	1.44186	5.82721	1.17728
Au	4.32558	5.82721	1.17728
Au	0.00000	0.00000	3.53184
Au	2.88372	0.00000	3.53184
Au	5.76744	0.00000	3.53184
Au	-1.44186	2.49737	3.53184
Au	1.44186	2.49737	3.53184
Au	4.32558	2.49737	3.53184
Au	-2.88372	4.99475	3.53184
Au	0.00000	4.99475	3.53184
Au	2.88372	4.99475	3.53184
Au	0.00000	1.66492	5.88639
Au	2.88372	1.66492	5.88639
Au	5.76744	1.66492	5.88639
Au	-1.44186	4.16229	5.88639
Au	1.44186	4.16229	5.88639
Au	4.32558	4.16229	5.88639
Au	-2.88372	6.65966	5.88639
Au	0.00000	6.65966	5.88639
Au	2.88372	6.65966	5.88639
Au	1.44186	0.83246	8.24095
Au	-0.00000	-0.00000	10.59550
Au	4.32558	0.83246	8.24095
Au	2.88372	-0.00000	10.59550
Au	7.20931	0.83246	8.24095
Au	5.76745	-0.00000	10.59550
Au	-0.00000	3.32984	8.24095
Au	-1.44186	2.49738	10.59550
Au	2.88372	3.32984	8.24095
Au	1.44186	2.49738	10.59550
Au	5.76745	3.32984	8.24095
Au	4.32558	2.49738	10.59550
Au	-1.44186	5.82721	8.24095
Au	-2.88372	4.99475	10.59550
Au	1.44186	5.82721	8.24095
Au	-0.00000	4.99475	10.59550
Au	4.32558	5.82721	8.24095
Au	2.88372	4.99475	10.59550
C	1.61258	2.62248	22.39669
C	1.51407	3.69405	21.57998
C	1.48928	3.69013	20.12545
C	1.55995	2.61214	19.29897
C	1.53529	2.60755	17.84880
C	1.43646	3.68025	17.01830
C	1.41179	3.67486	15.56377

C	1.48260	2.59797	14.75116
H	1.68562	1.61078	22.01060
H	1.44442	4.67896	22.04025
H	1.40370	4.67853	19.67814
H	1.64553	1.62458	19.75002
H	1.60560	1.61711	17.40142
H	1.36602	4.67152	17.46190
H	1.32642	4.65683	15.09984
H	1.56883	1.58885	15.14129
S	1.44186	1.87738	12.98550
S	1.63183	3.37462	24.16177
Au	-0.00000	-0.00000	26.55177
Au	-0.00000	1.66492	28.90632
Au	2.88372	-0.00000	26.55177
Au	2.88372	1.66492	28.90632
Au	5.76745	-0.00000	26.55177
Au	5.76745	1.66492	28.90632
Au	-1.44186	2.49738	26.55177
Au	-1.44186	4.16230	28.90632
Au	1.44186	2.49738	26.55177
Au	1.44186	4.16230	28.90632
Au	4.32558	2.49738	26.55177
Au	4.32558	4.16230	28.90632
Au	-2.88372	4.99475	26.55177
Au	-2.88372	6.65967	28.90632
Au	-0.00000	4.99475	26.55177
Au	-0.00000	6.65967	28.90632
Au	2.88372	4.99475	26.55177
Au	2.88372	6.65967	28.90632
Au	4.32558	5.82721	31.26088
Au	7.20930	5.82721	31.26088
Au	10.09302	5.82721	31.26088
Au	2.88372	8.32458	31.26088
Au	5.76744	8.32458	31.26088
Au	8.65116	8.32458	31.26088
Au	1.44186	10.82196	31.26088
Au	4.32558	10.82196	31.26088
Au	7.20930	10.82196	31.26088
Au	2.88372	4.99475	33.61543
Au	5.76744	4.99475	33.61543
Au	8.65116	4.99475	33.61543
Au	1.44186	7.49213	33.61543
Au	4.32558	7.49213	33.61543
Au	7.20930	7.49213	33.61543
Au	-0.00000	9.98950	33.61543
Au	2.88372	9.98950	33.61543
Au	5.76744	9.98950	33.61543
Au	2.88372	6.65967	35.96999
Au	5.76744	6.65967	35.96999
Au	8.65116	6.65967	35.96999
Au	1.44186	9.15704	35.96999
Au	4.32558	9.15704	35.96999
Au	7.20930	9.15704	35.96999
Au	-0.00000	11.65442	35.96999
Au	2.88372	11.65442	35.96999
Au	5.76744	11.65442	35.96999

Atomic co-ordinates of the two-probe system of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface: Arrangement 1(d)

ATOM	X (Å)	Y (Å)	Z (Å)
Au	1.44186	0.83246	1.17728
Au	4.32558	0.83246	1.17728
Au	7.20930	0.83246	1.17728
Au	-0.00000	3.32983	1.17728
Au	2.88372	3.32983	1.17728
Au	5.76744	3.32983	1.17728
Au	-1.44186	5.82721	1.17728
Au	1.44186	5.82721	1.17728
Au	4.32558	5.82721	1.17728
Au	0.00000	0.00000	3.53184
Au	2.88372	0.00000	3.53184
Au	5.76744	0.00000	3.53184
Au	-1.44186	2.49737	3.53184
Au	1.44186	2.49737	3.53184
Au	4.32558	2.49737	3.53184
Au	-2.88372	4.99475	3.53184
Au	0.00000	4.99475	3.53184
Au	2.88372	4.99475	3.53184
Au	0.00000	1.66492	5.88639
Au	2.88372	1.66492	5.88639
Au	5.76744	1.66492	5.88639
Au	-1.44186	4.16229	5.88639
Au	1.44186	4.16229	5.88639
Au	4.32558	4.16229	5.88639
Au	-2.88372	6.65966	5.88639
Au	0.00000	6.65966	5.88639
Au	2.88372	6.65966	5.88639
Au	1.44186	0.83246	8.24095
Au	-0.00000	-0.00000	10.59550
Au	4.32558	0.83246	8.24095
Au	2.88372	-0.00000	10.59550
Au	7.20931	0.83246	8.24095
Au	5.76745	-0.00000	10.59550
Au	-0.00000	3.32984	8.24095
Au	-1.44186	2.49738	10.59550
Au	2.88372	3.32984	8.24095
Au	1.44186	2.49738	10.59550
Au	5.76745	3.32984	8.24095
Au	4.32558	2.49738	10.59550
Au	-1.44186	5.82721	8.24095
Au	-2.88372	4.99475	10.59550
Au	1.44186	5.82721	8.24095
Au	-0.00000	4.99475	10.59550
Au	4.32558	5.82721	8.24095
Au	2.88372	4.99475	10.59550
C	1.44186	2.49738	13.99586
C	1.44186	3.70266	14.64314
C	1.44186	3.91204	16.07552
C	1.44186	2.98495	17.07793
C	1.44186	3.21825	18.50881
C	1.44186	4.41595	19.16380

