

Supplementary Material

Assessing the Importance of Multireference Correlation in Predicting Reversed Conductance Decay

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Section S1. XYZ coordinates for all systems in Angstroms.

p1 Electrodes (1-layer)

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#1 Phenyl ring (p1)

Al	-3.4007400000	0.0000000000	0.0000000000
C	-1.4344500000	0.0000000000	0.0000000000
H	-1.2268100000	0.0000000000	2.1606600000
H	-1.2268100000	0.0000000000	-2.1606600000
C	-0.6992200000	0.0000000000	1.2090300000
C	-0.6992200000	0.0000000000	-1.2090400000
C	0.6992200000	0.0000000000	1.2090300000
C	0.6992200000	0.0000000000	-1.2090400000
H	1.2268100000	0.0000000000	2.1606600000
H	1.2268100000	0.0000000000	-2.1606600000
C	1.4344500000	0.0000000000	0.0000000000
Al	3.4007400000	0.0000000000	0.0000000000

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#2 Phenyl ring (p1)

Al	-5.5659700000	0.0000000000	0.0000500000
C	-3.6047800000	-0.0001000000	0.0000000000
H	-3.3858500000	2.0513000000	0.6758600000
H	-3.3857400000	-2.0514800000	-0.6758700000
C	-2.8639300000	1.1464600000	0.3727700000
C	-2.8638800000	-1.1466100000	-0.3727800000
C	-1.4679900000	1.1496600000	0.3732100000
C	-1.4679300000	-1.1497400000	-0.3732300000
H	-0.9326800000	2.0388200000	0.6911100000
H	-0.9325800000	-2.0388700000	-0.6911500000
C	-0.7425500000	-0.0000200000	-0.0000100000
C	0.7425500000	0.0000200000	-0.0000100000
H	0.9325700000	2.0388700000	-0.6911300000
H	0.9326900000	-2.0388200000	0.6911200000
C	1.4679300000	1.1497400000	-0.3732200000
C	1.4679900000	-1.1496600000	0.3732100000
C	2.8638700000	1.1466200000	-0.3727800000
C	2.8639400000	-1.1464600000	0.3727600000
H	3.3857400000	2.0514900000	-0.6758700000
H	3.3858500000	-2.0513000000	0.6758600000
C	3.6047800000	0.0001000000	-0.0000100000
Al	5.5659700000	0.0000200000	0.0000600000

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#3 Phenyl ring (p1)

Al	-7.7345300000	0.0000700000	-0.0001000000
C	-5.7738600000	0.0000100000	-0.0000500000
H	-5.5550200000	-2.1231200000	-0.3954000000
H	-5.5549700000	2.1231400000	0.3953000000
C	-5.0328100000	-1.1858600000	-0.2164400000
C	-5.0327800000	1.1858700000	0.2163400000
C	-3.6370400000	-1.1885600000	-0.2187500000
C	-3.6370100000	1.1885500000	0.2186400000
H	-3.1021400000	-2.1118500000	-0.4184600000
H	-3.1020900000	2.1118300000	0.4183400000
C	-2.9107600000	-0.0000100000	-0.0000500000
C	-1.4265000000	-0.0000200000	-0.0000600000
H	-1.2281100000	-1.9490000000	0.9113000000
H	-1.2281000000	1.9489700000	-0.9113700000
C	-0.6969500000	1.1004400000	-0.4925100000
C	-0.6969500000	-1.1004800000	0.4924200000
C	0.6969500000	1.1004400000	-0.4925200000
C	0.6969500000	-1.1004800000	0.4924300000
H	1.2280900000	-1.9490100000	0.9113100000
H	1.2281000000	1.9489800000	-0.9113700000
C	1.4265100000	-0.0000200000	-0.0000500000
C	2.9107400000	-0.0000100000	-0.0000300000
H	3.1021000000	2.1122400000	0.4163800000
H	3.1021700000	-2.1122400000	-0.4164600000
C	3.6370000000	1.1887500000	0.2175700000

C	3.6370400000	-1.1887500000	-0.2176400000
C	5.0327700000	1.1860800000	0.2152800000
C	5.0328000000	-1.1860400000	-0.2153200000
H	5.5549400000	2.1235300000	0.3933400000
H	5.5550000000	-2.1234700000	-0.3933800000
C	5.7738700000	0.0000300000	-0.0000200000
Al	7.7345300000	0.0000400000	-0.0000500000

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#4 Phenyl ring (p1)

Al	-9.9010800000	-0.0000200000	0.0000000000
C	-7.9404500000	-0.0000200000	0.0000100000
H	-7.7224900000	2.1549700000	-0.1375000000
H	-7.7224800000	-2.1550000000	0.1375200000
C	-7.1996400000	1.2028500000	-0.0814900000
C	-7.1996400000	-1.2028800000	0.0815000000
C	-5.8038900000	1.2060200000	-0.0814000000
C	-5.8038900000	-1.2060500000	0.0814100000
H	-5.2684500000	2.1497400000	-0.1173100000
H	-5.2684500000	-2.1497600000	0.1173200000
C	-5.0778600000	-0.0000100000	0.0000100000
C	-3.5936800000	-0.0000100000	0.0000000000
H	-3.3942400000	1.6406200000	-1.3923600000
H	-3.3942300000	-1.6406300000	1.3923700000
C	-2.8640600000	0.9325700000	-0.7637800000
C	-2.8640600000	-0.9325800000	0.7637800000
C	-1.4698400000	0.9330700000	-0.7632600000
C	-1.4698300000	-0.9330700000	0.7632700000
H	-0.9380400000	1.6417600000	-1.3900300000
H	-0.9380300000	-1.6417600000	1.3900400000
C	-0.7408000000	0.0000000000	0.0000000000
C	0.7430900000	0.0000000000	0.0000000000
H	0.9376900000	2.1512200000	-0.0104800000
H	0.9377000000	-2.1512200000	0.0104800000
C	1.4711800000	1.2060400000	-0.0149200000
C	1.4711900000	-1.2060300000	0.0149200000
C	2.8654800000	1.2061600000	-0.0107200000
C	2.8654900000	-1.2061500000	0.0107100000
H	3.3988600000	2.1510900000	-0.0347800000
H	3.3988700000	-2.1510800000	0.0347600000
C	3.5933700000	0.0000100000	-0.0000100000
C	5.0776900000	0.0000100000	-0.0000100000
H	5.2661400000	-1.6778100000	-1.3482800000
H	5.2661500000	1.6778200000	1.3482600000
C	5.8028400000	0.9519300000	0.7450900000
C	5.8028400000	-0.9519100000	-0.7451100000
C	7.1987800000	0.9485800000	0.7442600000
C	7.1987800000	-0.9485600000	-0.7442900000
H	7.7208000000	-1.6935900000	-1.3405800000
H	7.7208100000	1.6936200000	1.3405400000
C	7.9398300000	0.0000100000	-0.0000200000

Al 9.9000000000 0.0000500000 -0.0000700000

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#5 Phenyl ring (p1)

Al	-12.0695900000	0.0005500000	-0.0010200000
C	-10.1090500000	0.0002800000	-0.0007900000
H	-9.8913300000	-2.1555500000	-0.1249100000
H	-9.8907700000	2.1560400000	0.1233800000
C	-9.3683600000	-1.2031700000	-0.0748300000
C	-9.3680500000	1.2035300000	0.0732000000
C	-7.9726300000	-1.2065100000	-0.0747200000
C	-7.9723200000	1.2065000000	0.0729600000
H	-7.4373700000	-2.1505200000	-0.1047000000
H	-7.4368000000	2.1503800000	0.1029000000
C	-7.2463400000	-0.0001000000	-0.0009300000
C	-5.7621600000	-0.0002400000	-0.0009100000
H	-5.5627700000	-1.6512600000	-1.3809400000
H	-5.5626900000	1.6507100000	1.3792000000
C	-5.0325600000	-0.9386100000	-0.7576200000
C	-5.0324900000	0.9379900000	0.7559300000
C	-3.6383300000	-0.9392300000	-0.7569700000
C	-3.6382700000	0.9382800000	0.7555600000
H	-3.1062900000	-1.6526400000	-1.3781600000
H	-3.1061400000	1.6515400000	1.3768700000
C	-2.9092700000	-0.0005800000	-0.0006000000
C	-1.4253800000	-0.0007000000	-0.0003400000
H	-1.2307700000	2.1504600000	-0.0111500000
H	-1.2307600000	-2.1518700000	0.0106700000
C	-0.6972400000	-1.2067200000	-0.0030000000
C	-0.6972100000	1.2053300000	0.0027200000
C	0.6971500000	1.2053300000	-0.0002300000
C	0.6971500000	-1.2067300000	0.0006200000
H	1.2305800000	-2.1518900000	-0.0150000000
H	1.2306700000	2.1504400000	0.0157300000
C	1.4253300000	-0.0007200000	0.0003500000
C	2.9092600000	-0.0005800000	0.0007100000
H	3.1061300000	1.6546600000	-1.3730100000
H	3.1063600000	-1.6558600000	1.3743900000
C	3.6382600000	0.9400500000	-0.7532800000
C	3.6383400000	-0.9410000000	0.7548400000
C	5.0324700000	0.9398000000	-0.7536100000
C	5.0325800000	-0.9403700000	0.7554900000
H	5.5626800000	1.6539200000	-1.3752600000
H	5.5628000000	-1.6544400000	1.3771700000
C	5.7621600000	-0.0001700000	0.0010600000
C	7.2463700000	0.0000000000	0.0010800000
H	7.4368500000	2.1507600000	-0.0968900000
H	7.4374300000	-2.1507000000	0.0991300000
C	7.9723600000	1.2068000000	-0.0695300000
C	7.9726700000	-1.2066000000	0.0717200000
C	9.3680900000	1.2038300000	-0.0696900000

C	9.368400000	-1.203250000	0.071860000
H	9.890810000	2.156480000	-0.117220000
H	9.891390000	-2.155750000	0.119350000
C	10.109080000	0.000390000	0.001090000
Al	12.069630000	0.000420000	0.001550000

P1 Electrodes (2-layer)

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#1 Ring (p1-2)

Al	-5.89953	0.00000	0.00000
Al	-3.40074	0.00000	0.00000
C	-1.43445	0.00000	0.00000
H	-1.22681	0.00000	-2.16066
H	-1.22681	0.00000	2.16066
C	-0.69922	0.00000	-1.20904
C	-0.69922	0.00000	1.20903
C	0.69922	0.00000	-1.20904
C	0.69922	0.00000	1.20903
H	1.22681	0.00000	-2.16066
H	1.22681	0.00000	2.16066
C	1.43445	0.00000	0.00000
Al	3.40074	0.00000	0.00000
Al	5.89953	0.00000	0.00000

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#2 Phenyl ring (p1-2)

Al	-8.06476	0.00000	0.00000
Al	-5.56597	0.00000	0.00005
C	-3.60478	-0.00010	0.00000
H	-3.38585	2.05130	0.67586
H	-3.38574	-2.05148	-0.67587
C	-2.86393	1.14646	0.37277
C	-2.86388	-1.14661	-0.37278
C	-1.46799	1.14966	0.37321
C	-1.46793	-1.14974	-0.37323
H	-0.93268	2.03882	0.69111
H	-0.93258	-2.03887	-0.69115
C	-0.74255	-0.00002	-0.00001
C	0.74255	0.00002	-0.00001
H	0.93257	2.03887	-0.69113
H	0.93269	-2.03882	0.69112
C	1.46793	1.14974	-0.37322
C	1.46799	-1.14966	0.37321
C	2.86387	1.14662	-0.37278
C	2.86394	-1.14646	0.37276
H	3.38574	2.05149	-0.67587
H	3.38585	-2.05130	0.67586
C	3.60478	0.00010	-0.00001
Al	5.56597	0.00002	0.00006
Al	8.06476	0.00000	0.00000

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#3 Phenyl ring (p1-2)

Al	-10.23332	0.00000	0.00000
Al	-7.73453	0.00007	-0.00010
C	-5.77386	0.00001	-0.00005
H	-5.55502	-2.12312	-0.39540
H	-5.55497	2.12314	0.39530
C	-5.03281	-1.18586	-0.21644
C	-5.03278	1.18587	0.21634
C	-3.63704	-1.18856	-0.21875
C	-3.63701	1.18855	0.21864
H	-3.10214	-2.11185	-0.41846
H	-3.10209	2.11183	0.41834
C	-2.91076	-0.00001	-0.00005
C	-1.42650	-0.00002	-0.00006
H	-1.22811	-1.94900	0.91130
H	-1.22810	1.94897	-0.91137
C	-0.69695	-1.10048	0.49242
C	-0.69695	1.10044	-0.49251
C	0.69695	-1.10048	0.49243
C	0.69695	1.10044	-0.49252
H	1.22809	-1.94901	0.91131
H	1.22810	1.94898	-0.91137
C	1.42651	-0.00002	-0.00005
C	2.91074	-0.00001	-0.00003
H	3.10210	2.11224	0.41638
H	3.10217	-2.11224	-0.41646
C	3.63700	1.18875	0.21757
C	3.63704	-1.18875	-0.21764
C	5.03277	1.18608	0.21528
C	5.03280	-1.18604	-0.21532
H	5.55494	2.12353	0.39334
H	5.55500	-2.12347	-0.39338
C	5.77387	0.00003	-0.00002
Al	7.73453	0.00004	-0.00005
Al	10.23332	0.00000	0.00000

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#4 Phenyl ring (p1-2)

Al	-12.39987	0.00000	0.00000
Al	-9.90108	-0.00002	0.00000
C	-7.94045	-0.00002	0.00001
H	-7.72249	2.15497	-0.13750
H	-7.72248	-2.15500	0.13752
C	-7.19964	1.20285	-0.08149
C	-7.19964	-1.20288	0.08150
C	-5.80389	1.20602	-0.08140
C	-5.80389	-1.20605	0.08141
H	-5.26845	2.14974	-0.11731
H	-5.26845	-2.14976	0.11732

C	-5.07786	-0.00001	0.00001
C	-3.59368	-0.00001	0.00000
H	-3.39424	1.64062	-1.39236
H	-3.39423	-1.64063	1.39237
C	-2.86406	0.93257	-0.76378
C	-2.86406	-0.93258	0.76378
C	-1.46984	0.93307	-0.76326
C	-1.46983	-0.93307	0.76327
H	-0.93804	1.64176	-1.39003
H	-0.93803	-1.64176	1.39004
C	-0.74080	0.00000	0.00000
C	0.74309	0.00000	0.00000
H	0.93769	2.15122	-0.01048
H	0.93770	-2.15122	0.01048
C	1.47118	1.20604	-0.01492
C	1.47119	-1.20603	0.01492
C	2.86548	1.20616	-0.01072
C	2.86549	-1.20615	0.01071
H	3.39886	2.15109	-0.03478
H	3.39887	-2.15108	0.03476
C	3.59337	0.00001	-0.00001
C	5.07769	0.00001	-0.00001
H	5.26614	-1.67781	-1.34828
H	5.26615	1.67782	1.34826
C	5.80284	0.95193	0.74509
C	5.80284	-0.95191	-0.74511
C	7.19878	0.94858	0.74426
C	7.19878	-0.94856	-0.74429
H	7.72080	-1.69359	-1.34058
H	7.72081	1.69362	1.34054
C	7.93983	0.00001	-0.00002
Al	9.90000	0.00005	-0.00007
Al	12.39879	0.00000	0.00000

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#5 Phenyl ring (p1-6)

Al	-14.56838	0.00000	0.00000
Al	-12.06959	0.00055	-0.00102
C	-10.10905	0.00028	-0.00079
H	-9.89133	-2.15555	-0.12491
H	-9.89077	2.15604	0.12338
C	-9.36836	-1.20317	-0.07483
C	-9.36805	1.20353	0.07320
C	-7.97263	-1.20651	-0.07472
C	-7.97232	1.20650	0.07296
H	-7.43737	-2.15052	-0.10470
H	-7.43680	2.15038	0.10290
C	-7.24634	-0.00010	-0.00093
C	-5.76216	-0.00024	-0.00091
H	-5.56277	-1.65126	-1.38094
H	-5.56269	1.65071	1.37920

C	-5.03256	-0.93861	-0.75762
C	-5.03249	0.93799	0.75593
C	-3.63833	-0.93923	-0.75697
C	-3.63827	0.93828	0.75556
H	-3.10629	-1.65264	-1.37816
H	-3.10614	1.65154	1.37687
C	-2.90927	-0.00058	-0.00060
C	-1.42538	-0.00070	-0.00034
H	-1.23077	2.15046	-0.01115
H	-1.23076	-2.15187	0.01067
C	-0.69724	-1.20672	-0.00300
C	-0.69721	1.20533	0.00272
C	0.69715	1.20533	-0.00023
C	0.69715	-1.20673	0.00062
H	1.23058	-2.15189	-0.01500
H	1.23067	2.15044	0.01573
C	1.42533	-0.00072	0.00035
C	2.90926	-0.00058	0.00071
H	3.10613	1.65466	-1.37301
H	3.10636	-1.65586	1.37439
C	3.63826	0.94005	-0.75328
C	3.63834	-0.94100	0.75484
C	5.03247	0.93980	-0.75361
C	5.03258	-0.94037	0.75549
H	5.56268	1.65392	-1.37526
H	5.56280	-1.65444	1.37717
C	5.76216	-0.00017	0.00106
C	7.24637	0.00000	0.00108
H	7.43685	2.15076	-0.09689
H	7.43743	-2.15070	0.09913
C	7.97236	1.20680	-0.06953
C	7.97267	-1.20660	0.07172
C	9.36809	1.20383	-0.06969
C	9.36840	-1.20325	0.07186
H	9.89081	2.15648	-0.11722
H	9.89139	-2.15575	0.11935
C	10.10908	0.00039	0.00109
Al	12.06963	0.00042	0.00155
Al	14.56842	0.00000	0.00000

P1 Electrodes (4-layer)

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#1 Phenyl ring (p1-4)

Al	-10.89711	0.00000	0.00000
Al	-8.39832	0.00000	0.00000
Al	-5.89953	0.00000	0.00000
Al	-3.40074	0.00000	0.00000
C	-1.43445	0.00000	0.00000
H	-1.22681	0.00000	-2.16066
H	-1.22681	0.00000	2.16066

C	-0.69922	0.00000	-1.20904
C	-0.69922	0.00000	1.20903
C	0.69922	0.00000	-1.20904
C	0.69922	0.00000	1.20903
H	1.22681	0.00000	-2.16066
H	1.22681	0.00000	2.16066
C	1.43445	0.00000	0.00000
Al	3.40074	0.00000	0.00000
Al	5.89953	0.00000	0.00000
Al	8.39832	0.00000	0.00000
Al	10.89711	0.00000	0.00000

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#2 Phenyl ring (p1-4)

Al	-13.06234	0.00000	0.00000
Al	-10.56355	0.00000	0.00000
Al	-8.06476	0.00000	0.00000
Al	-5.56597	0.00000	0.00005
C	-3.60478	-0.00010	0.00000
H	-3.38585	2.05130	0.67586
H	-3.38574	-2.05148	-0.67587
C	-2.86393	1.14646	0.37277
C	-2.86388	-1.14661	-0.37278
C	-1.46799	1.14966	0.37321
C	-1.46793	-1.14974	-0.37323
H	-0.93268	2.03882	0.69111
H	-0.93258	-2.03887	-0.69115
C	-0.74255	-0.00002	-0.00001
C	0.74255	0.00002	-0.00001
H	0.93257	2.03887	-0.69113
H	0.93269	-2.03882	0.69112
C	1.46793	1.14974	-0.37322
C	1.46799	-1.14966	0.37321
C	2.86387	1.14662	-0.37278
C	2.86394	-1.14646	0.37276
H	3.38574	2.05149	-0.67587
H	3.38585	-2.05130	0.67586
C	3.60478	0.00010	-0.00001
Al	5.56597	0.00002	0.00006
Al	8.06476	0.00000	0.00000
Al	10.56355	0.00000	0.00000
Al	13.06234	0.00000	0.00000

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#3 Phenyl ring (p1-4)

Al	-15.23090	0.00000	0.00000
Al	-12.73211	0.00000	0.00000
Al	-10.23332	0.00000	0.00000
Al	-7.73453	0.00007	-0.00010
C	-5.77386	0.00001	-0.00005
H	-5.55502	-2.12312	-0.39540

H	-5.55497	2.12314	0.39530
C	-5.03281	-1.18586	-0.21644
C	-5.03278	1.18587	0.21634
C	-3.63704	-1.18856	-0.21875
C	-3.63701	1.18855	0.21864
H	-3.10214	-2.11185	-0.41846
H	-3.10209	2.11183	0.41834
C	-2.91076	-0.00001	-0.00005
C	-1.42650	-0.00002	-0.00006
H	-1.22811	-1.94900	0.91130
H	-1.22810	1.94897	-0.91137
C	-0.69695	1.10044	-0.49251
C	-0.69695	-1.10048	0.49242
C	0.69695	1.10044	-0.49252
C	0.69695	-1.10048	0.49243
H	1.22809	-1.94901	0.91131
H	1.22810	1.94898	-0.91137
C	1.42651	-0.00002	-0.00005
C	2.91074	-0.00001	-0.00003
H	3.10210	2.11224	0.41638
H	3.10217	-2.11224	-0.41646
C	3.63700	1.18875	0.21757
C	3.63704	-1.18875	-0.21764
C	5.03277	1.18608	0.21528
C	5.03280	-1.18604	-0.21532
H	5.55494	2.12353	0.39334
H	5.55500	-2.12347	-0.39338
C	5.77387	0.00003	-0.00002
Al	7.73453	0.00004	-0.00005
Al	10.23332	0.00000	0.00000
Al	12.73211	0.00000	0.00000
Al	15.23090	0.00000	0.00000

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#4 Phenyl ring (p1-4)

Al	-17.39745	0.00000	0.00000
Al	-14.89866	0.00000	0.00000
Al	-12.39987	0.00000	0.00000
Al	-9.90108	-0.00002	0.00000
C	-7.94045	-0.00002	0.00001
H	-7.72249	2.15497	-0.13750
H	-7.72248	-2.15500	0.13752
C	-7.19964	-1.20288	0.08150
C	-7.19964	1.20285	-0.08149
C	-5.80389	-1.20605	0.08141
C	-5.80389	1.20602	-0.08140
H	-5.26845	-2.14976	0.11732
H	-5.26845	2.14974	-0.11731
C	-5.07786	-0.00001	0.00001
C	-3.59368	-0.00001	0.00000
H	-3.39424	1.64062	-1.39236

H	-3.39423	-1.64063	1.39237
C	-2.86406	-0.93258	0.76378
C	-2.86406	0.93257	-0.76378
C	-1.46984	0.93307	-0.76326
C	-1.46983	-0.93307	0.76327
H	-0.93804	1.64176	-1.39003
H	-0.93803	-1.64176	1.39004
C	-0.74080	0.00000	0.00000
C	0.74309	0.00000	0.00000
H	0.93769	2.15122	-0.01048
H	0.93770	-2.15122	0.01048
C	1.47118	1.20604	-0.01492
C	1.47119	-1.20603	0.01492
C	2.86548	1.20616	-0.01072
C	2.86549	-1.20615	0.01071
H	3.39886	2.15109	-0.03478
H	3.39887	-2.15108	0.03476
C	3.59337	0.00001	-0.00001
C	5.07769	0.00001	-0.00001
H	5.26614	-1.67781	-1.34828
H	5.26615	1.67782	1.34826
C	5.80284	-0.95191	-0.74511
C	5.80284	0.95193	0.74509
C	7.19878	-0.94856	-0.74429
C	7.19878	0.94858	0.74426
H	7.72080	-1.69359	-1.34058
H	7.72081	1.69362	1.34054
C	7.93983	0.00001	-0.00002
Al	9.90000	0.00005	-0.00007
Al	12.39879	0.00000	0.00000
Al	14.89758	0.00000	0.00000
Al	17.39637	0.00000	0.00000

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#5 Phenyl ring (p1-4)

Al	-19.56596	0.00000	0.00000
Al	-17.06717	0.00000	0.00000
Al	-14.56838	0.00000	0.00000
Al	-12.06959	0.00055	-0.00102
C	-10.10905	0.00028	-0.00079
H	-9.89133	-2.15555	-0.12491
H	-9.89077	2.15604	0.12338
C	-9.36836	-1.20317	-0.07483
C	-9.36805	1.20353	0.07320
C	-7.97263	-1.20651	-0.07472
C	-7.97232	1.20650	0.07296
H	-7.43737	-2.15052	-0.10470
H	-7.43680	2.15038	0.10290
C	-7.24634	-0.00010	-0.00093
C	-5.76216	-0.00024	-0.00091
H	-5.56277	-1.65126	-1.38094

