

Supplementary data

Molecular modeling and simulation for the design of molecular diodes using density functional theory.

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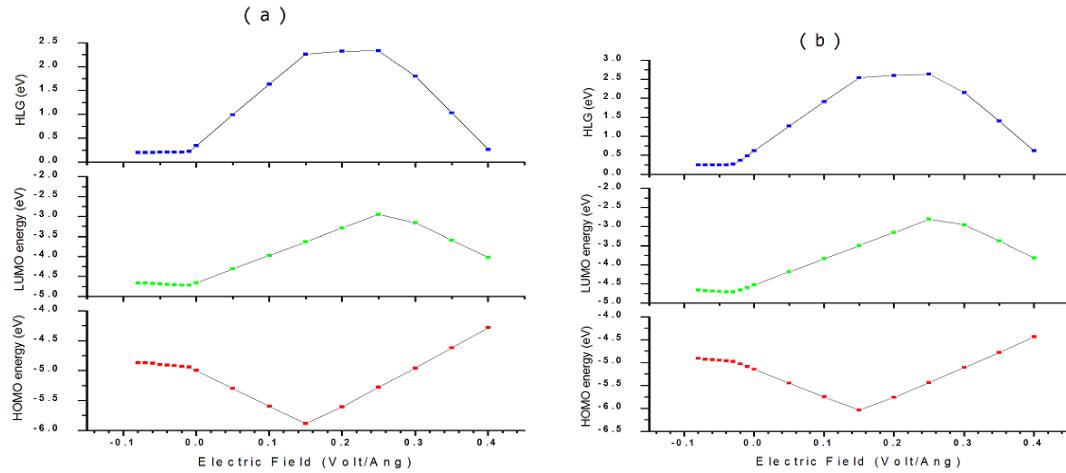


Figure S1. Effect of Electric field on the HOMO energy, LUMO energy and HOMO-LUMO gap of TCNQ- σ - DBTTF with (a) B3PW91 and (b) MPW1PW91functionals

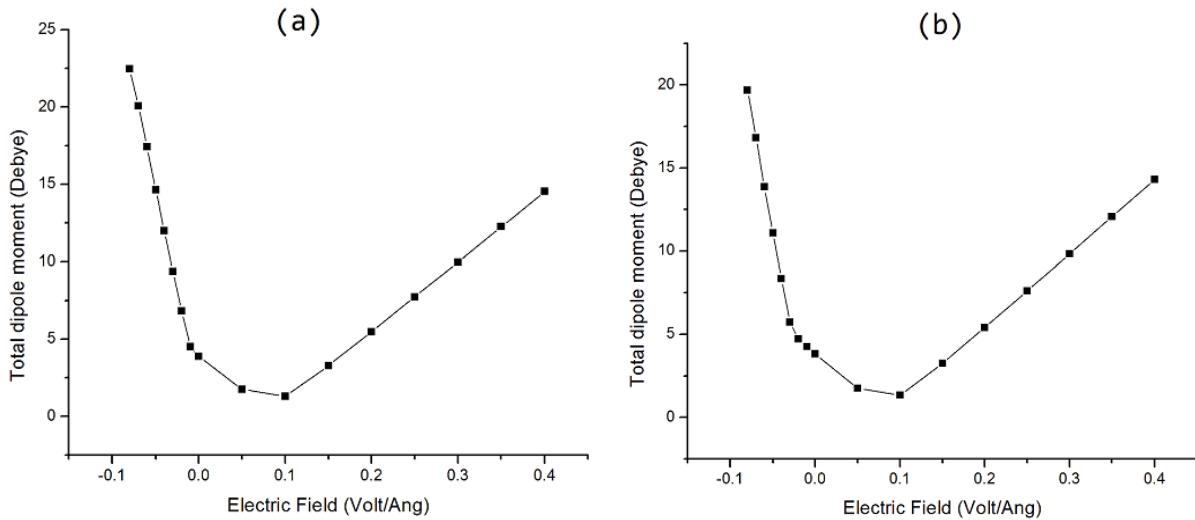


Figure S2. Electric field effect on the total dipole moment of TCNQ- σ - DBTTF with (a) B3PW91 and (b) MPW1PW91functionals

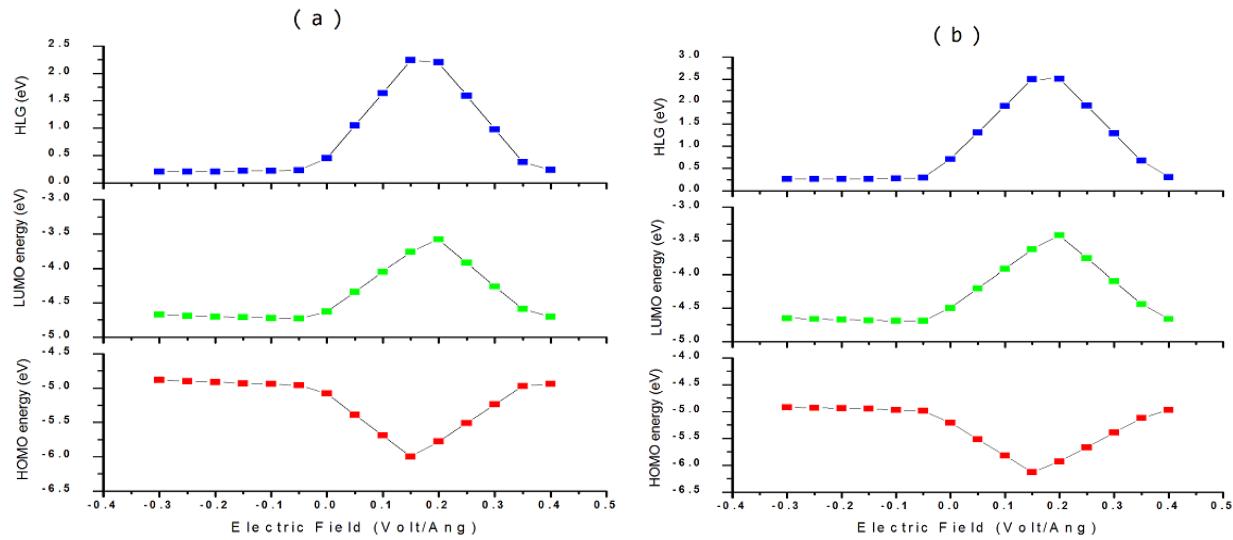


Figure S3. Effect of Electric field on the HOMO energy, LUMO energy and HOMO-LUMO gap of TCNQ- σ -Tetracene with (a) B3PW91 and (b) MPW1PW91functionals

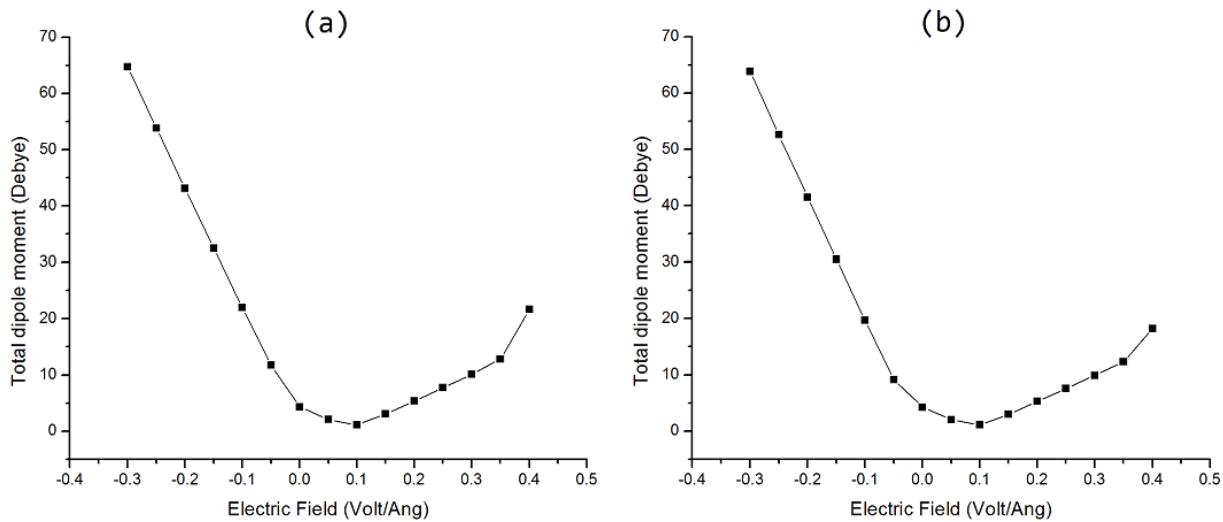


Figure S4. Electric field effect on the total dipole moment of TCNQ- σ -Tetracene with (a) B3PW91 and (b) MPW1PW91functionals

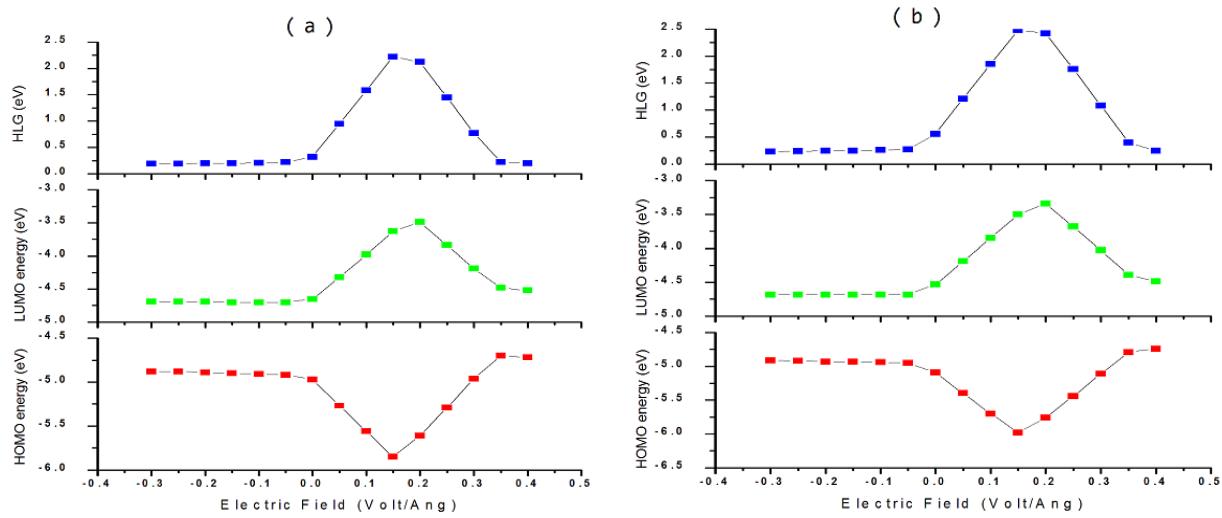


Figure S5. Effect of Electric field on the HOMO energy, LUMO energy and HOMO-LUMO gap of TCNQ- σ - ADT with (a) B3PW91 and (b) MPW1PW91functionals

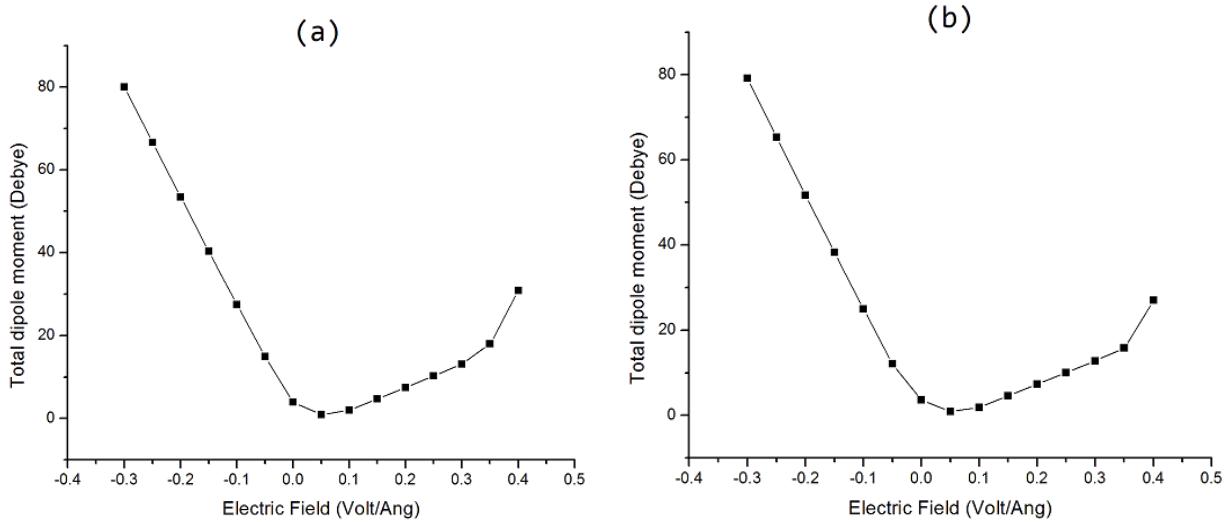


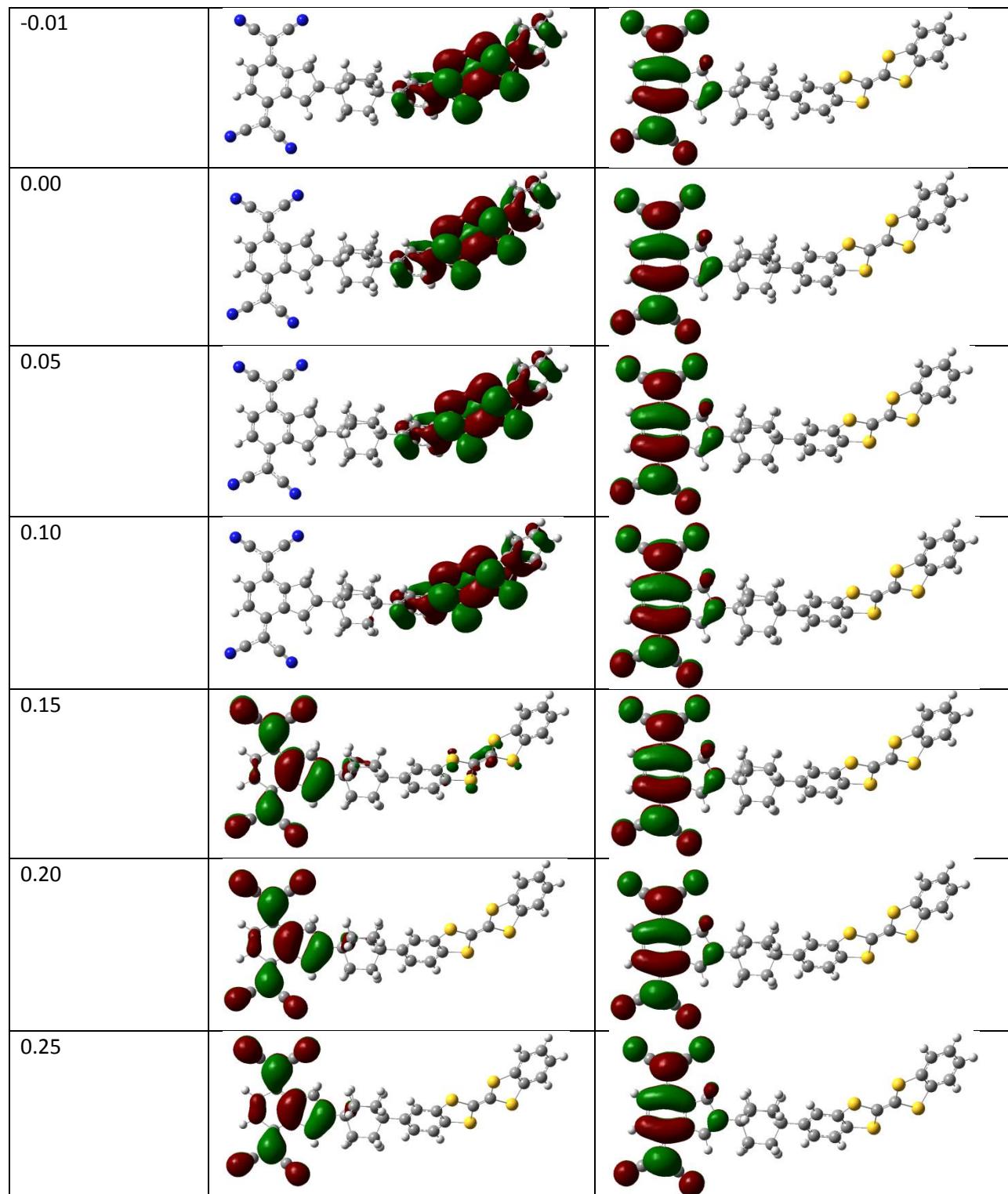
Figure S6. Electric field effect on the total dipole moment of TCNQ- σ - ADT with (a) B3PW91 and (b) MPW1PW91functionals

Table S1. HOMO energy (E_{HOMO}), LUMO energy (E_{LUMO}), HOMO-LUMO gap ($E_{\text{HOMO}}-E_{\text{LUMO}}$) and the total dipole moment of TCNQ- σ -DBTTF system under various electric fields with B3PW91/MPW1PW91 functionals.

Electric Field (V/Å)	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{\text{HOMO}}-E_{\text{LUMO}}$ (eV)	Total dipole moment (Debye)
-0.08	-4.87/-4.91	-4.67/-4.66	0.20/0.25	22.47/19.69
-0.07	-4.87/-4.93	-4.67/-4.68	0.20/0.25	20.08/16.81
-0.06	-4.88/-4.94	-4.68/-4.69	0.20/0.25	17.42/13.86
-0.05	-4.90/-4.95	-4.69/-4.70	0.21/0.25	14.64/11.09
-0.04	-4.91/-4.96	-4.70/-4.71	0.21/0.25	11.99/8.35
-0.03	-4.92/-4.98	-4.71/-4.71	0.21/0.27	9.39/5.73
-0.02	-4.93/-5.03	-4.72/-4.66	0.21/0.37	6.83/4.72
-0.01	-4.94/-5.09	-4.72/-4.60	0.22/0.49	4.53/4.26
0.00	-5.00/-5.15	-4.66/-4.53	0.34/0.62	3.89/3.82
0.05	-5.30/-5.45	-4.31/-4.18	0.99/1.27	1.76/1.75
0.10	-5.60/-5.75	-3.97/-3.84	1.63/1.91	1.32/1.35
0.15	-5.89/-6.04	-3.63/-3.50	2.26/2.54	3.29/3.26
0.20	-5.61/-5.76	-3.29/-3.16	2.32/2.60	5.49/5.42
0.25	-5.28/-5.44	-2.95/-2.81	2.33/2.63	7.73/7.62
0.30	-4.96/-5.11	-3.16/-2.96	1.80/2.15	9.98/9.84
0.35	-4.62/-4.78	-3.59/-3.38	1.03/1.40	12.25/12.06
0.40	-4.28/-4.44	-4.02/-3.82	0.26/0.62	14.54/14.30

Table S2. Spatial distribution of the HOMO and LUMO of TCNQ- σ -DBTTF system under various electric fields with B3LYP functional.