C	1.44186	4.66457	20.58955
C	1.44186	3.73305	21.59290
H	1.44186	1.59452	14.60515
H	1.44186	4.60430	14.03269
H	1.44186	4.96272	16.36441
H	1.44186	1.93043	16.79960
H	1.44186	2.30863	19.11007
H	1.44186	5.32145	18.55800
H	1.44186	5.72125	20.87391
H	1.44186	2.67550	21.33353
S	1.44186	4.71809	23.11139
S	1.44186	1.51234	12.47738
Au	-0.00000	-0.00000	24.99327
Au	-0.00000	1.66492	27.34782
Au	2.88372	-0.00000	24.99327
Au	2.88372	1.66492	27.34782
Au	5.76745	-0.00000	24.99327
Au	5.76745	1.66492	27.34782
Au	-1.44186	2.49738	24.99327
Au	-1.44186	4.16230	27.34782
Au	1.44186	2.49738	24.99327
Au	1.44186	4.16230	27.34782
Au	4.32558	2.49738	24.99327
Au	4.32558	4.16230	27.34782
Au	-2.88372	4.99475	24.99327
Au	-2.88372	6.65967	27.34782
Au	-0.00000	4.99475	24.99327
Au	-0.00000	6.65967	27.34782
Au	2.88372	4.99475	24.99327
Au	2.88372	6.65967	27.34782
Au	4.32558	5.82721	29.70238
Au	7.20930	5.82721	29.70238
Au	10.09302	5.82721	29.70238
Au	2.88372	8.32458	29.70238
Au	5.76744	8.32458	29.70238
Au	8.65116	8.32458	29.70238
Au	1.44186	10.82196	29.70238
Au	4.32558	10.82196	29.70238
Au	7.20930	10.82196	29.70238
Au	2.88372	4.99475	32.05693
Au	5.76744	4.99475	32.05693
Au	8.65116	4.99475	32.05693
Au	1.44186	7.49213	32.05693
Au	4.32558	7.49213	32.05693
Au	7.20930	7.49213	32.05693
Au	-0.00000	9.98950	32.05693
Au	2.88372	9.98950	32.05693
Au	5.76744	9.98950	32.05693
Au	2.88372	6.65967	34.41149
Au	5.76744	6.65967	34.41149
Au	8.65116	6.65967	34.41149
Au	1.44186	9.15704	34.41149
Au	4.32558	9.15704	34.41149
Au	7.20930	9.15704	34.41149
Au	-0.00000	11.65442	34.41149
Au	2.88372	11.65442	34.41149
Au	5.76744	11.65442	34.41149

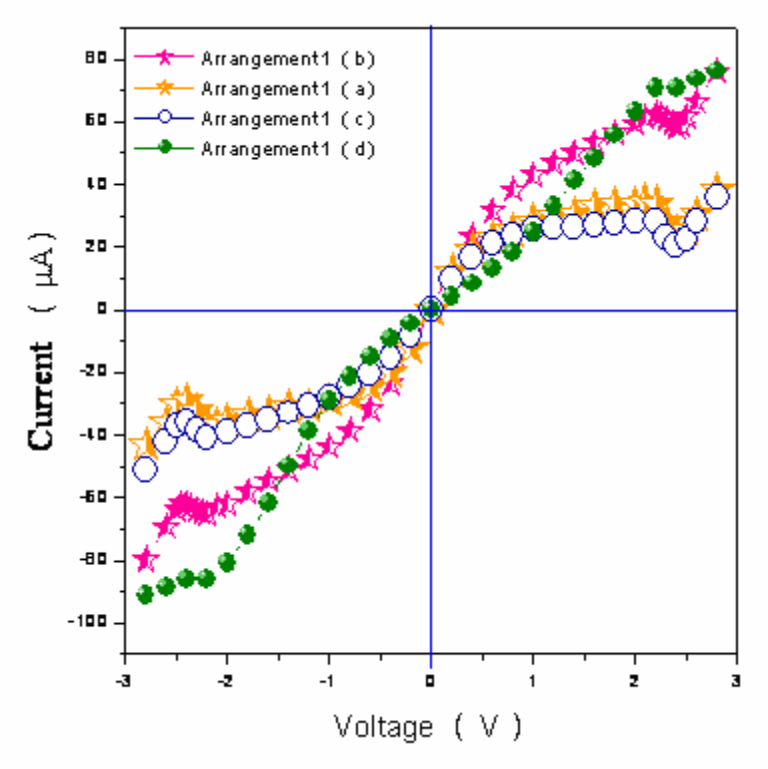


Figure S1. Current-voltage (*I-V*) characteristic of all four arrangements of the two probe system of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface.