H	-5.56269	1.65071	1.37920
C	-5.03256	-0.93861	-0.75762
C	-5.03249	0.93799	0.75593
C	-3.63833	-0.93923	-0.75697
C	-3.63827	0.93828	0.75556
H	-3.10629	-1.65264	-1.37816
H	-3.10614	1.65154	1.37687
C	-2.90927	-0.00058	-0.00060
C	-1.42538	-0.00070	-0.00034
H	-1.23077	2.15046	-0.01115
H	-1.23076	-2.15187	0.01067
C	-0.69724	-1.20672	-0.00300
C	-0.69721	1.20533	0.00272
C	0.69715	-1.20673	0.00062
C	0.69715	1.20533	-0.00023
H	1.23058	-2.15189	-0.01500
H	1.23067	2.15044	0.01573
C	1.42533	-0.00072	0.00035
C	2.90926	-0.00058	0.00071
H	3.10613	1.65466	-1.37301
H	3.10636	-1.65586	1.37439
C	3.63826	0.94005	-0.75328
C	3.63834	-0.94100	0.75484
C	5.03247	0.93980	-0.75361
C	5.03258	-0.94037	0.75549
H	5.56268	1.65392	-1.37526
H	5.56280	-1.65444	1.37717
C	5.76216	-0.00017	0.00106
C	7.24637	0.00000	0.00108
H	7.43685	2.15076	-0.09689
H	7.43743	-2.15070	0.09913
C	7.97236	1.20680	-0.06953
C	7.97267	-1.20660	0.07172
C	9.36809	1.20383	-0.06969
C	9.36840	-1.20325	0.07186
H	9.89081	2.15648	-0.11722
H	9.89139	-2.15575	0.11935
C	10.10908	0.00039	0.00109
Al	12.06963	0.00042	0.00155
Al	14.56842	0.00000	0.00000
Al	17.06721	0.00000	0.00000
Al	19.56600	0.00000	0.00000

P1 Electrodes (6-layer)

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#1 Phenyl ring (p1-6)

Al	-15.89469	0.00000	0.00000
Al	-13.39590	0.00000	0.00000
Al	-10.89711	0.00000	0.00000
Al	-8.39832	0.00000	0.00000
Al	-5.89953	0.00000	0.00000

Al	-3.40074	0.00000	0.00000
C	-1.43445	0.00000	0.00000
H	-1.22681	0.00000	2.16066
H	-1.22681	0.00000	-2.16066
C	-0.69922	0.00000	1.20903
C	-0.69922	0.00000	-1.20904
C	0.69922	0.00000	1.20903
C	0.69922	0.00000	-1.20904
H	1.22681	0.00000	2.16066
H	1.22681	0.00000	-2.16066
C	1.43445	0.00000	0.00000
Al	3.40074	0.00000	0.00000
Al	5.89953	0.00000	0.00000
Al	8.39832	0.00000	0.00000
Al	10.89711	0.00000	0.00000
Al	13.39590	0.00000	0.00000
Al	15.89469	0.00000	0.00000

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#2 Phenyl ring (p1-6)

Al	-18.05992	0.00000	0.00000
Al	-15.56113	0.00000	0.00000
Al	-13.06234	0.00000	0.00000
Al	-10.56355	0.00000	0.00000
Al	-8.06476	0.00000	0.00000
Al	-5.56597	0.00000	0.00005
C	-3.60478	-0.00010	0.00000
H	-3.38585	2.05130	0.67586
H	-3.38574	-2.05148	-0.67587
C	-2.86393	1.14646	0.37277
C	-2.86388	-1.14661	-0.37278
C	-1.46799	1.14966	0.37321
C	-1.46793	-1.14974	-0.37323
H	-0.93268	2.03882	0.69111
H	-0.93258	-2.03887	-0.69115
C	-0.74255	-0.00002	-0.00001
C	0.74255	0.00002	-0.00001
H	0.93257	2.03887	-0.69113
H	0.93269	-2.03882	0.69112
C	1.46793	1.14974	-0.37322
C	1.46799	-1.14966	0.37321
C	2.86387	1.14662	-0.37278
C	2.86394	-1.14646	0.37276
H	3.38574	2.05149	-0.67587
H	3.38585	-2.05130	0.67586
C	3.60478	0.00010	-0.00001
Al	5.56597	0.00002	0.00006
Al	8.06476	0.00000	0.00000
Al	10.56355	0.00000	0.00000
Al	13.06234	0.00000	0.00000
Al	15.56113	0.00000	0.00000

Al	18.05992	0.00000	0.00000
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#3 Phenyl ring (p1-6)

Al	-20.22848	0.00000	0.00000
Al	-17.72969	0.00000	0.00000
Al	-15.23090	0.00000	0.00000
Al	-12.73211	0.00000	0.00000
Al	-10.23332	0.00000	0.00000
Al	-7.73453	0.00007	-0.00010
C	-5.77386	0.00001	-0.00005
H	-5.55502	-2.12312	-0.39540
H	-5.55497	2.12314	0.39530
C	-5.03281	-1.18586	-0.21644
C	-5.03278	1.18587	0.21634
C	-3.63704	-1.18856	-0.21875
C	-3.63701	1.18855	0.21864
H	-3.10214	-2.11185	-0.41846
H	-3.10209	2.11183	0.41834
C	-2.91076	-0.00001	-0.00005
C	-1.42650	-0.00002	-0.00006
H	-1.22811	-1.94900	0.91130
H	-1.22810	1.94897	-0.91137
C	-0.69695	-1.10048	0.49242
C	-0.69695	1.10044	-0.49251
C	0.69695	-1.10048	0.49243
C	0.69695	1.10044	-0.49252
H	1.22809	-1.94901	0.91131
H	1.22810	1.94898	-0.91137
C	1.42651	-0.00002	-0.00005
C	2.91074	-0.00001	-0.00003
H	3.10210	2.11224	0.41638
H	3.10217	-2.11224	-0.41646
C	3.63700	1.18875	0.21757
C	3.63704	-1.18875	-0.21764
C	5.03277	1.18608	0.21528
C	5.03280	-1.18604	-0.21532
H	5.55494	2.12353	0.39334
H	5.55500	-2.12347	-0.39338
C	5.77387	0.00003	-0.00002
Al	7.73453	0.00004	-0.00005
Al	10.23332	0.00000	0.00000
Al	12.73211	0.00000	0.00000
Al	15.23090	0.00000	0.00000
Al	17.72969	0.00000	0.00000
Al	20.22848	0.00000	0.00000

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#4 Phenyl ring (p1-6)

Al	-22.39503	0.00000	0.00000
Al	-19.89624	0.00000	0.00000

Al	-17.39745	0.00000	0.00000
Al	-14.89866	0.00000	0.00000
Al	-12.39987	0.00000	0.00000
Al	-9.90108	-0.00002	0.00000
C	-7.94045	-0.00002	0.00001
H	-7.72249	2.15497	-0.13750
H	-7.72248	-2.15500	0.13752
C	-7.19964	1.20285	-0.08149
C	-7.19964	-1.20288	0.08150
C	-5.80389	1.20602	-0.08140
C	-5.80389	-1.20605	0.08141
H	-5.26845	2.14974	-0.11731
H	-5.26845	-2.14976	0.11732
C	-5.07786	-0.00001	0.00001
C	-3.59368	-0.00001	0.00000
H	-3.39424	1.64062	-1.39236
H	-3.39423	-1.64063	1.39237
C	-2.86406	0.93257	-0.76378
C	-2.86406	-0.93258	0.76378
C	-1.46984	0.93307	-0.76326
C	-1.46983	-0.93307	0.76327
H	-0.93804	1.64176	-1.39003
H	-0.93803	-1.64176	1.39004
C	-0.74080	0.00000	0.00000
C	0.74309	0.00000	0.00000
H	0.93769	2.15122	-0.01048
H	0.93770	-2.15122	0.01048
C	1.47118	1.20604	-0.01492
C	1.47119	-1.20603	0.01492
C	2.86548	1.20616	-0.01072
C	2.86549	-1.20615	0.01071
H	3.39886	2.15109	-0.03478
H	3.39887	-2.15108	0.03476
C	3.59337	0.00001	-0.00001
C	5.07769	0.00001	-0.00001
H	5.26614	-1.67781	-1.34828
H	5.26615	1.67782	1.34826
C	5.80284	0.95193	0.74509
C	5.80284	-0.95191	-0.74511
C	7.19878	0.94858	0.74426
C	7.19878	-0.94856	-0.74429
H	7.72080	-1.69359	-1.34058
H	7.72081	1.69362	1.34054
C	7.93983	0.00001	-0.00002
Al	9.90000	0.00005	-0.00007
Al	12.39879	0.00000	0.00000
Al	14.89758	0.00000	0.00000
Al	17.39637	0.00000	0.00000
Al	19.89516	0.00000	0.00000

Al	22.39395	0.00000	0.00000
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#5 Phenyl ring (p1-6)

Al	-24.56354	0.00000	0.00000
Al	-22.06475	0.00000	0.00000
Al	-19.56596	0.00000	0.00000
Al	-17.06717	0.00000	0.00000
Al	-14.56838	0.00000	0.00000
Al	-12.06959	0.00055	-0.00102
C	-10.10905	0.00028	-0.00079
H	-9.89133	-2.15555	-0.12491
H	-9.89077	2.15604	0.12338
C	-9.36836	-1.20317	-0.07483
C	-9.36805	1.20353	0.07320
C	-7.97263	-1.20651	-0.07472
C	-7.97232	1.20650	0.07296
H	-7.43737	-2.15052	-0.10470
H	-7.43680	2.15038	0.10290
C	-7.24634	-0.00010	-0.00093
C	-5.76216	-0.00024	-0.00091
H	-5.56277	-1.65126	-1.38094
H	-5.56269	1.65071	1.37920
C	-5.03256	-0.93861	-0.75762
C	-5.03249	0.93799	0.75593
C	-3.63833	-0.93923	-0.75697
C	-3.63827	0.93828	0.75556
H	-3.10629	-1.65264	-1.37816
H	-3.10614	1.65154	1.37687
C	-2.90927	-0.00058	-0.00060
C	-1.42538	-0.00070	-0.00034
H	-1.23077	2.15046	-0.01115
H	-1.23076	-2.15187	0.01067
C	-0.69724	-1.20672	-0.00300
C	-0.69721	1.20533	0.00272
C	0.69715	1.20533	-0.00023
C	0.69715	-1.20673	0.00062
H	1.23058	-2.15189	-0.01500
H	1.23067	2.15044	0.01573
C	1.42533	-0.00072	0.00035
C	2.90926	-0.00058	0.00071
H	3.10613	1.65466	-1.37301
H	3.10636	-1.65586	1.37439
C	3.63826	0.94005	-0.75328
C	3.63834	-0.94100	0.75484
C	5.03247	0.93980	-0.75361
C	5.03258	-0.94037	0.75549
H	5.56268	1.65392	-1.37526
H	5.56280	-1.65444	1.37717
C	5.76216	-0.00017	0.00106
C	7.24637	0.00000	0.00108

H	7.43685	2.15076	-0.09689
H	7.43743	-2.15070	0.09913
C	7.97236	1.20680	-0.06953
C	7.97267	-1.20660	0.07172
C	9.36809	1.20383	-0.06969
C	9.36840	-1.20325	0.07186
H	9.89081	2.15648	-0.11722
H	9.89139	-2.15575	0.11935
C	10.10908	0.00039	0.00109
Al	12.06963	0.00042	0.00155
Al	14.56842	0.00000	0.00000
Al	17.06721	0.00000	0.00000
Al	19.56600	0.00000	0.00000
Al	22.06479	0.00000	0.00000
Al	24.56358	0.00000	0.00000

pX2 Electrodes (1-layer)

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#1 Phenyl ring (pX2)

Al	-3.9631700000	0.0000000000	1.6494700000
Al	-3.9631600000	0.0000000000	-1.6494700000
C	-2.8741900000	0.0000000000	0.0000000000
C	-1.4749400000	0.0000000000	0.0000000000
H	-1.2100400000	0.0000000000	-2.1746500000
H	-1.2100400000	0.0000000000	2.1746500000
C	-0.6795700000	0.0000000000	-1.2285700000
C	-0.6795700000	0.0000000000	1.2285700000
C	0.6795700000	0.0000000000	-1.2285700000
C	0.6795700000	0.0000000000	1.2285700000
H	1.2100400000	0.0000000000	-2.1746500000
H	1.2100400000	0.0000000000	2.1746500000
C	1.4749400000	0.0000000000	0.0000000000
C	2.8741900000	0.0000000000	0.0000000000
Al	3.9631600000	0.0000000000	-1.6494700000
Al	3.9631700000	0.0000000000	1.6494700000

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#2 Phenyl ring (pX2)

Al	-6.1382800000	1.6418100000	-0.0000200000
Al	-6.1377300000	-1.6425700000	-0.0000100000
C	-5.0488800000	-0.0002000000	-0.0000100000
C	-3.6398800000	0.0000400000	-0.0000100000
H	-3.3740700000	2.1689800000	-0.0000100000
H	-3.3733500000	-2.1688200000	-0.0000100000
C	-2.8482500000	1.2207300000	-0.0000100000
C	-2.8478500000	-1.2203900000	-0.0000100000
C	-1.4822800000	1.2199000000	-0.0000100000
C	-1.4818800000	-1.2191100000	-0.0000100000
H	-0.9734900000	2.1754900000	-0.0000100000
H	-0.9727000000	-2.1745100000	-0.0000100000

C	-0.7103400000	0.0005100000	-0.0000100000
C	0.7103400000	0.0005100000	-0.0000100000
H	0.9727000000	-2.1745100000	-0.0000100000
H	0.9734900000	2.1754900000	-0.0000100000
C	1.4818800000	-1.2191100000	-0.0000100000
C	1.4822800000	1.2199000000	-0.0000100000
C	2.8478500000	-1.2203900000	-0.0000100000
C	2.8482500000	1.2207300000	-0.0000100000
H	3.3733500000	-2.1688200000	-0.0000100000
H	3.3740700000	2.1689800000	-0.0000100000
C	3.6398800000	0.0000400000	-0.0000100000
C	5.0488800000	-0.0002000000	-0.0000100000
Al	6.1377300000	-1.6425700000	-0.0000200000
Al	6.1382800000	1.6418100000	-0.0000200000

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#3 Phenyl ring (pX2)

Al	-8.3196900000	-1.6374400000	0.0000000000
Al	-8.3187200000	1.6393300000	0.0000000000
C	-7.2293200000	0.0006200000	-0.0000100000
C	-5.8132300000	0.0002000000	-0.0000100000
H	-5.5504900000	-2.1660900000	-0.0000100000
H	-5.5492000000	2.1663300000	-0.0000100000
C	-5.0256700000	-1.2172500000	-0.0000100000
C	-5.0249500000	1.2171800000	-0.0000100000
C	-3.6551600000	-1.2154800000	-0.0000200000
C	-3.6544300000	1.2145900000	-0.0000200000
H	-3.1468400000	-2.1717000000	-0.0000200000
H	-3.1454800000	2.1704900000	-0.0000200000
C	-2.8899900000	-0.0006600000	-0.0000200000
C	-1.4529000000	-0.0008800000	-0.0000200000
H	-1.1924500000	2.1666700000	-0.0000200000
H	-1.1924000000	-2.1684800000	-0.0000200000
C	-0.6874100000	-1.2111800000	-0.0000200000
C	-0.6874100000	1.2093800000	-0.0000200000
C	0.6874100000	-1.2111800000	-0.0000200000
C	0.6874100000	1.2093800000	-0.0000200000
H	1.1923900000	-2.1684800000	-0.0000200000
H	1.1924500000	2.1666700000	-0.0000200000
C	1.4529000000	-0.0008800000	-0.0000200000
C	2.8899900000	-0.0006700000	-0.0000200000
H	3.1454800000	2.1704800000	-0.0000200000
H	3.1468400000	-2.1717000000	-0.0000100000
C	3.6544300000	1.2145900000	-0.0000200000
C	3.6551600000	-1.2154800000	-0.0000100000
C	5.0249500000	1.2171800000	-0.0000200000
C	5.0256700000	-1.2172500000	-0.0000100000
H	5.5492000000	2.1663300000	-0.0000100000
H	5.5504900000	-2.1660900000	-0.0000100000
C	5.8132300000	0.0002000000	-0.0000100000
C	7.2293200000	0.0006200000	-0.0000100000

Al	8.318720000	1.639330000	0.000000000
Al	8.319690000	-1.637440000	0.000010000

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#4 Phenyl ring (pX2)

Al	10.52941	-1.71596	0.00000
Al	10.52555	1.72723	0.00000
C	9.44798	0.00443	0.00000
C	8.02552	0.00279	0.00000
H	7.75423	-2.16464	0.00000
H	7.74909	2.16962	0.00000
C	7.23355	-1.21015	0.00000
C	7.23071	1.21388	0.00000
C	5.85925	-1.21138	0.00000
C	5.85642	1.21184	0.00000
H	5.35126	-2.16802	0.00000
H	5.34618	2.16727	0.00000
C	5.09792	-0.00066	0.00000
C	3.64661	-0.00233	0.00000
H	3.39243	-2.16636	0.00000
H	3.38754	2.16112	0.00000
C	2.88814	-1.20834	0.00000
C	2.88541	1.20196	0.00000
C	1.50676	-1.20899	0.00000
C	1.50404	1.19945	0.00000
H	1.00365	-2.16782	0.00000
H	0.99876	2.15713	0.00000
C	0.74822	-0.00563	0.00000
C	-0.71062	-0.00733	0.00000
H	-0.96104	-2.17010	0.00000
H	-0.96618	2.15485	0.00000
C	-1.46638	-1.21244	0.00000
C	-1.46923	1.19599	0.00000
C	-2.84776	-1.21503	0.00000
C	-2.85061	1.19526	0.00000
H	-3.34979	-2.17423	0.00000
H	-3.35495	2.15325	0.00000
C	-3.60904	-0.01078	0.00000
C	-5.06037	-0.01246	0.00000
H	-5.30877	-2.18039	0.00000
H	-5.31360	2.15489	0.00000
C	-5.81894	-1.22492	0.00000
C	-5.82166	1.19829	0.00000
C	-7.19323	-1.22687	0.00000
C	-7.19595	1.19716	0.00000
H	-7.71170	-2.18257	0.00000
H	-7.71659	2.15167	0.00000
C	-7.98797	-0.01574	0.00000
C	-9.41045	-0.01735	0.00000
Al	-10.49191	1.70260	0.00000

Al -10.48827 -1.73974 0.00000

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#5 Phenyl ring (pX2)

Al	-12.7010800000	-1.6302000000	-0.0000600000
Al	-12.7002700000	1.6399900000	-0.0004200000
C	-11.6088400000	0.0046500000	-0.0001600000
C	-10.1826200000	0.0043300000	-0.0000600000
H	-9.9243700000	-2.1586400000	0.0001600000
H	-9.9236900000	2.1672300000	-0.0002200000
C	-9.4010500000	-1.2088800000	0.0001000000
C	-9.4006600000	1.2173000000	-0.0001100000
C	-8.0242700000	-1.2060000000	0.0001700000
C	-8.0238800000	1.2139800000	-0.0000300000
H	-7.5158500000	-2.1623600000	0.0002900000
H	-7.5151200000	2.1701600000	-0.0000800000
C	-7.2676300000	0.0038700000	0.0001100000
C	-5.8082800000	0.0037600000	0.0001700000
H	-5.5556900000	2.1655900000	0.0001200000
H	-5.5556200000	-2.1580900000	0.0002500000
C	-5.0523500000	1.2071400000	0.0001600000
C	-5.0523400000	-1.1996200000	0.0002400000
C	-3.6677700000	1.2059300000	0.0002000000
C	-3.6677600000	-1.1983900000	0.0002800000
H	-3.1635700000	2.1642200000	0.0001900000
H	-3.1635500000	-2.1566700000	0.0003200000
C	-2.9152500000	0.0037700000	0.0002600000
C	-1.4451300000	0.0037800000	0.0002800000
H	-1.1965700000	-2.1562000000	0.0003400000
H	-1.1965600000	2.1637500000	0.0002200000
C	-0.6931400000	-1.1975100000	0.0003200000
C	-0.6931300000	1.2050600000	0.0002500000
C	0.6931300000	-1.1975100000	0.0003200000
C	0.6931400000	1.2050600000	0.0002500000
H	1.1965600000	-2.1562100000	0.0003500000
H	1.1965800000	2.1637500000	0.0002300000
C	1.4451300000	0.0037700000	0.0002800000
C	2.9152500000	0.0037500000	0.0002600000
H	3.1635300000	-2.1566900000	0.0003400000
H	3.1635900000	2.1642000000	0.0001900000
C	3.6677500000	-1.1984100000	0.0002900000
C	3.6677800000	1.2059100000	0.0002000000
C	5.0523300000	-1.1996500000	0.0002500000
C	5.0523600000	1.2071100000	0.0001600000
H	5.5556100000	-2.1581200000	0.0002600000
H	5.5557100000	2.1655500000	0.0001200000
C	5.8082800000	0.0037200000	0.0001800000
C	7.2676300000	0.0038200000	0.0001200000
H	7.5151400000	2.1701100000	-0.0000600000
H	7.5158400000	-2.1624100000	0.0002800000
C	8.0238900000	1.2139300000	-0.0000100000

C	8.0242600000	-1.2060600000	0.0001700000
C	9.4006700000	1.2172400000	-0.0001000000
C	9.4010400000	-1.2089500000	0.0000900000
H	9.9237100000	2.1671600000	-0.0002000000
H	9.9243500000	-2.1587100000	0.0001400000
C	10.1826200000	0.0042700000	-0.0000600000
C	11.6088400000	0.0045700000	-0.0001600000
Al	12.7002700000	1.6399100000	-0.0004200000
Al	12.7010700000	-1.6302900000	-0.0000700000

pX2 Electrodes (2-layer)

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#1 Phenyl ring (pX2-2)

Al	-6.46196	0.00000	1.64947
Al	-6.46196	0.00000	-1.64947
Al	-3.96317	0.00000	1.64947
Al	-3.96316	0.00000	-1.64947
C	-2.87419	0.00000	0.00000
C	-1.47494	0.00000	0.00000
H	-1.21004	0.00000	2.17465
H	-1.21004	0.00000	-2.17465
C	-0.67957	0.00000	1.22857
C	-0.67957	0.00000	-1.22857
C	0.67957	0.00000	1.22857
C	0.67957	0.00000	-1.22857
H	1.21004	0.00000	2.17465
H	1.21004	0.00000	-2.17465
C	1.47494	0.00000	0.00000
C	2.87419	0.00000	0.00000
Al	3.96316	0.00000	-1.64947
Al	3.96317	0.00000	1.64947
Al	6.46195	0.00000	-1.64947
Al	6.46195	0.00000	1.64947

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#2 Phenyl rings (pX2-2)

Al	-8.63707	1.64181	-0.00002
Al	-8.63707	-1.64257	-0.00001
Al	-6.13828	1.64181	-0.00002
Al	-6.13773	-1.64257	-0.00001
C	-5.04888	-0.00020	-0.00001
C	-3.63988	0.00004	-0.00001
H	-3.37407	2.16898	-0.00001
H	-3.37335	-2.16882	-0.00001
C	-2.84825	1.22073	-0.00001
C	-2.84785	-1.22039	-0.00001
C	-1.48228	1.21990	-0.00001
C	-1.48188	-1.21911	-0.00001

H	-0.97349	2.17549	-0.00001
H	-0.97270	-2.17451	-0.00001
C	-0.71034	0.00051	-0.00001
C	0.71034	0.00051	-0.00001
H	0.97270	-2.17451	-0.00001
H	0.97349	2.17549	-0.00001
C	1.48188	-1.21911	-0.00001
C	1.48228	1.21990	-0.00001
C	2.84785	-1.22039	-0.00001
C	2.84825	1.22073	-0.00001
H	3.37335	-2.16882	-0.00001
H	3.37407	2.16898	-0.00001
C	3.63988	0.00004	-0.00001
C	5.04888	-0.00020	-0.00001
Al	6.13773	-1.64257	-0.00002
Al	6.13828	1.64181	-0.00002
Al	8.63707	1.64181	-0.00002
Al	8.63707	-1.64257	-0.00002

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#3 Phenyl rings (pX2-2)

Al	13.02820	-1.71596	0.00000
Al	13.02434	1.72723	0.00000
Al	10.52941	-1.71596	0.00000
Al	10.52555	1.72723	0.00000
C	9.44798	0.00443	0.00000
C	8.02552	0.00279	0.00000
H	7.75423	-2.16464	0.00000
H	7.74909	2.16962	0.00000
C	7.23355	-1.21015	0.00000
C	7.23071	1.21388	0.00000
C	5.85925	-1.21138	0.00000
C	5.85642	1.21184	0.00000
H	5.35126	-2.16802	0.00000
H	5.34618	2.16727	0.00000
C	5.09792	-0.00066	0.00000
C	3.64661	-0.00233	0.00000
H	3.39243	-2.16636	0.00000
H	3.38754	2.16112	0.00000
C	2.88814	-1.20834	0.00000
C	2.88541	1.20196	0.00000
C	1.50676	-1.20899	0.00000
C	1.50404	1.19945	0.00000
H	1.00365	-2.16782	0.00000
H	0.99876	2.15713	0.00000
C	0.74822	-0.00563	0.00000
C	-0.71062	-0.00733	0.00000
H	-0.96104	-2.17010	0.00000
H	-0.96618	2.15485	0.00000
C	-1.46638	-1.21244	0.00000
C	-1.46923	1.19599	0.00000

C	-2.84776	-1.21503	0.00000
C	-2.85061	1.19526	0.00000
H	-3.34979	-2.17423	0.00000
H	-3.35495	2.15325	0.00000
C	-3.60904	-0.01078	0.00000
C	-5.06037	-0.01246	0.00000
H	-5.30877	-2.18039	0.00000
H	-5.31360	2.15489	0.00000
C	-5.81894	-1.22492	0.00000
C	-5.82166	1.19829	0.00000
C	-7.19323	-1.22687	0.00000
C	-7.19595	1.19716	0.00000
H	-7.71170	-2.18257	0.00000
H	-7.71659	2.15167	0.00000
C	-7.98797	-0.01574	0.00000
C	-9.41045	-0.01735	0.00000
Al	-10.49191	1.70260	0.00000
Al	-10.48827	-1.73974	0.00000
Al	-12.99070	1.70260	0.00000
Al	-12.98710	-1.73974	0.00000