Electric Field (V/ \AA)	HOMO	LUMO
-0.08		
-0.07		
-0.06		
-0.05		
-0.04		
-0.03		
-0.02		



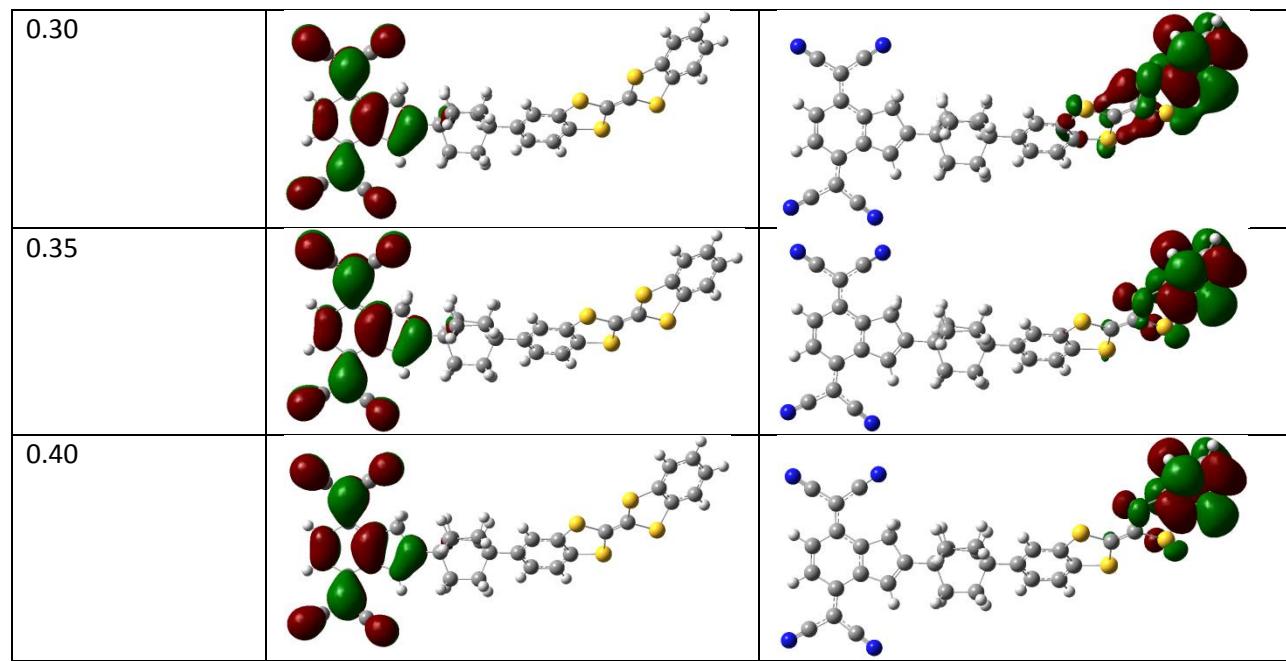
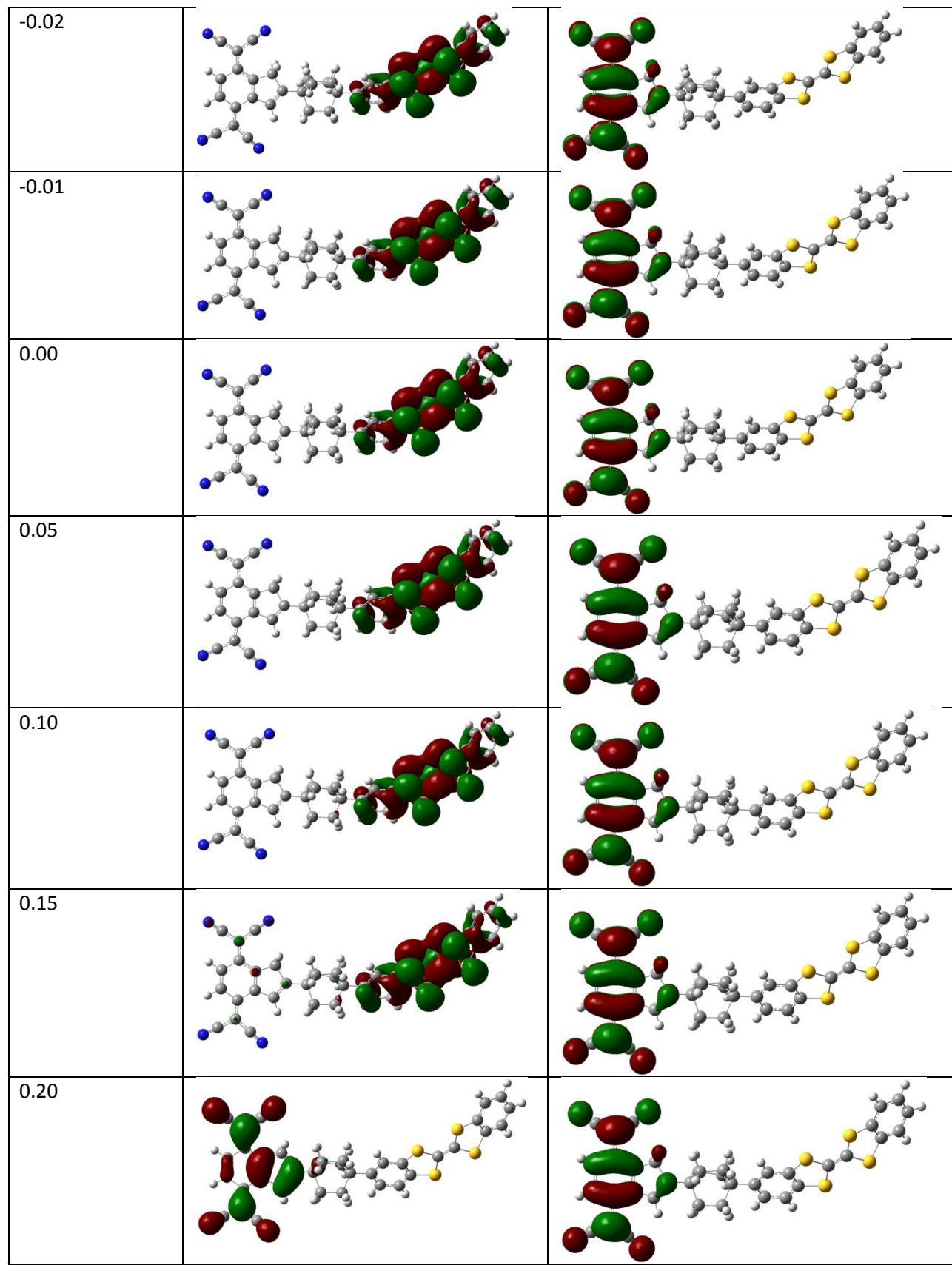


Table S3. Spatial distribution of the HOMO and LUMO of TCNQ- σ -DBTTF system under various electric fields with B3PW91 functional.

Electric Field (V/Å)	HOMO	LUMO
-0.08		
-0.07		
-0.06		
-0.05		
-0.04		
-0.03		



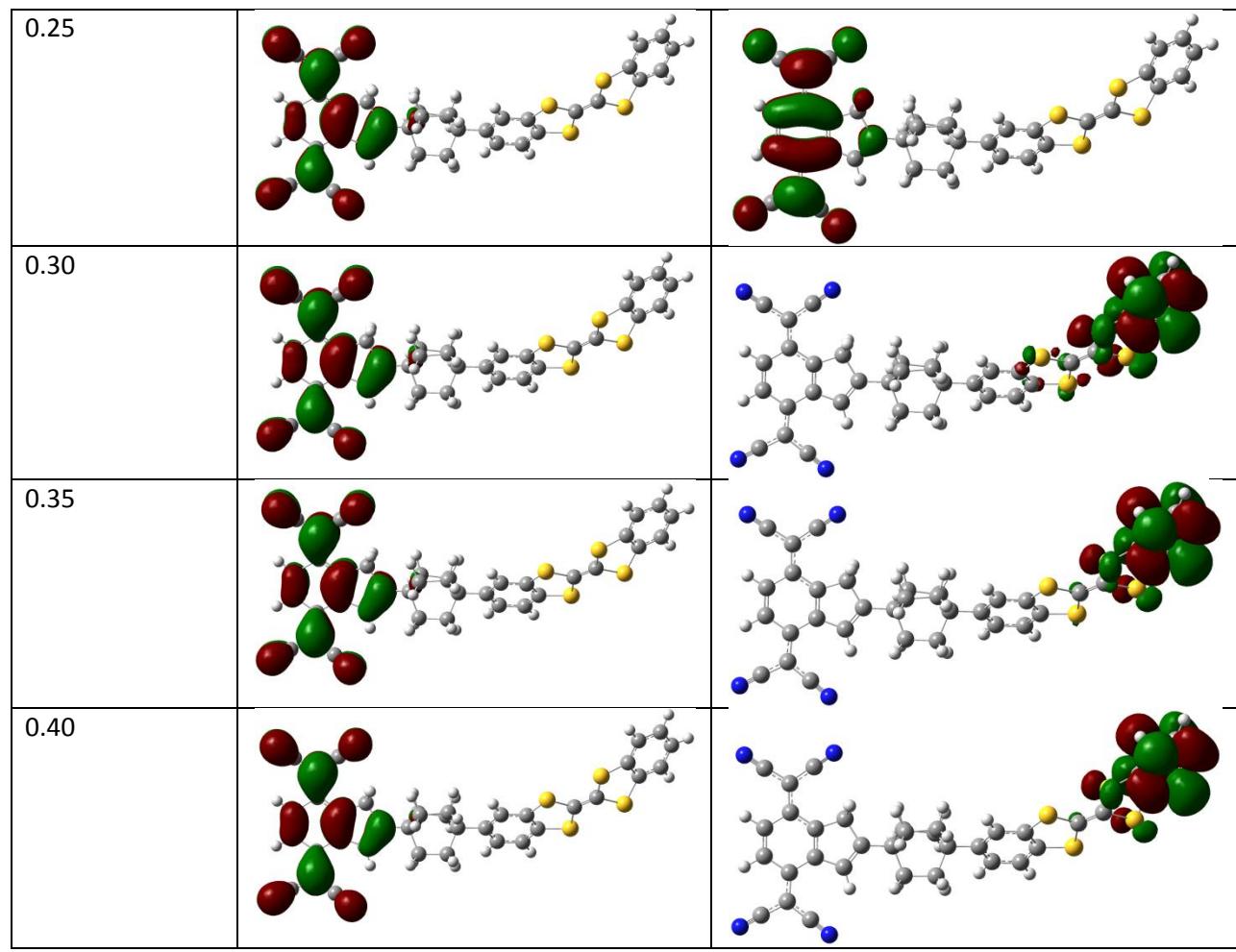
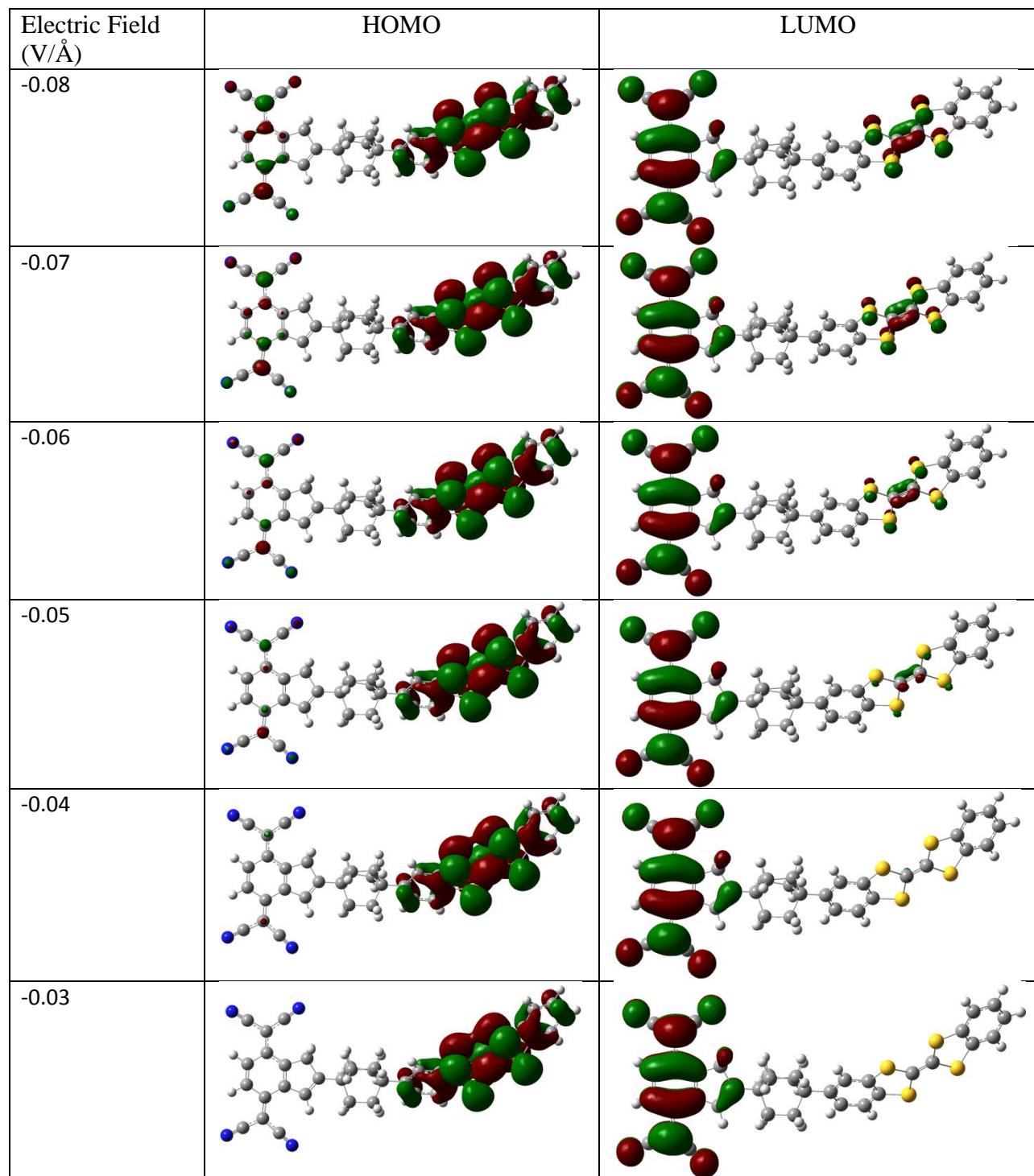
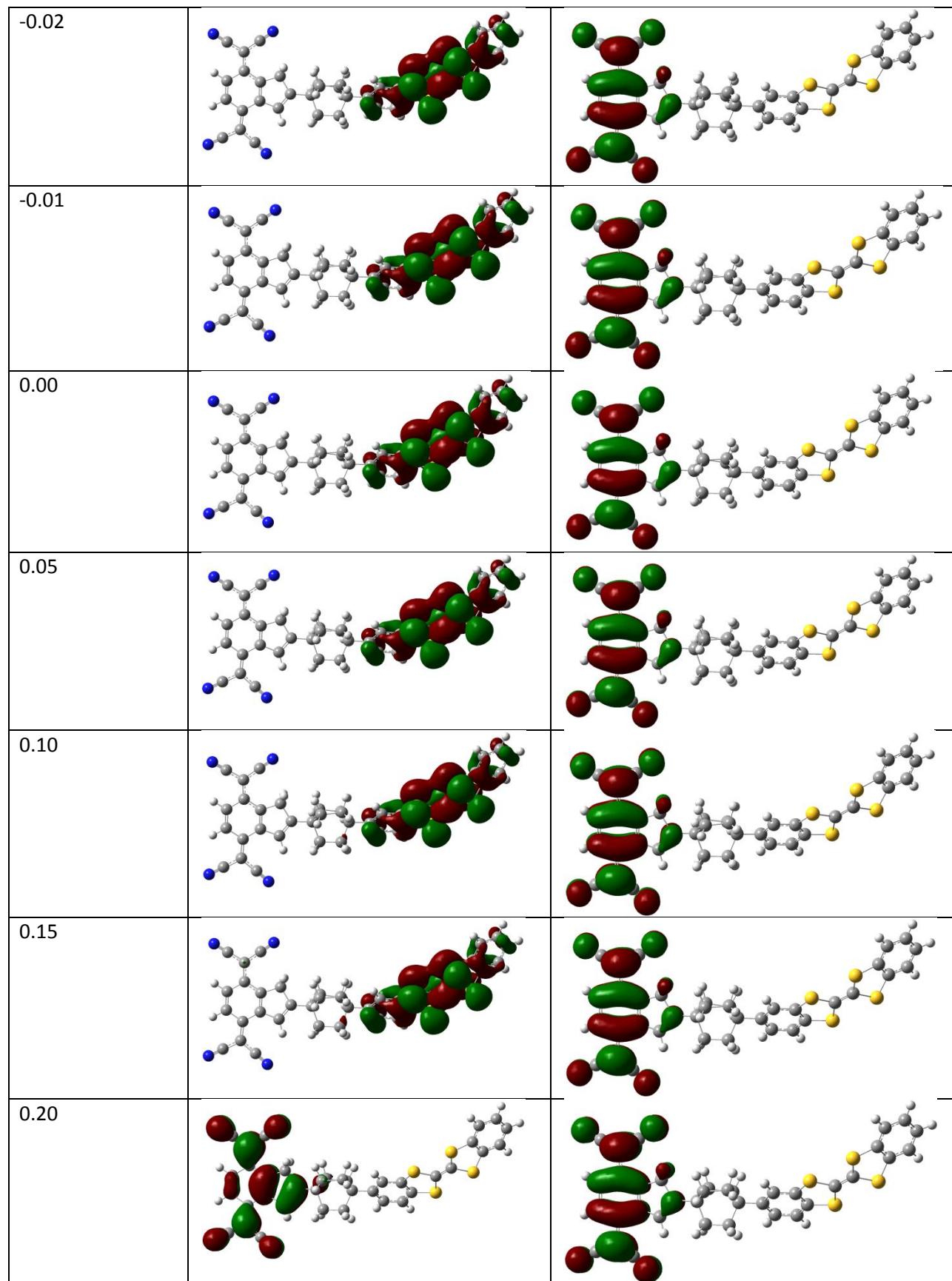


Table S4. Spatial distribution of the HOMO and LUMO of TCNQ- σ -DBTTF system under various electric fields with MPW1PW91 functional.