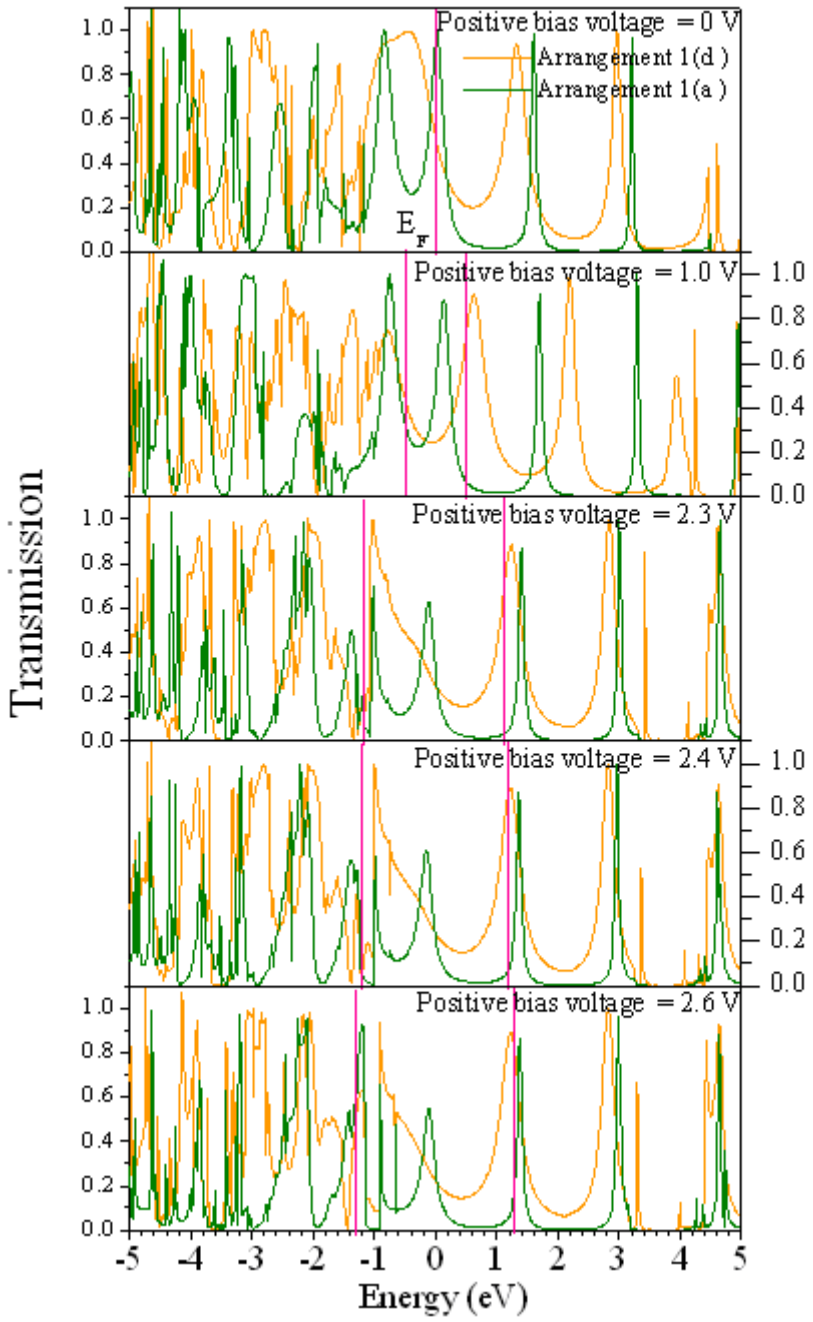


Figure S2: 2D view of Transmission spectra of the arrangement **1 (d)** and arrangement **1 (a)**, at bias voltage of 0.0 V, 1.0 V, 2.3 V, 2.4 V, and 2.6 V respectively. Pink lines indicate the bias window. A positive bias corresponds to electron current from left to right electrode.

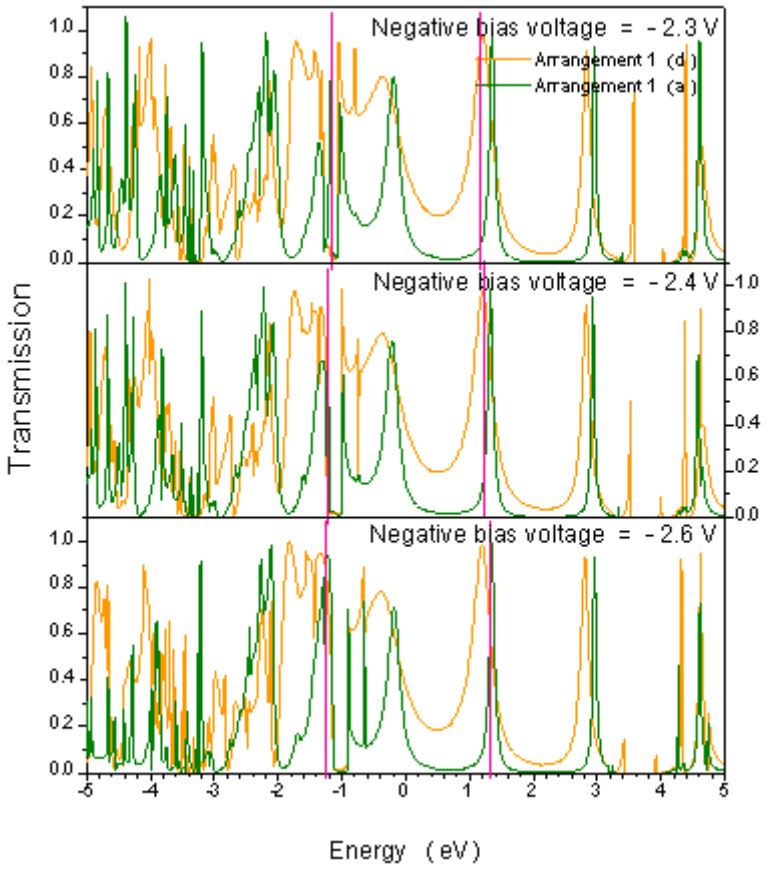


Figure S3: 2D view of Transmission spectra of the arrangement **1 (d)** and arrangement **1 (a)**, at bias voltage of -2.3 V, -2.4 V, and -2.6 V respectively. Pink lines indicate the bias window. A negative bias corresponds to electron current from right to left electrode.