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#4 Phenyl ring (pX2-2)

Al	-12.99025	-1.61944	0.23980
Al	-12.98898	1.61808	-0.24469
Al	-10.49146	-1.61944	0.23980
Al	-10.49019	1.61808	-0.24469
C	-9.39923	-0.00059	-0.00018
C	-7.97466	-0.00088	-0.00056
H	-7.71859	2.14291	-0.29610
H	-7.71856	-2.14471	0.29464
C	-7.19343	-1.20602	0.15723
C	-7.19339	1.20433	-0.15789
C	-5.81741	-1.20392	0.15158
C	-5.81741	1.20238	-0.15169
H	-5.29900	-2.14343	0.30514
H	-5.29897	2.14190	-0.30514
C	-5.06500	-0.00076	0.00013
C	-3.61139	-0.00063	0.00036
H	-3.37686	2.11567	0.43733
H	-3.37607	-2.11688	-0.43656
C	-2.86140	1.18821	0.21868
C	-2.86098	-1.18924	-0.21785
C	-1.47794	1.18777	0.21801
C	-1.47751	-1.18832	-0.21705
H	-0.95865	2.11377	0.43672
H	-0.95783	-2.11415	-0.43558
C	-0.73187	-0.00014	0.00042
C	0.72850	-0.00005	0.00045
H	0.95459	-2.10037	0.49819
H	0.95484	2.10017	-0.49774

C	1.47425	-1.18130	0.25273
C	1.47436	1.18108	-0.25214
C	2.85773	-1.18206	0.25328
C	2.85784	1.18166	-0.25299
H	3.37337	-2.10273	0.49874
H	3.37352	2.10221	-0.49876
C	3.60782	-0.00025	0.00012
C	5.06137	-0.00052	-0.00016
H	5.29421	-2.15035	-0.24981
H	5.29559	2.14918	0.24964
C	5.81326	-1.20749	-0.12068
C	5.81400	1.20601	0.12022
C	7.18926	-1.21001	-0.12719
C	7.19001	1.20773	0.12627
H	7.71414	-2.15193	-0.24182
H	7.71548	2.14933	0.24078
C	7.97082	-0.00136	-0.00062
C	9.39540	-0.00175	-0.00087
Al	10.48652	-1.62223	-0.23053
Al	10.48744	1.61815	0.22837
Al	12.98531	-1.62223	-0.23053
Al	12.98623	1.61815	0.22837

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#5 Phenyl ring (pX2-2)

Al	-15.19987	-1.63020	-0.00006
Al	-15.19906	1.63999	-0.00042
Al	-12.70108	-1.63020	-0.00006
Al	-12.70027	1.63999	-0.00042
C	-11.60884	0.00465	-0.00016
C	-10.18262	0.00433	-0.00006
H	-9.92437	-2.15864	0.00016
H	-9.92369	2.16723	-0.00022
C	-9.40105	-1.20888	0.00010
C	-9.40066	1.21730	-0.00011
C	-8.02427	-1.20600	0.00017
C	-8.02388	1.21398	-0.00003
H	-7.51585	-2.16236	0.00029
H	-7.51512	2.17016	-0.00008
C	-7.26763	0.00387	0.00011
C	-5.80828	0.00376	0.00017
H	-5.55569	2.16559	0.00012
H	-5.55562	-2.15809	0.00025
C	-5.05235	1.20714	0.00016
C	-5.05234	-1.19962	0.00024
C	-3.66777	1.20593	0.00020
C	-3.66776	-1.19839	0.00028
H	-3.16357	2.16422	0.00019
H	-3.16355	-2.15667	0.00032
C	-2.91525	0.00377	0.00026
C	-1.44513	0.00378	0.00028

H	-1.19657	-2.15620	0.00034
H	-1.19656	2.16375	0.00022
C	-0.69314	-1.19751	0.00032
C	-0.69313	1.20506	0.00025
C	0.69313	-1.19751	0.00032
C	0.69314	1.20506	0.00025
H	1.19656	-2.15621	0.00035
H	1.19658	2.16375	0.00023
C	1.44513	0.00377	0.00028
C	2.91525	0.00375	0.00026
H	3.16353	-2.15669	0.00034
H	3.16359	2.16420	0.00019
C	3.66775	-1.19841	0.00029
C	3.66778	1.20591	0.00020
C	5.05233	-1.19965	0.00025
C	5.05236	1.20711	0.00016
H	5.55561	-2.15812	0.00026
H	5.55571	2.16555	0.00012
C	5.80828	0.00372	0.00018
C	7.26763	0.00382	0.00012
H	7.51514	2.17011	-0.00006
H	7.51584	-2.16241	0.00028
C	8.02389	1.21393	-0.00001
C	8.02426	-1.20606	0.00017
C	9.40067	1.21724	-0.00010
C	9.40104	-1.20895	0.00009
H	9.92371	2.16716	-0.00020
H	9.92435	-2.15871	0.00014
C	10.18262	0.00427	-0.00006
C	11.60884	0.00457	-0.00016
Al	12.70027	1.63991	-0.00042
Al	12.70107	-1.63029	-0.00007
Al	15.19906	1.63991	-0.00042
Al	15.19986	-1.63029	-0.00007

pX2 Electrodes (4-layer)

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#1 Phenyl ring (pX2-4)

Al	-11.45954	0.00000	-1.64947
Al	-11.45954	0.00000	1.64947
Al	-8.96075	0.00000	-1.64947
Al	-8.96075	0.00000	1.64947
Al	-6.46196	0.00000	-1.64947
Al	-6.46196	0.00000	1.64947
Al	-3.96317	0.00000	1.64947
Al	-3.96316	0.00000	-1.64947
C	-2.87419	0.00000	0.00000
C	-1.47494	0.00000	0.00000
H	-1.21004	0.00000	-2.17465
H	-1.21004	0.00000	2.17465

C	-0.67957	0.00000	-1.22857
C	-0.67957	0.00000	1.22857
C	0.67957	0.00000	-1.22857
C	0.67957	0.00000	1.22857
H	1.21004	0.00000	-2.17465
H	1.21004	0.00000	2.17465
C	1.47494	0.00000	0.00000
C	2.87419	0.00000	0.00000
Al	3.96316	0.00000	-1.64947
Al	3.96317	0.00000	1.64947
Al	6.46195	0.00000	1.64947
Al	6.46195	0.00000	-1.64947
Al	8.96074	0.00000	1.64947
Al	8.96074	0.00000	-1.64947
Al	11.45953	0.00000	1.64947
Al	11.45953	0.00000	-1.64947

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#2 Phenyl ring (pX2-4)

Al	-13.63465	1.64181	-0.00002
Al	-13.63465	-1.64257	-0.00001
Al	-11.13586	1.64181	-0.00002
Al	-11.13586	-1.64257	-0.00001
Al	-8.63707	1.64181	-0.00002
Al	-8.63707	-1.64257	-0.00001
Al	-6.13828	1.64181	-0.00002
Al	-6.13773	-1.64257	-0.00001
C	-5.04888	-0.00020	-0.00001
C	-3.63988	0.00004	-0.00001
H	-3.37407	2.16898	-0.00001
H	-3.37335	-2.16882	-0.00001
C	-2.84825	1.22073	-0.00001
C	-2.84785	-1.22039	-0.00001
C	-1.48228	1.21990	-0.00001
C	-1.48188	-1.21911	-0.00001
H	-0.97349	2.17549	-0.00001
H	-0.97270	-2.17451	-0.00001
C	-0.71034	0.00051	-0.00001
C	0.71034	0.00051	-0.00001
H	0.97270	-2.17451	-0.00001
H	0.97349	2.17549	-0.00001
C	1.48188	-1.21911	-0.00001
C	1.48228	1.21990	-0.00001
C	2.84785	-1.22039	-0.00001
C	2.84825	1.22073	-0.00001
H	3.37335	-2.16882	-0.00001
H	3.37407	2.16898	-0.00001
C	3.63988	0.00004	-0.00001
C	5.04888	-0.00020	-0.00001
Al	6.13773	-1.64257	-0.00002
Al	6.13828	1.64181	-0.00002

Al	8.63707	1.64181	-0.00002
Al	8.63707	-1.64257	-0.00002
Al	11.13586	1.64181	-0.00002
Al	11.13586	-1.64257	-0.00002
Al	13.63465	1.64181	-0.00002
Al	13.63465	-1.64257	-0.00002

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#3 Phenyl ring (pX2-4)

Al	-15.81606	-1.63744	0.00000
Al	-15.81606	1.63933	0.00000
Al	-13.31727	-1.63744	0.00000
Al	-13.31727	1.63933	0.00000
Al	-10.81848	-1.63744	0.00000
Al	-10.81848	1.63933	0.00000
Al	-8.31969	-1.63744	0.00000
Al	-8.31872	1.63933	0.00000
C	-7.22932	0.00062	-0.00001
C	-5.81323	0.00020	-0.00001
H	-5.55049	-2.16609	-0.00001
H	-5.54920	2.16633	-0.00001
C	-5.02567	-1.21725	-0.00001
C	-5.02495	1.21718	-0.00001
C	-3.65516	-1.21548	-0.00002
C	-3.65443	1.21459	-0.00002
H	-3.14684	-2.17170	-0.00002
H	-3.14548	2.17049	-0.00002
C	-2.88999	-0.00066	-0.00002
C	-1.45290	-0.00088	-0.00002
H	-1.19245	2.16667	-0.00002
H	-1.19240	-2.16848	-0.00002
C	-0.68741	1.20938	-0.00002
C	-0.68741	-1.21118	-0.00002
C	0.68741	1.20938	-0.00002
C	0.68741	-1.21118	-0.00002
H	1.19239	-2.16848	-0.00002
H	1.19245	2.16667	-0.00002
C	1.45290	-0.00088	-0.00002
C	2.88999	-0.00067	-0.00002
H	3.14548	2.17048	-0.00002
H	3.14684	-2.17170	-0.00001
C	3.65443	1.21459	-0.00002
C	3.65516	-1.21548	-0.00001
C	5.02495	1.21718	-0.00002
C	5.02567	-1.21725	-0.00001
H	5.54920	2.16633	-0.00001
H	5.55049	-2.16609	-0.00001
C	5.81323	0.00020	-0.00001
C	7.22932	0.00062	-0.00001
Al	8.31872	1.63933	0.00000
Al	8.31969	-1.63744	0.00001

Al	10.81751	-1.63744	0.00001
Al	10.81751	1.63933	0.00000
Al	13.31630	-1.63744	0.00001
Al	13.31630	1.63933	0.00000
Al	15.81509	-1.63744	0.00001
Al	15.81509	1.63933	0.00000

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#4 Phenyl ring (pX2-4)

Al	18.02578	-1.71596	0.00000
Al	18.02192	1.72723	0.00000
Al	15.52699	-1.71596	0.00000
Al	15.52313	1.72723	0.00000
Al	13.02820	-1.71596	0.00000
Al	13.02434	1.72723	0.00000
Al	10.52941	-1.71596	0.00000
Al	10.52555	1.72723	0.00000
C	9.44798	0.00443	0.00000
C	8.02552	0.00279	0.00000
H	7.75423	-2.16464	0.00000
H	7.74909	2.16962	0.00000
C	7.23355	-1.21015	0.00000
C	7.23071	1.21388	0.00000
C	5.85925	-1.21138	0.00000
C	5.85642	1.21184	0.00000
H	5.35126	-2.16802	0.00000
H	5.34618	2.16727	0.00000
C	5.09792	-0.00066	0.00000
C	3.64661	-0.00233	0.00000
H	3.39243	-2.16636	0.00000
H	3.38754	2.16112	0.00000
C	2.88814	-1.20834	0.00000
C	2.88541	1.20196	0.00000
C	1.50676	-1.20899	0.00000
C	1.50404	1.19945	0.00000
H	1.00365	-2.16782	0.00000
H	0.99876	2.15713	0.00000
C	0.74822	-0.00563	0.00000
C	-0.71062	-0.00733	0.00000
H	-0.96104	-2.17010	0.00000
H	-0.96618	2.15485	0.00000
C	-1.46638	-1.21244	0.00000
C	-1.46923	1.19599	0.00000
C	-2.84776	-1.21503	0.00000
C	-2.85061	1.19526	0.00000
H	-3.34979	-2.17423	0.00000
H	-3.35495	2.15325	0.00000
C	-3.60904	-0.01078	0.00000
C	-5.06037	-0.01246	0.00000
H	-5.30877	-2.18039	0.00000
H	-5.31360	2.15489	0.00000

C	-5.81894	-1.22492	0.00000
C	-5.82166	1.19829	0.00000
C	-7.19323	-1.22687	0.00000
C	-7.19595	1.19716	0.00000
H	-7.71170	-2.18257	0.00000
H	-7.71659	2.15167	0.00000
C	-7.98797	-0.01574	0.00000
C	-9.41045	-0.01735	0.00000
Al	-10.49191	1.70260	0.00000
Al	-10.48827	-1.73974	0.00000
Al	-12.99070	1.70260	0.00000
Al	-12.98710	-1.73974	0.00000
Al	-15.48950	1.70260	0.00000
Al	-15.48590	-1.73974	0.00000
Al	-17.98830	1.70260	0.00000
Al	-17.98460	-1.73974	0.00000

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#5 Phenyl ring (pX2-4)

Al	-20.19745	-1.63020	-0.00006
Al	-20.19664	1.63999	-0.00042
Al	-17.69866	-1.63020	-0.00006
Al	-17.69785	1.63999	-0.00042
Al	-15.19987	-1.63020	-0.00006
Al	-15.19906	1.63999	-0.00042
Al	-12.70108	-1.63020	-0.00006
Al	-12.70027	1.63999	-0.00042
C	-11.60884	0.00465	-0.00016
C	-10.18262	0.00433	-0.00006
H	-9.92437	-2.15864	0.00016
H	-9.92369	2.16723	-0.00022
C	-9.40105	-1.20888	0.00010
C	-9.40066	1.21730	-0.00011
C	-8.02427	-1.20600	0.00017
C	-8.02388	1.21398	-0.00003
H	-7.51585	-2.16236	0.00029
H	-7.51512	2.17016	-0.00008
C	-7.26763	0.00387	0.00011
C	-5.80828	0.00376	0.00017
H	-5.55569	2.16559	0.00012
H	-5.55562	-2.15809	0.00025
C	-5.05235	1.20714	0.00016
C	-5.05234	-1.19962	0.00024
C	-3.66777	1.20593	0.00020
C	-3.66776	-1.19839	0.00028
H	-3.16357	2.16422	0.00019
H	-3.16355	-2.15667	0.00032
C	-2.91525	0.00377	0.00026
C	-1.44513	0.00378	0.00028
H	-1.19657	-2.15620	0.00034
H	-1.19656	2.16375	0.00022

C	-0.69314	-1.19751	0.00032
C	-0.69313	1.20506	0.00025
C	0.69313	-1.19751	0.00032
C	0.69314	1.20506	0.00025
H	1.19656	-2.15621	0.00035
H	1.19658	2.16375	0.00023
C	1.44513	0.00377	0.00028
C	2.91525	0.00375	0.00026
H	3.16353	-2.15669	0.00034
H	3.16359	2.16420	0.00019
C	3.66775	-1.19841	0.00029
C	3.66778	1.20591	0.00020
C	5.05233	-1.19965	0.00025
C	5.05236	1.20711	0.00016
H	5.55561	-2.15812	0.00026
H	5.55571	2.16555	0.00012
C	5.80828	0.00372	0.00018
C	7.26763	0.00382	0.00012
H	7.51514	2.17011	-0.00006
H	7.51584	-2.16241	0.00028
C	8.02389	1.21393	-0.00001
C	8.02426	-1.20606	0.00017
C	9.40067	1.21724	-0.00010
C	9.40104	-1.20895	0.00009
H	9.92371	2.16716	-0.00020
H	9.92435	-2.15871	0.00014
C	10.18262	0.00427	-0.00006
C	11.60884	0.00457	-0.00016
Al	12.70027	1.63991	-0.00042
Al	12.70107	-1.63029	-0.00007
Al	15.19906	1.63991	-0.00042
Al	15.19986	-1.63029	-0.00007
Al	17.69785	1.63991	-0.00042
Al	17.69865	-1.63029	-0.00007
Al	20.19664	1.63991	-0.00042
Al	20.19744	-1.63029	-0.00007

pX2 Electrodes (6-layer)

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#1 Phenyl ring (pX2-6)

Al	-16.45712	0.00000	1.64947
Al	-16.45712	0.00000	-1.64947
Al	-13.95833	0.00000	1.64947
Al	-13.95833	0.00000	-1.64947
Al	-11.45954	0.00000	1.64947
Al	-11.45954	0.00000	-1.64947
Al	-8.96075	0.00000	1.64947
Al	-8.96075	0.00000	-1.64947
Al	-6.46196	0.00000	1.64947
Al	-6.46196	0.00000	-1.64947

Al	-3.96317	0.00000	1.64947
Al	-3.96316	0.00000	-1.64947
C	-2.87419	0.00000	0.00000
C	-1.47494	0.00000	0.00000
H	-1.21004	0.00000	2.17465
H	-1.21004	0.00000	-2.17465
C	-0.67957	0.00000	1.22857
C	-0.67957	0.00000	-1.22857
C	0.67957	0.00000	1.22857
C	0.67957	0.00000	-1.22857
H	1.21004	0.00000	2.17465
H	1.21004	0.00000	-2.17465
C	1.47494	0.00000	0.00000
C	2.87419	0.00000	0.00000
Al	3.96316	0.00000	-1.64947
Al	3.96317	0.00000	1.64947
Al	6.46195	0.00000	-1.64947
Al	6.46195	0.00000	1.64947
Al	8.96074	0.00000	-1.64947
Al	8.96074	0.00000	1.64947
Al	11.45953	0.00000	-1.64947
Al	11.45953	0.00000	1.64947
Al	13.95832	0.00000	-1.64947
Al	13.95832	0.00000	1.64947
Al	16.45711	0.00000	-1.64947
Al	16.45711	0.00000	1.64947

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#2 Phenyl ring (pX2-6)

Al	-18.63223	-1.64257	-0.00001
Al	-18.63223	1.64181	-0.00002
Al	-16.13344	-1.64257	-0.00001
Al	-16.13344	1.64181	-0.00002
Al	-13.63465	-1.64257	-0.00001
Al	-13.63465	1.64181	-0.00002
Al	-11.13586	-1.64257	-0.00001
Al	-11.13586	1.64181	-0.00002
Al	-8.63707	-1.64257	-0.00001
Al	-8.63707	1.64181	-0.00002
Al	-6.13828	1.64181	-0.00002
Al	-6.13773	-1.64257	-0.00001
C	-5.04888	-0.00020	-0.00001
C	-3.63988	0.00004	-0.00001
H	-3.37407	2.16898	-0.00001
H	-3.37335	-2.16882	-0.00001
C	-2.84825	1.22073	-0.00001
C	-2.84785	-1.22039	-0.00001
C	-1.48228	1.21990	-0.00001
C	-1.48188	-1.21911	-0.00001
H	-0.97349	2.17549	-0.00001
H	-0.97270	-2.17451	-0.00001

C	-0.71034	0.00051	-0.00001
C	0.71034	0.00051	-0.00001
H	0.97270	-2.17451	-0.00001
H	0.97349	2.17549	-0.00001
C	1.48188	-1.21911	-0.00001
C	1.48228	1.21990	-0.00001
C	2.84785	-1.22039	-0.00001
C	2.84825	1.22073	-0.00001
H	3.37335	-2.16882	-0.00001
H	3.37407	2.16898	-0.00001
C	3.63988	0.00004	-0.00001
C	5.04888	-0.00020	-0.00001
Al	6.13773	-1.64257	-0.00002
Al	6.13828	1.64181	-0.00002
Al	8.63707	-1.64257	-0.00002
Al	8.63707	1.64181	-0.00002
Al	11.13586	-1.64257	-0.00002
Al	11.13586	1.64181	-0.00002
Al	13.63465	-1.64257	-0.00002
Al	13.63465	1.64181	-0.00002
Al	16.13344	-1.64257	-0.00002
Al	16.13344	1.64181	-0.00002
Al	18.63223	-1.64257	-0.00002
Al	18.63223	1.64181	-0.00002

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#3 Phenyl ring (pX2-6)

Al	-20.81364	1.63933	0.00000
Al	-20.81364	-1.63744	0.00000
Al	-18.31485	1.63933	0.00000
Al	-18.31485	-1.63744	0.00000
Al	-15.81606	1.63933	0.00000
Al	-15.81606	-1.63744	0.00000
Al	-13.31727	1.63933	0.00000
Al	-13.31727	-1.63744	0.00000
Al	-10.81848	1.63933	0.00000
Al	-10.81848	-1.63744	0.00000
Al	-8.31969	-1.63744	0.00000
Al	-8.31872	1.63933	0.00000
C	-7.22932	0.00062	-0.00001
C	-5.81323	0.00020	-0.00001
H	-5.55049	-2.16609	-0.00001
H	-5.54920	2.16633	-0.00001
C	-5.02567	-1.21725	-0.00001
C	-5.02495	1.21718	-0.00001
C	-3.65516	-1.21548	-0.00002
C	-3.65443	1.21459	-0.00002
H	-3.14684	-2.17170	-0.00002
H	-3.14548	2.17049	-0.00002
C	-2.88999	-0.00066	-0.00002
C	-1.45290	-0.00088	-0.00002

H	-1.19245	2.16667	-0.00002
H	-1.19240	-2.16848	-0.00002
C	-0.68741	-1.21118	-0.00002
C	-0.68741	1.20938	-0.00002
C	0.68741	-1.21118	-0.00002
C	0.68741	1.20938	-0.00002
H	1.19239	-2.16848	-0.00002
H	1.19245	2.16667	-0.00002
C	1.45290	-0.00088	-0.00002
C	2.88999	-0.00067	-0.00002
H	3.14548	2.17048	-0.00002
H	3.14684	-2.17170	-0.00001
C	3.65443	1.21459	-0.00002
C	3.65516	-1.21548	-0.00001
C	5.02495	1.21718	-0.00002
C	5.02567	-1.21725	-0.00001
H	5.54920	2.16633	-0.00001
H	5.55049	-2.16609	-0.00001
C	5.81323	0.00020	-0.00001
C	7.22932	0.00062	-0.00001
Al	8.31872	1.63933	0.00000
Al	8.31969	-1.63744	0.00001
Al	10.81751	1.63933	0.00000
Al	10.81751	-1.63744	0.00001
Al	13.31630	1.63933	0.00000
Al	13.31630	-1.63744	0.00001
Al	15.81509	1.63933	0.00000
Al	15.81509	-1.63744	0.00001
Al	18.31388	1.63933	0.00000
Al	18.31388	-1.63744	0.00001
Al	20.81267	1.63933	0.00000
Al	20.81267	-1.63744	0.00001

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#4 Phenyl ring (pX2-6)

Al	23.02336	-1.71596	0.00000
Al	23.01950	1.72723	0.00000
Al	20.52457	-1.71596	0.00000
Al	20.52071	1.72723	0.00000
Al	18.02578	-1.71596	0.00000
Al	18.02192	1.72723	0.00000
Al	15.52699	-1.71596	0.00000
Al	15.52313	1.72723	0.00000
Al	13.02820	-1.71596	0.00000
Al	13.02434	1.72723	0.00000
Al	10.52941	-1.71596	0.00000
Al	10.52555	1.72723	0.00000
C	9.44798	0.00443	0.00000
C	8.02552	0.00279	0.00000
H	7.75423	-2.16464	0.00000
H	7.74909	2.16962	0.00000

C	7.23355	-1.21015	0.00000
C	7.23071	1.21388	0.00000
C	5.85925	-1.21138	0.00000
C	5.85642	1.21184	0.00000
H	5.35126	-2.16802	0.00000
H	5.34618	2.16727	0.00000
C	5.09792	-0.00066	0.00000
C	3.64661	-0.00233	0.00000
H	3.39243	-2.16636	0.00000
H	3.38754	2.16112	0.00000
C	2.88814	-1.20834	0.00000
C	2.88541	1.20196	0.00000
C	1.50676	-1.20899	0.00000
C	1.50404	1.19945	0.00000
H	1.00365	-2.16782	0.00000
H	0.99876	2.15713	0.00000
C	0.74822	-0.00563	0.00000
C	-0.71062	-0.00733	0.00000
H	-0.96104	-2.17010	0.00000
H	-0.96618	2.15485	0.00000
C	-1.46638	-1.21244	0.00000
C	-1.46923	1.19599	0.00000
C	-2.84776	-1.21503	0.00000
C	-2.85061	1.19526	0.00000
H	-3.34979	-2.17423	0.00000
H	-3.35495	2.15325	0.00000
C	-3.60904	-0.01078	0.00000
C	-5.06037	-0.01246	0.00000
H	-5.30877	-2.18039	0.00000
H	-5.31360	2.15489	0.00000
C	-5.81894	-1.22492	0.00000
C	-5.82166	1.19829	0.00000
C	-7.19323	-1.22687	0.00000
C	-7.19595	1.19716	0.00000
H	-7.71170	-2.18257	0.00000
H	-7.71659	2.15167	0.00000
C	-7.98797	-0.01574	0.00000
C	-9.41045	-0.01735	0.00000
Al	-10.49191	1.70260	0.00000
Al	-10.48827	-1.73974	0.00000
Al	-12.99070	1.70260	0.00000
Al	-12.98710	-1.73974	0.00000
Al	-15.48950	1.70260	0.00000
Al	-15.48590	-1.73974	0.00000
Al	-17.98830	1.70260	0.00000
Al	-17.98460	-1.73974	0.00000
Al	-20.48710	1.70260	0.00000
Al	-20.48340	-1.73974	0.00000
Al	-22.98590	1.70260	0.00000