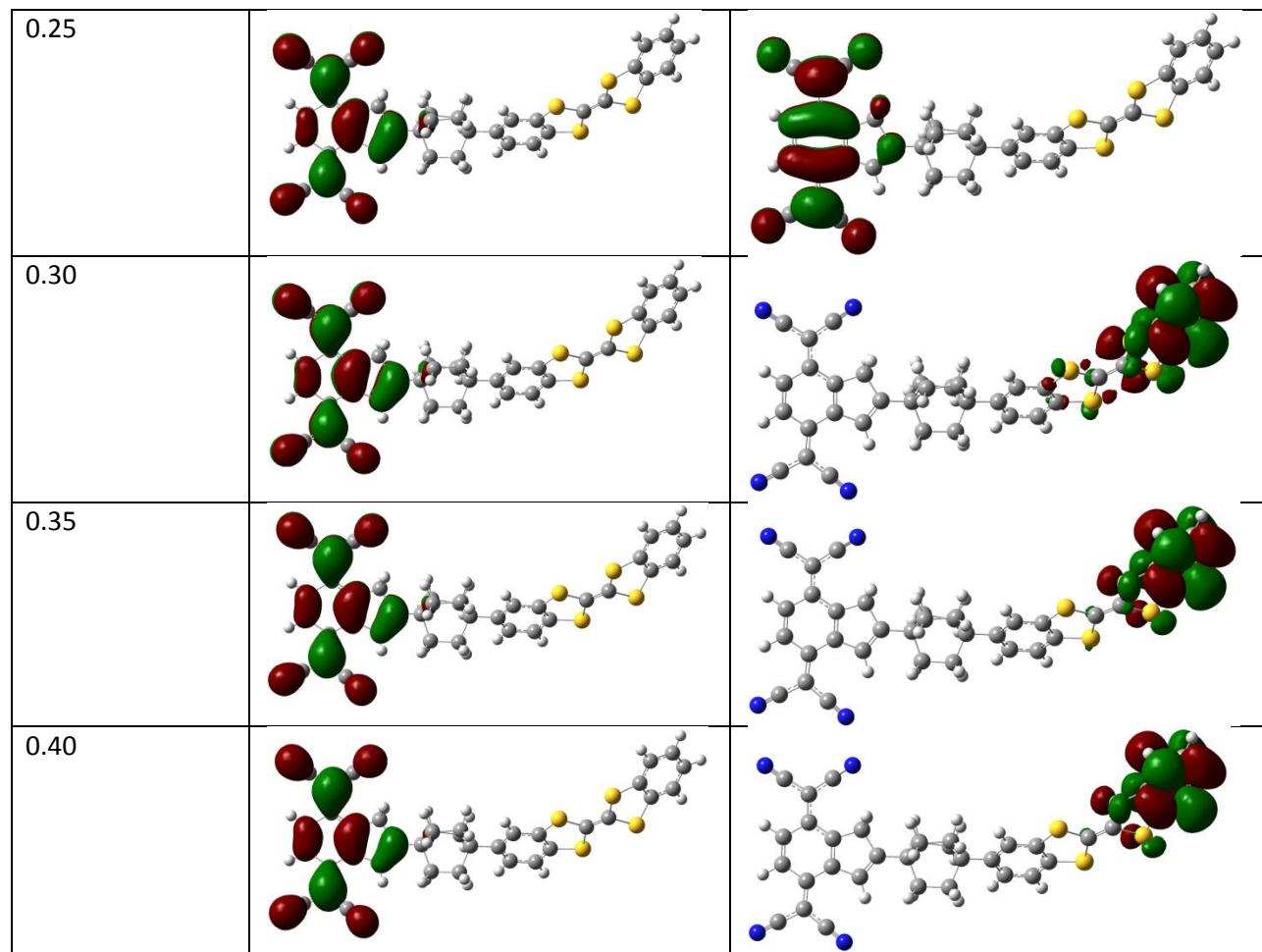


Table S5: Optimized parameters (bond lengths, bond angles and dihedral angles) of TCNQ- σ -DBTTF system without electric field and with an extreme electric field of 0.40 V/ \AA in reverse direction using B3LYP functional. Bond lengths are in Angstrom, bond angles and dihedral angles are in degree.

Optimized Parameters	Without Electric Field	With 0.40 V/ \AA Electric Field
R(1,2)	1.387	1.3812
R(1,6)	1.4557	1.4558
R(1,7)	1.4573	1.466
R(2,3)	1.4324	1.4393
R(2,9)	1.5051	1.5071
R(3,4)	1.4553	1.4522
R(3,15)	1.3967	1.3953
R(4,5)	1.3515	1.3552
R(4,10)	1.0843	1.085
R(5,6)	1.4524	1.4519
R(5,11)	1.0842	1.085
R(6,14)	1.3898	1.3902
R(7,8)	1.3585	1.353
R(7,12)	1.0781	1.0781
R(8,9)	1.5092	1.5086
R(8,24)	1.5069	1.5104
R(9,13)	1.097	1.0967
R(9,30)	1.0972	1.097
R(14,16)	1.4309	1.4278
R(14,17)	1.4267	1.4286
R(15,18)	1.4275	1.4263
R(15,19)	1.4243	1.4265
R(16,20)	1.1645	1.1645
R(17,21)	1.1648	1.1651
R(18,22)	1.1652	1.1647
R(19,23)	1.1656	1.1663
R(24,25)	1.5452	1.5448
R(24,28)	1.5536	1.5523
R(24,49)	1.5564	1.5542
R(25,26)	1.5529	1.554
R(25,31)	1.095	1.0936
R(25,32)	1.0961	1.0948
R(26,27)	1.5524	1.555
R(26,33)	1.0958	1.0967
R(26,34)	1.0932	1.0947
R(27,29)	1.5465	1.5461
R(27,50)	1.5538	1.5562
R(27,58)	1.5318	1.5297

R(28,29)	1.5538	1.5549
R(28,35)	1.0958	1.0949
R(28,36)	1.0946	1.0934
R(29,37)	1.0949	1.097
R(29,38)	1.0959	1.0977
R(39,40)	1.3994	1.3948
R(39,41)	1.7738	1.7805
R(39,55)	1.3951	1.3956
R(40,42)	1.7757	1.7828
R(40,56)	1.3962	1.3965
R(41,43)	1.7827	1.773
R(42,43)	1.7825	1.7717
R(43,44)	1.3493	1.3546
R(44,45)	1.7818	1.7885
R(44,46)	1.7818	1.7862
R(45,47)	1.7752	1.7735
R(46,48)	1.7752	1.7712
R(47,48)	1.4032	1.41
R(47,59)	1.3956	1.3957
R(48,60)	1.3955	1.3962
R(49,50)	1.5525	1.5528
R(49,51)	1.0958	1.0947
R(49,52)	1.0956	1.0943
R(50,53)	1.0946	1.0958
R(50,54)	1.0949	1.0964
R(55,57)	1.3925	1.3912
R(55,67)	1.0856	1.0857
R(56,58)	1.4015	1.4029
R(56,69)	1.0834	1.0833
R(57,58)	1.4065	1.4099
R(57,68)	1.0852	1.0843
R(59,61)	1.3956	1.3981
R(59,63)	1.0855	1.0864
R(60,62)	1.3956	1.3975
R(60,66)	1.0855	1.0858
R(61,62)	1.3963	1.3957
R(61,64)	1.0854	1.0875
R(62,65)	1.0854	1.0869
A(2,1,6)	120.8617	121.0558
A(2,1,7)	109.0871	108.6167
A(6,1,7)	130.0511	130.3274
A(1,2,3)	122.2348	122.3154
A(1,2,9)	108.1844	108.6366
A(3,2,9)	129.5807	129.048
A(2,3,4)	116.3703	116.1859
A(2,3,15)	124.9954	124.1106

A(4,3,15)	118.6343	119.7035
A(3,4,5)	122.0576	122.0039
A(3,4,10)	118.2888	118.5062
A(5,4,10)	119.6536	119.4897
A(4,5,6)	122.2065	122.3507
A(4,5,11)	119.5655	119.3634
A(6,5,11)	118.228	118.2855
A(1,6,5)	116.2691	116.0785
A(1,6,14)	125.1133	124.7254
A(5,6,14)	118.6176	119.1955
A(1,7,8)	109.9465	110.0673
A(1,7,12)	124.7461	124.2145
A(8,7,12)	125.307	125.717
A(7,8,9)	108.8298	108.981
A(7,8,24)	127.8211	127.8149
A(9,8,24)	123.338	123.1926
A(2,9,8)	103.952	103.698
A(2,9,13)	111.9771	111.6248
A(2,9,30)	112.1447	111.7401
A(8,9,13)	112.102	112.5367
A(8,9,30)	111.7884	112.2446
A(13,9,30)	105.0788	105.1954
A(6,14,16)	120.9999	121.9082
A(6,14,17)	125.3114	124.0291
A(16,14,17)	113.6888	114.0609
A(3,15,18)	121.393	122.3615
A(3,15,19)	123.7679	123.2305
A(18,15,19)	114.8391	114.4068
A(8,24,25)	112.0786	112.1352
A(8,24,28)	111.1994	111.2277
A(8,24,49)	110.1833	110.4527
A(25,24,28)	107.6658	107.506
A(25,24,49)	108.0864	107.8845
A(28,24,49)	107.4509	107.4392
A(24,25,26)	110.7527	110.9699
A(24,25,31)	109.7423	109.7734
A(24,25,32)	109.1271	109.2161
A(26,25,31)	110.0485	109.9085
A(26,25,32)	110.5114	110.414
A(31,25,32)	106.5649	106.4533
A(25,26,27)	110.9495	110.6834
A(25,26,33)	110.7414	110.8626
A(25,26,34)	109.9317	109.9653
A(27,26,33)	108.6182	108.573
A(27,26,34)	110.3224	110.4534
A(33,26,34)	106.1623	106.2029

A(26,27,29)	107.0024	107.2191
A(26,27,50)	108.0634	108.0917
A(26,27,58)	110.9649	110.9196
A(29,27,50)	107.4455	107.6839
A(29,27,58)	113.1622	113.1717
A(50,27,58)	109.9956	109.5717
A(24,28,29)	110.6159	110.8995
A(24,28,35)	108.7318	108.759
A(24,28,36)	110.2038	110.1025
A(29,28,35)	110.7519	110.5965
A(29,28,36)	109.8368	109.7775
A(35,28,36)	106.6177	106.6099
A(27,29,28)	111.1146	110.807
A(27,29,37)	109.8413	109.874
A(27,29,38)	109.4531	109.4029
A(28,29,37)	109.5355	109.6477
A(28,29,38)	110.0002	110.1334
A(37,29,38)	106.7991	106.895
A(40,39,41)	116.7797	116.6963
A(40,39,55)	119.3384	119.4811
A(41,39,55)	123.8594	123.8141
A(39,40,42)	116.4137	116.2027
A(39,40,56)	120.6728	121.0401
A(42,40,56)	122.8905	122.7483
A(39,41,43)	94.9186	95.823
A(40,42,43)	95.0259	96.0028
A(41,43,42)	113.912	114.5386
A(41,43,44)	123.0413	122.6894
A(42,43,44)	123.0173	122.7439
A(43,44,45)	123.0217	123.8805
A(43,44,46)	122.9959	123.6551
A(45,44,46)	113.9522	112.4639
A(44,45,47)	95.0838	94.4286
A(44,46,48)	95.0877	94.4325
A(45,47,48)	116.5141	116.0317
A(45,47,59)	123.2434	123.9347
A(48,47,59)	120.2208	119.9836
A(46,48,47)	116.5029	116.248
A(46,48,60)	123.2363	123.7785
A(47,48,60)	120.2383	119.9216
A(24,49,50)	110.5061	110.9559
A(24,49,51)	109.2405	109.3351
A(24,49,52)	109.4415	109.3152
A(50,49,51)	110.2733	110.1466
A(50,49,52)	110.6021	110.3329
A(51,49,52)	106.6924	106.6528

A(27,50,49)	111.1016	110.6561
A(27,50,53)	109.3066	109.2836
A(27,50,54)	109.2519	109.3338
A(49,50,53)	110.2067	110.2813
A(49,50,54)	110.4687	110.7549
A(53,50,54)	106.3843	106.4299
A(39,55,57)	119.6125	119.1858
A(39,55,67)	120.311	120.6999
A(57,55,67)	120.0763	120.1142
A(40,56,58)	120.7319	120.4929
A(40,56,69)	118.6333	119.4007
A(58,56,69)	120.6343	120.1062
A(55,57,58)	121.9527	122.4156
A(55,57,68)	118.0833	118.1755
A(58,57,68)	119.9629	119.4087
A(27,58,56)	122.3142	122.4807
A(27,58,57)	119.9847	120.1243
A(56,58,57)	117.6882	117.3832
A(47,59,61)	119.3781	119.7971
A(47,59,63)	120.1896	119.759
A(61,59,63)	120.432	120.4398
A(48,60,62)	119.3763	119.7985
A(48,60,66)	120.1887	119.7869
A(62,60,66)	120.4348	120.4108
A(59,61,62)	120.3976	120.2179
A(59,61,64)	119.4711	119.5373
A(62,61,64)	120.1305	120.2344
A(60,62,61)	120.3879	120.2763
A(60,62,65)	119.4796	119.4016
A(61,62,65)	120.1318	120.3127
D(6,1,2,3)	0.0954	-0.1277
D(6,1,2,9)	179.963	179.9246
D(7,1,2,3)	-179.916	179.7565
D(7,1,2,9)	-0.0484	-0.1912
D(2,1,6,5)	-0.0621	0.8906
D(2,1,6,14)	179.9156	-178.8241
D(7,1,6,5)	179.952	-178.9654
D(7,1,6,14)	-0.0703	1.3199
D(2,1,7,8)	0.122	0.2293
D(2,1,7,12)	-179.6449	-179.3867
D(6,1,7,8)	-179.8908	-179.9009
D(6,1,7,12)	0.3422	0.4832
D(1,2,3,4)	-0.0791	-0.6783
D(1,2,3,15)	179.9578	179.2728
D(9,2,3,4)	-179.9159	179.2579
D(9,2,3,15)	0.1209	-0.791

D(1,2,9,8)	-0.0327	0.0927
D(1,2,9,13)	-121.2533	-121.3058
D(1,2,9,30)	120.8999	121.2021
D(3,2,9,8)	179.8221	-179.8503
D(3,2,9,13)	58.6015	58.7511
D(3,2,9,30)	-59.2454	-58.741
D(2,3,4,5)	0.0345	0.7124
D(2,3,4,10)	-179.9659	-179.4281
D(15,3,4,5)	-179.9999	-179.241
D(15,3,4,10)	-0.0003	0.6185
D(2,3,15,18)	179.9929	-179.8482
D(2,3,15,19)	-0.031	-0.2604
D(4,3,15,18)	0.0305	0.1013
D(4,3,15,19)	-179.9934	179.6891
D(3,4,5,6)	-0.0068	0.0673
D(3,4,5,11)	-179.9898	179.8288
D(10,4,5,6)	179.9936	-179.7908
D(10,4,5,11)	0.0106	-0.0294
D(4,5,6,1)	0.0188	-0.8668
D(4,5,6,14)	-179.9604	178.8645
D(11,5,6,1)	-179.998	179.3693
D(11,5,6,14)	0.0228	-0.8993
D(1,6,14,16)	-179.9727	179.9451
D(1,6,14,17)	-0.0014	0.4512
D(5,6,14,16)	0.0045	0.2386
D(5,6,14,17)	179.9758	-179.2552
D(1,7,8,9)	-0.1414	-0.1656
D(1,7,8,24)	-178.9499	-178.9485
D(12,7,8,9)	179.624	179.4432
D(12,7,8,24)	0.8155	0.6603
D(7,8,9,2)	0.1077	0.0484
D(7,8,9,13)	121.2448	120.8335
D(7,8,9,30)	-121.0635	-120.721
D(24,8,9,2)	178.9811	178.8995
D(24,8,9,13)	-59.8818	-60.3155
D(24,8,9,30)	57.8099	58.13
D(7,8,24,25)	-1.3777	-0.731
D(7,8,24,28)	-121.9466	-121.1541
D(7,8,24,49)	119.0228	119.6364
D(9,8,24,25)	179.9722	-179.3556
D(9,8,24,28)	59.4033	60.2212
D(9,8,24,49)	-59.6273	-58.9882
D(8,24,25,26)	-174.0501	-173.9914
D(8,24,25,31)	-52.3493	-52.3028
D(8,24,25,32)	64.0785	64.0593
D(28,24,25,26)	-51.4531	-51.4323

D(28,24,25,31)	70.2477	70.2563
D(28,24,25,32)	-173.3244	-173.3816
D(49,24,25,26)	64.3387	64.1614
D(49,24,25,31)	-173.9605	-174.15
D(49,24,25,32)	-57.5327	-57.7879
D(8,24,28,29)	-172.9417	-172.9309
D(8,24,28,35)	65.2349	65.241
D(8,24,28,36)	-51.2889	-51.2322
D(25,24,28,29)	63.9215	63.951
D(25,24,28,35)	-57.902	-57.8772
D(25,24,28,36)	-174.4258	-174.3503
D(49,24,28,29)	-52.2878	-51.9368
D(49,24,28,35)	-174.1113	-173.7649
D(49,24,28,36)	69.3649	69.7619
D(8,24,49,50)	-174.5344	-174.6462
D(8,24,49,51)	63.9745	63.669
D(8,24,49,52)	-52.5013	-52.7414
D(25,24,49,50)	-51.7597	-51.7643
D(25,24,49,51)	-173.2508	-173.4491
D(25,24,49,52)	70.2734	70.1405
D(28,24,49,50)	64.1724	63.8732
D(28,24,49,51)	-57.3187	-57.8115
D(28,24,49,52)	-173.7945	-174.2219
D(24,25,26,27)	-11.1888	-11.0019
D(24,25,26,33)	109.5106	109.5441
D(24,25,26,34)	-133.4927	-133.3159
D(31,25,26,27)	-132.7096	-132.6114
D(31,25,26,33)	-12.0102	-12.0654
D(31,25,26,34)	104.9865	105.0746
D(32,25,26,27)	109.8673	110.2457
D(32,25,26,33)	-129.4333	-129.2083
D(32,25,26,34)	-12.4367	-12.0683
D(25,26,27,29)	64.6002	64.6041
D(25,26,27,50)	-50.8344	-51.2325
D(25,26,27,58)	-171.5074	-171.3754
D(33,26,27,29)	-57.347	-57.2958
D(33,26,27,50)	-172.7817	-173.1324
D(33,26,27,58)	66.5453	66.7248
D(34,26,27,29)	-173.3232	-173.3676
D(34,26,27,50)	71.2421	70.7958
D(34,26,27,58)	-49.4309	-49.3471
D(26,27,29,28)	-52.0075	-52.0833
D(26,27,29,37)	69.353	69.2381
D(26,27,29,38)	-173.6911	-173.7002
D(50,27,29,28)	63.8393	64.0236
D(50,27,29,37)	-174.8002	-174.655