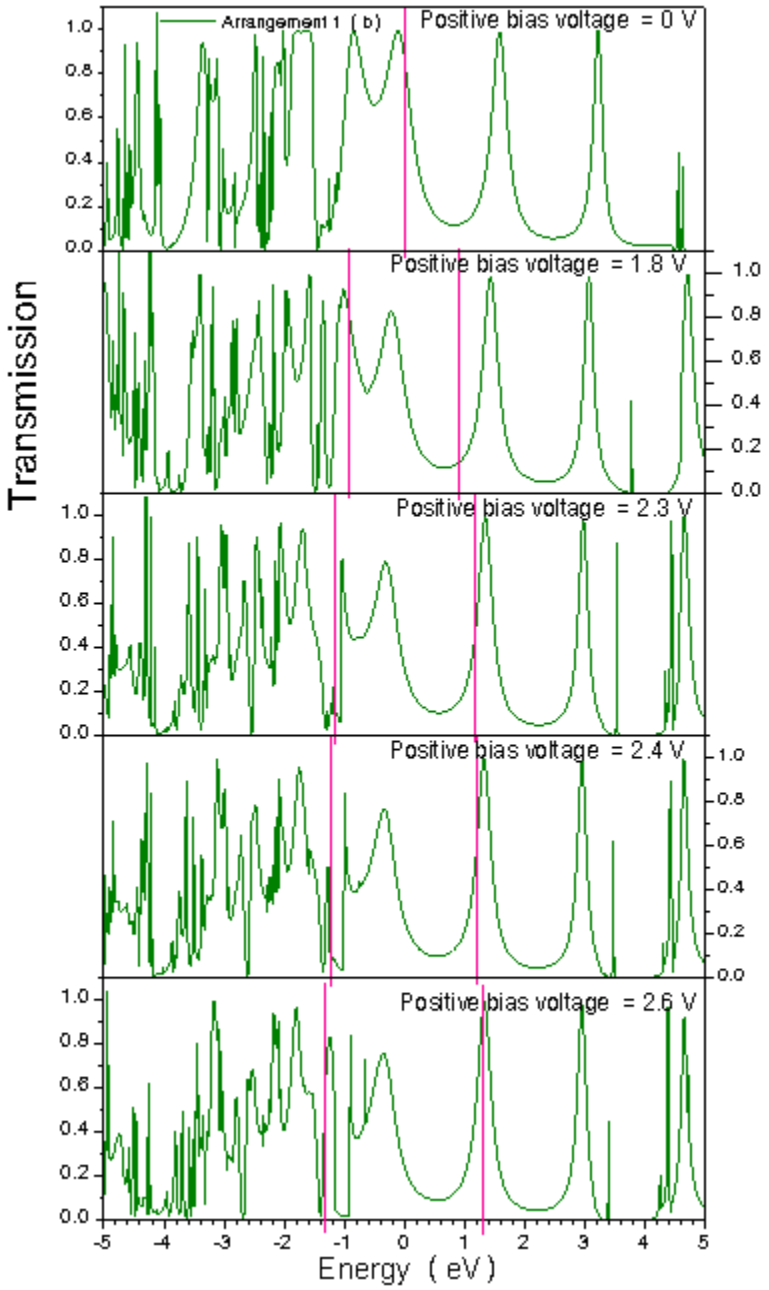


Figure S4: 2D view of Transmission spectra of the arrangement **1(b)**, at bias voltage of 0 V, 1.8 V, 2.3 V, 2.4 V, and 2.6 V respectively. Pink lines indicate the bias window. A positive bias corresponds to electron current from left to right electrode.

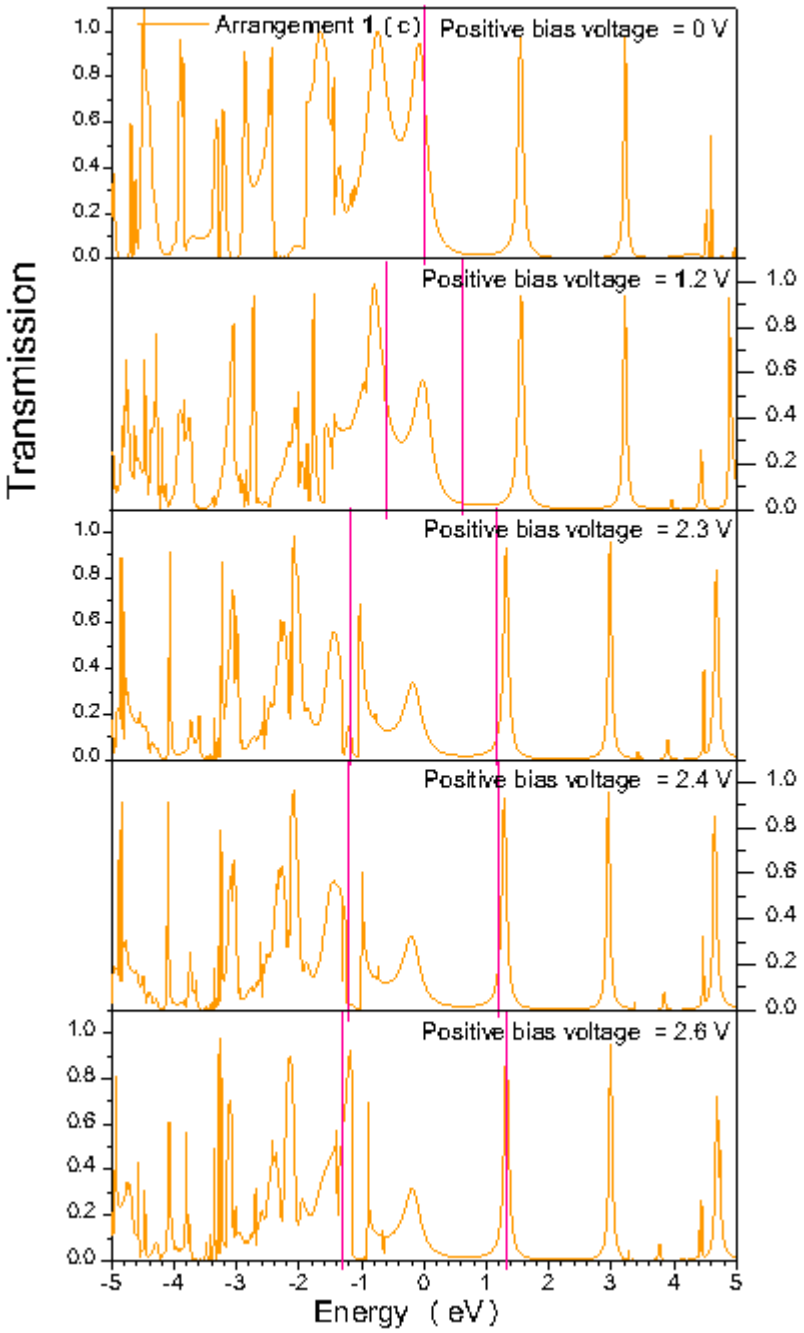


Figure S5: 2D view of Transmission spectra of the arrangement **1(c)**, at bias voltage of 0 V, 1.2 V, 2.3 V, 2.4 V, and 2.6 V respectively. Pink lines indicate the bias window. A positive bias corresponds to electron current from left to right electrode.