Al	-22.98220	-1.73974	0.00000
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#5 Phenyl ring (pX2-6)

Al	-25.19503	-1.63020	-0.00006
Al	-25.19422	1.63999	-0.00042
Al	-22.69624	-1.63020	-0.00006
Al	-22.69543	1.63999	-0.00042
Al	-20.19745	-1.63020	-0.00006
Al	-20.19664	1.63999	-0.00042
Al	-17.69866	-1.63020	-0.00006
Al	-17.69785	1.63999	-0.00042
Al	-15.19987	-1.63020	-0.00006
Al	-15.19906	1.63999	-0.00042
Al	-12.70108	-1.63020	-0.00006
Al	-12.70027	1.63999	-0.00042
C	-11.60884	0.00465	-0.00016
C	-10.18262	0.00433	-0.00006
H	-9.92437	-2.15864	0.00016
H	-9.92369	2.16723	-0.00022
C	-9.40105	-1.20888	0.00010
C	-9.40066	1.21730	-0.00011
C	-8.02427	-1.20600	0.00017
C	-8.02388	1.21398	-0.00003
H	-7.51585	-2.16236	0.00029
H	-7.51512	2.17016	-0.00008
C	-7.26763	0.00387	0.00011
C	-5.80828	0.00376	0.00017
H	-5.55569	2.16559	0.00012
H	-5.55562	-2.15809	0.00025
C	-5.05235	1.20714	0.00016
C	-5.05234	-1.19962	0.00024
C	-3.66777	1.20593	0.00020
C	-3.66776	-1.19839	0.00028
H	-3.16357	2.16422	0.00019
H	-3.16355	-2.15667	0.00032
C	-2.91525	0.00377	0.00026
C	-1.44513	0.00378	0.00028
H	-1.19657	-2.15620	0.00034
H	-1.19656	2.16375	0.00022
C	-0.69314	-1.19751	0.00032
C	-0.69313	1.20506	0.00025
C	0.69313	-1.19751	0.00032
C	0.69314	1.20506	0.00025
H	1.19656	-2.15621	0.00035
H	1.19658	2.16375	0.00023
C	1.44513	0.00377	0.00028
C	2.91525	0.00375	0.00026
H	3.16353	-2.15669	0.00034
H	3.16359	2.16420	0.00019
C	3.66775	-1.19841	0.00029

C	3.66778	1.20591	0.00020
C	5.05233	-1.19965	0.00025
C	5.05236	1.20711	0.00016
H	5.55561	-2.15812	0.00026
H	5.55571	2.16555	0.00012
C	5.80828	0.00372	0.00018
C	7.26763	0.00382	0.00012
H	7.51514	2.17011	-0.00006
H	7.51584	-2.16241	0.00028
C	8.02389	1.21393	-0.00001
C	8.02426	-1.20606	0.00017
C	9.40067	1.21724	-0.00010
C	9.40104	-1.20895	0.00009
H	9.92371	2.16716	-0.00020
H	9.92435	-2.15871	0.00014
C	10.18262	0.00427	-0.00006
C	11.60884	0.00457	-0.00016
Al	12.70027	1.63991	-0.00042
Al	15.19906	1.63991	-0.00042
Al	17.69785	1.63991	-0.00042
Al	20.19664	1.63991	-0.00042
Al	22.69543	1.63991	-0.00042
Al	25.19422	1.63991	-0.00042
Al	12.70107	-1.63029	-0.00007
Al	15.19986	-1.63029	-0.00007
Al	17.69865	-1.63029	-0.00007
Al	20.19744	-1.63029	-0.00007
Al	22.69623	-1.63029	-0.00007
Al	25.19502	-1.63029	-0.00007

pX2 Electrodes (Twisted)

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#5 Phenyl ring twisted (pX2)

Al	-12.7010800000	-1.6302000000	-0.0000600000
Al	-12.7002700000	1.6399900000	-0.0004200000
C	-11.6088400000	0.0046500000	-0.0001600000
C	-10.1826200000	0.0043300000	-0.0000600000
H	-9.9243700000	-2.1586400000	0.0001600000
H	-9.9236900000	2.1672300000	-0.0002200000
C	-9.4010500000	-1.2088800000	0.0001000000
C	-9.4006600000	1.2173000000	-0.0001100000
C	-8.0242700000	-1.2060000000	0.0001700000
C	-8.0238800000	1.2139800000	-0.0000300000
H	-7.5158500000	-2.1623600000	0.0002900000
H	-7.5151200000	2.1701600000	-0.0000800000
C	-7.2676300000	0.0038700000	0.0001100000
C	-5.8082072974	0.0041386208	0.0147246038
H	-5.5662505078	-1.9034350115	-1.0051049181
H	-5.5449394469	1.9115565918	1.0294942241
C	-5.0582560311	-1.0578629304	-0.5591172876

C	-5.0463644132	1.0657411981	0.5734275454
C	-3.6737395425	-1.0571360070	-0.5724159864
C	-3.6618599914	1.0643152262	0.5589805887
H	-3.1742937121	-1.9028016172	-1.0284114057
H	-3.1529464512	1.9097282616	1.0048742670
C	-2.9153226064	0.0033956676	-0.0142616312
C	-1.4451300000	0.0037800000	0.0002800000
H	-1.1965700000	-2.1562000000	0.0003400000
H	-1.1965600000	2.1637500000	0.0002200000
C	-0.6931400000	-1.1975100000	0.0003200000
C	-0.6931300000	1.2050600000	0.0002500000
C	0.6931300000	-1.1975100000	0.0003200000
C	0.6931400000	1.2050600000	0.0002500000
H	1.1965600000	-2.1562100000	0.0003500000
H	1.1965800000	2.1637500000	0.0002300000
C	1.4451300000	0.0037700000	0.0002800000
C	2.9153548282	0.0210125588	0.0023445570
H	3.1460162830	-1.6273819490	1.4018926263
H	3.1812776577	1.6634949383	-1.3979245761
C	3.6580066053	-0.9035641900	0.7802077134
C	3.6776240330	0.9276101748	-0.7777301139
C	5.0424761001	-0.9210568951	0.7789671972
C	5.0621134067	0.9119758782	-0.7805516180
H	5.5379110747	-1.6570678951	1.3992796129
H	5.5732351838	1.6359323607	-1.4023313203
C	5.8081748274	-0.0135849814	-0.0019040785
C	7.2676300000	0.0038200000	0.0001200000
H	7.5151400000	2.1701100000	-0.0000600000
H	7.5158400000	-2.1624100000	0.0002800000
C	8.0238900000	1.2139300000	-0.0000100000
C	8.0242600000	-1.2060600000	0.0001700000
C	9.4006700000	1.2172400000	-0.0001000000
C	9.4010400000	-1.2089500000	0.0000900000
H	9.9237100000	2.1671600000	-0.0002000000
H	9.9243500000	-2.1587100000	0.0001400000
C	10.1826200000	0.0042700000	-0.0000600000
C	11.6088400000	0.0045700000	-0.0001600000
Al	12.7002700000	1.6399100000	-0.0004200000
Al	12.7010700000	-1.6302900000	-0.0000700000

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#5 Phenyl ring twisted (pX2-2)

Al	-15.1998700000	-1.6302000000	-0.0000600000
Al	-15.1990600000	1.6399900000	-0.0004200000
Al	-12.7010800000	-1.6302000000	-0.0000600000
Al	-12.7002700000	1.6399900000	-0.0004200000
C	-11.6088400000	0.0046500000	-0.0001600000
C	-10.1826200000	0.0043300000	-0.0000600000
H	-9.9243700000	-2.1586400000	0.0001600000
H	-9.9236900000	2.1672300000	-0.0002200000
C	-9.4010500000	-1.2088800000	0.0001000000

C	-9.4006600000	1.2173000000	-0.0001100000
C	-8.0242700000	-1.2060000000	0.0001700000
C	-8.0238800000	1.2139800000	-0.0000300000
H	-7.5158500000	-2.1623600000	0.0002900000
H	-7.5151200000	2.1701600000	-0.0000800000
C	-7.2676300000	0.0038700000	0.0001100000
C	-5.8082072974	0.0041386208	0.0147246038
H	-5.5662505078	-1.9034350115	-1.0051049181
H	-5.5449394469	1.9115565918	1.0294942241
C	-5.0582560311	-1.0578629304	-0.5591172876
C	-5.0463644132	1.0657411981	0.5734275454
C	-3.6737395425	-1.0571360070	-0.5724159864
C	-3.6618599914	1.0643152262	0.5589805887
H	-3.1742937121	-1.9028016172	-1.0284114057
H	-3.1529464512	1.9097282616	1.0048742670
C	-2.9153226064	0.0033956676	-0.0142616312
C	-1.4451300000	0.0037800000	0.0002800000
H	-1.1965700000	-2.1562000000	0.0003400000
H	-1.1965600000	2.1637500000	0.0002200000
C	-0.6931400000	-1.1975100000	0.0003200000
C	-0.6931300000	1.2050600000	0.0002500000
C	0.6931300000	-1.1975100000	0.0003200000
C	0.6931400000	1.2050600000	0.0002500000
H	1.1965600000	-2.1562100000	0.0003500000
H	1.1965800000	2.1637500000	0.0002300000
C	1.4451300000	0.0037700000	0.0002800000
C	2.9153548282	0.0210125588	0.0023445570
H	3.1460162830	-1.6273819490	1.4018926263
H	3.1812776577	1.6634949383	-1.3979245761
C	3.6580066053	-0.9035641900	0.7802077134
C	3.6776240330	0.9276101748	-0.7777301139
C	5.0424761001	-0.9210568951	0.7789671972
C	5.0621134067	0.9119758782	-0.7805516180
H	5.5379110747	-1.6570678951	1.3992796129
H	5.5732351838	1.6359323607	-1.4023313203
C	5.8081748274	-0.0135849814	-0.0019040785
C	7.2676300000	0.0038200000	0.0001200000
H	7.5151400000	2.1701100000	-0.0000600000
H	7.5158400000	-2.1624100000	0.0002800000
C	8.0238900000	1.2139300000	-0.0000100000
C	8.0242600000	-1.2060600000	0.0001700000
C	9.4006700000	1.2172400000	-0.0001000000
C	9.4010400000	-1.2089500000	0.0000900000
H	9.9237100000	2.1671600000	-0.0002000000
H	9.9243500000	-2.1587100000	0.0001400000
C	10.1826200000	0.0042700000	-0.0000600000
C	11.6088400000	0.0045700000	-0.0001600000
Al	12.7002700000	1.6399100000	-0.0004200000
Al	12.7010700000	-1.6302900000	-0.0000700000
Al	15.1990600000	1.6399100000	-0.0004200000
Al	15.1998600000	-1.6302900000	-0.0000700000

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#5 Phenyl ring twisted (pX2-4)

Al	-20.1974500000	-1.6302000000	-0.0000600000
Al	-20.1966400000	1.6399900000	-0.0004200000
Al	-17.6986600000	-1.6302000000	-0.0000600000
Al	-17.6978500000	1.6399900000	-0.0004200000
Al	-15.1998700000	-1.6302000000	-0.0000600000
Al	-15.1990600000	1.6399900000	-0.0004200000
Al	-12.7010800000	-1.6302000000	-0.0000600000
Al	-12.7002700000	1.6399900000	-0.0004200000
C	-11.6088400000	0.0046500000	-0.0001600000
C	-10.1826200000	0.0043300000	-0.0000600000
H	-9.9243700000	-2.1586400000	0.0001600000
H	-9.9236900000	2.1672300000	-0.0002200000
C	-9.4010500000	-1.2088800000	0.0001000000
C	-9.4006600000	1.2173000000	-0.0001100000
C	-8.0242700000	-1.2060000000	0.0001700000
C	-8.0238800000	1.2139800000	-0.0000300000
H	-7.5158500000	-2.1623600000	0.0002900000
H	-7.5151200000	2.1701600000	-0.0000800000
C	-7.2676300000	0.0038700000	0.0001100000
C	-5.8082072974	0.0041386208	0.0147246038
H	-5.5662505078	-1.9034350115	-1.0051049181
H	-5.5449394469	1.9115565918	1.0294942241
C	-5.0582560311	-1.0578629304	-0.5591172876
C	-5.0463644132	1.0657411981	0.5734275454
C	-3.6737395425	-1.0571360070	-0.5724159864
C	-3.6618599914	1.0643152262	0.5589805887
H	-3.1742937121	-1.9028016172	-1.0284114057
H	-3.1529464512	1.9097282616	1.0048742670
C	-2.9153226064	0.0033956676	-0.0142616312
C	-1.4451300000	0.0037800000	0.0002800000
H	-1.1965700000	-2.1562000000	0.0003400000
H	-1.1965600000	2.1637500000	0.0002200000
C	-0.6931400000	-1.1975100000	0.0003200000
C	-0.6931300000	1.2050600000	0.0002500000
C	0.6931300000	-1.1975100000	0.0003200000
C	0.6931400000	1.2050600000	0.0002500000
H	1.1965600000	-2.1562100000	0.0003500000
H	1.1965800000	2.1637500000	0.0002300000
C	1.4451300000	0.0037700000	0.0002800000
C	2.9153548282	0.0210125588	0.0023445570
H	3.1460162830	-1.6273819490	1.4018926263
H	3.1812776577	1.6634949383	-1.3979245761
C	3.6580066053	-0.9035641900	0.7802077134
C	3.6776240330	0.9276101748	-0.7777301139
C	5.0424761001	-0.9210568951	0.7789671972
C	5.0621134067	0.9119758782	-0.7805516180
H	5.5379110747	-1.6570678951	1.3992796129
H	5.5732351838	1.6359323607	-1.4023313203

C	5.8081748274	-0.0135849814	-0.0019040785
C	7.2676300000	0.0038200000	0.0001200000
H	7.5151400000	2.1701100000	-0.0000600000
H	7.5158400000	-2.1624100000	0.0002800000
C	8.0238900000	1.2139300000	-0.0000100000
C	8.0242600000	-1.2060600000	0.0001700000
C	9.4006700000	1.2172400000	-0.0001000000
C	9.4010400000	-1.2089500000	0.0000900000
H	9.9237100000	2.1671600000	-0.0002000000
H	9.9243500000	-2.1587100000	0.0001400000
C	10.1826200000	0.0042700000	-0.0000600000
C	11.6088400000	0.0045700000	-0.0001600000
Al	12.7002700000	1.6399100000	-0.0004200000
Al	12.7010700000	-1.6302900000	-0.0000700000
Al	15.1990600000	1.6399100000	-0.0004200000
Al	15.1998600000	-1.6302900000	-0.0000700000
Al	17.6978500000	1.6399100000	-0.0004200000
Al	17.6986500000	-1.6302900000	-0.0000700000
Al	20.1966400000	1.6399100000	-0.0004200000
Al	20.1974400000	-1.6302900000	-0.0000700000

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#5 Phenyl ring twisted (pX2-6)

Al	-25.1950300000	-1.6302000000	-0.0000600000
Al	-25.1942200000	1.6399900000	-0.0004200000
Al	-22.6962400000	-1.6302000000	-0.0000600000
Al	-22.6954300000	1.6399900000	-0.0004200000
Al	-20.1974500000	-1.6302000000	-0.0000600000
Al	-20.1966400000	1.6399900000	-0.0004200000
Al	-17.6986600000	-1.6302000000	-0.0000600000
Al	-17.6978500000	1.6399900000	-0.0004200000
Al	-15.1998700000	-1.6302000000	-0.0000600000
Al	-15.1990600000	1.6399900000	-0.0004200000
Al	-12.7010800000	-1.6302000000	-0.0000600000
Al	-12.7002700000	1.6399900000	-0.0004200000
C	-11.6088400000	0.0046500000	-0.0001600000
C	-10.1826200000	0.0043300000	-0.0000600000
H	-9.9243700000	-2.1586400000	0.0001600000
H	-9.9236900000	2.1672300000	-0.0002200000
C	-9.4010500000	-1.2088800000	0.0001000000
C	-9.4006600000	1.2173000000	-0.0001100000
C	-8.0242700000	-1.2060000000	0.0001700000
C	-8.0238800000	1.2139800000	-0.0000300000
H	-7.5158500000	-2.1623600000	0.0002900000
H	-7.5151200000	2.1701600000	-0.0000800000
C	-7.2676300000	0.0038700000	0.0001100000
C	-5.8082072974	0.0041386208	0.0147246038
H	-5.5662505078	-1.9034350115	-1.0051049181
H	-5.5449394469	1.9115565918	1.0294942241
C	-5.0582560311	-1.0578629304	-0.5591172876
C	-5.0463644132	1.0657411981	0.5734275454

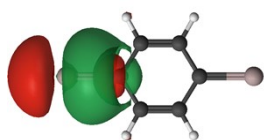
C	-3.6737395425	-1.0571360070	-0.5724159864
C	-3.6618599914	1.0643152262	0.5589805887
H	-3.1742937121	-1.9028016172	-1.0284114057
H	-3.1529464512	1.9097282616	1.0048742670
C	-2.9153226064	0.0033956676	-0.0142616312
C	-1.4451300000	0.0037800000	0.0002800000
H	-1.1965700000	-2.1562000000	0.0003400000
H	-1.1965600000	2.1637500000	0.0002200000
C	-0.6931400000	-1.1975100000	0.0003200000
C	-0.6931300000	1.2050600000	0.0002500000
C	0.6931300000	-1.1975100000	0.0003200000
C	0.6931400000	1.2050600000	0.0002500000
H	1.1965600000	-2.1562100000	0.0003500000
H	1.1965800000	2.1637500000	0.0002300000
C	1.4451300000	0.0037700000	0.0002800000
C	2.9153548282	0.0210125588	0.0023445570
H	3.1460162830	-1.6273819490	1.4018926263
H	3.1812776577	1.6634949383	-1.3979245761
C	3.6580066053	-0.9035641900	0.7802077134
C	3.6776240330	0.9276101748	-0.7777301139
C	5.0424761001	-0.9210568951	0.7789671972
C	5.0621134067	0.9119758782	-0.7805516180
H	5.5379110747	-1.6570678951	1.3992796129
H	5.5732351838	1.6359323607	-1.4023313203
C	5.8081748274	-0.0135849814	-0.0019040785
C	7.2676300000	0.0038200000	0.0001200000
H	7.5151400000	2.1701100000	-0.0000600000
H	7.5158400000	-2.1624100000	0.0002800000
C	8.0238900000	1.2139300000	-0.0000100000
C	8.0242600000	-1.2060600000	0.0001700000
C	9.4006700000	1.2172400000	-0.0001000000
C	9.4010400000	-1.2089500000	0.0000900000
H	9.9237100000	2.1671600000	-0.0002000000
H	9.9243500000	-2.1587100000	0.0001400000
C	10.1826200000	0.0042700000	-0.0000600000
C	11.6088400000	0.0045700000	-0.0001600000
Al	12.7002700000	1.6399100000	-0.0004200000
Al	12.7010700000	-1.6302900000	-0.0000700000
Al	15.1990600000	1.6399100000	-0.0004200000
Al	15.1998600000	-1.6302900000	-0.0000700000
Al	17.6978500000	1.6399100000	-0.0004200000
Al	17.6986500000	-1.6302900000	-0.0000700000
Al	20.1966400000	1.6399100000	-0.0004200000
Al	20.1974400000	-1.6302900000	-0.0000700000
Al	22.6954300000	1.6399100000	-0.0004200000
Al	22.6962300000	-1.6302900000	-0.0000700000
Al	25.1942200000	1.6399100000	-0.0004200000
Al	25.1950200000	-1.6302900000	-0.0000700000

Section S2. Active Space Orbitals for All Systems Studied

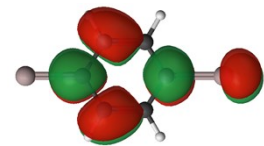
pP 1-Ring

(12e, 12o) CAS

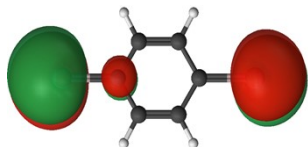
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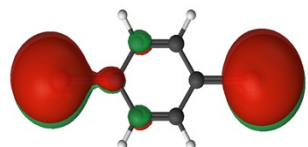
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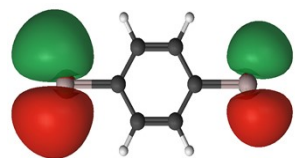
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9

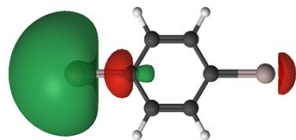


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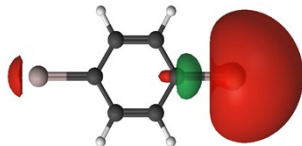


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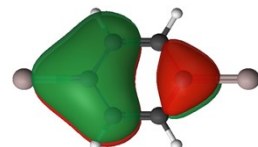
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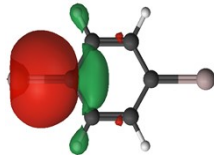
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4



3

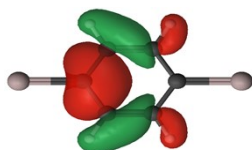
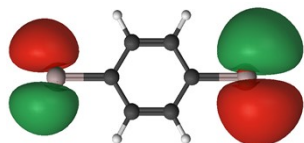


2



1

Orb.	Occ.
12	0.02
11	0.04
10	0.06
9	0.06
8	0.07
7	0.07
6	1.87
5	1.87
4	1.97
3	1.98
2	2.0
1	2.0

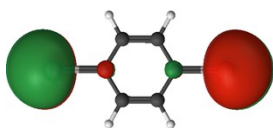


pP 1-Ring

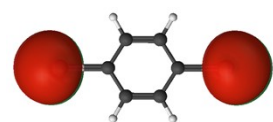
(8e, 8o) CAS

1-layer electrode

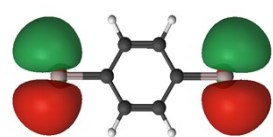
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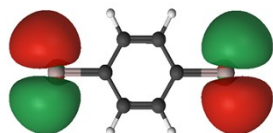
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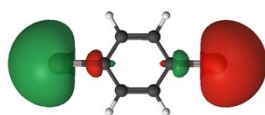
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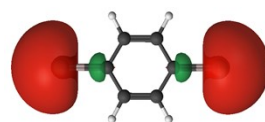
5



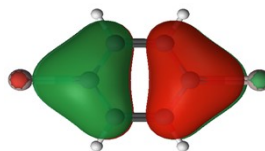
4



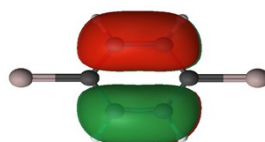
3



2



1



Orb.	Occ.
8	0.06
7	0.06
6	0.07
5	0.07
4	1.87
3	1.87

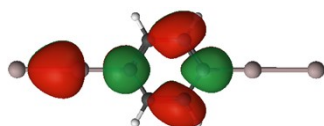
2	2.0
1	2.0

pP 1-Ring

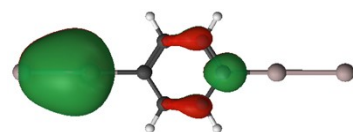
(8e, 8o) CAS

2-layer electrode

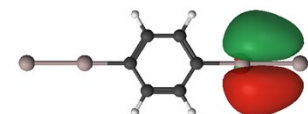
8



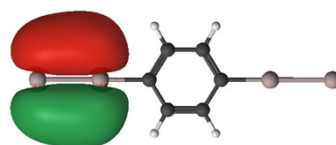
7



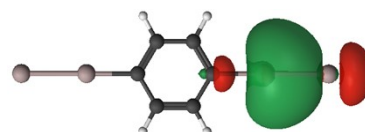
6



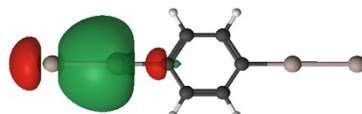
4

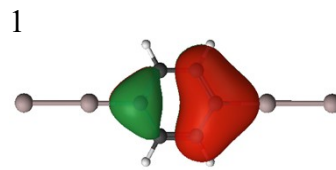
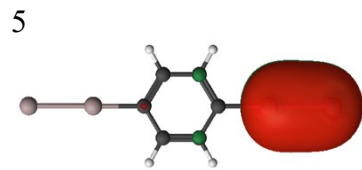