D(50,27,29,38)	-57.8443	-57.5933
D(58,27,29,28)	-174.5394	-174.7168
D(58,27,29,37)	-53.1789	-53.3953
D(58,27,29,38)	63.7771	63.6664
D(26,27,50,49)	63.3294	63.4786
D(26,27,50,53)	-58.5063	-58.1467
D(26,27,50,54)	-174.5427	-174.2709
D(29,27,50,49)	-51.8145	-52.0542
D(29,27,50,53)	-173.6502	-173.6796
D(29,27,50,54)	70.3134	70.1963
D(58,27,50,49)	-175.3944	-175.5367
D(58,27,50,53)	62.7699	62.8379
D(58,27,50,54)	-53.2665	-53.2862
D(26,27,58,56)	-123.9245	-123.7784
D(26,27,58,57)	57.4144	57.5056
D(29,27,58,56)	-3.625	-3.2252
D(29,27,58,57)	177.7139	178.0587
D(50,27,58,56)	116.5522	116.9637
D(50,27,58,57)	-62.1088	-61.7524
D(24,28,29,27)	-10.2147	-10.3037
D(24,28,29,37)	-131.754	-131.7584
D(24,28,29,38)	111.1491	110.883
D(35,28,29,27)	110.4129	110.4431
D(35,28,29,37)	-11.1265	-11.0116
D(35,28,29,38)	-128.2234	-128.3702
D(36,28,29,27)	-132.0835	-132.1927
D(36,28,29,37)	106.3772	106.3526
D(36,28,29,38)	-10.7197	-11.0059
D(41,39,40,42)	-0.0111	-0.0537
D(41,39,40,56)	-178.3176	-178.9985
D(55,39,40,42)	178.332	178.925
D(55,39,40,56)	0.0255	-0.0198
D(40,39,41,43)	-10.0736	-5.0092
D(55,39,41,43)	171.6658	176.0608
D(40,39,55,57)	-0.4014	-0.2087
D(40,39,55,67)	179.4637	179.7279
D(41,39,55,57)	177.8172	178.6931
D(41,39,55,67)	-2.3176	-1.3703
D(39,40,42,43)	10.0922	5.0925
D(56,40,42,43)	-171.6424	-175.9825
D(39,40,56,58)	0.4946	0.3215
D(39,40,56,69)	-179.2508	-179.5013
D(42,40,56,58)	-177.6991	-178.5528
D(42,40,56,69)	2.5554	1.6243
D(39,41,43,42)	16.6723	8.3646
D(39,41,43,44)	-165.2466	-173.5147

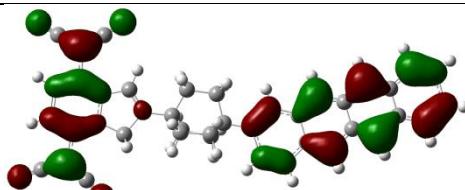
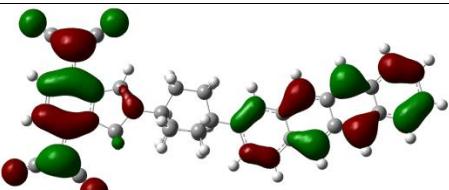
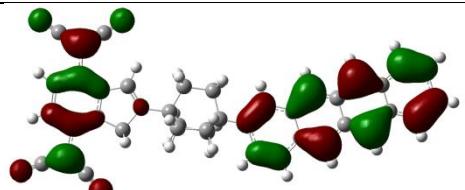
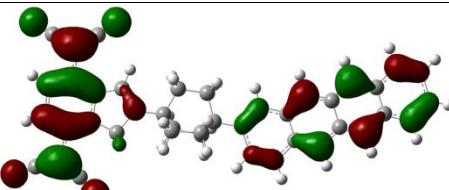
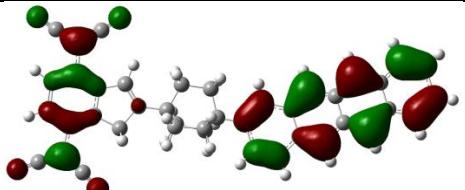
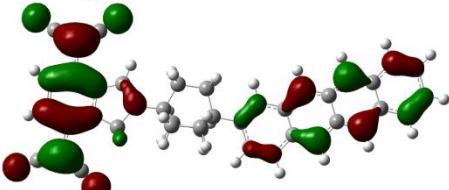
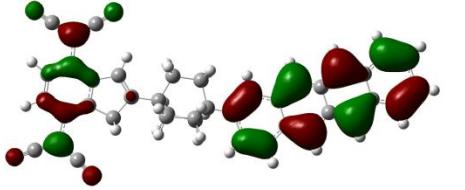
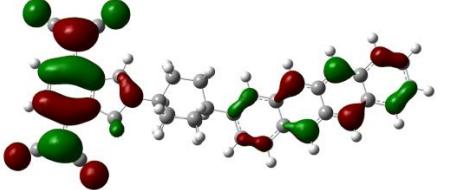
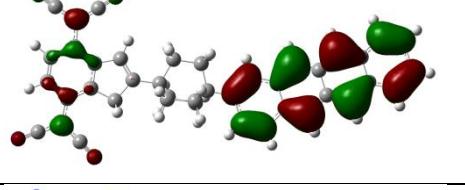
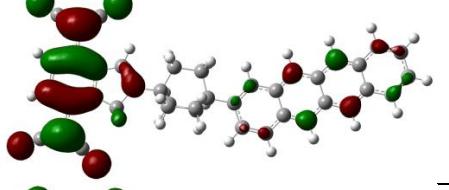
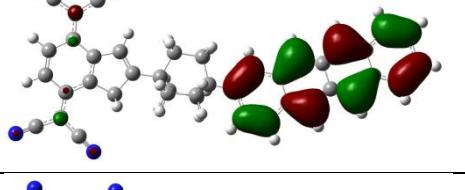
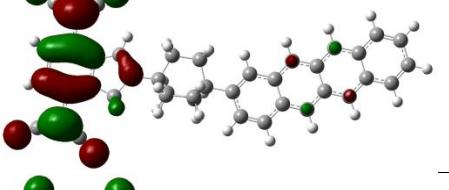
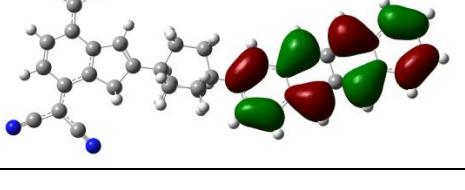
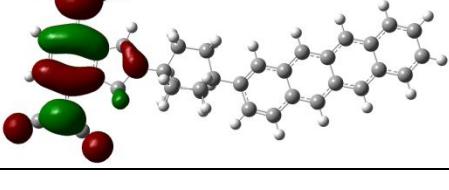
D(40,42,43,41)	-16.6957	-8.4012
D(40,42,43,44)	165.2227	173.4792
D(41,43,44,45)	0.0157	1.0513
D(41,43,44,46)	-177.8635	-178.6686
D(42,43,44,45)	177.9236	179.0186
D(42,43,44,46)	0.0444	-0.7012
D(43,44,45,47)	165.5174	155.914
D(46,44,45,47)	-16.4288	-24.3383
D(43,44,46,48)	-165.4989	-155.8447
D(45,44,46,48)	16.4468	24.4069
D(44,45,47,48)	9.8943	14.6674
D(44,45,47,59)	-171.8034	-167.9124
D(44,46,48,47)	-9.953	-14.9404
D(44,46,48,60)	171.7735	167.6892
D(45,47,48,46)	0.0406	0.1764
D(45,47,48,60)	178.3692	177.6547
D(59,47,48,46)	-178.3162	-177.3525
D(59,47,48,60)	0.0124	0.1257
D(45,47,59,61)	-177.9648	-176.8384
D(45,47,59,63)	2.2177	3.8964
D(48,47,59,61)	0.2771	0.4853
D(48,47,59,63)	-179.5404	-178.78
D(46,48,60,62)	177.92	176.6397
D(46,48,60,66)	-2.2526	-4.0632
D(47,48,60,62)	-0.2916	-0.6391
D(47,48,60,66)	179.5358	178.6581
D(24,49,50,27)	-10.492	-10.3914
D(24,49,50,53)	110.8177	110.6444
D(24,49,50,54)	-131.9102	-131.8067
D(51,49,50,27)	110.3862	110.8172
D(51,49,50,53)	-128.3041	-128.147
D(51,49,50,54)	-11.032	-10.5981
D(52,49,50,27)	-131.8401	-131.7
D(52,49,50,53)	-10.5305	-10.6642
D(52,49,50,54)	106.7417	106.8847
D(39,55,57,58)	0.2721	0.1444
D(39,55,57,68)	179.9057	179.9631
D(67,55,57,58)	-179.5933	-179.7926
D(67,55,57,68)	0.0402	0.0262
D(40,56,58,27)	-179.3036	-179.1259
D(40,56,58,57)	-0.6133	-0.3766
D(69,56,58,27)	0.4367	0.6957
D(69,56,58,57)	179.127	179.445
D(55,57,58,27)	178.9564	178.9279
D(55,57,58,56)	0.2343	0.1477
D(68,57,58,27)	-0.6705	-0.8887

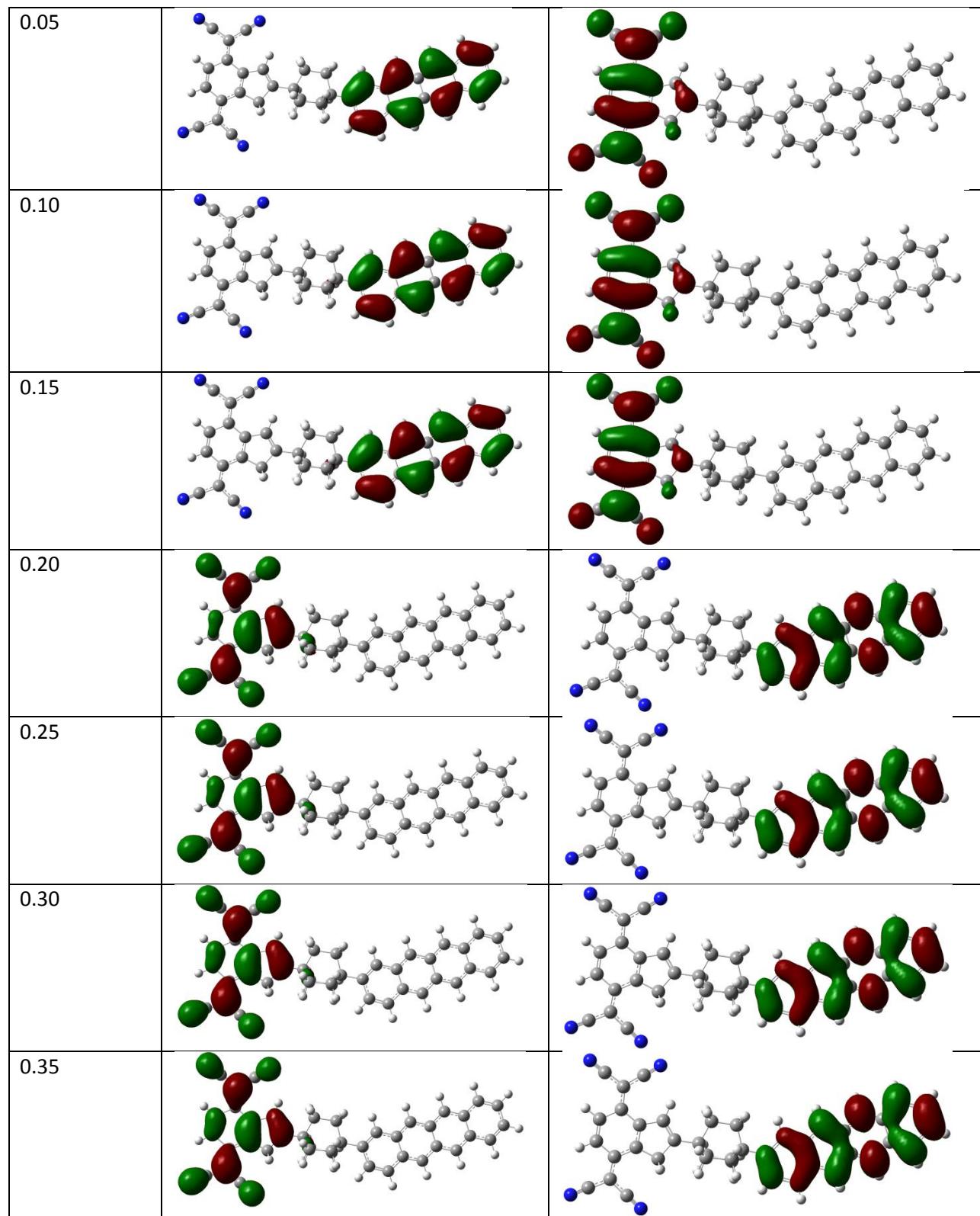
D(68,57,58,56)	-179.3926	-179.6689
D(47,59,61,62)	-0.2876	-0.5839
D(47,59,61,64)	-179.9665	-179.4151
D(63,59,61,62)	179.5294	178.6762
D(63,59,61,64)	-0.1495	-0.1549
D(48,60,62,61)	0.282	0.5438
D(48,60,62,65)	179.9714	179.4349
D(66,60,62,61)	-179.545	-178.7489
D(66,60,62,65)	0.1444	0.1422
D(59,61,62,60)	0.0079	0.0692
D(59,61,62,65)	-179.6794	-178.8117
D(64,61,62,60)	179.6846	178.8921
D(64,61,62,65)	-0.0027	0.0112

Table S6. HOMO energy (E_{HOMO}), LUMO energy (E_{LUMO}), HOMO-LUMO gap ($E_{\text{HOMO}}-E_{\text{LUMO}}$) and the total dipole moment of TCNQ- σ -Tetracene system under various electric fields with B3PW91/MPW1PW91 functionals.

Electric Field (V/Å)	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{\text{HOMO}}-E_{\text{LUMO}}$ (eV)	Total dipole moment (Debye)
-0.30	-4.88/-4.92	-4.67/-4.65	0.21/0.27	64.77/63.85
-0.25	-4.90/-4.93	-4.69/-4.66	0.21/0.27	53.87/52.60
-0.20	-4.91/-4.94	-4.70/-4.67	0.21/0.27	43.12/41.50
-0.15	-4.93/-4.95	-4.71/-4.68	0.22/0.27	32.51/30.54
-0.10	-4.94/-4.97	-4.72/-4.69	0.22/0.28	22.03/19.72
-0.05	-4.96/-4.99	-4.73/-4.69	0.23/0.30	11.74/9.17
0.00	-5.08/-5.21	-4.63/-4.50	0.45/0.71	4.35/4.26
0.05	-5.39/-5.52	-4.34/-4.21	1.05/1.31	2.07/2.04
0.10	-5.69/-5.82	-4.05/-3.92	1.64/1.90	1.11/1.08
0.15	-6.00/-6.13	-3.76/-3.63	2.24/2.50	3.07/3.00
0.20	-5.78/-5.93	-3.58/-3.42	2.20/2.51	5.37/5.27
0.25	-5.51/-5.67	-3.92/-3.76	1.59/1.91	7.72/7.58
0.30	-5.24/-5.39	-4.26/-4.10	0.98/1.29	10.12/9.92
0.35	-4.97/-5.12	-4.59/-4.44	0.38/0.68	12.83/12.33
0.40	-4.94/-4.97	-4.70/-4.66	0.24/0.31	21.66/18.23

Table S7. Spatial distribution of the HOMO and LUMO of TCNQ- σ -Tetracene system under various electric fields with B3LYP functional.

Electric Field (V/ \AA)	HOMO	LUMO
-0.30		
-0.25		
-0.20		
-0.15		
-0.10		
-0.05		
0.00		