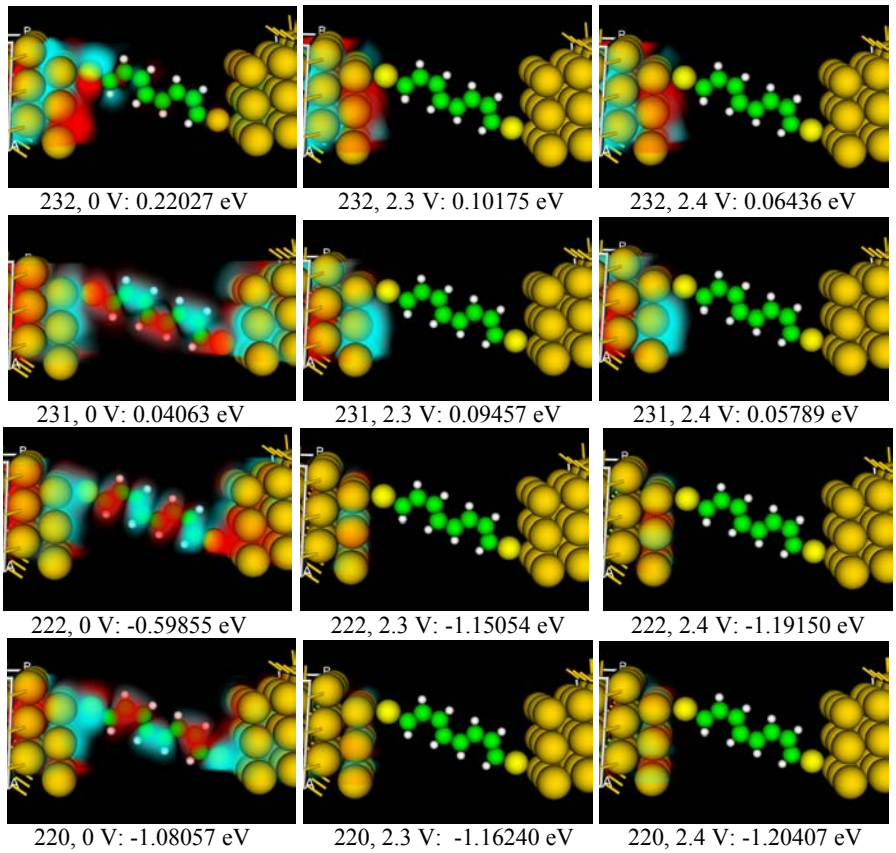


Figure S6: MPSH states of the arrangement **1 (b)** contributing to the bias window at the bias voltage of 0 V, 2.3 V and 2.4 V, respectively. A positive bias corresponds to electron current from left to right electrode.

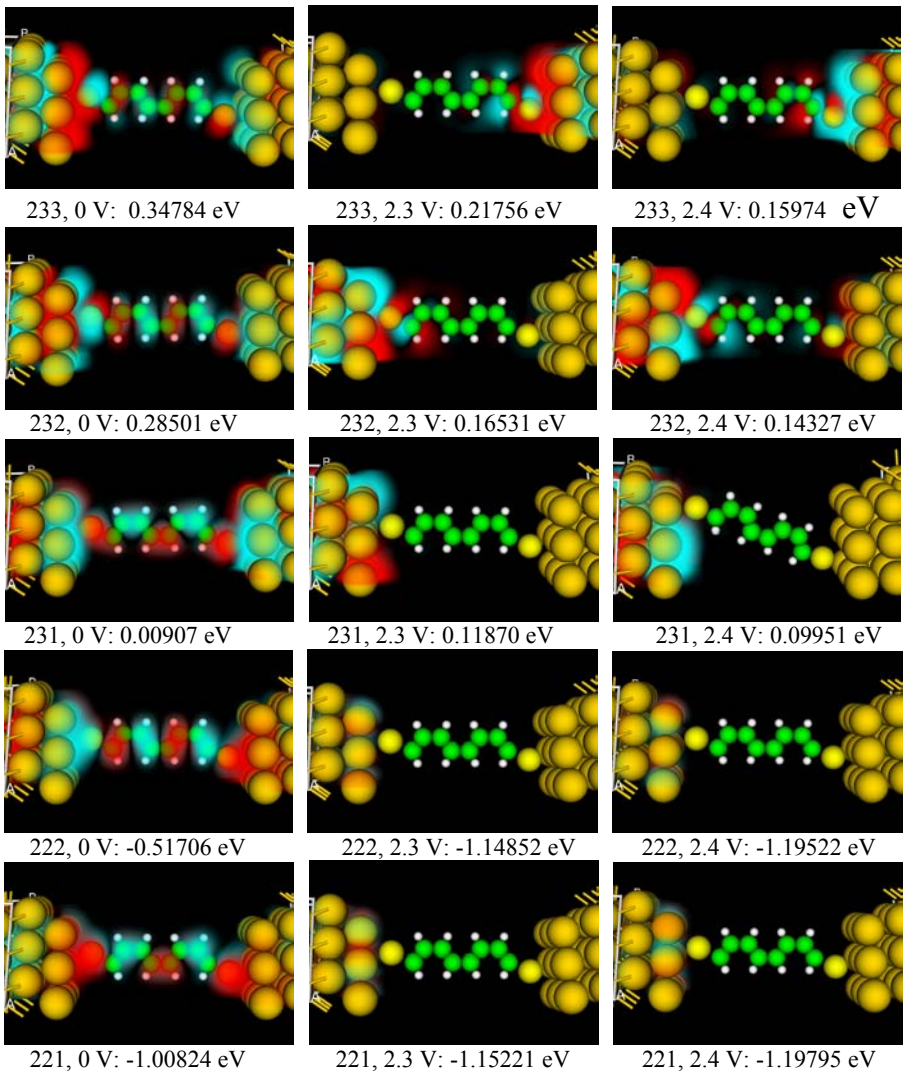


Figure S7: MPSH states of the arrangement **1 (c)** contributing to the bias window at the bias voltage of 0 V, 2.3 V and 2.4 V, respectively. A positive bias corresponds to electron current from left to right electrode.