3



2



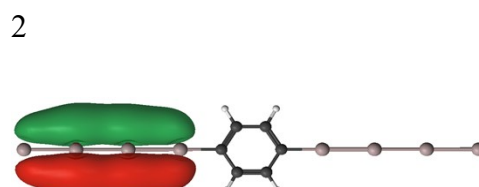
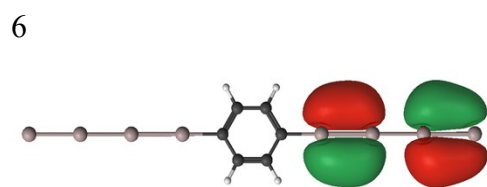
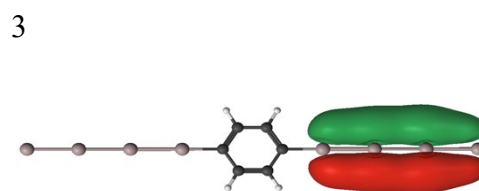
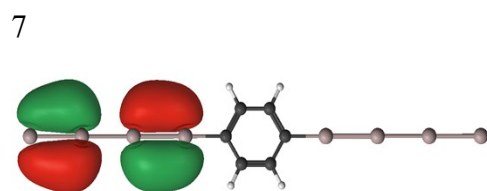
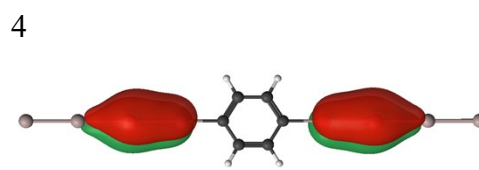
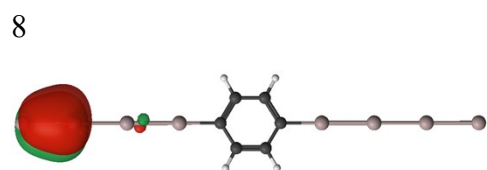


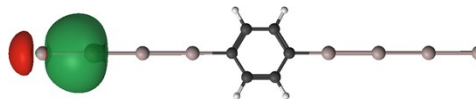
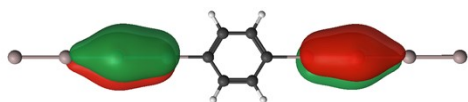
Orb.	Occ.
8	0.04
7	0.05
6	0.05
5	1.0
4	1.0
3	1.95
2	1.95
1	1.96

pP 1-Ring

(8e, 8o) CAS

4-layer electrode





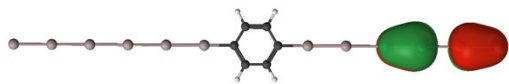
Orb.	Occ.
8	0.05
7	0.47
6	0.5
5	0.95
4	1.04
3	1.5
2	1.53
1	1.96

pP 1-Ring

(8e, 8o) CAS

6-layer electrode

8



7

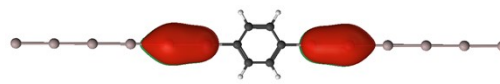


6

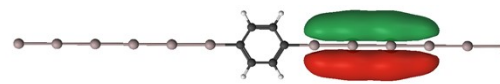


5

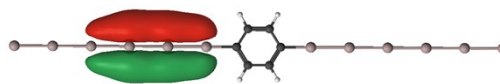
4



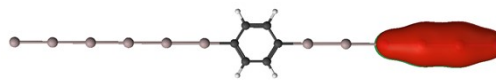
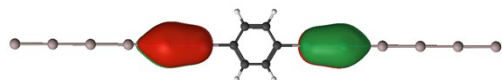
3



2



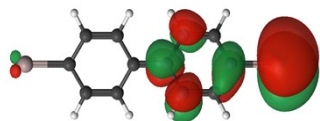
1



Orb.	Occ.
8	0.34
7	0.46
6	0.52
5	0.95
4	1.05
3	1.48
2	1.54
1	1.66

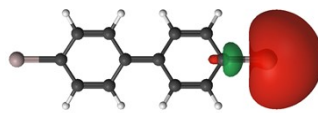
pP 2-Ring (12e, 12o) CAS

12



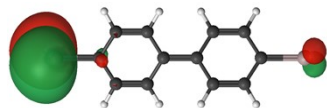
11

6



5

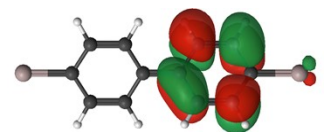
Orb.	Occ.
12	0.06
11	0.06
10	0.07



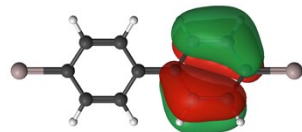
10



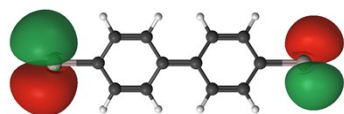
4



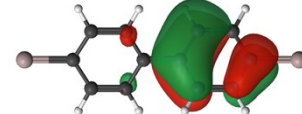
9



3



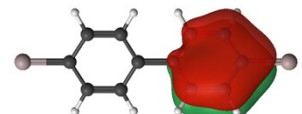
8



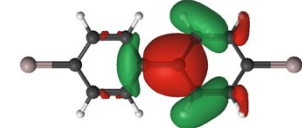
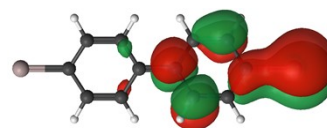
2



7



1



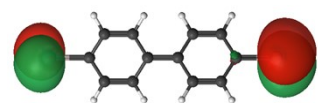
9	0.07
8	0.07
7	0.07
6	1.87
5	1.87
4	1.94
3	1.94
2	1.99
1	2.0

pP 2-Ring

(8e, 8o) CAS

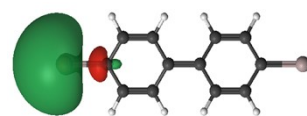
1-layer electrode

8

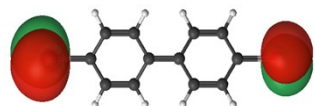


7

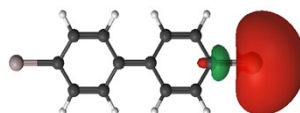
4



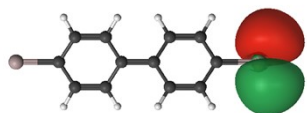
3



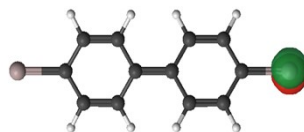
6



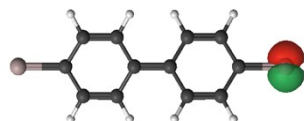
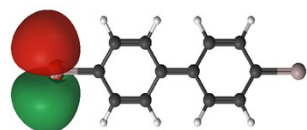
2



5



1



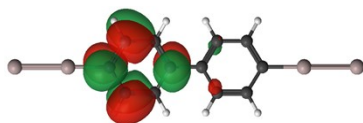
Orb.	Occ.
8	0.06
7	0.06
6	0.07
5	0.07
4	1.87
3	1.87
2	2.0
1	2.0

pP 2-Ring

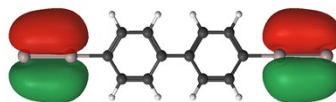
(8e, 8o) CAS

2-layer electrode

8

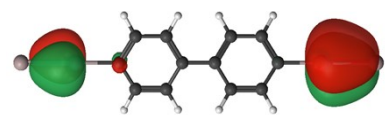


4

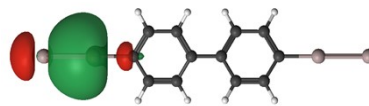


7

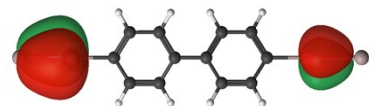
3



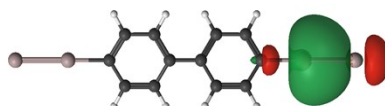
6



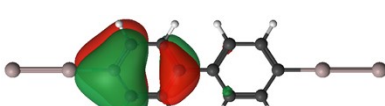
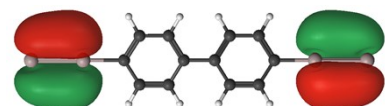
2



5



1



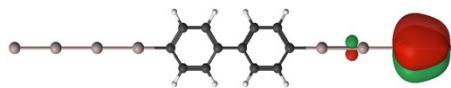
Orb.	Occ.
8	0.04
7	0.05
6	0.05
5	1.0
4	1.0
3	1.95
2	1.95
1	1.96

pP 2-Ring

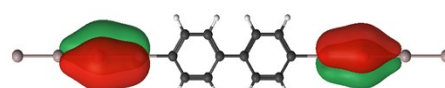
(8e, 8o) CAS

4-layer electrode

8

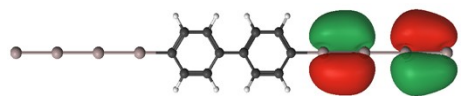


4

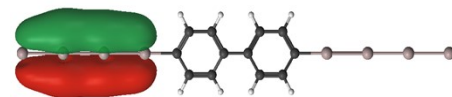


7

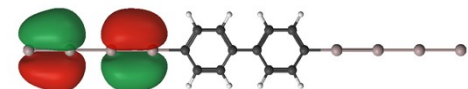
3



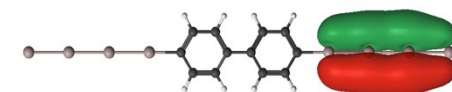
6



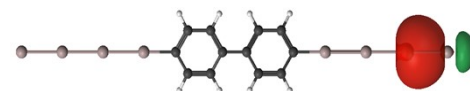
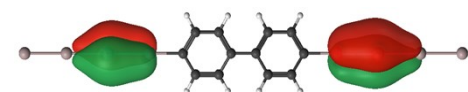
2



5



1



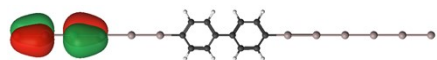
Orb.	Occ.
8	0.05
7	0.47
6	0.5
5	0.99
4	1.01
3	1.50
2	1.53
1	1.96

pP 2-Ring

(8e, 8o) CAS

6-layer electrode

8

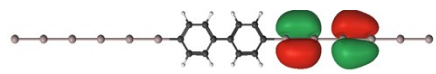


7

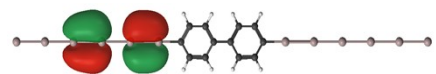
4



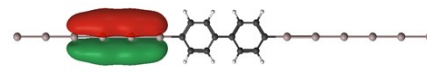
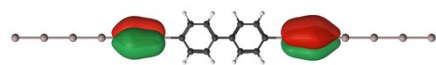
3



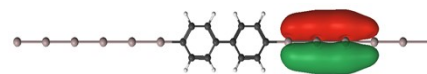
6



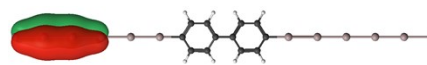
5



2



1

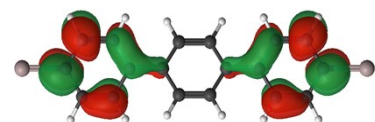


Orb.	Occ.
8	0.34
7	0.47
6	0.53
5	0.99
4	1.01
3	1.47
2	1.53
1	1.66

pP 3-Ring

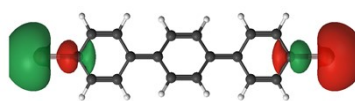
(12e, 12o) CAS

12

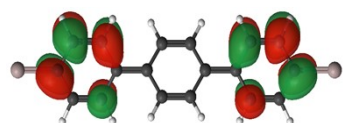


11

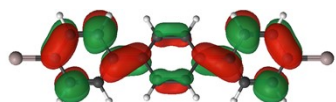
6



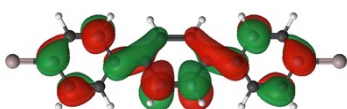
5



10



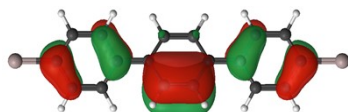
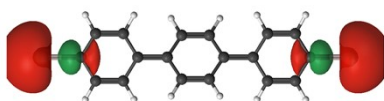
9



8



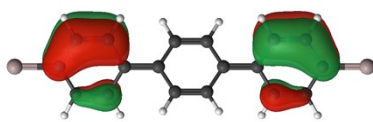
7



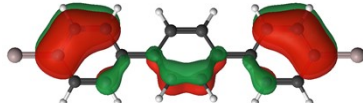
4



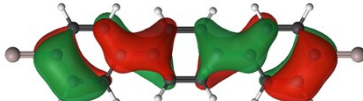
3



2



1



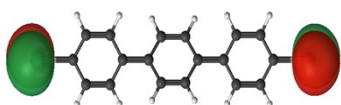
Orb.	Occ.
12	0.07
11	0.07
10	0.07
9	0.07
8	0.17
7	1.0
6	1.0
5	1.86
4	1.92
3	1.92
2	1.92
1	1.94

pP 3-Ring

(8e, 8o) CAS

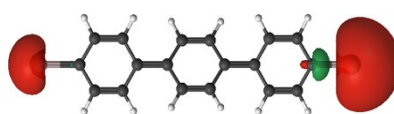
1-layer electrode

8

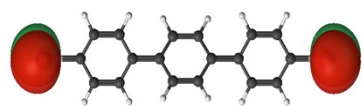


7

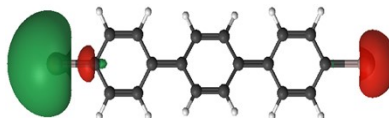
4



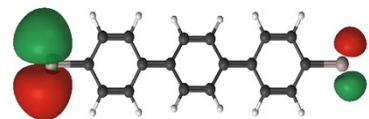
3



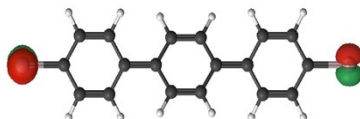
6



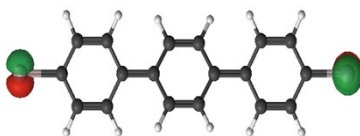
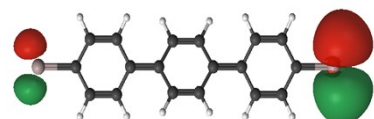
2



5



1



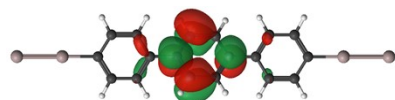
Orb.	Occ.
8	0.06
7	0.06
6	0.07
5	0.07
4	1.87
3	1.87
2	2.0
1	2.0

pP 3-Ring

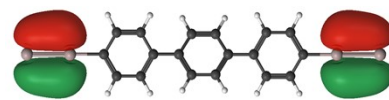
(8e, 8o) CAS

2-layer electrode

8

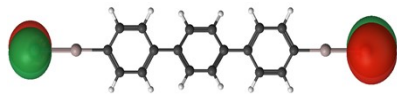


4

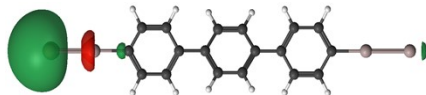


7

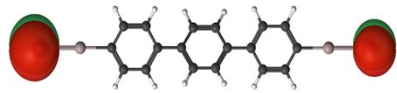
3



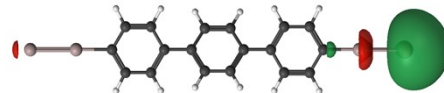
6



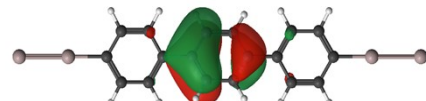
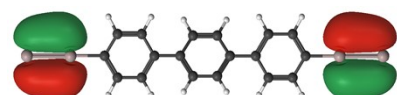
2



5



1



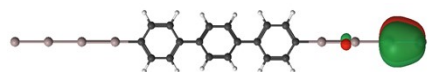
Orb.	Occ.
8	0.04
7	0.08
6	0.08
5	1.0
4	1.0
3	1.92
2	1.92
1	1.96

pP 3-Ring

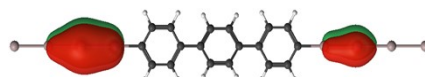
(8e, 8o) CAS

4-layer electrode

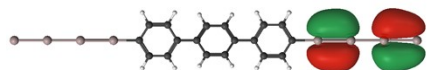
8



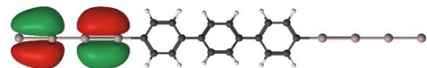
4



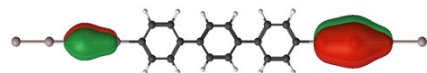
7



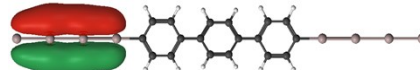
6



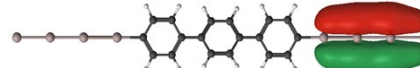
5



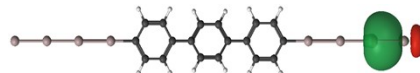
3



2



1



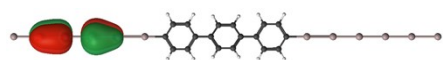
Orb.	Occ.
8	0.05
7	0.47
6	0.5
5	0.99
4	1.0
3	1.50
2	1.53
1	1.96

pP 3-Ring

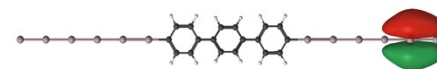
(8e, 8o) CAS

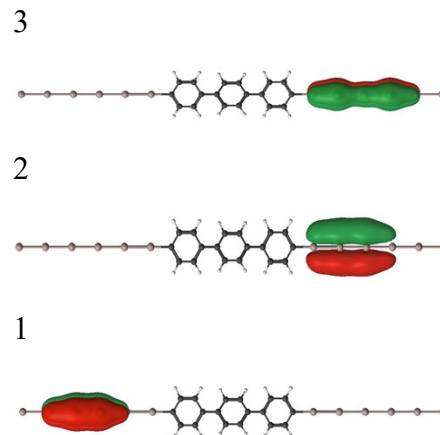
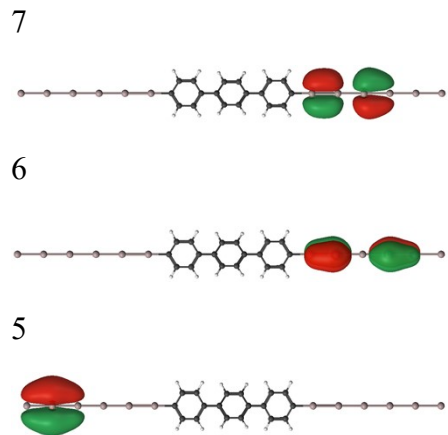
6-layer electrode

8



4



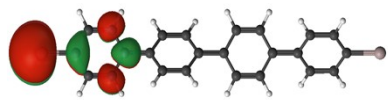


Orb.	Occ.
8	0.35
7	0.47
6	0.75
5	1.0
4	1.0
3	1.25
2	1.53
1	1.65

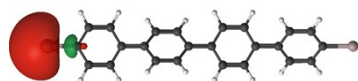
pP 4-Ring
(12e, 12o) CAS

12

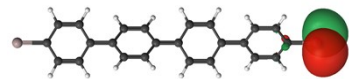
6



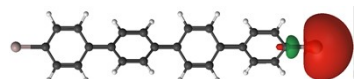
11



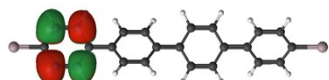
5



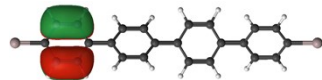
10



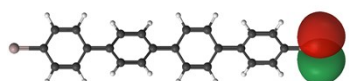
4



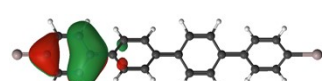
9



3



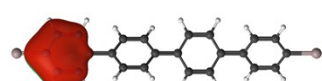
8



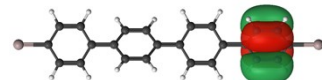
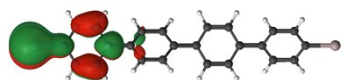
2



7



1



Orb.	Occ.
12	0.06
11	0.06
10	0.07
9	0.07
8	0.07
7	0.07
6	1.87
5	1.87
4	1.94
3	1.94
2	1.99
1	2.0

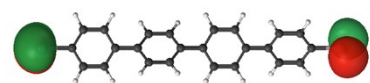
pP 4-Ring

(8e, 8o) CAS

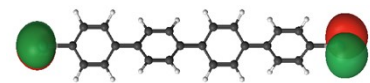
1-layer electrode

8

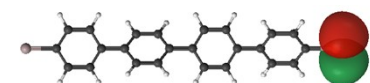
4



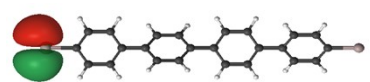
7



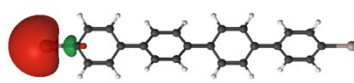
6



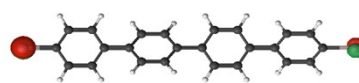
5



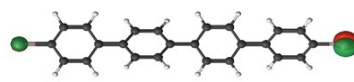
3



2



1



Orb.	Occ.
8	0.06
7	0.06
6	0.07
5	0.07
4	1.87
3	1.87
2	2.0
1	2.0

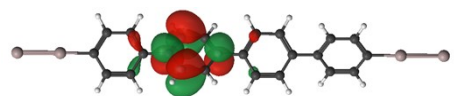
pP 4-Ring

(8e, 8o) CAS

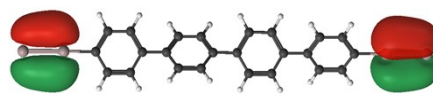
2-layer electrode

8

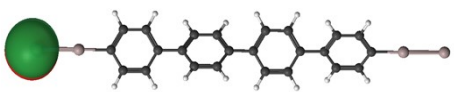
4



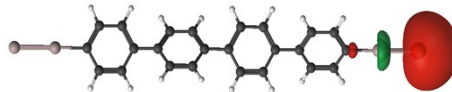
7



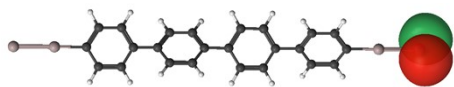
3



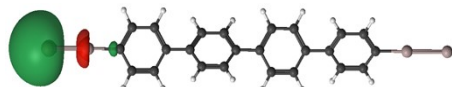
6



2



5



1

Orb.	Occ.
8	0.04
7	0.08
6	0.08
5	1.0
4	1.0
3	1.92
2	1.92
1	1.96

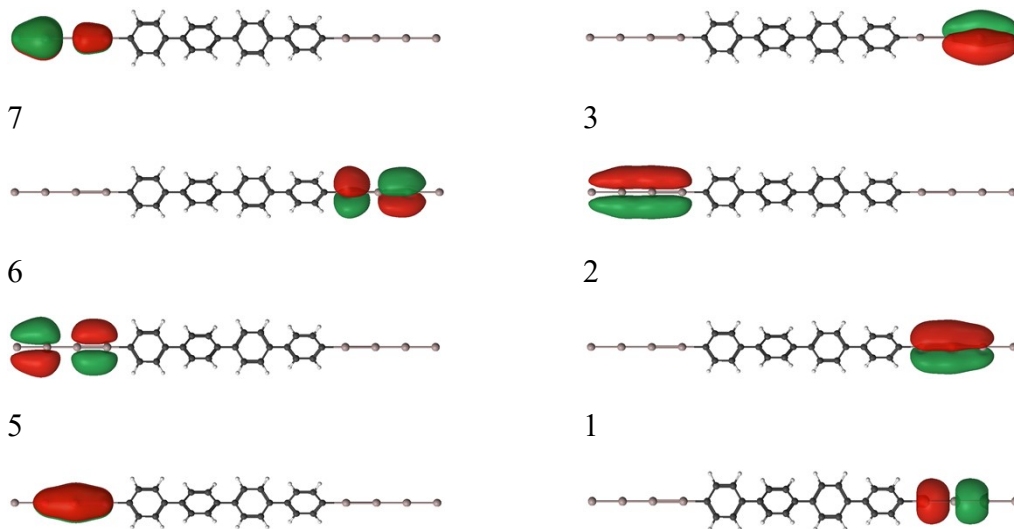
pP 4-Ring

(8e, 8o) CAS

4-layer electrode

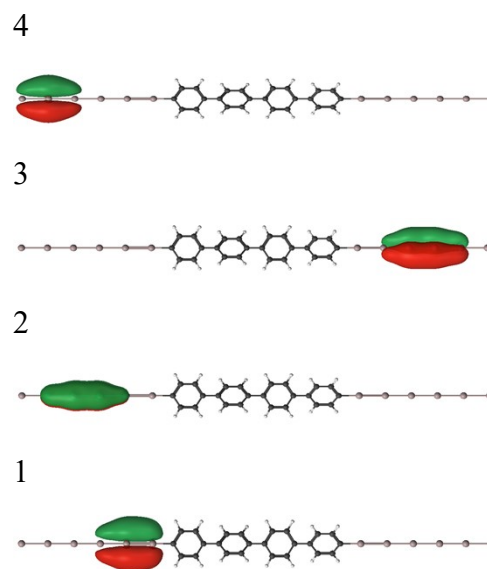
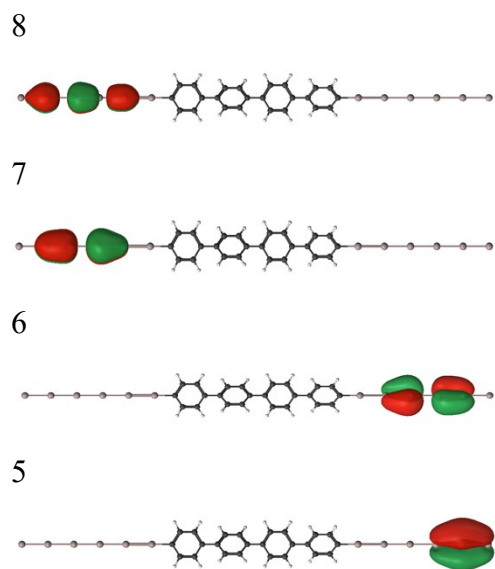
8