0.40

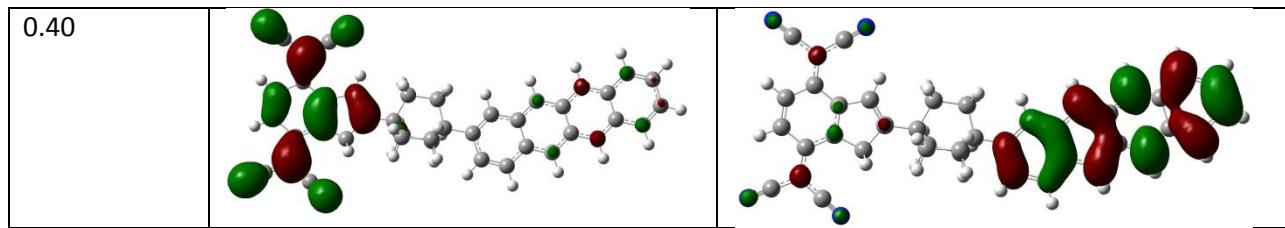
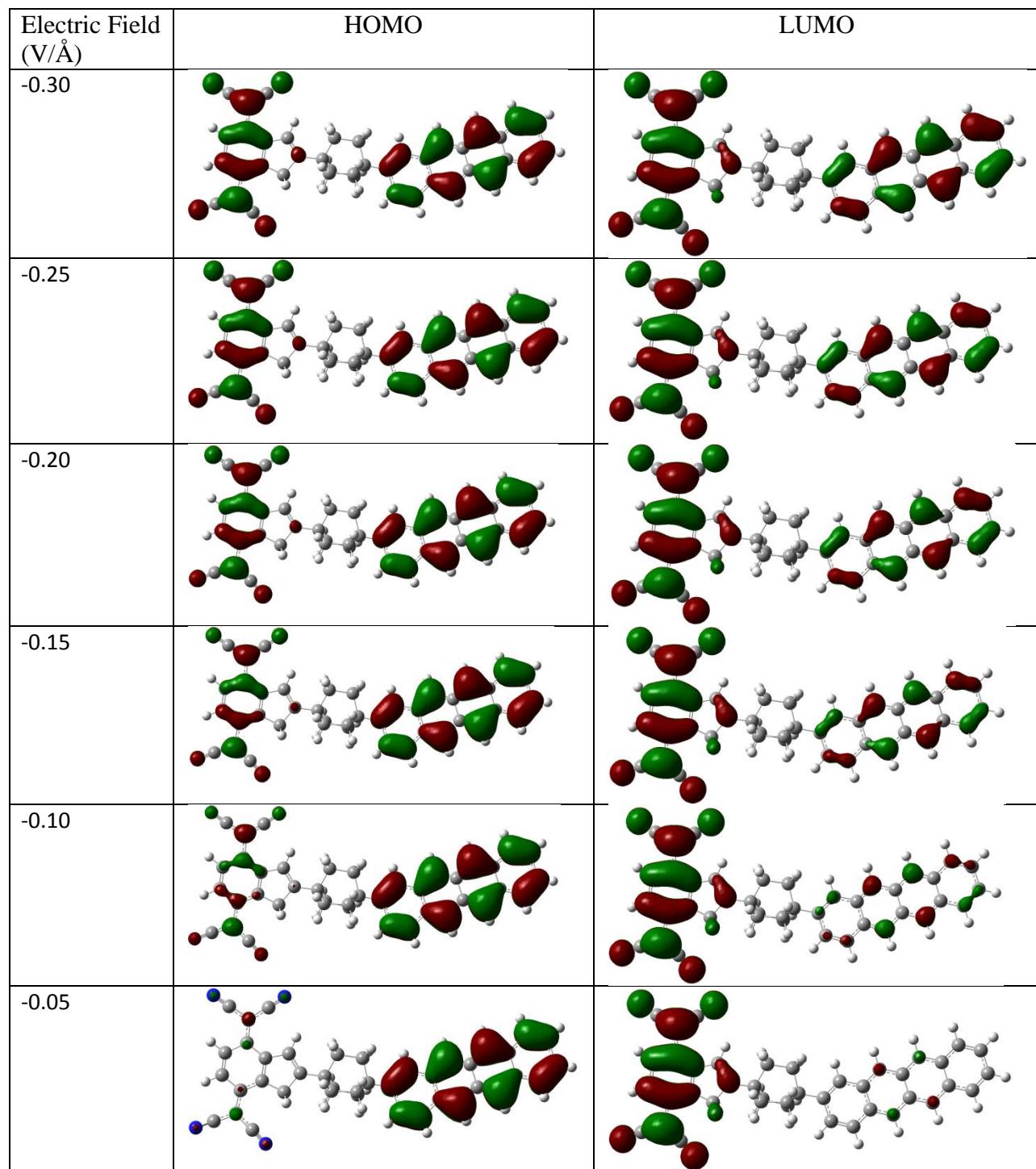
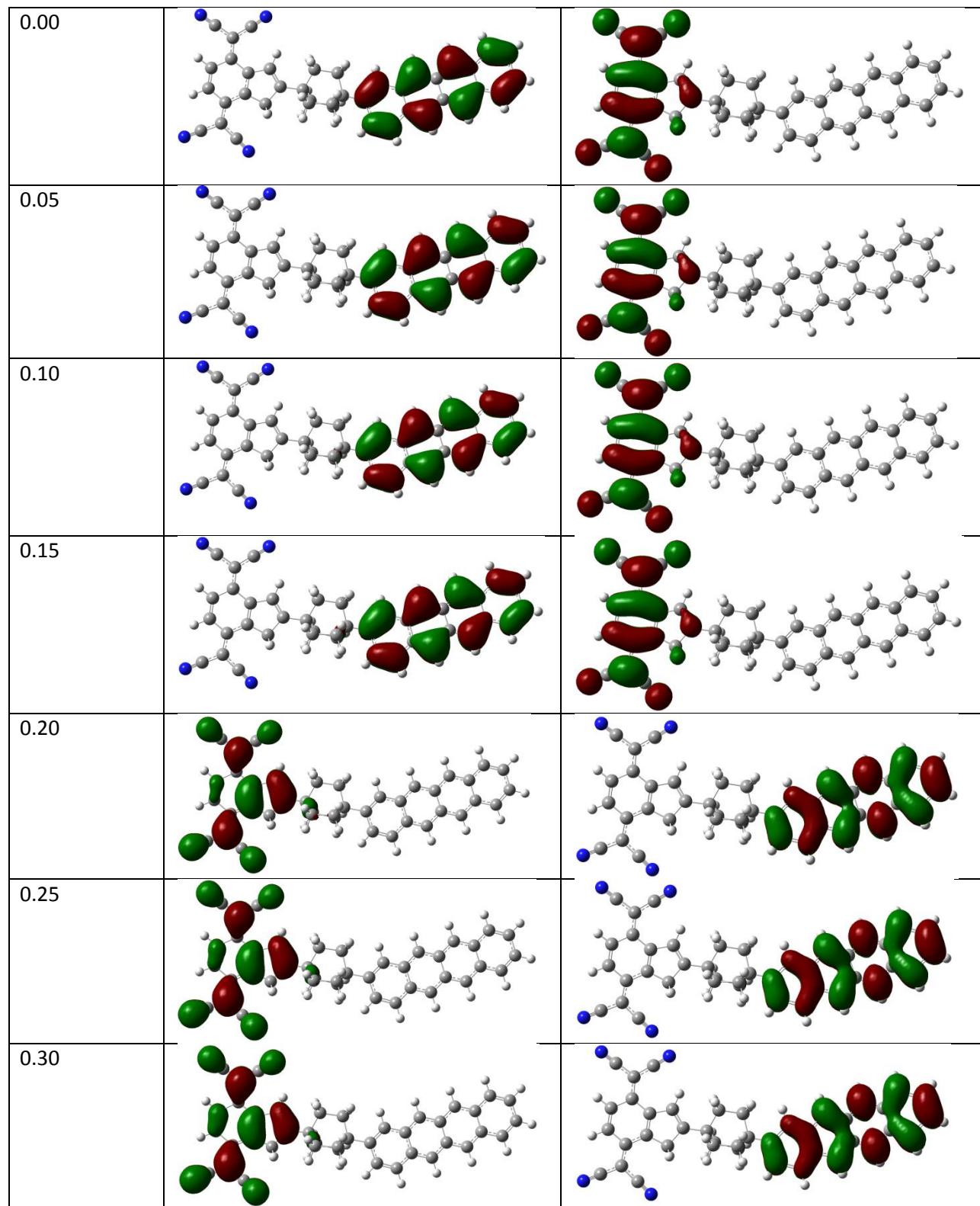


Table S8. Spatial distribution of the HOMO and LUMO of TCNQ- σ -Tetracene system under various electric fields with B3PW91 functional.





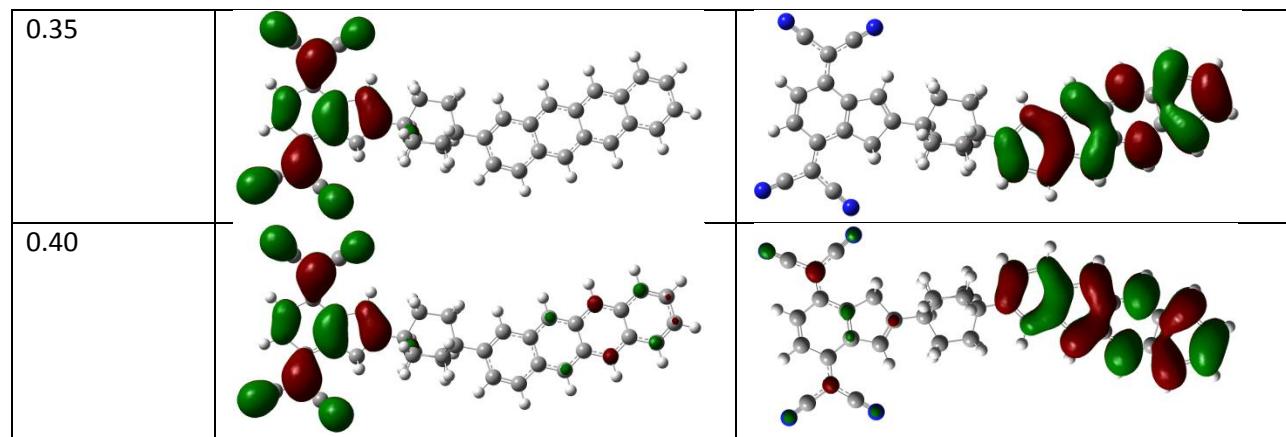
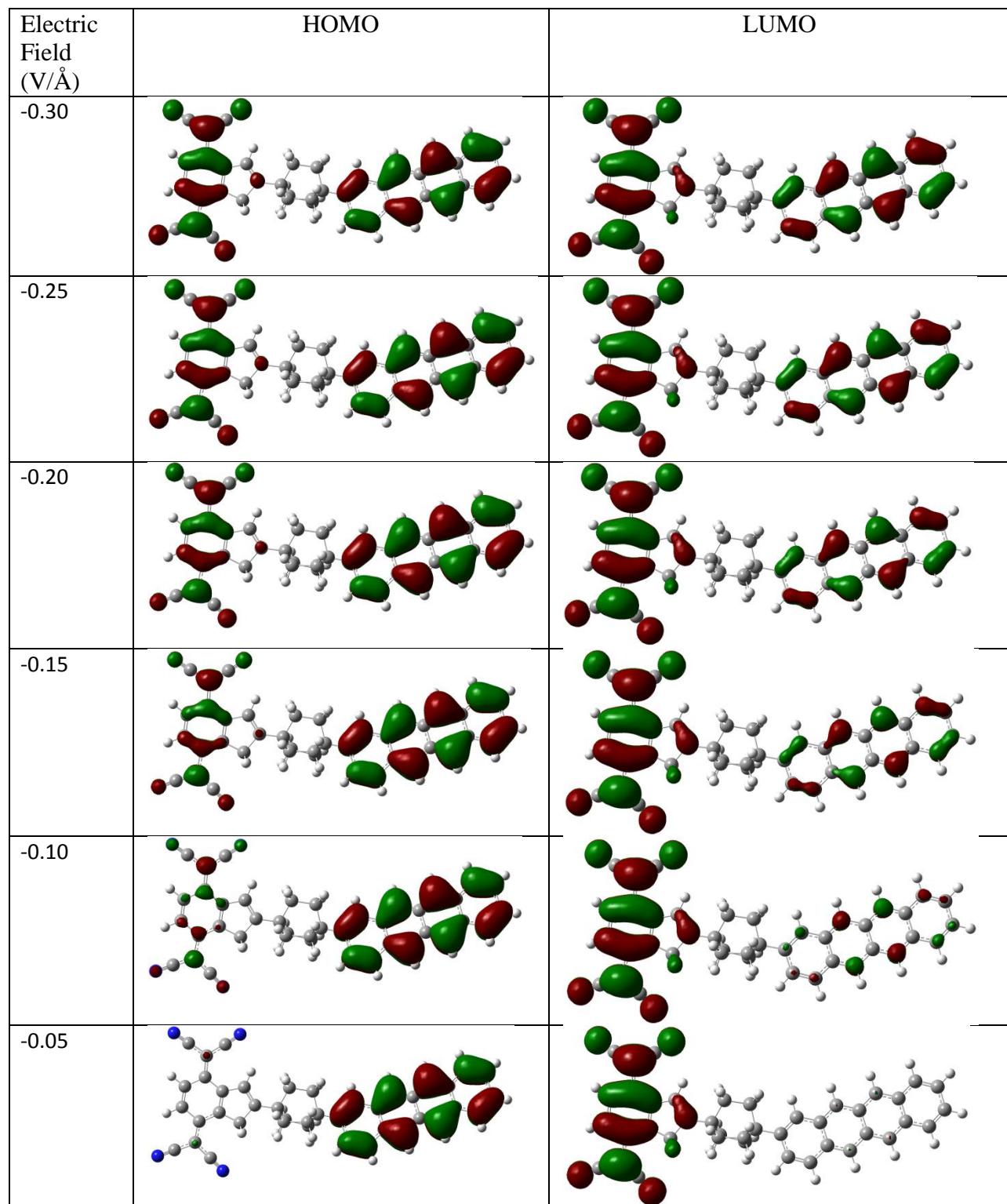
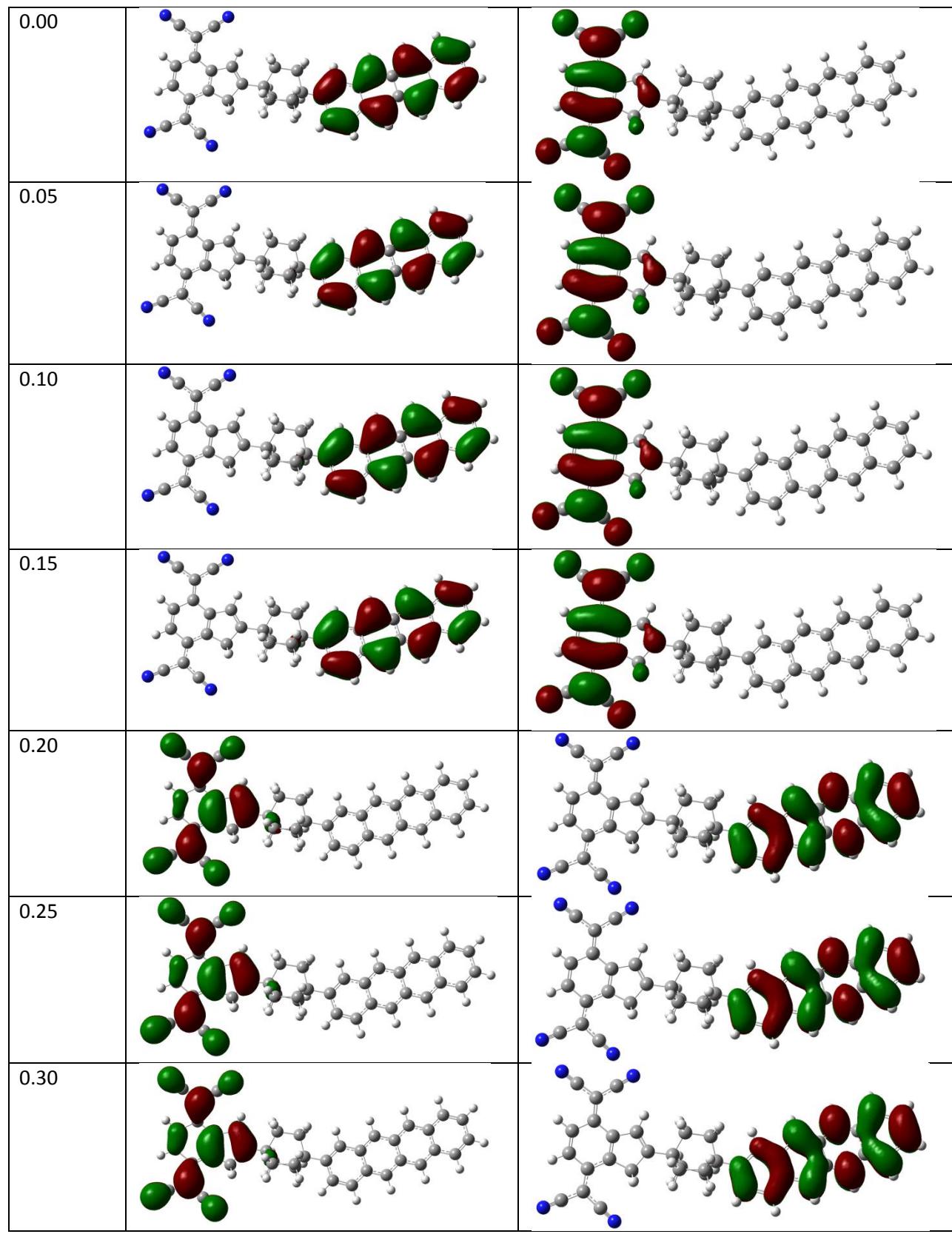


Table S9. Spatial distribution of the HOMO and LUMO of TCNQ- σ -Tetracene system under various electric fields with MPW1PW91 functional.





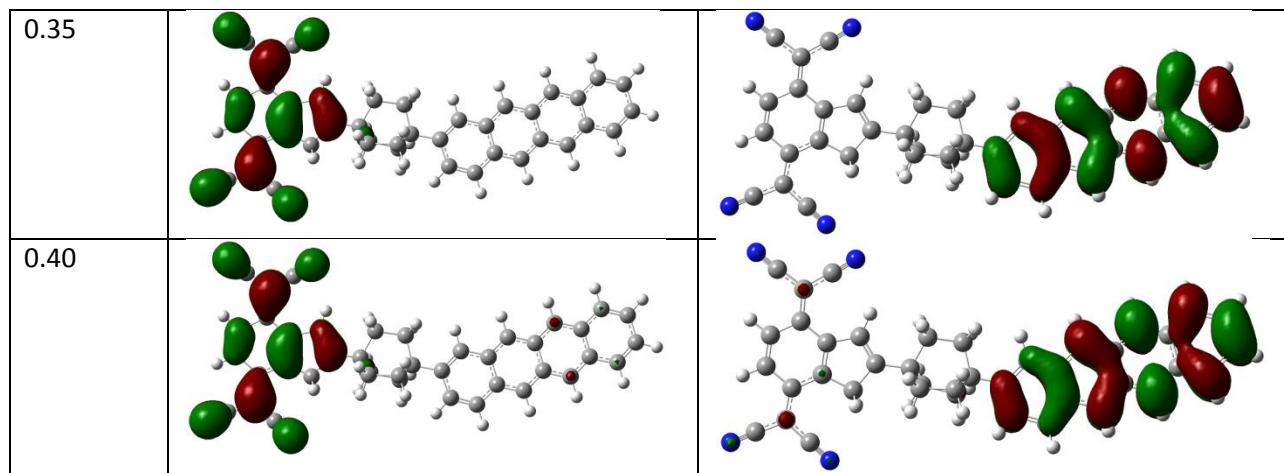


Table S10: Optimized parameters (bond lengths, bond angles and dihedral angles) of TCNQ- σ -Tetracene system without electric field and with an extreme electric field of 0.40 V/ \AA in reverse direction using B3LYP functional. Bond lengths are in Angstrom, bond angles and dihedral angles are in degree.