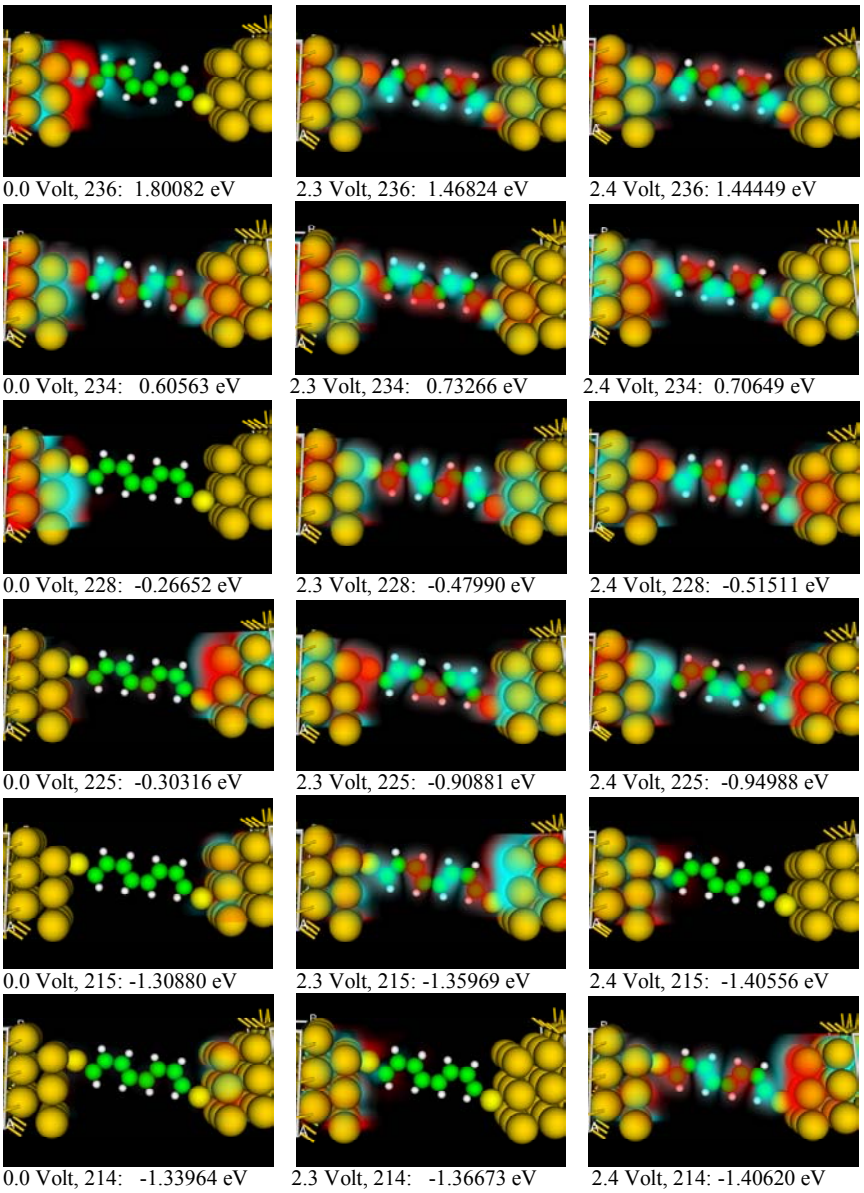


Figure S8: MPSH states of the arrangement **1(d)** contributing to the bias window at the bias voltage of 0 V, 2.3 V and 2.4 V, respectively. A positive bias corresponds to electron current from left to right electrode.

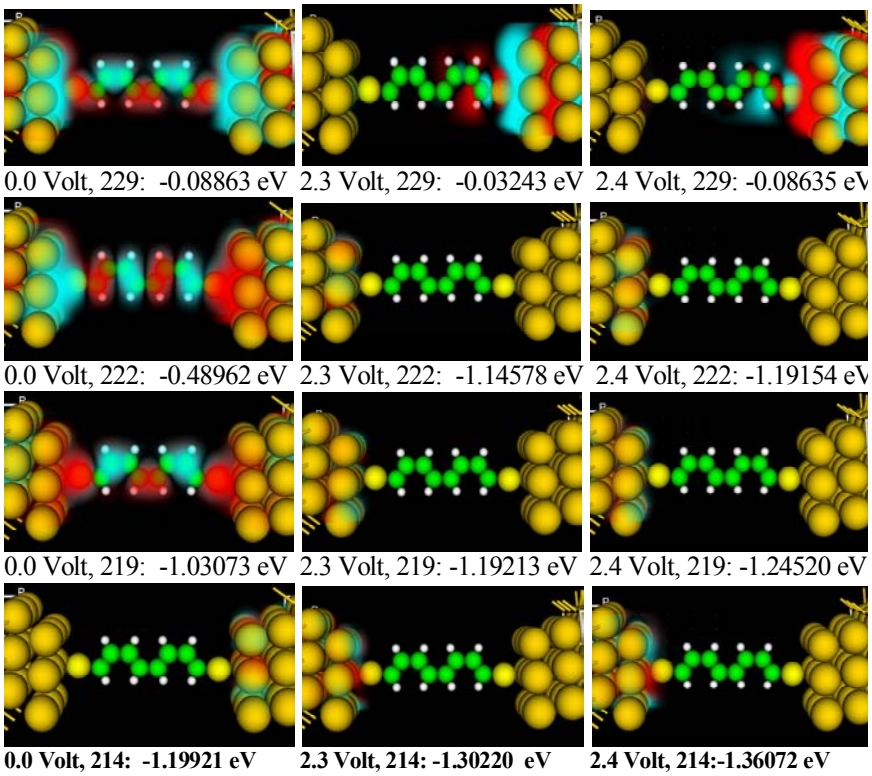


Figure S9: MPSH states of the arrangement **1(a)** contributing to the bias window at the bias voltage of 0 V, 2.3 V and 2.4 V, respectively. A positive bias corresponds to electron current from left to right electrode.

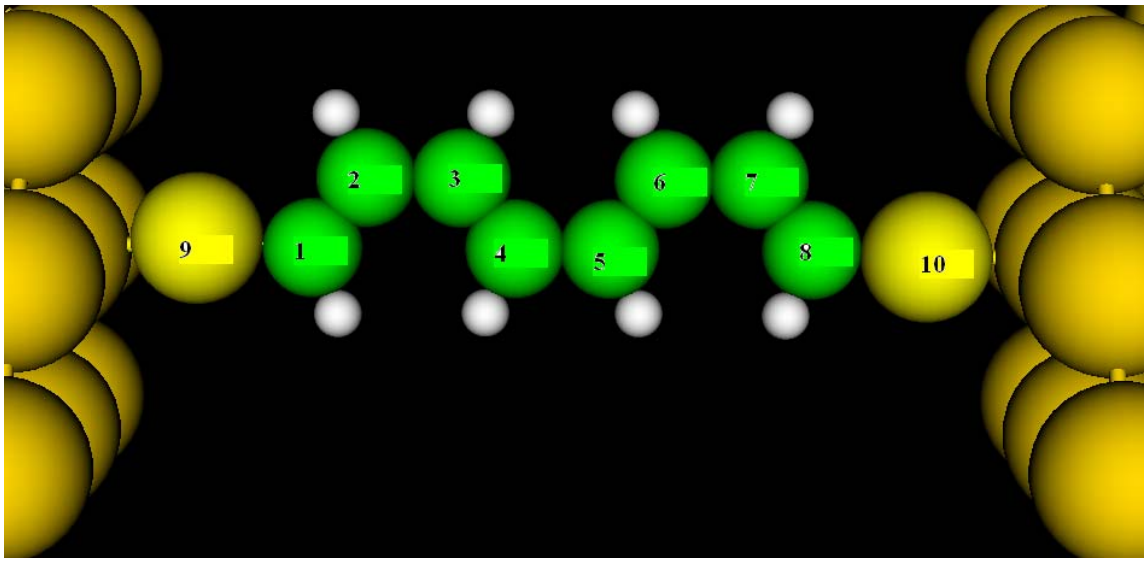


Figure S10. Selected view of the arrangement 1(a).