4



Orb.	Occ.
8	0.04
7	0.23
6	0.36
5	0.96
4	1.0
3	1.64
2	1.77
1	2.0

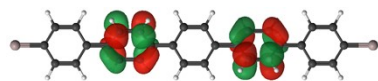
pP 4-Ring
(8e, 8o) CAS
6-layer electrode



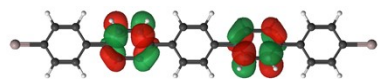
Orb.	Occ.
8	0.02
7	0.31
6	0.35
5	1.0
4	1.0
3	1.65
2	1.67
1	2.0

pP 5-Ring
(12e, 12o) CAS

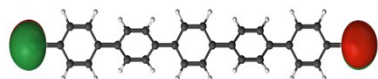
12



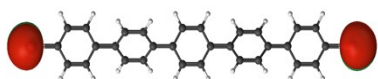
11



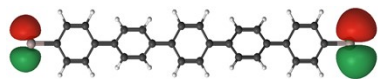
10



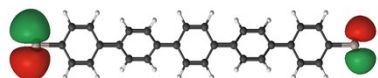
9



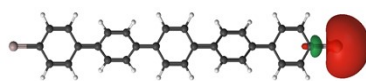
8



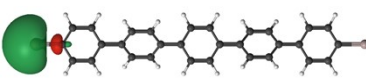
7



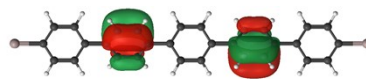
6



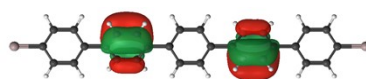
5



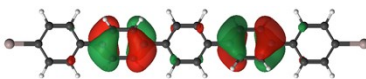
4



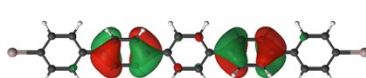
3



2



1



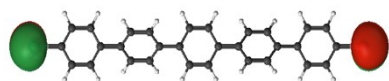
Orb.	Occ.
12	0.05
11	0.05
10	0.06
9	0.06
8	0.07
7	0.07
6	1.87
5	1.87
4	1.96
3	1.96
2	1.99
1	2.0

pP 5-Ring

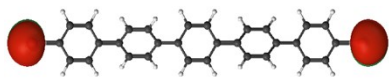
(8e, 8o) CAS

1-layer electrode

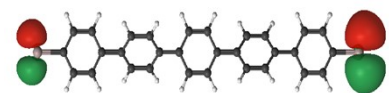
8



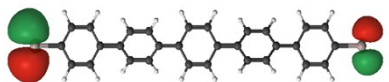
7



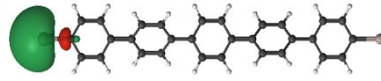
6



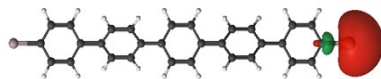
5



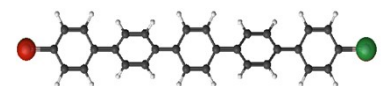
4



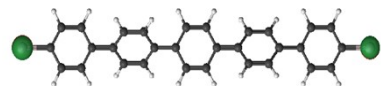
3



2



1

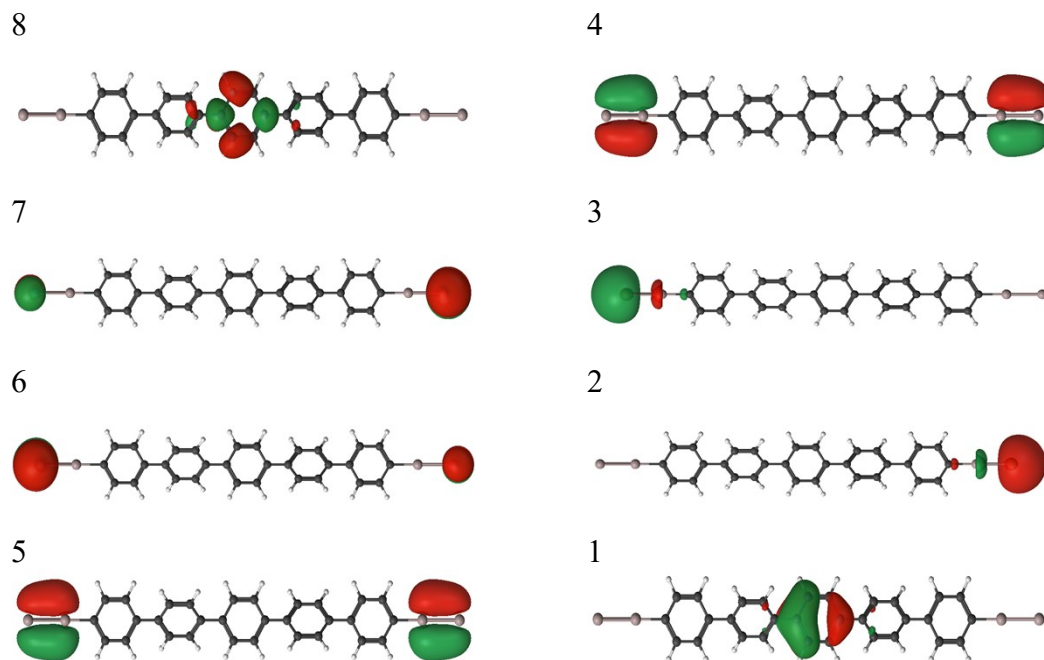


Orb.	Occ.
8	0.06
7	0.06
6	0.07
5	0.07
4	1.87
3	1.87
2	2.0
1	2.0

pP 5-Ring

(8e, 8o) CAS

2-layer electrode

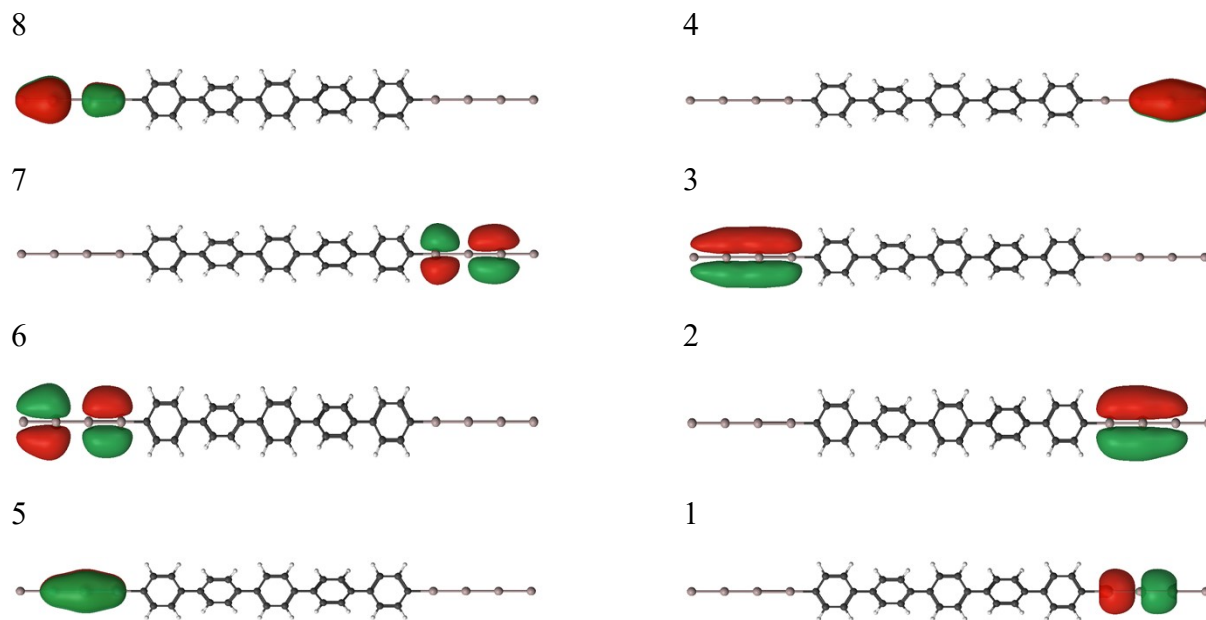


Orb.	Occ.
8	0.04
7	0.08
6	0.08
5	1.0
4	1.0
3	1.92
2	1.92
1	1.96

pP 5-Ring

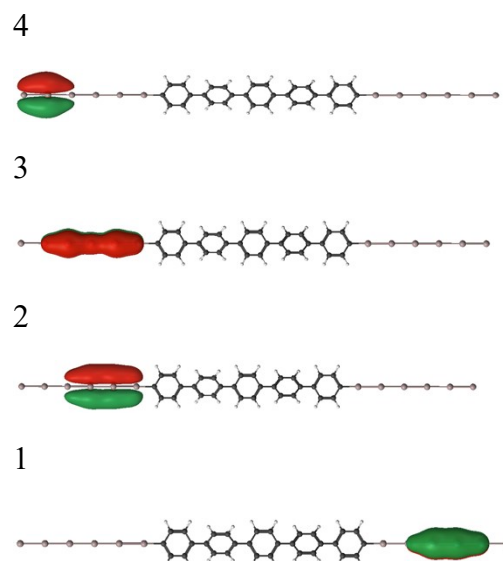
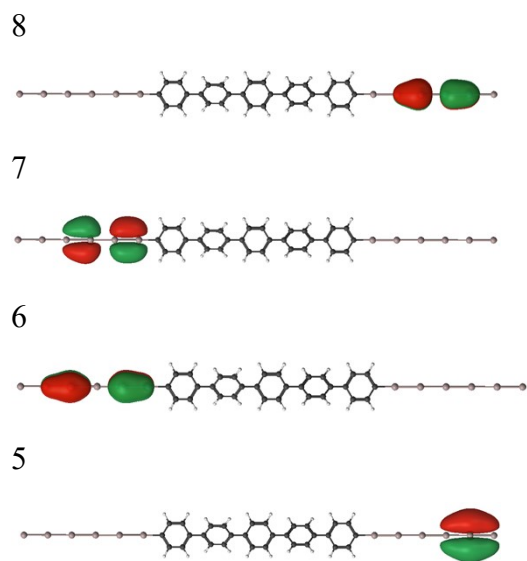
(8e, 8o) CAS

4-layer electrode



Orb.	Occ.
8	0.04
7	0.23
6	0.36
5	0.96
4	1.00
3	1.64
2	1.77
1	2.0

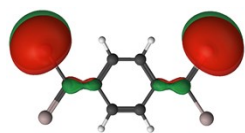
pP 5-Ring
(8e, 8o) CAS
6-layer electrode



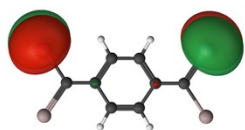
Orb.	Occ.
8	0.35
7	0.47
6	0.75
5	1.0
4	1.0
3	1.25
2	1.53
1	1.65

pX2 1-Ring
(12e, 12o) CAS

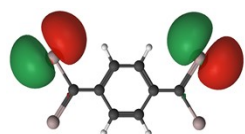
12



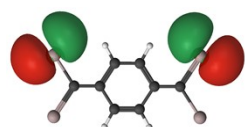
11



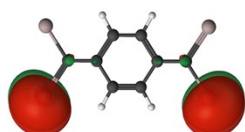
10



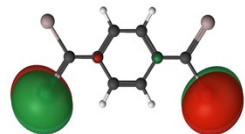
9



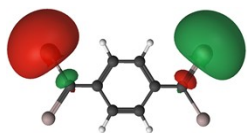
8



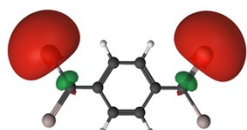
7



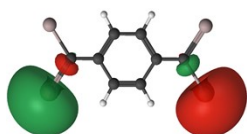
6



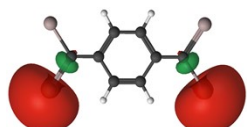
5



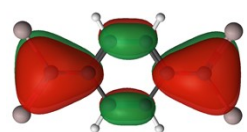
4



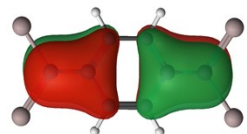
3



2



1



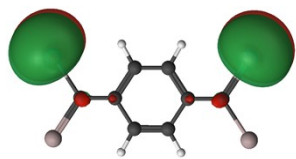
Orb.	Occ.
12	0.06
11	0.06
10	0.07
9	0.07
8	0.08
7	0.08
6	1.87
5	1.87
4	1.92
3	1.92
2	2.0
1	2.0

pX2 1-Ring

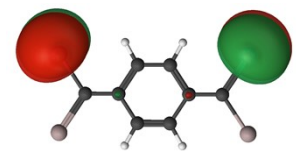
(8e, 8o) CAS

1-layer electrode

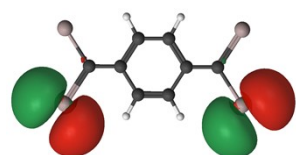
8



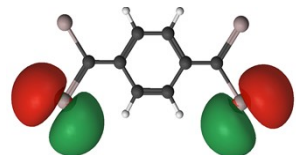
7



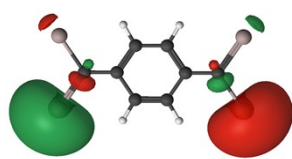
6



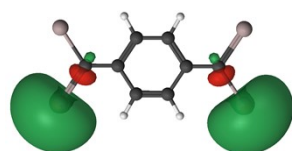
5



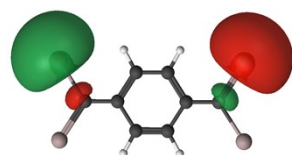
4



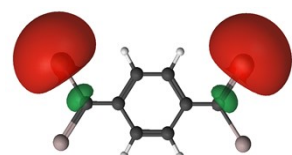
3



2



1

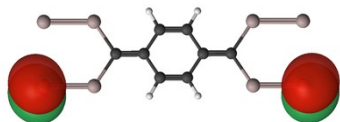


Orb.	Occ.
8	0.08
7	0.08
6	0.09
5	0.09
4	1.91
3	1.91
2	1.92
1	1.92

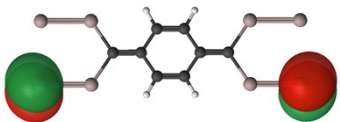
pX2 1-Ring
(8e, 8o) CAS

2-layer electrode

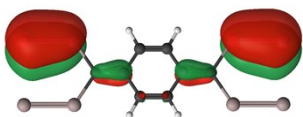
8



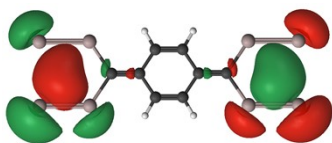
7



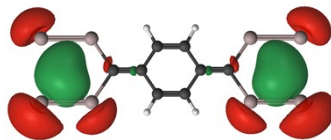
6



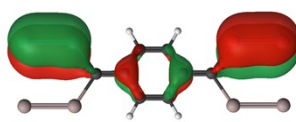
5



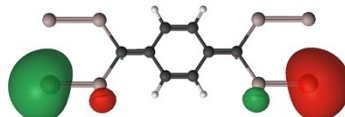
4



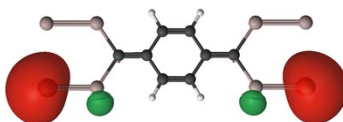
3



2



1



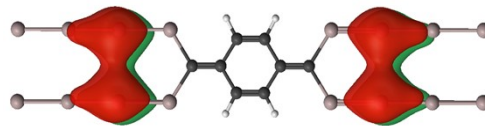
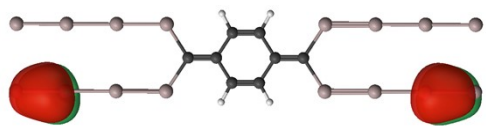
Orb.	Occ.
8	0.08
7	0.08
6	0.74
5	0.98
4	1.01
3	1.26
2	1.93
1	1.93

pX2 1-Ring

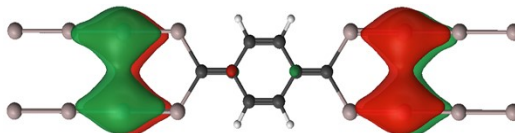
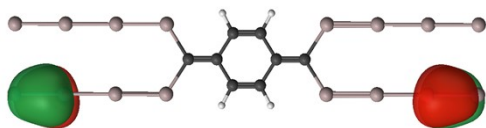
(8e, 8o) CAS

4-layer electrode

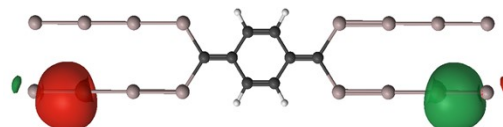
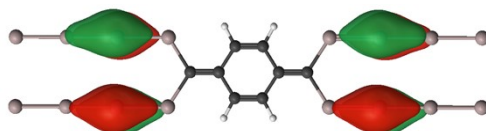
8 4



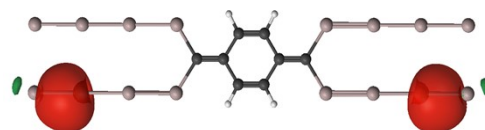
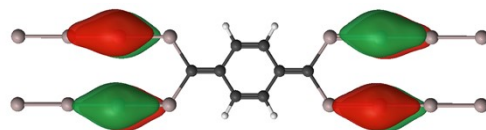
7 3



6 2



5 1

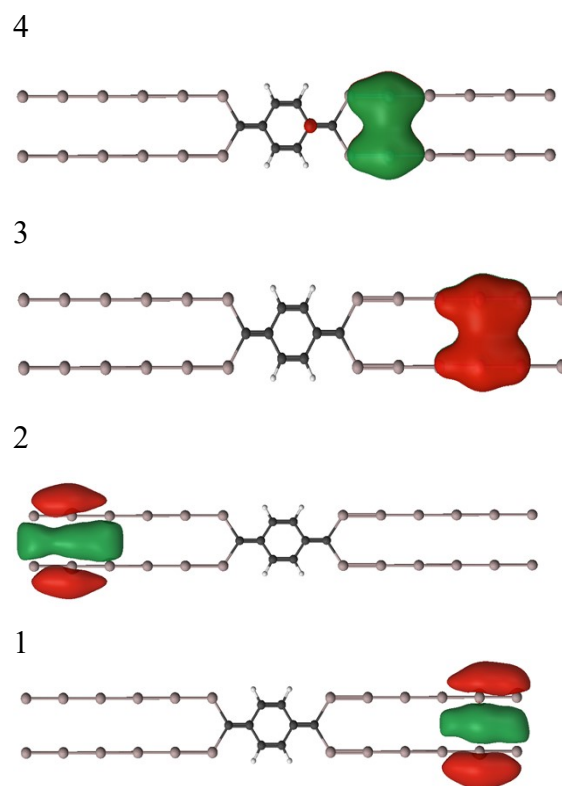
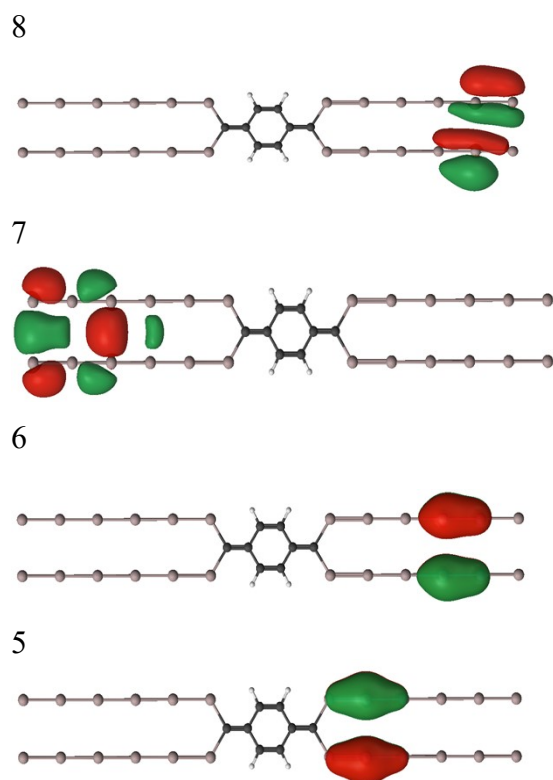


Orb.	Occ.
8	0.04
7	0.04
6	0.31
5	0.31
4	1.68
3	1.7
2	1.96
1	1.96

pX2 1-Ring

(8e, 8o) CAS

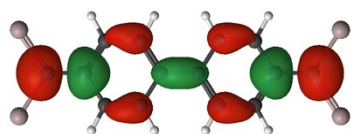
6-layer electrode



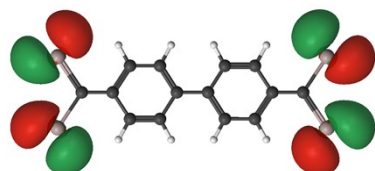
Orb.	Occ.
8	0.07
7	0.12
6	0.23
5	0.36
4	1.64
3	1.76
2	1.88
1	1.93

pX2 2-Ring
(12e, 12o) CAS

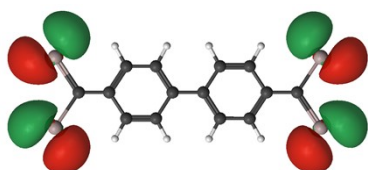
12



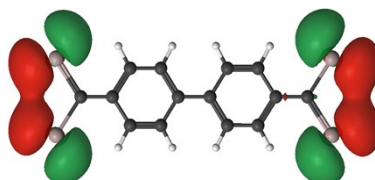
11



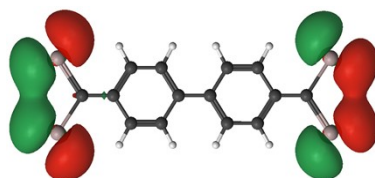
10



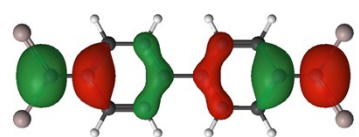
9



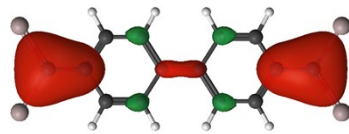
8



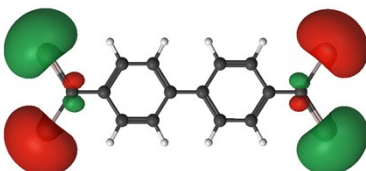
7



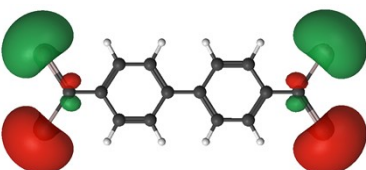
6



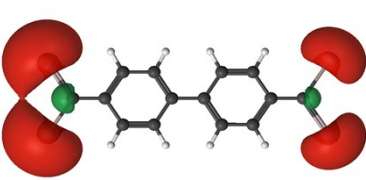
5



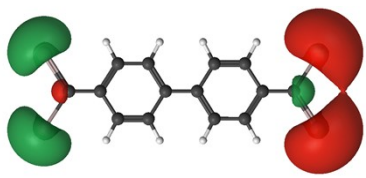
4



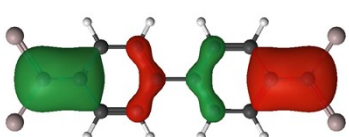
3



2



1



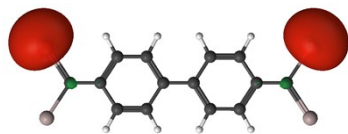
Orb.	Occ.
12	0.07
11	0.08
10	0.08
9	0.1
8	0.1
7	0.1
6	1.9
5	1.91
4	1.91
3	1.91
2	1.91
1	1.92

pX2 2-Ring

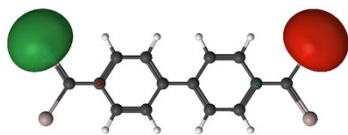
(8e, 8o) CAS

1-layer electrode

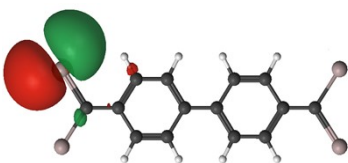
8



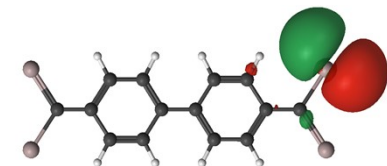
7



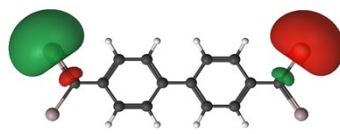
6



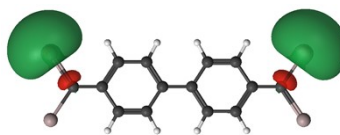
5



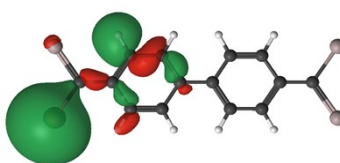
4



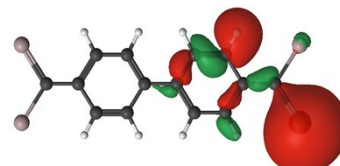
3



2



1



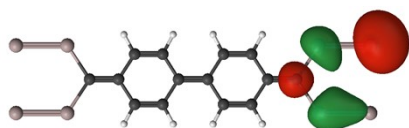
Orb.	Occ.
8	0.06
7	0.06
6	0.07
5	0.07
4	1.87
3	1.87
2	2.0
1	2.0