Optimized Parameters	Without Electric Field	With 0.40 V/ \AA Electric Field
R(1,2)	1.3871	1.3846
R(1,6)	1.4557	1.4543
R(1,7)	1.4572	1.4629
R(2,3)	1.4321	1.4386
R(2,9)	1.5049	1.5074
R(3,4)	1.4553	1.4521
R(3,15)	1.3968	1.3969
R(4,5)	1.3514	1.3555
R(4,10)	1.0843	1.085
R(5,6)	1.4525	1.4504
R(5,11)	1.0842	1.0849
R(6,14)	1.3898	1.3929
R(7,8)	1.3586	1.3544
R(7,12)	1.078	1.0778
R(8,9)	1.5091	1.5094
R(8,24)	1.5068	1.511
R(9,13)	1.0969	1.0968
R(9,30)	1.0972	1.097
R(14,16)	1.4309	1.4273
R(14,17)	1.4267	1.4277
R(15,18)	1.4274	1.4245
R(15,19)	1.4243	1.4263
R(16,20)	1.1645	1.1647
R(17,21)	1.1648	1.1656
R(18,22)	1.1652	1.1652
R(19,23)	1.1656	1.1657
R(24,25)	1.5445	1.5449
R(24,28)	1.5551	1.5529
R(24,39)	1.5557	1.5536
R(25,26)	1.554	1.5555
R(25,31)	1.095	1.0938
R(25,32)	1.096	1.0949
R(26,27)	1.5445	1.5444
R(26,33)	1.0956	1.0971
R(26,34)	1.0946	1.0963
R(27,29)	1.5546	1.5566
R(27,40)	1.5534	1.5554
R(27,50)	1.5289	1.5271

R(28,29)	1.5534	1.5552
R(28,35)	1.0958	1.095
R(28,36)	1.095	1.0937
R(29,37)	1.0949	1.0961
R(29,38)	1.0945	1.0956
R(39,40)	1.5527	1.5545
R(39,41)	1.0959	1.0947
R(39,42)	1.0956	1.0945
R(40,43)	1.0957	1.0966
R(40,44)	1.0938	1.0952
R(45,46)	1.3643	1.3656
R(45,50)	1.4421	1.4425
R(45,61)	1.0855	1.0845
R(46,47)	1.4325	1.4299
R(46,62)	1.087	1.087
R(47,48)	1.4483	1.4509
R(47,51)	1.3913	1.3942
R(48,49)	1.4349	1.4327
R(48,52)	1.3923	1.3968
R(49,50)	1.3717	1.376
R(49,63)	1.0846	1.0843
R(51,54)	1.4109	1.409
R(51,60)	1.0876	1.0881
R(52,53)	1.411	1.41
R(52,64)	1.0877	1.0874
R(53,54)	1.4522	1.456
R(53,59)	1.4098	1.4117
R(54,55)	1.4096	1.411
R(55,56)	1.0876	1.0887
R(55,57)	1.393	1.395
R(57,58)	1.4514	1.4541
R(57,69)	1.4336	1.4317
R(58,59)	1.393	1.3955
R(58,66)	1.4337	1.4317
R(59,65)	1.0876	1.0879
R(66,67)	1.3669	1.3724
R(66,70)	1.0869	1.0877
R(67,68)	1.4302	1.4274
R(67,72)	1.086	1.0882
R(68,69)	1.3668	1.3726
R(68,73)	1.086	1.0891
R(69,71)	1.0869	1.0887
A(2,1,6)	120.8276	121.0459
A(2,1,7)	109.1011	108.669
A(6,1,7)	130.0714	130.2851
A(1,2,3)	122.2659	122.0232

A(1,2,9)	108.1692	108.5162
A(3,2,9)	129.5649	129.4606
A(2,3,4)	116.3675	116.4359
A(2,3,15)	125.0178	124.1828
A(4,3,15)	118.6147	119.3812
A(3,4,5)	122.0495	121.9631
A(3,4,10)	118.2967	118.5159
A(5,4,10)	119.6538	119.521
A(4,5,6)	122.212	122.2213
A(4,5,11)	119.5628	119.3363
A(6,5,11)	118.2251	118.4423
A(1,6,5)	116.2774	116.3099
A(1,6,14)	125.1142	124.5338
A(5,6,14)	118.6084	119.1562
A(1,7,8)	109.9333	110.1532
A(1,7,12)	124.7449	124.2673
A(8,7,12)	125.3215	125.5791
A(7,8,9)	108.8277	108.9143
A(7,8,24)	127.9229	127.6246
A(9,8,24)	123.2468	123.4589
A(2,9,8)	103.9682	103.7468
A(2,9,13)	112.1057	111.7214
A(2,9,30)	112.0253	111.6674
A(8,9,13)	112.0861	112.5412
A(8,9,30)	111.7841	112.2622
A(13,9,30)	105.0729	105.1042
A(6,14,16)	121.0019	122.0076
A(6,14,17)	125.3106	124.3445
A(16,14,17)	113.6875	113.6477
A(3,15,18)	121.3935	122.1873
A(3,15,19)	123.7955	122.8948
A(18,15,19)	114.811	114.9179
A(8,24,25)	112.1713	112.1581
A(8,24,28)	110.8192	110.9433
A(8,24,39)	110.3886	110.6234
A(25,24,28)	107.6464	107.4601
A(25,24,39)	107.9902	107.778
A(28,24,39)	107.6555	107.6914
A(24,25,26)	110.9314	111.0604
A(24,25,31)	109.7113	109.7226
A(24,25,32)	109.1459	109.2129
A(26,25,31)	109.9656	109.9073
A(26,25,32)	110.4837	110.4008
A(31,25,32)	106.4992	106.4255
A(25,26,27)	111.0673	110.9331
A(25,26,33)	110.2176	110.289

A(25,26,34)	109.6272	109.6515
A(27,26,33)	109.3872	109.3325
A(27,26,34)	109.7742	109.8048
A(33,26,34)	106.6672	106.7381
A(26,27,29)	107.3402	107.5615
A(26,27,40)	106.9684	107.1579
A(26,27,50)	113.2699	113.3845
A(29,27,40)	108.2793	108.2686
A(29,27,50)	110.0134	109.7802
A(40,27,50)	110.7721	110.5088
A(24,28,29)	110.5117	110.877
A(24,28,35)	108.6941	108.7873
A(24,28,36)	110.0601	110.08
A(29,28,35)	110.8621	110.6499
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A(35,28,36)	106.6343	106.6066
A(27,29,28)	111.2254	110.8146
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A(27,29,38)	109.5528	109.6539
A(28,29,37)	110.4476	110.6094
A(28,29,38)	110.06	110.0076
A(37,29,38)	106.361	106.4218
A(24,39,40)	110.551	110.9277
A(24,39,41)	109.1646	109.2891
A(24,39,42)	109.5329	109.5077
A(40,39,41)	110.2604	110.1112
A(40,39,42)	110.5494	110.2643
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A(27,40,39)	111.0287	110.6768
A(27,40,43)	108.4498	108.4202
A(27,40,44)	110.4479	110.6502
A(39,40,43)	110.6699	110.8133
A(39,40,44)	109.8848	109.9326
A(43,40,44)	106.243	106.2496
A(46,45,50)	121.9926	122.44
A(46,45,61)	118.8426	118.9087
A(50,45,61)	119.1646	118.6512
A(45,46,47)	121.2191	121.0501
A(45,46,62)	120.2635	120.2505
A(47,46,62)	118.5174	118.6994
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A(49,48,52)	122.0093	122.2268

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A(27,50,45)	118.8684	118.7646
A(27,50,49)	123.2841	123.8375
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A(47,51,60)	119.3584	119.0679
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A(48,52,53)	121.8669	122.129
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A(53,52,64)	118.8105	118.857
A(52,53,54)	118.8757	118.9081
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A(54,53,59)	118.8311	118.5809
A(51,54,53)	118.7973	118.6017
A(51,54,55)	122.3262	122.6112
A(53,54,55)	118.8766	118.7871
A(54,55,56)	118.868	118.5842
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A(55,57,58)	119.2513	119.0263
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A(53,59,58)	121.8987	122.2233
A(53,59,65)	118.8541	118.5867
A(58,59,65)	119.2472	119.19
A(58,66,67)	121.0169	121.5293
A(58,66,70)	118.3794	118.0563
A(67,66,70)	120.6037	120.4144
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A(66,67,72)	120.1672	120.0739
A(68,67,72)	119.3167	119.7249
A(67,68,69)	120.5095	120.2567
A(67,68,73)	119.3142	119.6144
A(69,68,73)	120.1763	120.1289
A(57,69,68)	121.0189	121.5109
A(57,69,71)	118.3855	118.0303
A(68,69,71)	120.5956	120.4589
D(6,1,2,3)	-0.095	-0.1726
D(6,1,2,9)	179.9383	179.8861
D(7,1,2,3)	179.9208	179.8314
D(7,1,2,9)	-0.0458	-0.1099

D(2,1,6,5)	0.1299	0.3128
D(2,1,6,14)	-179.7862	-179.5437
D(7,1,6,5)	-179.8897	-179.6921
D(7,1,6,14)	0.1942	0.4514
D(2,1,7,8)	0.193	0.2375
D(2,1,7,12)	-179.6189	-179.5391
D(6,1,7,8)	-179.7891	-179.7581
D(6,1,7,12)	0.3989	0.4653
D(1,2,3,4)	0.0241	-0.0452
D(1,2,3,15)	-179.9106	-179.9845
D(9,2,3,4)	179.983	179.8827
D(9,2,3,15)	0.0483	-0.0567
D(1,2,9,8)	-0.0985	-0.0384
D(1,2,9,13)	-121.379	-121.5234
D(1,2,9,30)	120.7753	121.0837
D(3,2,9,8)	179.9381	-179.9739
D(3,2,9,13)	58.6576	58.541
D(3,2,9,30)	-59.1881	-58.8519
D(2,3,4,5)	0.0055	0.113
D(2,3,4,10)	-179.9869	-179.9131
D(15,3,4,5)	179.9446	-179.9446
D(15,3,4,10)	-0.0478	0.0294
D(2,3,15,18)	179.976	179.9752
D(2,3,15,19)	0.0088	-0.0349
D(4,3,15,18)	0.0426	0.0375
D(4,3,15,19)	-179.9245	-179.9726
D(3,4,5,6)	0.0372	0.04
D(3,4,5,11)	179.9837	179.9411
D(10,4,5,6)	-179.9706	-179.9336
D(10,4,5,11)	-0.0241	-0.0325
D(4,5,6,1)	-0.1024	-0.2491
D(4,5,6,14)	179.8194	179.6156
D(11,5,6,1)	179.9504	179.849
D(11,5,6,14)	-0.1278	-0.2863
D(1,6,14,16)	-179.9944	-179.9876
D(1,6,14,17)	0.0976	0.1953
D(5,6,14,16)	0.0914	0.1597
D(5,6,14,17)	-179.8167	-179.6575
D(1,7,8,9)	-0.2544	-0.2596
D(1,7,8,24)	-179.6742	-179.7232
D(12,7,8,9)	179.5562	179.5133
D(12,7,8,24)	0.1364	0.0497
D(7,8,9,2)	0.2176	0.1847
D(7,8,9,13)	121.5113	121.1195
D(7,8,9,30)	-120.8179	-120.5369
D(24,8,9,2)	179.6703	179.6755

D(24,8,9,13)	-59.036	-59.3898
D(24,8,9,30)	58.6348	58.9539
D(7,8,24,25)	1.8013	1.914
D(7,8,24,28)	-118.541	-118.268
D(7,8,24,39)	122.283	122.2794
D(9,8,24,25)	-177.542	-177.4777
D(9,8,24,28)	62.1157	62.3403
D(9,8,24,39)	-57.0603	-57.1124
D(8,24,25,26)	-175.1496	-175.0484
D(8,24,25,31)	-53.4562	-53.3358
D(8,24,25,32)	62.8858	62.9622
D(28,24,25,26)	-52.9831	-52.8617
D(28,24,25,31)	68.7103	68.8509
D(28,24,25,32)	-174.9477	-174.8511
D(39,24,25,26)	62.9887	62.9488
D(39,24,25,31)	-175.3179	-175.3386
D(39,24,25,32)	-58.9758	-59.0406
D(8,24,28,29)	-173.7932	-173.6903
D(8,24,28,35)	64.337	64.4106
D(8,24,28,36)	-52.1043	-52.0623
D(25,24,28,29)	63.2071	63.3717
D(25,24,28,35)	-58.6628	-58.5274
D(25,24,28,36)	-175.104	-175.0003
D(39,24,28,29)	-52.9845	-52.496
D(39,24,28,35)	-174.8544	-174.3951
D(39,24,28,36)	68.7044	69.1321
D(8,24,39,40)	-174.2903	-174.4275
D(8,24,39,41)	64.2555	63.9809
D(8,24,39,42)	-52.2333	-52.4982
D(25,24,39,40)	-51.3348	-51.4801
D(25,24,39,41)	-172.789	-173.0717
D(25,24,39,42)	70.7222	70.4493
D(28,24,39,40)	64.631	64.1784
D(28,24,39,41)	-56.8231	-57.4132
D(28,24,39,42)	-173.3119	-173.8923
D(24,25,26,27)	-9.0501	-9.0653
D(24,25,26,33)	112.3457	112.2204
D(24,25,26,34)	-130.5358	-130.5179
D(31,25,26,27)	-130.5945	-130.6699
D(31,25,26,33)	-9.1986	-9.3843
D(31,25,26,34)	107.9198	107.8774
D(32,25,26,27)	112.1301	112.2298
D(32,25,26,33)	-126.4741	-126.4845
D(32,25,26,34)	-9.3556	-9.2228
D(25,26,27,29)	63.1072	63.1875
D(25,26,27,40)	-52.9208	-53.0327

D(25,26,27,50)	-175.2543	-175.2404
D(33,26,27,29)	-58.774	-58.659
D(33,26,27,40)	-174.802	-174.8792
D(33,26,27,50)	62.8645	62.9131
D(34,26,27,29)	-175.4932	-175.4498
D(34,26,27,40)	68.4788	68.33
D(34,26,27,50)	-53.8548	-53.8778
D(26,27,29,28)	-52.6661	-52.5307
D(26,27,29,37)	69.3921	69.5727
D(26,27,29,38)	-174.5649	-174.1618
D(40,27,29,28)	62.4925	62.9574
D(40,27,29,37)	-175.4493	-174.9392
D(40,27,29,38)	-59.4063	-58.6737
D(50,27,29,28)	-176.3216	-176.3255
D(50,27,29,37)	-54.2634	-54.2221
D(50,27,29,38)	61.7796	62.0434
D(26,27,40,39)	64.5426	64.3775
D(26,27,40,43)	-57.2547	-57.3575
D(26,27,40,44)	-173.3004	-173.5062
D(29,27,40,39)	-50.8589	-51.3737
D(29,27,40,43)	-172.6563	-173.1087
D(29,27,40,44)	71.2981	70.7426
D(50,27,40,39)	-171.5745	-171.6369
D(50,27,40,43)	66.6282	66.6281
D(50,27,40,44)	-49.4175	-49.5205
D(26,27,50,45)	179.9345	-179.7261
D(26,27,50,49)	-0.8789	-0.3534
D(29,27,50,45)	-59.9381	-59.4045
D(29,27,50,49)	119.2485	119.9682
D(40,27,50,45)	59.7429	59.9489
D(40,27,50,49)	-121.0704	-120.6784
D(24,28,29,27)	-8.9369	-9.3069
D(24,28,29,37)	-130.1916	-130.6018
D(24,28,29,38)	112.6667	112.1163
D(35,28,29,27)	111.647	111.4962
D(35,28,29,37)	-9.6077	-9.7986
D(35,28,29,38)	-126.7494	-127.0805
D(36,28,29,27)	-130.6632	-131.1311
D(36,28,29,37)	108.0821	107.574
D(36,28,29,38)	-9.0596	-9.7079
D(24,39,40,27)	-10.9653	-10.607
D(24,39,40,43)	109.5267	109.7098
D(24,39,40,44)	-133.4492	-133.1426
D(41,39,40,27)	109.8387	110.5014
D(41,39,40,43)	-129.6693	-129.1818
D(41,39,40,44)	-12.6452	-12.0343

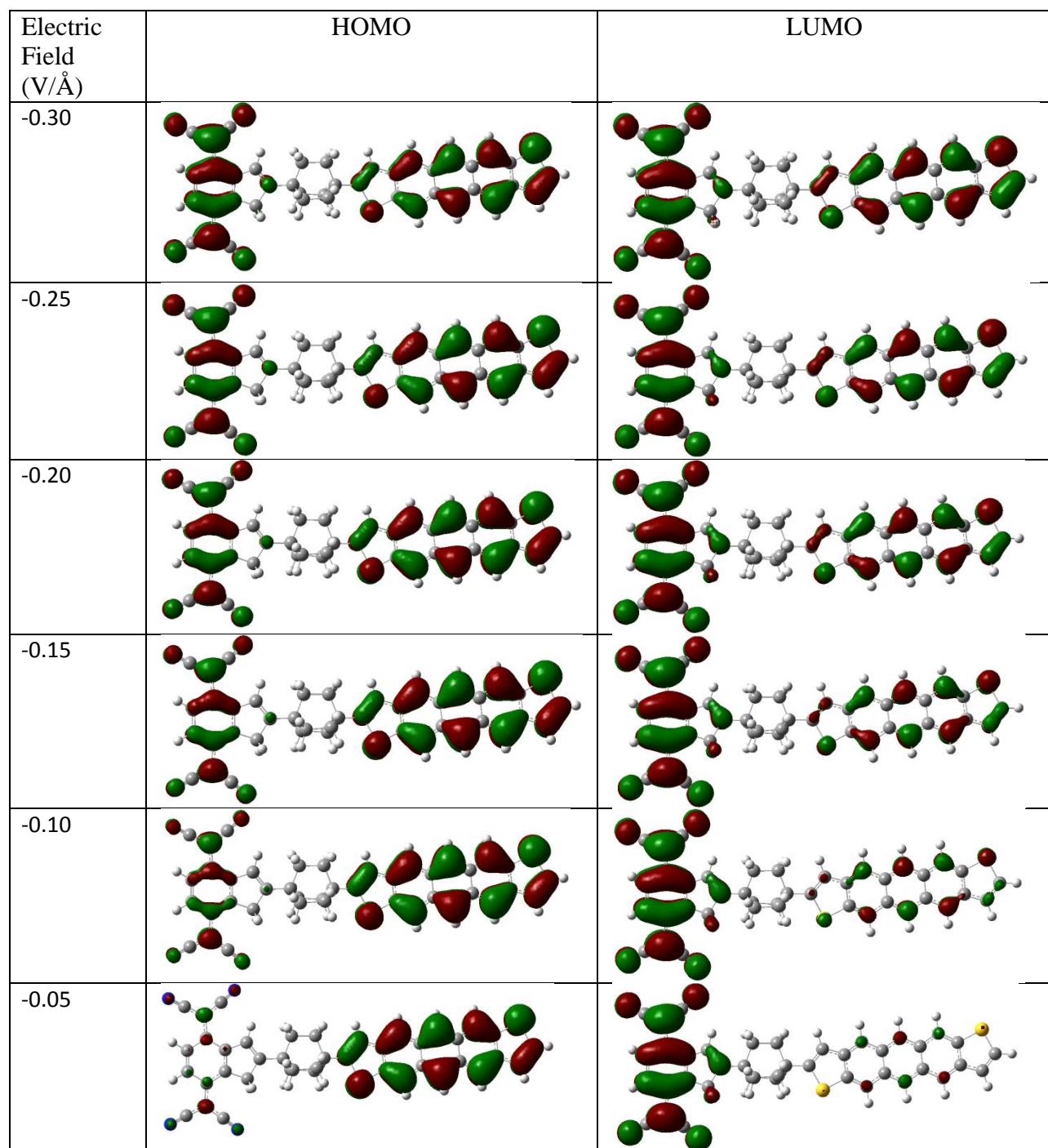
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D(42,39,40,43)	-11.9313	-11.7766
D(42,39,40,44)	105.0928	105.3709
D(50,45,46,47)	-0.0024	0.0103
D(50,45,46,62)	-179.9434	-179.9394
D(61,45,46,47)	179.8311	179.8566
D(61,45,46,62)	-0.1099	-0.0931
D(46,45,50,27)	179.3374	179.5575
D(46,45,50,49)	0.1064	0.1444
D(61,45,50,27)	-0.4955	-0.2891
D(61,45,50,49)	-179.7266	-179.7023
D(45,46,47,48)	-0.0356	-0.0848
D(45,46,47,51)	-179.9483	179.9793
D(62,46,47,48)	179.9063	179.8657
D(62,46,47,51)	-0.0063	-0.0702
D(46,47,48,49)	-0.0277	0.0073
D(46,47,48,52)	-179.9613	-179.9849
D(51,47,48,49)	179.8878	179.9453
D(51,47,48,52)	-0.0458	-0.0469
D(46,47,51,54)	179.902	179.9551
D(46,47,51,60)	-0.0623	-0.0295
D(48,47,51,54)	-0.0091	0.0204
D(48,47,51,60)	-179.9734	-179.9642
D(47,48,49,50)	0.137	0.1533
D(47,48,49,63)	-179.6938	-179.7517
D(52,48,49,50)	-179.9314	-179.8547
D(52,48,49,63)	0.2377	0.2403
D(47,48,52,53)	0.0507	0.0226
D(47,48,52,64)	-179.983	-179.9804
D(49,48,52,53)	-179.8807	-179.9694
D(49,48,52,64)	0.0856	0.0277
D(48,49,50,27)	-179.3677	-179.6055
D(48,49,50,45)	-0.1733	-0.2248
D(63,49,50,27)	0.4565	0.2968
D(63,49,50,45)	179.651	179.6775
D(47,51,54,53)	0.058	0.0297
D(47,51,54,55)	-179.9167	-179.9675
D(60,51,54,53)	-179.9775	-179.9857
D(60,51,54,55)	0.0477	0.0171
D(48,52,53,54)	-0.0016	0.0274
D(48,52,53,59)	179.9674	-179.9773
D(64,52,53,54)	-179.9681	-179.9697
D(64,52,53,59)	0.001	0.0256
D(52,53,54,51)	-0.0526	-0.0534
D(52,53,54,55)	179.923	179.9439
D(59,53,54,51)	179.9772	179.9511