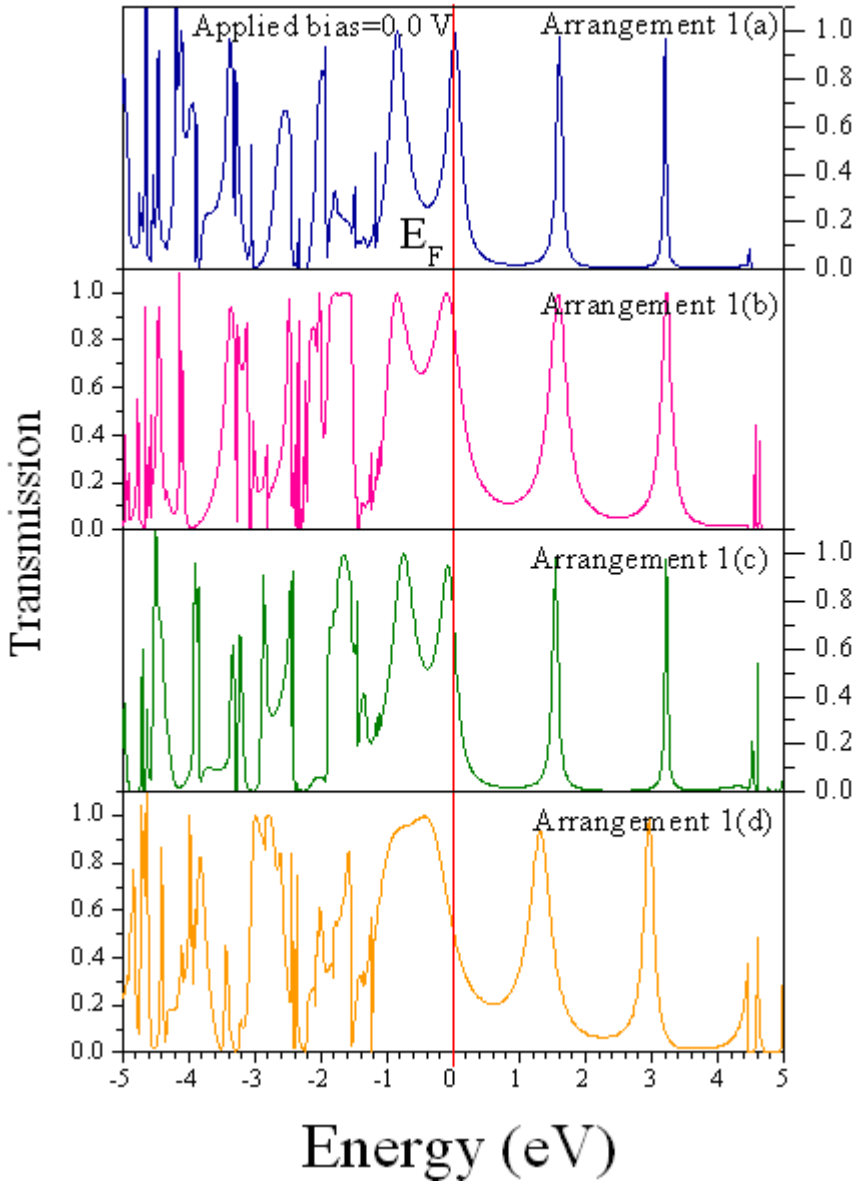
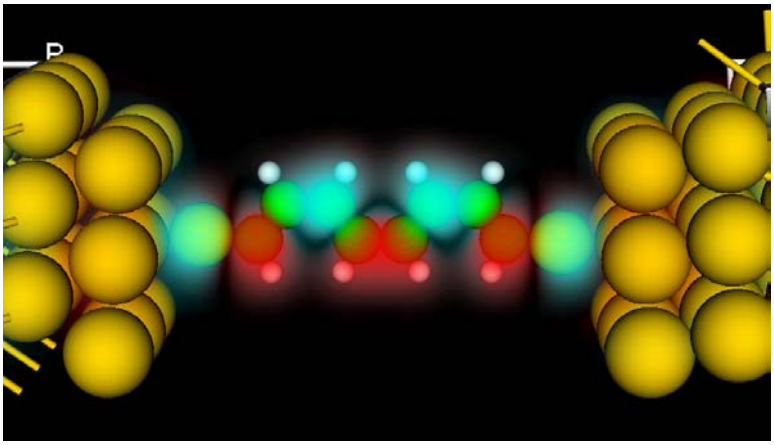
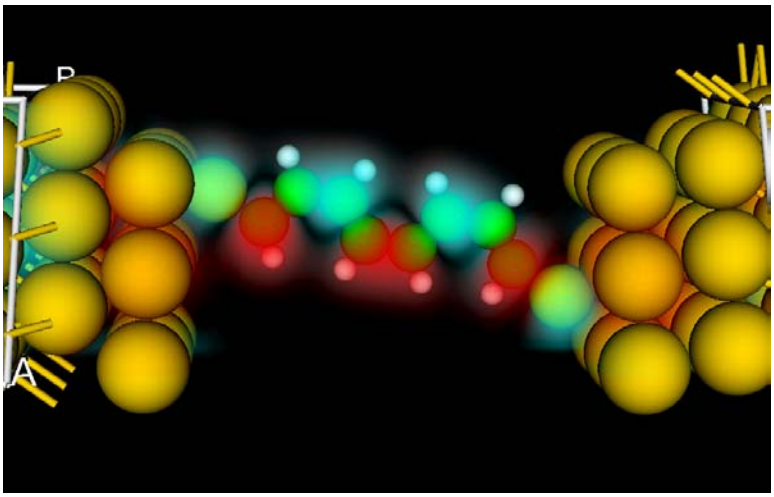


Figure S11. Zero bias transmission spectra of 1(a), 1(b), 1(c) and 1(d).