pX2 2-Ring

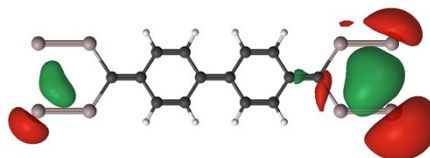
(8e, 8o) CAS

2-layer electrode

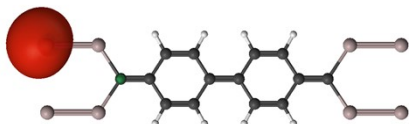
8



4



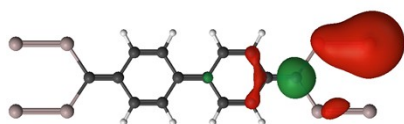
7



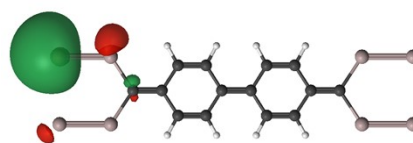
3



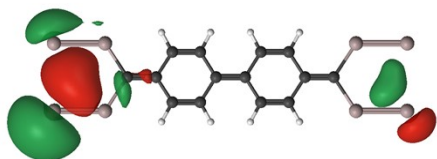
6



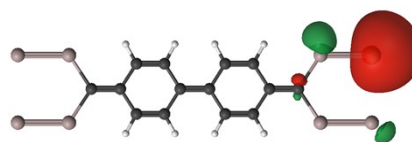
2



5



1



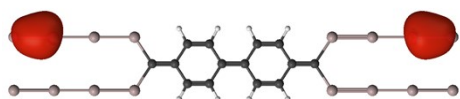
Orb.	Occ.
8	0.06
7	0.09
6	0.11
5	1.0
4	1.0
3	1.91
2	1.92
1	1.92

pX2 2-Ring

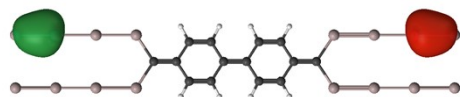
(8e, 8o) CAS

4-layer electrode

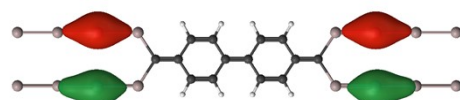
8



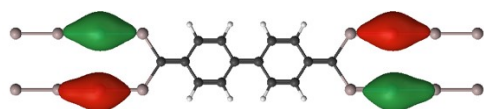
7



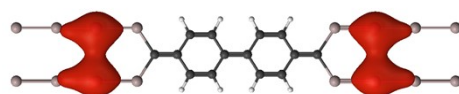
6



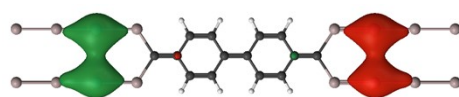
5



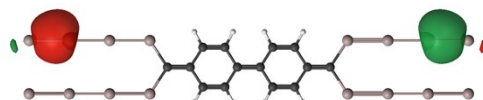
4



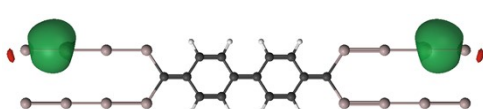
3



2



1



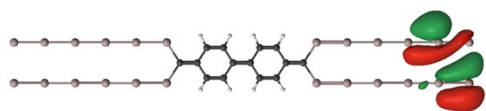
Orb.	Occ.
8	0.04
7	0.04
6	0.30
5	0.30
4	1.69
3	1.71
2	1.96
1	1.96

pX2 2-Ring

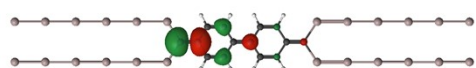
(8e, 8o) CAS

6-layer electrode

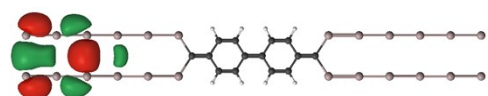
8



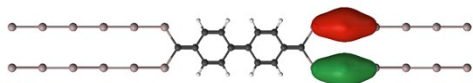
7



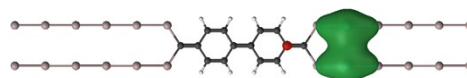
6



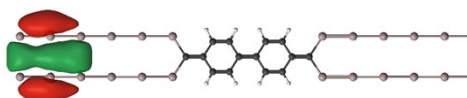
5



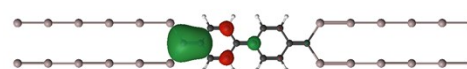
4



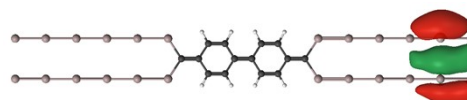
3



2



1

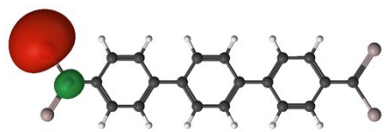


Orb.	Occ.
8	0.08
7	0.08
6	0.12
5	0.35
4	1.65
3	1.88
2	1.92
1	1.92

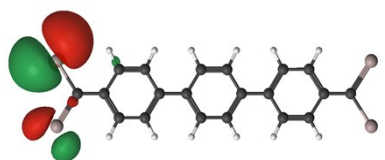
pX2 3-Ring

(12e, 12o) CAS

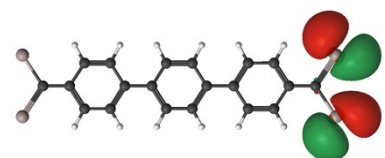
12



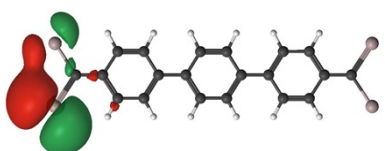
11



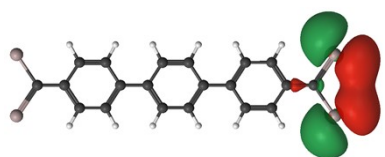
10



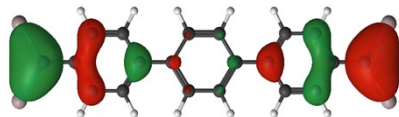
9



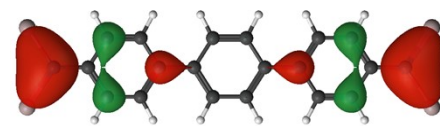
8



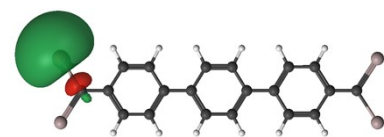
7



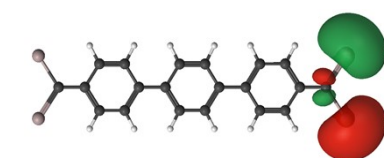
6



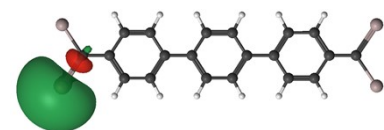
5



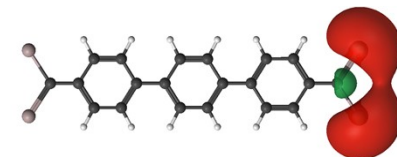
4



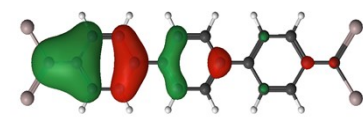
3



2



1



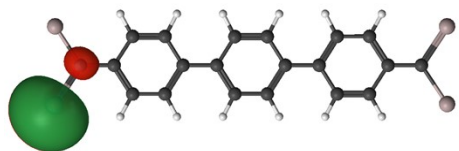
Orb.	Occ.
12	0.06
11	0.07
10	0.08
9	0.09
8	0.1
7	0.8
6	1.21
5	1.87
4	1.91
3	1.91
2	1.91
1	2.0

pX2 3-Ring

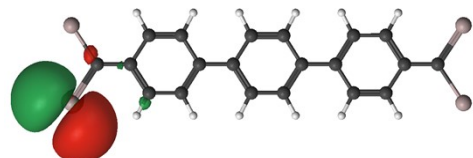
(8e, 8o) CAS

1-layer electrode

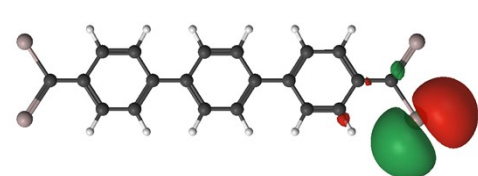
8



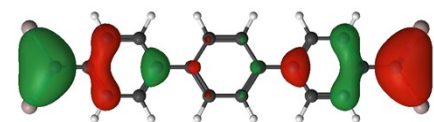
7



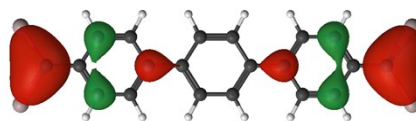
6



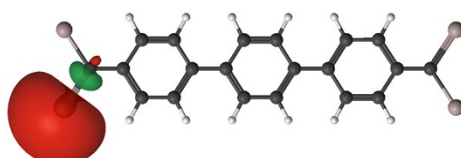
5



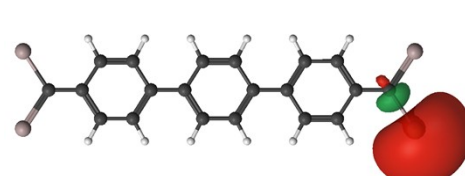
4



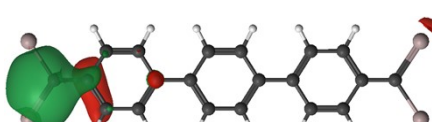
3



2



1



Orb.	Occ.
8	0.06
7	0.07
6	0.09
5	0.8
4	1.2
3	1.87
2	1.91
1	2.0

pX2 3-Ring

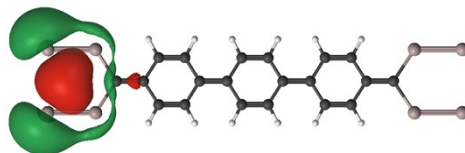
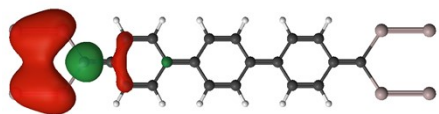
(8e, 8o) CAS

2-layer

electrode

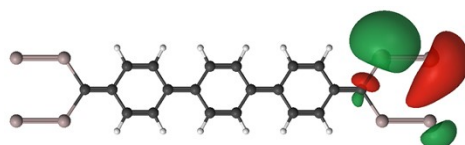
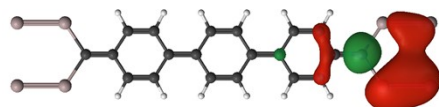
8

4



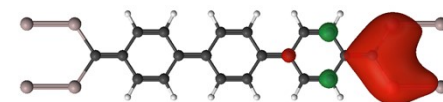
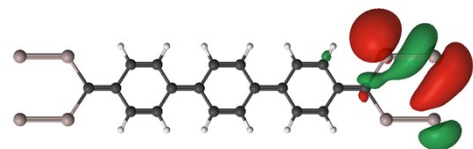
7

3



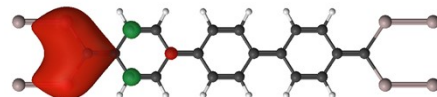
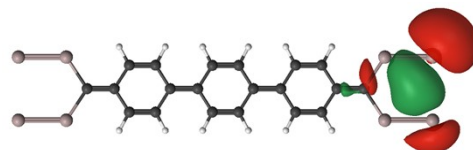
6

2



5

1

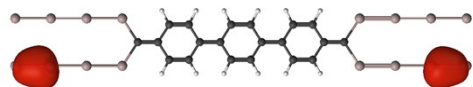


Orb.	Occ.
8	0.1
7	0.11
6	0.13
5	1.0
4	1.0
3	1.87
2	1.89
1	1.90

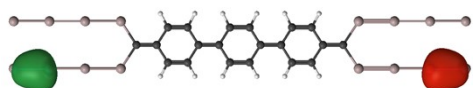
pX2 3-Ring

(8e, 8o) CAS
4-layer electrode

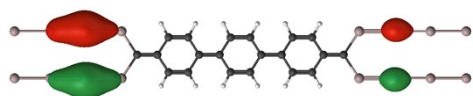
8



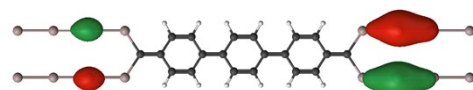
7



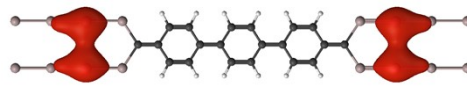
6



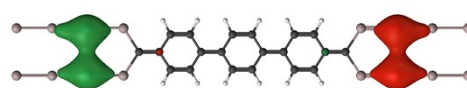
5



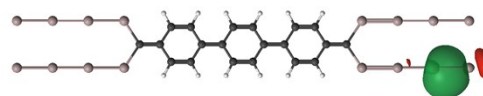
4



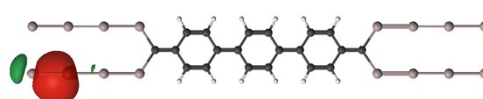
3



2



1

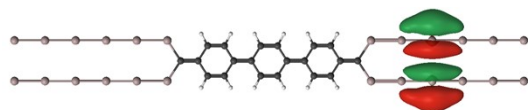


Orb.	Occ.
8	0.04
7	0.04
6	0.29
5	0.29
4	1.70
3	1.72
2	1.96
1	1.96

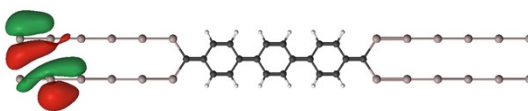
pX2 3-Ring

(8e, 8o) CAS
6-layer electrode

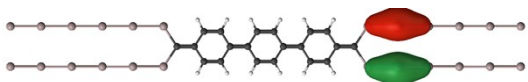
8



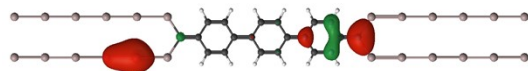
7



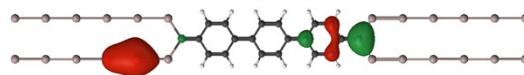
6



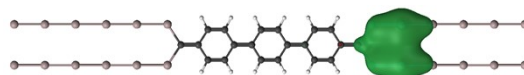
5



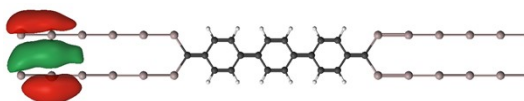
4



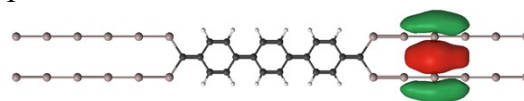
3



2



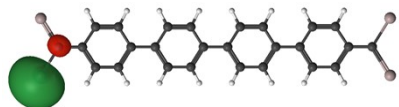
1



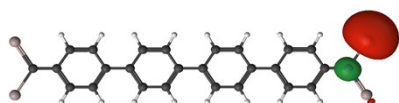
Orb.	Occ.
8	0.06
7	0.08
6	0.31
5	0.92
4	1.07
3	1.71
2	1.92
1	1.94

pX2 4-Ring
(12e, 12o) CAS

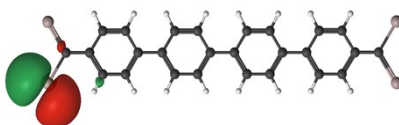
12



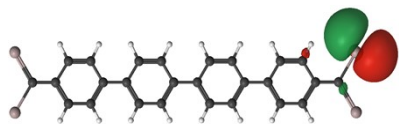
11



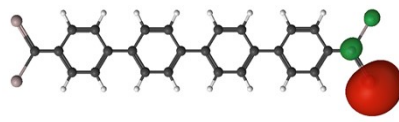
10



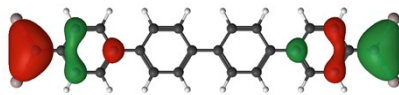
9



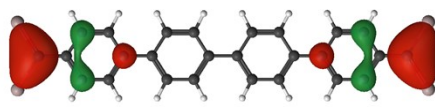
8



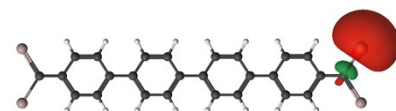
7



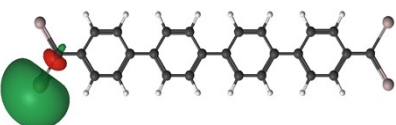
6



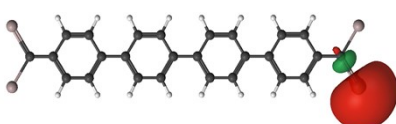
5



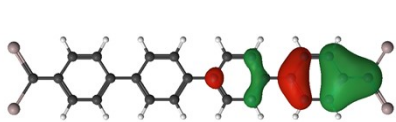
4



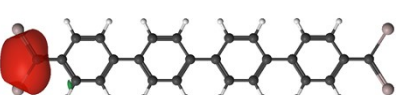
3



2



1



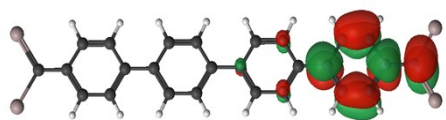
Orb.	Occ.
12	0.06
11	0.06
10	0.07
9	0.07
8	0.08
7	0.95
6	1.06
5	1.87
4	1.87
3	1.92
2	2.0
1	2.0

pX2 4-Ring

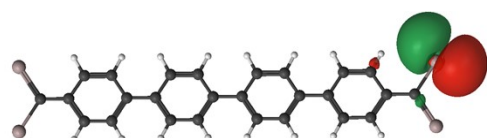
(8e, 8o) CAS

1-layer electrode

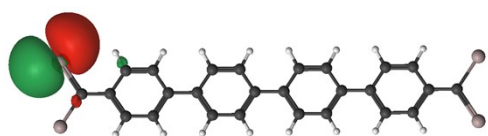
8



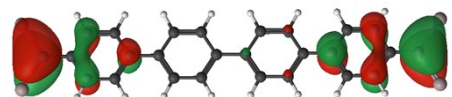
7



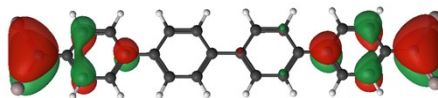
6



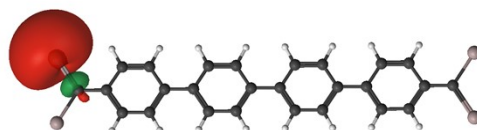
5



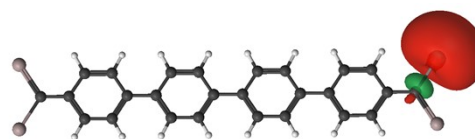
4



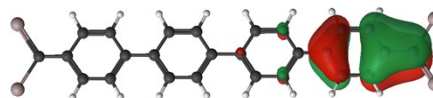
3



2



1



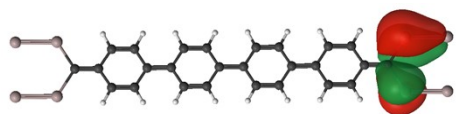
Orb.	Occ.
8	0.07
7	0.09
6	0.09
5	0.93
4	1.07
3	1.91
2	1.91
1	1.93

pX2 4-Ring

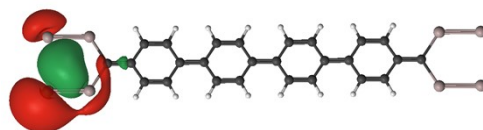
(8e, 8o) CAS

2-layer electrode

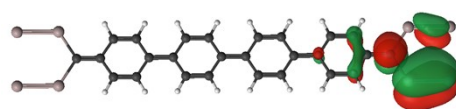
8



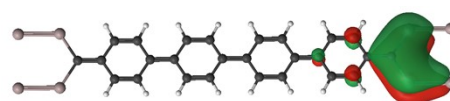
4



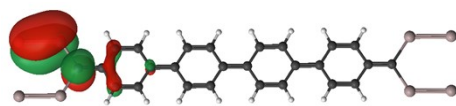
7



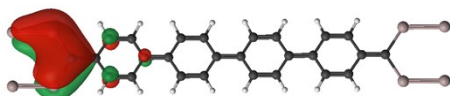
3



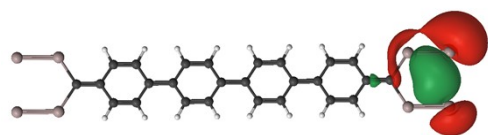
6



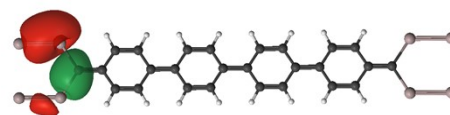
2



5



1



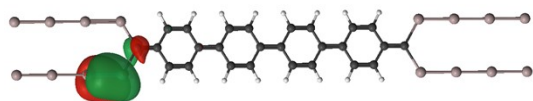
Orb.	Occ.
8	0.02
7	0.12
6	0.14
5	1.0
4	1.0
3	1.86
2	1.87
1	2.0

pX2 4-Ring

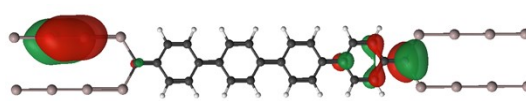
(8e, 8o) CAS

4-layer electrode

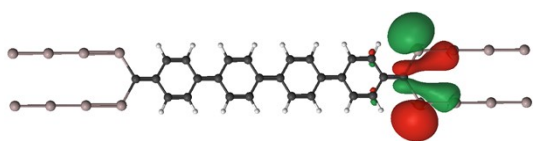
8



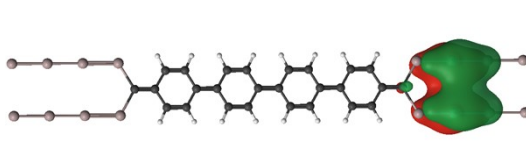
4



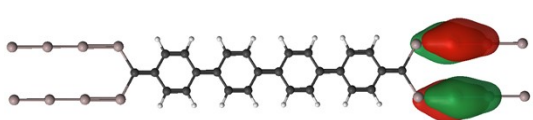
7



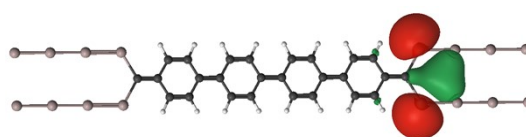
3



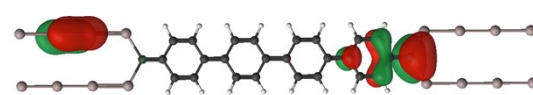
6



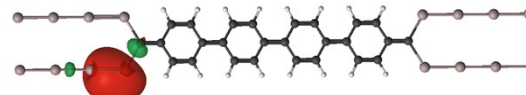
2



5



1



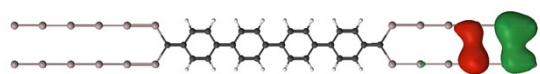
Orb.	Occ.
8	0.03
7	0.34
6	0.37
5	0.97
4	1.02
3	1.64
2	1.66
1	1.97

pX2 4-Ring

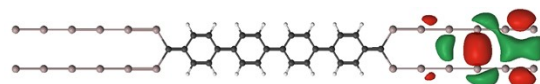
(8e, 8o) CAS

6-layer electrode

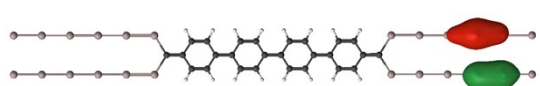
8



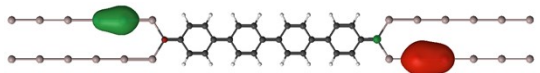
7



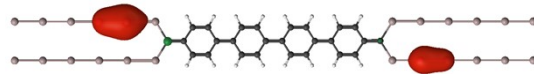
6



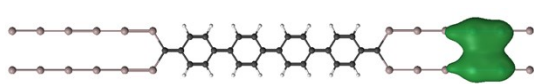
5



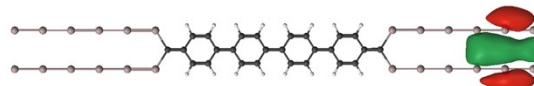
4



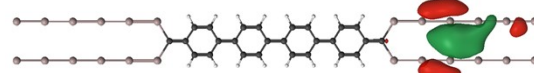
3



2



1

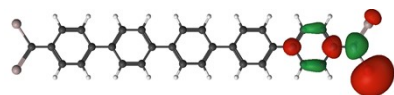


Orb.	Occ.
8	0.06
7	0.11
6	0.23
5	0.99
4	1.01
3	1.71
2	1.90
1	1.99

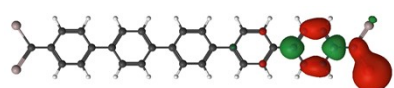
pX2 5-Ring

(12e, 12o) CAS

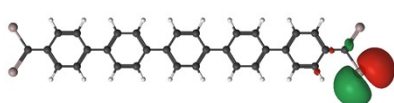
12



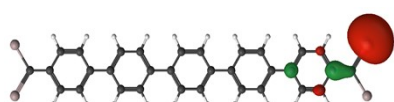
11



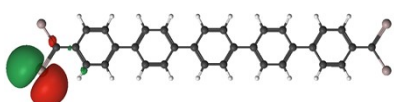
10



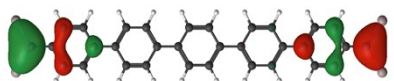
9



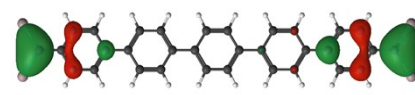
8



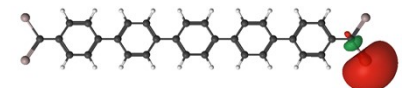
7



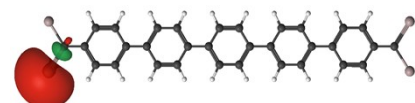
6



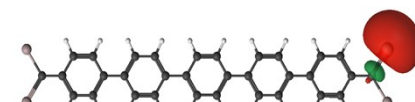
5



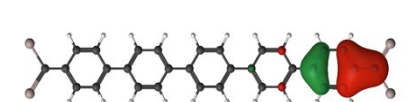
4



3



2



1



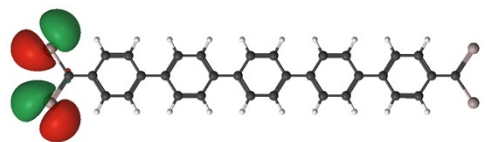
Orb.	Occ.
12	0.06
11	0.06
10	0.07
9	0.08
8	0.09
7	0.98
6	1.02
5	1.87
4	1.91
3	1.92
2	1.94
1	2.0