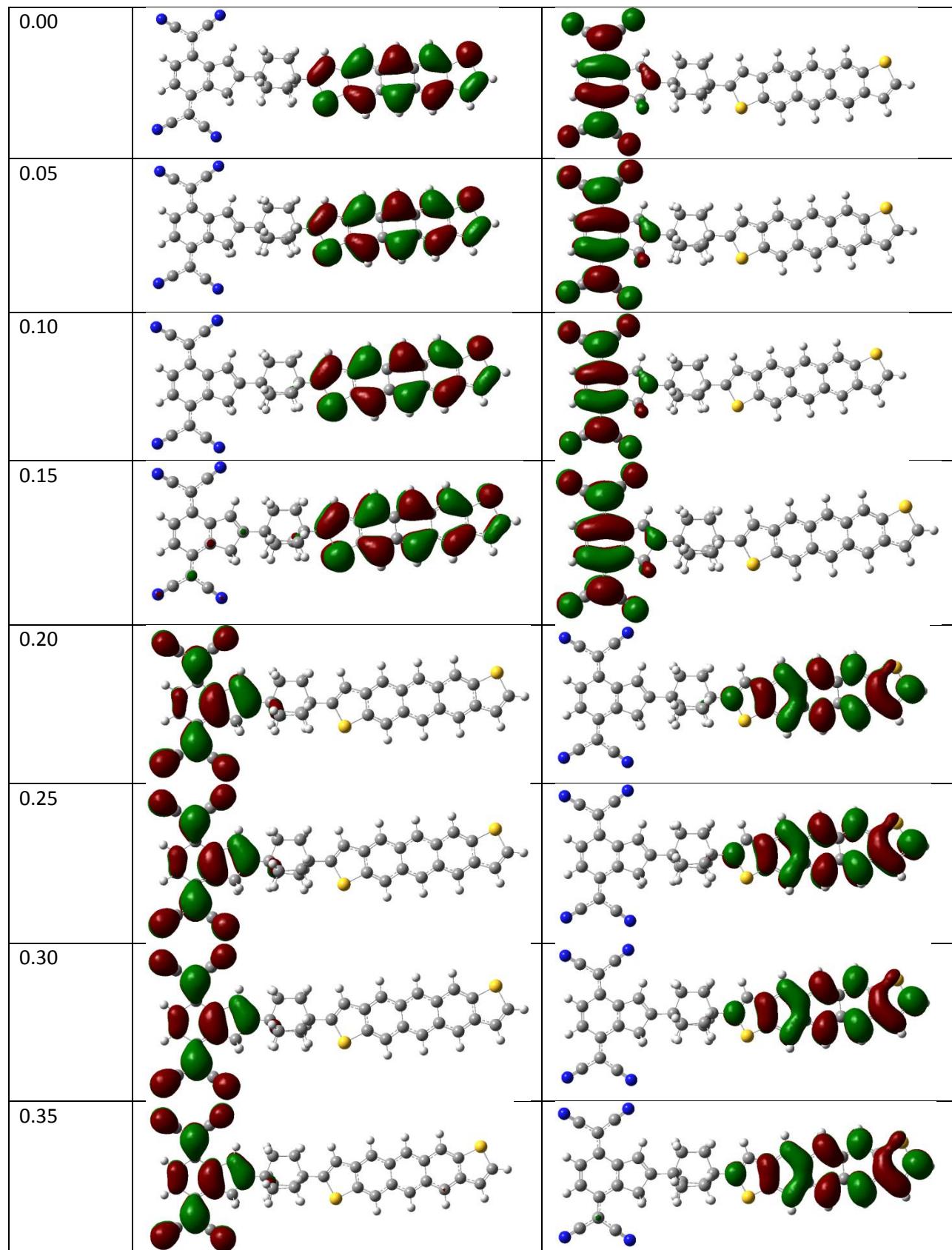
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D(52,53,59,58)	-179.9234	-179.961
D(52,53,59,65)	0.0518	0.0222
D(54,53,59,58)	0.0456	0.0343
D(54,53,59,65)	-179.9792	-179.9825
D(51,54,55,56)	-0.0042	0.0283
D(51,54,55,57)	179.983	-179.9764
D(53,54,55,56)	-179.979	-179.9689
D(53,54,55,57)	0.0083	0.0264
D(54,55,57,58)	0.0325	0.0169
D(54,55,57,69)	-179.9642	-179.9833
D(56,55,57,58)	-179.9803	-179.9879
D(56,55,57,69)	0.023	0.0119
D(55,57,58,59)	-0.0345	-0.0349
D(55,57,58,66)	179.9804	179.9758
D(69,57,58,59)	179.9623	179.9653
D(69,57,58,66)	-0.0228	-0.0239
D(55,57,69,68)	-179.996	-179.9862
D(55,57,69,71)	0.0039	0.0188
D(58,57,69,68)	0.0073	0.0136
D(58,57,69,71)	-179.9928	-179.9814
D(57,58,59,53)	-0.005	0.0088
D(57,58,59,65)	-179.9801	-179.9742
D(66,58,59,53)	179.9795	179.9976
D(66,58,59,65)	0.0044	0.0145
D(57,58,66,67)	0.0233	0.0188
D(57,58,66,70)	-179.9875	-179.9972
D(59,58,66,67)	-179.9614	-179.9701
D(59,58,66,70)	0.0279	0.0139
D(58,66,67,68)	-0.0077	-0.0024
D(58,66,67,72)	179.9953	179.9883
D(70,66,67,68)	-179.9967	-179.986
D(70,66,67,72)	0.0062	0.0047
D(66,67,68,69)	-0.0087	-0.0089
D(66,67,68,73)	179.9964	179.9844
D(72,67,68,69)	179.9884	-179.9996
D(72,67,68,73)	-0.0066	-0.0063
D(67,68,69,57)	0.0086	0.0029
D(67,68,69,71)	-179.9913	179.9978
D(73,68,69,57)	-179.9965	-179.9904
D(73,68,69,71)	0.0037	0.0045

Table S11. HOMO energy (E_{HOMO}), LUMO energy (E_{LUMO}), HOMO-LUMO gap ($E_{\text{HOMO}} - E_{\text{LUMO}}$) and the total dipole moment of TCNQ- σ - ADT system under various electric fields with B3PW91/MPW1PW91 functionals.

Electric Field (V/Å)	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{\text{HOMO}} - E_{\text{LUMO}}$ (eV)	Total dipole moment (Debye)
-0.30	-4.88/-4.91	-4.69/-4.68	0.19/0.23	79.99/79.14
-0.25	-4.88/-4.92	-4.69/-4.68	0.19/0.24	66.58/65.30
-0.20	-4.89/-4.93	-4.69/-4.68	0.20/0.25	53.35/51.65
-0.15	-4.90/-4.93	-4.70/-4.68	0.20/0.25	40.31/38.20
-0.10	-4.91/-4.94	-4.70/-4.68	0.21/0.26	27.48/24.97
-0.05	-4.92/-4.95	-4.70/-4.68	0.22/0.27	14.93/12.08
0.00	-4.97/-5.09	-4.65/-4.53	0.32/0.56	3.90/3.58
0.05	-5.27/-5.40	-4.32/-4.19	0.95/1.21	0.91/0.90
0.10	-5.56/-5.70	-3.98/-3.85	1.58/1.85	1.94/1.89
0.15	-5.85/-5.98	-3.63/-3.50	2.22/2.48	4.68/4.58
0.20	-5.61/-5.76	-3.49/-3.34	2.12/2.42	7.46/7.30
0.25	-5.29/-5.44	-3.84/-3.68	1.45/1.76	10.27/10.05
0.30	-4.96/-5.11	-4.19/-4.03	0.77/1.08	13.14/12.84
0.35	-4.70/-4.79	-4.48/-4.39	0.22/0.40	18.06/15.80
0.40	-4.72/-4.74	-4.52/-4.49	0.20/0.25	30.94/27.07

Table S12. Spatial distribution of the HOMO and LUMO of TCNQ- σ - ADT under various electric fields with B3LYP functional.





0.40

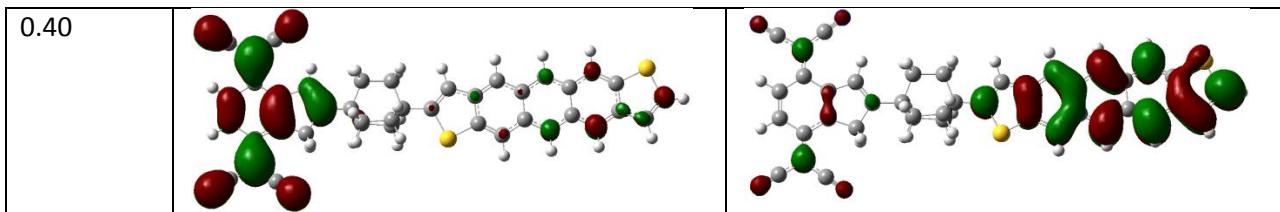


Table S13. Spatial distribution of the HOMO and LUMO of TCNQ- σ - ADT under various electric fields with B3PW91 functional.

Electric Field (V/ \AA)	HOMO	LUMO
-0.30		
-0.25		
-0.20		
-0.15		
-0.10		
-0.05		
0.00		

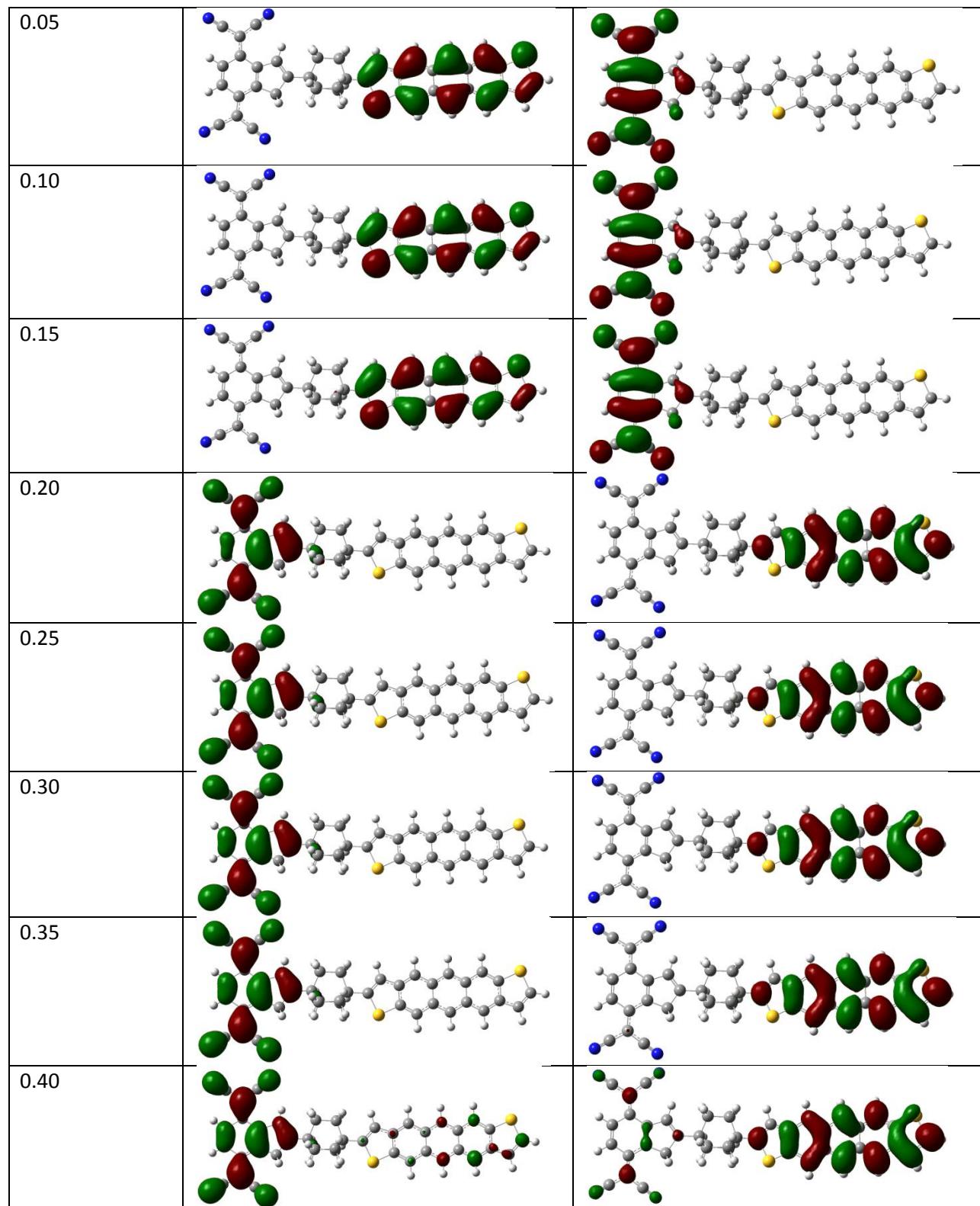


Table S14. Spatial distribution of the HOMO and LUMO of TCNQ- σ - ADT under various electric fields with MPW1PW91 functional.

Electric Field (V/ \AA)	HOMO	LUMO
-0.30		
-0.25		
-0.20		
-0.15		
-0.10		
-0.05		
0.00		

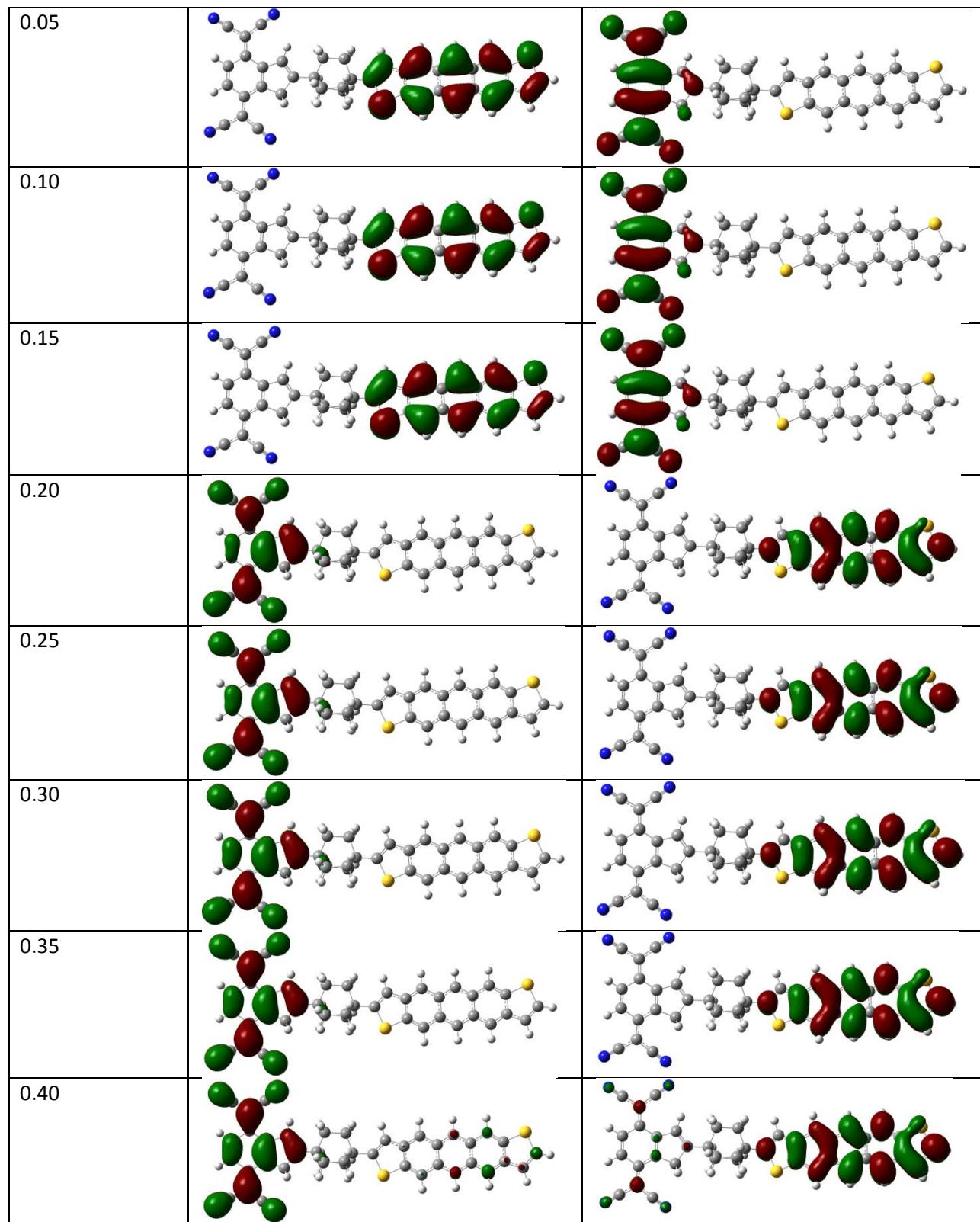


Table S15: Optimized parameters (bond lengths, bond angles and dihedral angles) of TCNQ- σ -ADT system without electric field and with an extreme electric field of 0.40 V/ \AA in reverse direction using B3LYP functional. Bond lengths are in Angstrom, bond angles and dihedral angles are in degree.