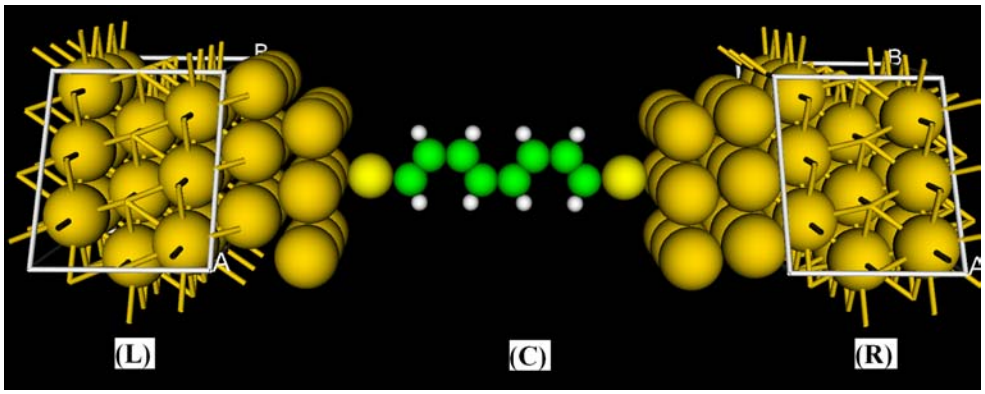


0.0 Volt, 237, 1(a): 1.5 eV (approximately)

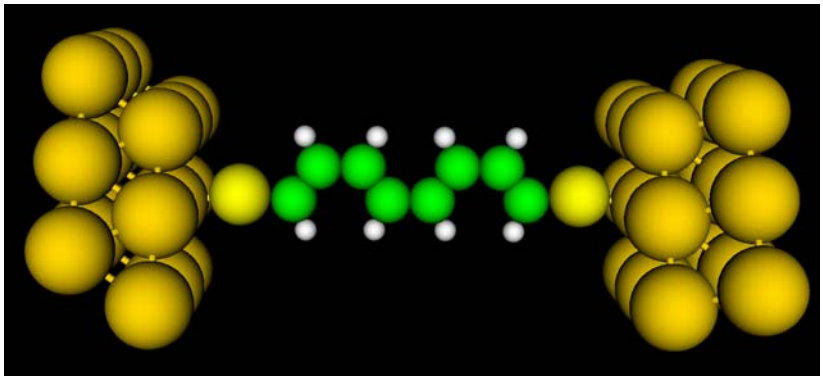


0.0 Volt, 235, 1(d): 1.5 eV (approximately)

Figure S12: MPSH state corresponding to the transmission peak at 1.5 eV (approximately) in 1(a) and 1(d)

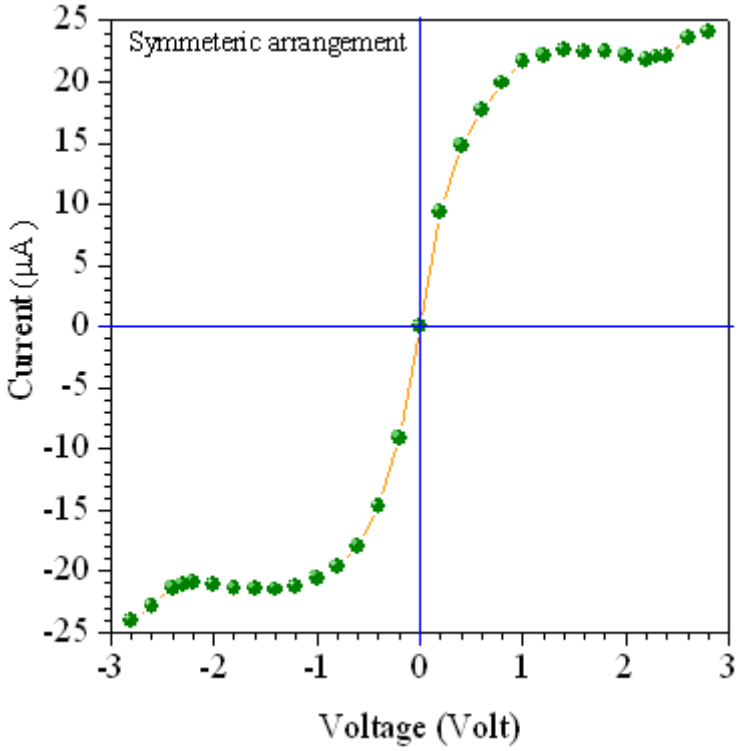


(a)

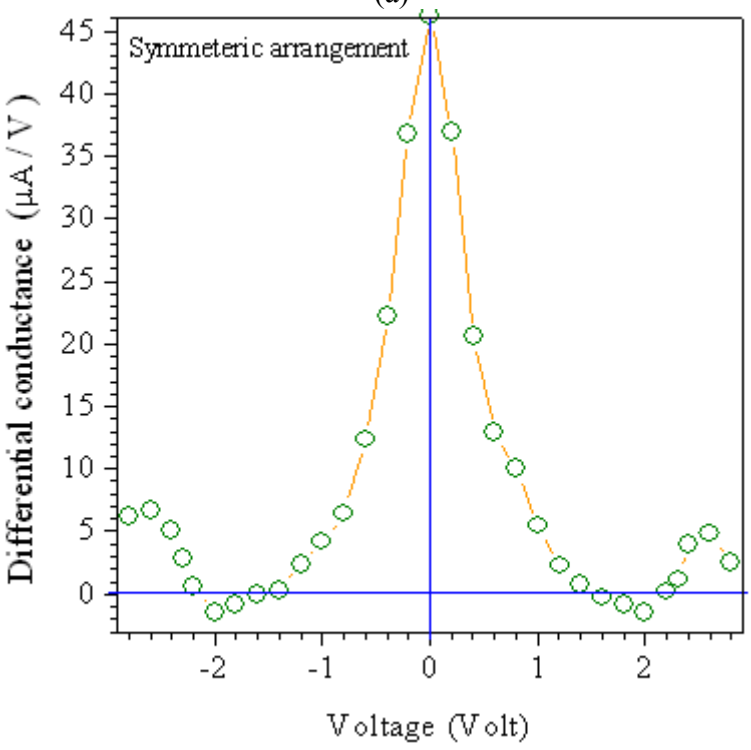


(b)

Figure S13: (a) Symmetric arrangement of the two-probe system of thiol-ended trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface. (b) Selected view of the symmetric arrangement of the two-probe system of thiol-ended trimer unit of cis-polyacetylene self-assembled on Au (111) surface.



(a)



(b)

Figure S14: (a) Current-voltage *(I-V)* characteristic of the symmetric arrangement of two probe system of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface. (b) Differential conductance (dI/dV) versus voltage (V) plot of the symmetric arrangement of trimer unit of cis-polyacetylene self-assembled on Au (1 1 1) surface.