pX2 5-Ring

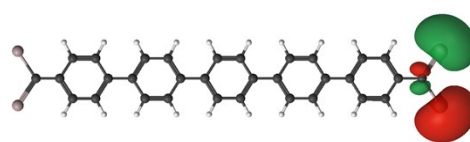
(8e, 8o) CAS

1-layer electrode

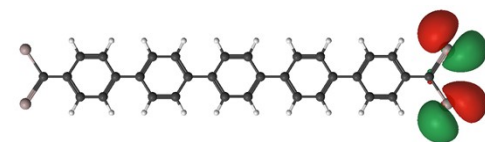
8



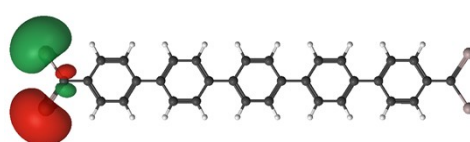
4



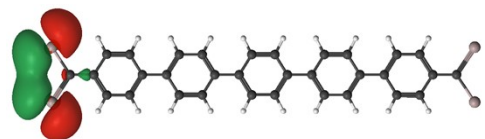
7



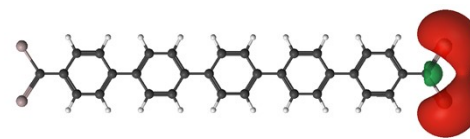
3



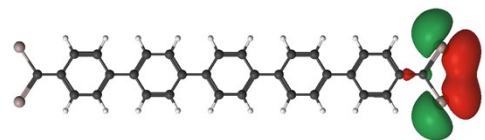
6



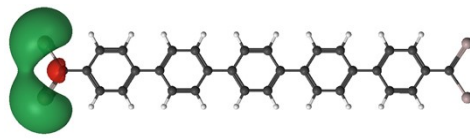
2



5



1



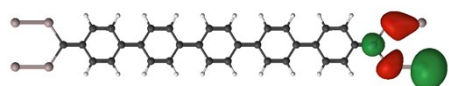
Orb.	Occ.
8	0.08
7	0.08
6	0.1
5	0.1
4	1.91
3	1.91
2	1.91
1	1.91

pX2 5-Ring

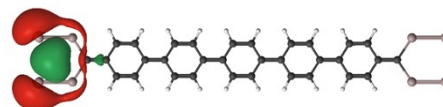
(8e, 8o) CAS

2-layer electrode

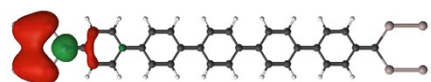
8



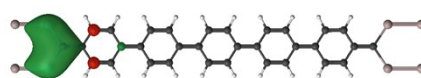
4



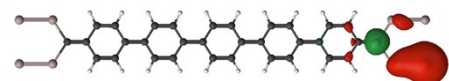
7



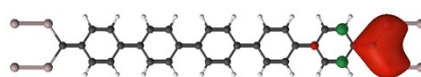
3



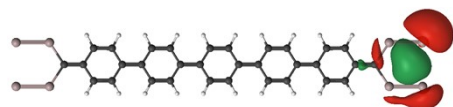
6



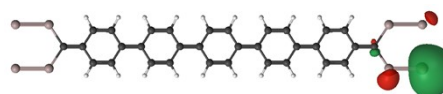
2



5



1



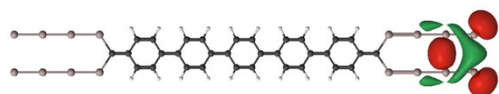
Orb.	Occ.
8	0.06
7	0.1
6	0.11
5	1.0
4	1.0
3	1.90
2	1.91
1	1.92

pX2 5-Ring

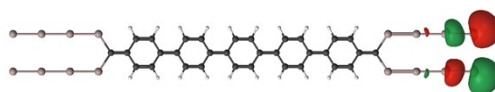
(8e, 8o) CAS

4-layer electrode

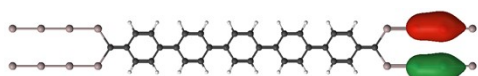
8



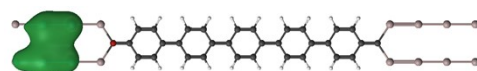
4



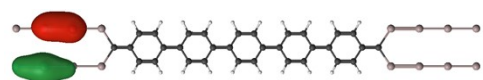
7



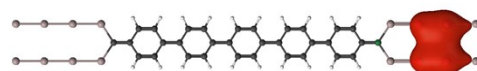
3



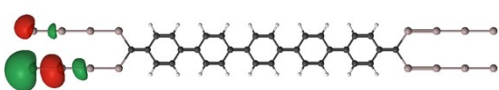
6



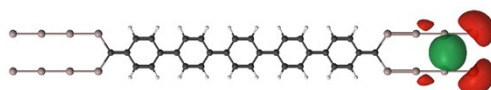
2



5



1



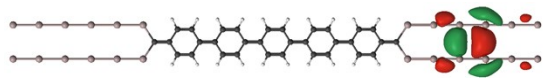
Orb.	Occ.
8	0.18
7	0.29
6	0.32
5	1.0
4	1.0
3	168
2	1.71
1	1.82

pX2 5-Ring

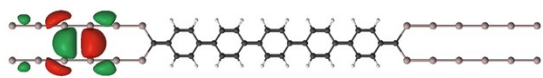
(8e, 8o) CAS

6-layer electrode

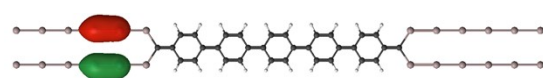
8



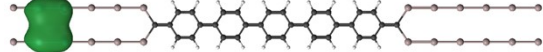
7



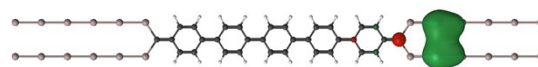
6



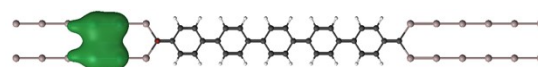
5



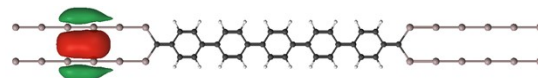
4



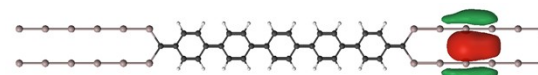
3



2



1



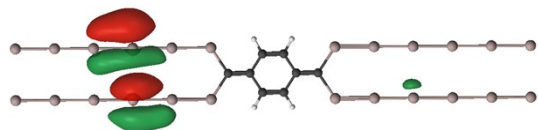
Orb.	Occ.
8	0.07
7	0.14
6	0.31
5	0.99
4	1.0
3	1.7
2	1.86
1	1.93

pX2 1-Ring Reoptimized Active Space

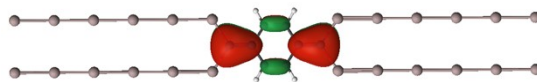
(8e, 8o) CAS

6-layer electrode

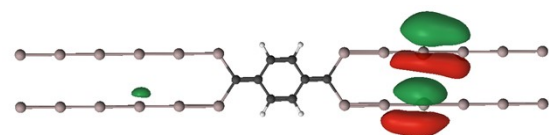
8



4



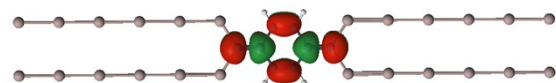
7



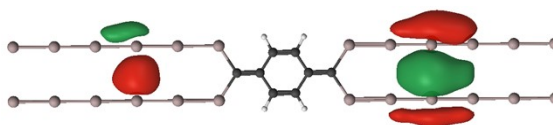
3



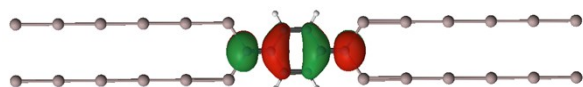
6



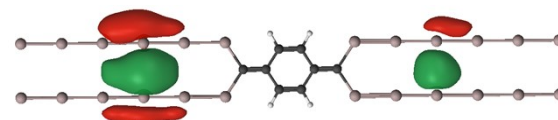
2



5



1



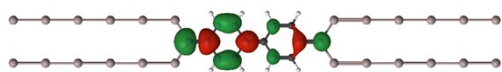
Orb.	Occ.
8	0.06
7	0.06
6	0.06
5	0.12
4	1.88
3	1.93
2	1.94
1	1.94

pX2 2-Ring Reoptimized Active Space

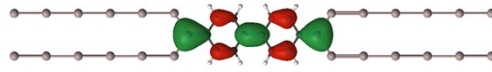
(8e, 8o) CAS

6-layer electrode

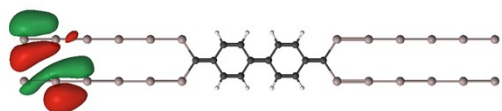
8



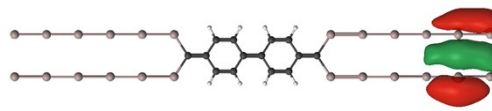
4



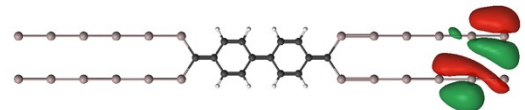
7



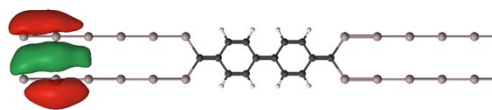
3



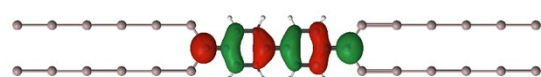
6



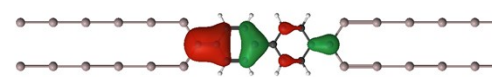
2



5



1



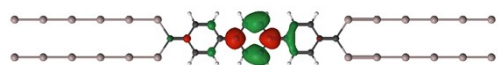
Orb.	Occ.
8	0.07
7	0.08
6	0.08
5	0.23
4	1.78
3	1.92
2	1.92
1	1.93

pX2 3-Ring Reoptimized Active Space

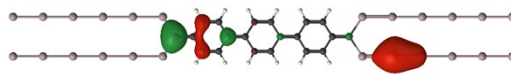
(8e, 8o) CAS

6-layer electrode

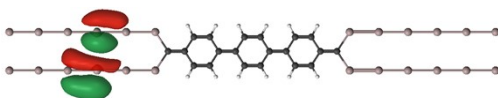
8



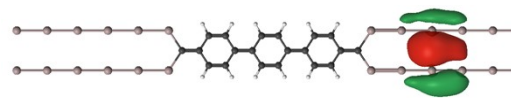
4



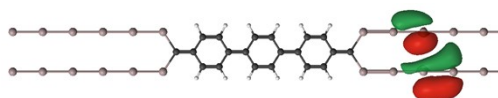
7



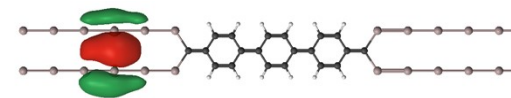
3



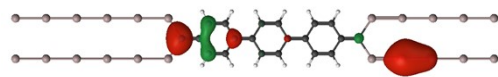
6



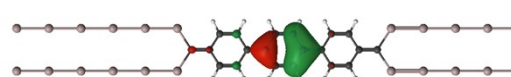
2



5



1



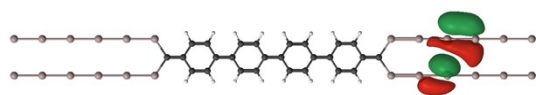
Orb.	Occ.
8	0.04
7	0.05
6	0.06
5	0.92
4	1.08
3	1.94
2	1.95
1	1.96

pX2 4-Ring Reoptimized Active Space

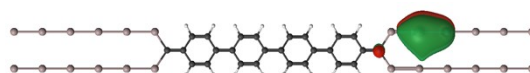
(8e, 8o) CAS

6-layer electrode

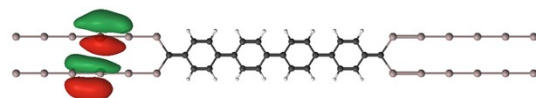
8



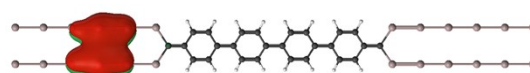
4



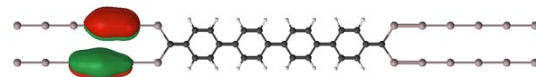
7



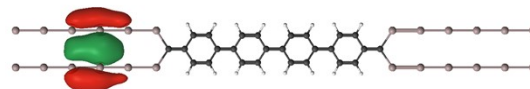
3



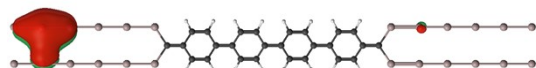
6



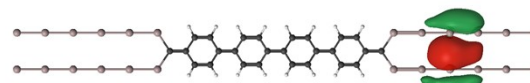
2



5



1



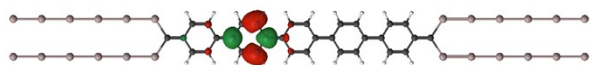
Orb.	Occ.
8	0.06
7	0.07
6	0.22
5	0.99
4	1.0
3	1.79
2	1.93
1	1.94

pX2 5-Ring Reoptimized Active Space

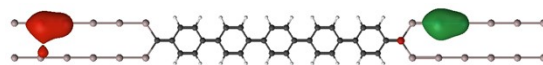
(8e, 8o) CAS

6-layer electrode

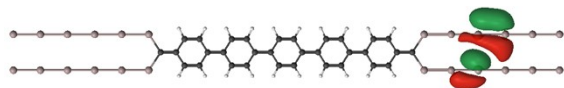
8



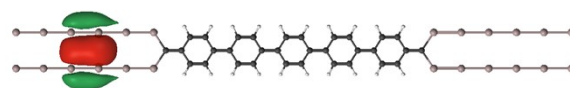
4



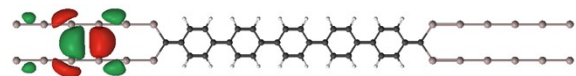
7



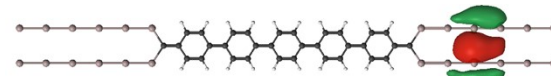
3



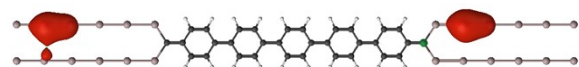
6



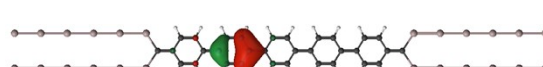
2



5



1

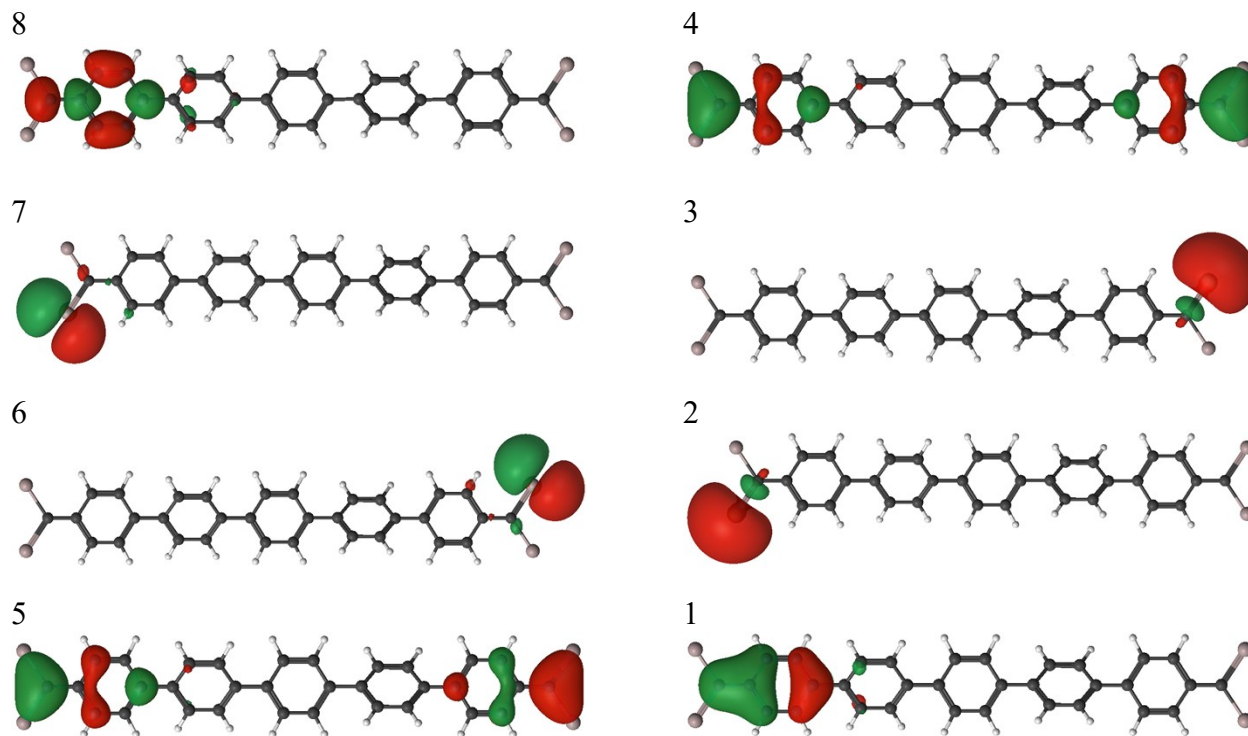


Orb.	Occ.
8	0.04
7	0.06
6	0.13
5	1.0
4	1.0
3	1.87
2	1.94
1	1.96

pX2 5-Ring Twisted Active Space

(8e, 8o) CAS

1-layer electrode



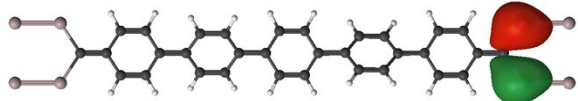
Orb.	Occ.
8	0.06
7	0.09
6	0.09
5	0.99
4	1.01
3	1.91
2	1.91
1	1.94

pX2 5-Ring Twisted Active Space

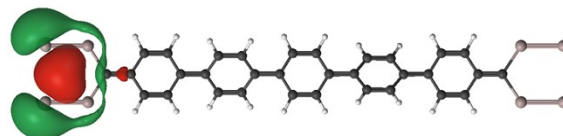
(8e, 8o) CAS

2-layer electrode

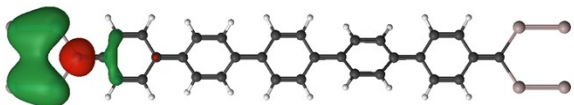
8



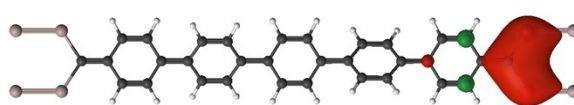
4



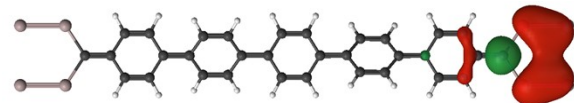
7



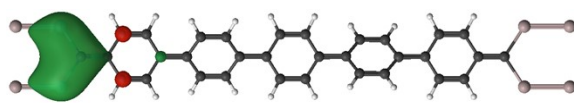
3



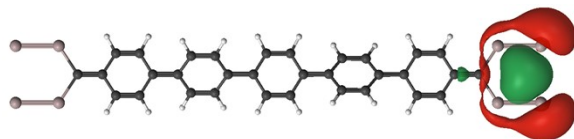
6



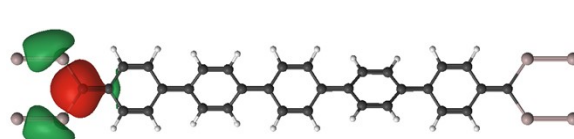
2



5



1



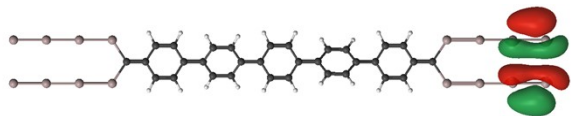
Orb.	Occ.
8	0.02
7	0.10
6	0.10
5	1.00
4	1.00
3	1.89
2	1.91
1	2.00

pX2 5-Ring Twisted Active Space

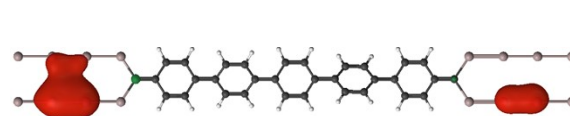
(8e, 8o) CAS

4-layer electrode

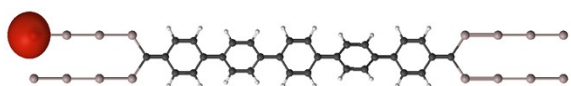
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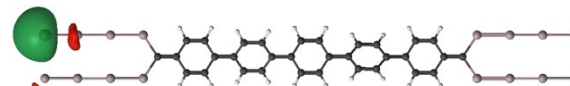
4



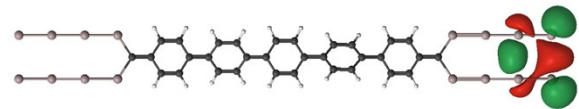
7



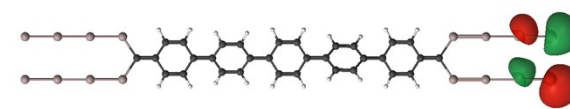
3



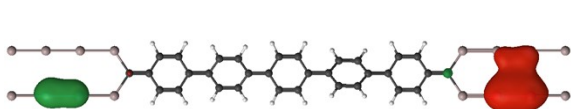
6



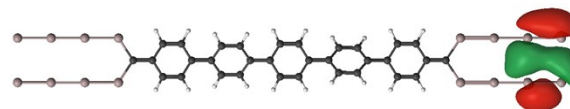
2



5



1

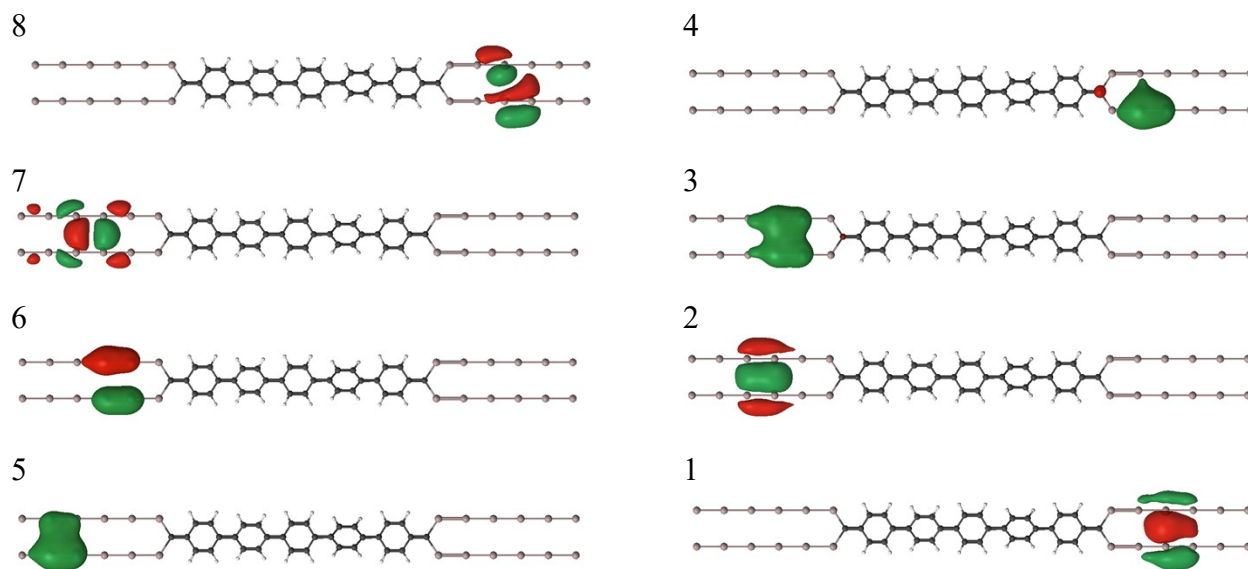


Orb.	Occ.
8	0.04
7	0.08
6	0.09
5	1.00
4	1.00
3	1.92
2	1.93
1	1.94

pX2 5-Ring Twisted Active Space

(8e, 8o) CAS

6-layer electrode



Orb.	Occ.
8	0.06
7	0.14
6	0.31
5	0.99
4	1.00
3	1.70
2	1.86
1	1.94