Optimized Parameters	Without Electric Field	With 0.40 V/ \AA Electric Field
R(1,2)	1.3869	1.3859
R(1,6)	1.4555	1.4542
R(1,7)	1.4574	1.4626
R(2,3)	1.4324	1.4374
R(2,9)	1.505	1.5074
R(3,4)	1.4551	1.4511
R(3,15)	1.3968	1.399
R(4,5)	1.3515	1.356
R(4,10)	1.0843	1.085
R(5,6)	1.4524	1.4499
R(5,11)	1.0842	1.0849
R(6,14)	1.3899	1.3939
R(7,8)	1.3584	1.3551
R(7,12)	1.0781	1.0779
R(8,9)	1.5092	1.5096
R(8,24)	1.5073	1.5123
R(9,13)	1.0969	1.0967
R(9,30)	1.0972	1.097
R(14,16)	1.4308	1.4264
R(14,17)	1.4267	1.4276
R(15,18)	1.4275	1.4237
R(15,19)	1.4243	1.4258
R(16,20)	1.1646	1.165
R(17,21)	1.1649	1.1654
R(18,22)	1.1652	1.1655
R(19,23)	1.1656	1.1658
R(24,25)	1.5445	1.5447
R(24,28)	1.5554	1.5535
R(24,39)	1.5559	1.5537
R(25,26)	1.5533	1.555
R(25,31)	1.0949	1.0936
R(25,32)	1.0956	1.0945
R(26,27)	1.5459	1.5472
R(26,33)	1.0953	1.0963
R(26,34)	1.0945	1.0957
R(27,29)	1.5541	1.5562
R(27,40)	1.5533	1.5555
R(27,72)	1.5108	1.5095

R(28,29)	1.5533	1.5556
R(28,35)	1.0957	1.0948
R(28,36)	1.0948	1.0937
R(29,37)	1.0946	1.0956
R(29,38)	1.095	1.0963
R(39,40)	1.5525	1.5551
R(39,41)	1.0956	1.0945
R(39,42)	1.0954	1.0944
R(40,43)	1.0953	1.096
R(40,44)	1.0942	1.0956
R(45,46)	1.4423	1.4455
R(45,47)	1.3695	1.3735
R(45,71)	1.7651	1.7538
R(46,48)	1.3791	1.3864
R(46,70)	1.4445	1.4388
R(47,50)	1.4274	1.4242
R(47,56)	1.0861	1.0863
R(48,49)	1.4233	1.4187
R(48,57)	1.0869	1.0868
R(49,50)	1.4527	1.4561
R(49,55)	1.4019	1.4091
R(50,51)	1.3994	1.4013
R(51,52)	1.0875	1.088
R(51,53)	1.4028	1.4045
R(53,54)	1.4524	1.4571
R(53,62)	1.4221	1.4188
R(54,55)	1.4006	1.3986
R(54,59)	1.4264	1.4314
R(55,58)	1.0875	1.0879
R(59,60)	1.3705	1.3722
R(59,63)	1.0861	1.0866
R(60,61)	1.4441	1.4408
R(60,65)	1.769	1.7849
R(61,62)	1.3797	1.3882
R(61,67)	1.4456	1.4405
R(62,64)	1.0869	1.0879
R(65,66)	1.7607	1.768
R(66,67)	1.3527	1.359
R(66,68)	1.0819	1.0825
R(67,69)	1.0841	1.0862
R(70,72)	1.3575	1.3638
R(70,73)	1.0833	1.0827
R(71,72)	1.7874	1.79
A(2,1,6)	120.8632	120.9364
A(2,1,7)	109.0756	108.63
A(6,1,7)	130.0612	130.4336

A(1,2,3)	122.2419	121.9779
A(1,2,9)	108.1994	108.537
A(3,2,9)	129.5588	129.4851
A(2,3,4)	116.3615	116.5862
A(2,3,15)	124.993	124.0743
A(4,3,15)	118.6455	119.3395
A(3,4,5)	122.0593	121.8946
A(3,4,10)	118.2868	118.5964
A(5,4,10)	119.6539	119.509
A(4,5,6)	122.2089	122.1815
A(4,5,11)	119.5646	119.3385
A(6,5,11)	118.2265	118.4801
A(1,6,5)	116.2652	116.4233
A(1,6,14)	125.1182	124.5499
A(5,6,14)	118.6166	119.0268
A(1,7,8)	109.9471	110.1764
A(1,7,12)	124.7045	124.2452
A(8,7,12)	125.3483	125.5782
A(7,8,9)	108.8326	108.9228
A(7,8,24)	127.8998	127.6451
A(9,8,24)	123.2654	123.4309
A(2,9,8)	103.9449	103.7333
A(2,9,13)	112.092	111.732
A(2,9,30)	112.0413	111.6804
A(8,9,13)	112.0802	112.4992
A(8,9,30)	111.8101	112.2321
A(13,9,30)	105.0745	105.1638
A(6,14,16)	121.0049	121.9684
A(6,14,17)	125.2969	124.1828
A(16,14,17)	113.6982	113.8488
A(3,15,18)	121.3839	122.2081
A(3,15,19)	123.7787	122.9508
A(18,15,19)	114.8374	114.841
A(8,24,25)	111.9656	111.9998
A(8,24,28)	110.7679	110.8532
A(8,24,39)	110.3581	110.5926
A(25,24,28)	107.8264	107.6262
A(25,24,39)	108.0632	107.8337
A(28,24,39)	107.7066	107.7659
A(24,25,26)	110.9937	111.149
A(24,25,31)	109.6601	109.7029
A(24,25,32)	109.0925	109.18
A(26,25,31)	109.9801	109.8348
A(26,25,32)	110.4292	110.3243
A(31,25,32)	106.5808	106.5389
A(25,26,27)	110.7368	110.6141

A(25,26,33)	110.4895	110.5079
A(25,26,34)	110.0147	110.03
A(27,26,33)	109.1339	109.0802
A(27,26,34)	109.5964	109.6393
A(33,26,34)	106.7823	106.8901
A(26,27,29)	107.7995	108.0169
A(26,27,40)	107.625	107.8214
A(26,27,72)	111.4061	111.4526
A(29,27,40)	108.1706	108.0725
A(29,27,72)	110.6828	110.4755
A(40,27,72)	111.012	110.8719
A(24,28,29)	110.5898	110.9626
A(24,28,35)	108.7366	108.8205
A(24,28,36)	110.0659	110.1204
A(29,28,35)	110.771	110.5296
A(29,28,36)	109.9358	109.6674
A(35,28,36)	106.6585	106.6444
A(27,29,28)	110.8689	110.4884
A(27,29,37)	109.1435	109.3359
A(27,29,38)	109.2701	109.2368
A(28,29,37)	110.6449	110.7726
A(28,29,38)	110.3923	110.3812
A(37,29,38)	106.4075	106.5337
A(24,39,40)	110.627	111.021
A(24,39,41)	109.2545	109.3984
A(24,39,42)	109.4247	109.4019
A(40,39,41)	110.2029	110.0114
A(40,39,42)	110.5279	110.2198
A(41,39,42)	106.7158	106.6869
A(27,40,39)	110.7778	110.445
A(27,40,43)	108.5866	108.6345
A(27,40,44)	109.9421	110.0305
A(39,40,43)	110.8371	110.9576
A(39,40,44)	110.2179	110.2132
A(43,40,44)	106.3715	106.4721
A(46,45,47)	122.1178	121.9116
A(46,45,71)	110.6732	110.8836
A(47,45,71)	127.2089	127.2047
A(45,46,48)	119.2731	118.9643
A(45,46,70)	111.5581	111.4602
A(48,46,70)	129.1688	129.5755
A(45,47,50)	119.4377	119.7479
A(45,47,56)	121.4637	121.0829
A(50,47,56)	119.0986	119.1692
A(46,48,49)	120.6934	120.964
A(46,48,57)	120.3157	119.9723

A(49,48,57)	118.9909	119.0637
A(48,49,50)	119.2358	119.2327
A(48,49,55)	121.922	122.3448
A(50,49,55)	118.8421	118.4225
A(47,50,49)	119.2421	119.1795
A(47,50,51)	121.736	121.8341
A(49,50,51)	119.0219	118.9864
A(50,51,52)	118.9867	118.6929
A(50,51,53)	122.1506	122.5031
A(52,51,53)	118.8628	118.804
A(51,53,54)	118.8424	118.6007
A(51,53,62)	121.88	122.1559
A(54,53,62)	119.2775	119.2433
A(53,54,55)	118.986	118.9247
A(53,54,59)	119.2644	118.8648
A(55,54,59)	121.7497	122.2105
A(49,55,54)	122.157	122.5626
A(49,55,58)	118.8848	118.4829
A(54,55,58)	118.9582	118.9545
A(54,59,60)	119.4831	119.7354
A(54,59,63)	119.0937	118.7606
A(60,59,63)	121.4232	121.504
A(59,60,61)	122.0098	122.2067
A(59,60,65)	127.2198	127.5285
A(61,60,65)	110.7703	110.2647
A(60,61,62)	119.2591	118.7902
A(60,61,67)	111.4806	111.7925
A(62,61,67)	129.2603	129.4173
A(53,62,61)	120.7061	121.1595
A(53,62,64)	119.0221	118.7873
A(61,62,64)	120.2719	120.0532
A(60,65,66)	90.6357	90.935
A(65,66,67)	113.8965	112.884
A(65,66,68)	118.7106	119.3251
A(67,66,68)	127.3928	127.7909
A(61,67,66)	113.2168	114.1238
A(61,67,69)	123.266	122.6023
A(66,67,69)	123.5172	123.2739
A(46,70,72)	114.6285	114.7698
A(46,70,73)	122.1442	122.6783
A(72,70,73)	123.2274	122.5519
A(45,71,72)	91.3969	91.6236
A(27,72,70)	129.0634	129.6054
A(70,72,71)	111.743	111.2625
D(6,1,2,3)	-0.0532	-0.1018
D(6,1,2,9)	179.9596	179.9323

D(7,1,2,3)	179.9599	179.9073
D(7,1,2,9)	-0.0272	-0.0586
D(2,1,6,5)	0.1068	0.1688
D(2,1,6,14)	-179.8328	-179.7383
D(7,1,6,5)	-179.9094	-179.8425
D(7,1,6,14)	0.151	0.2503
D(2,1,7,8)	0.1571	0.1933
D(2,1,7,12)	-179.6944	-179.6475
D(6,1,7,8)	-179.8282	-179.7964
D(6,1,7,12)	0.3203	0.3628
D(1,2,3,4)	-0.0175	-0.0057
D(1,2,3,15)	-179.985	-179.9666
D(9,2,3,4)	179.9667	179.9525
D(9,2,3,15)	-0.0008	-0.0084
D(1,2,9,8)	-0.0954	-0.0783
D(1,2,9,13)	-121.3469	-121.5103
D(1,2,9,30)	120.8037	121.0062
D(3,2,9,8)	179.9187	179.9591
D(3,2,9,13)	58.6672	58.5271
D(3,2,9,30)	-59.1822	-58.9563
D(2,3,4,5)	0.0307	0.0399
D(2,3,4,10)	-179.9759	-179.9756
D(15,3,4,5)	-179.9996	-179.9973
D(15,3,4,10)	-0.0062	-0.0128
D(2,3,15,18)	179.9931	179.996
D(2,3,15,19)	-0.0011	0.0079
D(4,3,15,18)	0.0262	0.0361
D(4,3,15,19)	-179.9679	-179.952
D(3,4,5,6)	0.0279	0.0351
D(3,4,5,11)	179.9844	179.9698
D(10,4,5,6)	-179.9654	-179.9493
D(10,4,5,11)	-0.0089	-0.0146
D(4,5,6,1)	-0.0952	-0.1369
D(4,5,6,14)	179.8485	179.7756
D(11,5,6,1)	179.9478	179.9278
D(11,5,6,14)	-0.1085	-0.1596
D(1,6,14,16)	-179.9934	-179.9662
D(1,6,14,17)	0.0767	0.1302
D(5,6,14,16)	0.0683	0.1289
D(5,6,14,17)	-179.8616	-179.7747
D(1,7,8,9)	-0.2172	-0.2424
D(1,7,8,24)	-179.6845	-179.8416
D(12,7,8,9)	179.6332	179.5958
D(12,7,8,24)	0.1659	-0.0034
D(7,8,9,2)	0.1925	0.1976
D(7,8,9,13)	121.4519	121.1143

D(7,8,9,30)	-120.8617	-120.5153
D(24,8,9,2)	179.6899	179.8174
D(24,8,9,13)	-59.0507	-59.2659
D(24,8,9,30)	58.6356	59.1045
D(7,8,24,25)	1.448	1.9904
D(7,8,24,28)	-118.9488	-118.2336
D(7,8,24,39)	121.8638	122.2989
D(9,8,24,25)	-177.9491	-177.5553
D(9,8,24,28)	61.6541	62.2207
D(9,8,24,39)	-57.5332	-57.2468
D(8,24,25,26)	-175.6384	-175.5475
D(8,24,25,31)	-53.9203	-53.881
D(8,24,25,32)	62.4604	62.5235
D(28,24,25,26)	-53.5437	-53.4602
D(28,24,25,31)	68.1744	68.2062
D(28,24,25,32)	-175.4449	-175.3892
D(39,24,25,26)	62.6189	62.5503
D(39,24,25,31)	-175.663	-175.7832
D(39,24,25,32)	-59.2822	-59.3787
D(8,24,28,29)	-174.4161	-174.2649
D(8,24,28,35)	63.75	63.9094
D(8,24,28,36)	-52.7482	-52.6509
D(25,24,28,29)	62.7526	62.9398
D(25,24,28,35)	-59.0812	-58.8858
D(25,24,28,36)	-175.5794	-175.4461
D(39,24,28,29)	-53.6431	-53.1152
D(39,24,28,35)	-175.4769	-174.9409
D(39,24,28,36)	68.0249	68.4988
D(8,24,39,40)	-175.2615	-175.5948
D(8,24,39,41)	63.2487	62.8052
D(8,24,39,42)	-53.2536	-53.7313
D(25,24,39,40)	-52.532	-52.8261
D(25,24,39,41)	-174.0218	-174.4261
D(25,24,39,42)	69.4759	69.0375
D(28,24,39,40)	63.7086	63.0929
D(28,24,39,41)	-57.7812	-58.5071
D(28,24,39,42)	-174.2835	-175.0435
D(24,25,26,27)	-8.0584	-8.0027
D(24,25,26,33)	112.9809	112.9
D(24,25,26,34)	-129.363	-129.2908
D(31,25,26,27)	-129.5892	-129.5921
D(31,25,26,33)	-8.5499	-8.6894
D(31,25,26,34)	109.1062	109.1198
D(32,25,26,27)	113.0593	113.2583
D(32,25,26,33)	-125.9013	-125.839
D(32,25,26,34)	-8.2452	-8.0298

D(25,26,27,29)	62.8322	62.8241
D(25,26,27,40)	-53.6331	-53.7413
D(25,26,27,72)	-175.547	-175.6401
D(33,26,27,29)	-59.006	-58.923
D(33,26,27,40)	-175.4713	-175.4883
D(33,26,27,72)	62.6148	62.6128
D(34,26,27,29)	-175.6167	-175.657
D(34,26,27,40)	67.9179	67.7777
D(34,26,27,72)	-53.9959	-54.1212
D(26,27,29,28)	-53.4535	-53.2447
D(26,27,29,37)	68.6707	68.9202
D(26,27,29,38)	-175.3461	-174.8563
D(40,27,29,28)	62.6551	63.1574
D(40,27,29,37)	-175.2207	-174.6777
D(40,27,29,38)	-59.2375	-58.4542
D(72,27,29,28)	-175.5223	-175.3834
D(72,27,29,37)	-53.3981	-53.2186
D(72,27,29,38)	62.5851	63.0049
D(26,27,40,39)	63.6059	63.2636
D(26,27,40,43)	-58.3308	-58.6439
D(26,27,40,44)	-174.3296	-174.8395
D(29,27,40,39)	-52.6161	-53.2655
D(29,27,40,43)	-174.5528	-175.1729
D(29,27,40,44)	69.4484	68.6314
D(72,27,40,39)	-174.2359	-174.4789
D(72,27,40,43)	63.8275	63.6136
D(72,27,40,44)	-52.1714	-52.582
D(26,27,72,70)	0.1344	0.2417
D(29,27,72,70)	120.0651	120.3384
D(40,27,72,70)	-119.797	-119.8748
D(24,28,29,27)	-8.0203	-8.4084
D(24,28,29,37)	-129.2642	-129.7254
D(24,28,29,38)	113.2135	112.5245
D(35,28,29,27)	112.6087	112.413
D(35,28,29,37)	-8.6353	-8.904
D(35,28,29,38)	-126.1576	-126.6541
D(36,28,29,27)	-129.7648	-130.2873
D(36,28,29,37)	108.9912	108.3957
D(36,28,29,38)	-8.5311	-9.3544
D(24,39,40,27)	-9.133	-8.5763
D(24,39,40,43)	111.476	111.9513
D(24,39,40,44)	-131.036	-130.3654
D(41,39,40,27)	111.7954	112.6643
D(41,39,40,43)	-127.5956	-126.8081
D(41,39,40,44)	-10.1076	-9.1248
D(42,39,40,27)	-130.4911	-129.9614

D(42,39,40,43)	-9.8822	-9.4338
D(42,39,40,44)	107.6059	108.2495
D(47,45,46,48)	0.0363	0.0272
D(47,45,46,70)	-179.8795	-179.8978
D(71,45,46,48)	179.9506	179.9367
D(71,45,46,70)	0.0348	0.0117
D(46,45,47,50)	0.0197	0.0285
D(46,45,47,56)	179.969	179.9802
D(71,45,47,50)	-179.8796	-179.8654
D(71,45,47,56)	0.0696	0.0863
D(46,45,71,72)	-0.1171	-0.0929
D(47,45,71,72)	179.7918	179.8106
D(45,46,48,49)	-0.0635	-0.0661
D(45,46,48,57)	-179.989	-179.9927
D(70,46,48,49)	179.8354	179.8433
D(70,46,48,57)	-0.0901	-0.0833
D(45,46,70,72)	0.1039	0.1123
D(45,46,70,73)	-179.8718	-179.8857
D(48,46,70,72)	-179.8013	-179.8025
D(48,46,70,73)	0.223	0.1994
D(45,47,50,49)	-0.047	-0.0445
D(45,47,50,51)	179.906	179.9144
D(56,47,50,49)	-179.9975	-179.9972
D(56,47,50,51)	-0.0445	-0.0383
D(46,48,49,50)	0.0358	0.0496
D(46,48,49,55)	-179.8928	-179.8916
D(57,48,49,50)	179.9623	179.9769
D(57,48,49,55)	0.0337	0.0357
D(48,49,50,47)	0.0202	0.0065
D(48,49,50,51)	-179.9341	-179.9536
D(55,49,50,47)	179.9511	179.95
D(55,49,50,51)	-0.0033	-0.0101
D(48,49,55,54)	179.9004	179.9193
D(48,49,55,58)	-0.0463	-0.0337
D(50,49,55,54)	-0.0285	-0.0223
D(50,49,55,58)	-179.9753	-179.9754
D(47,50,51,52)	0.0573	0.0503
D(47,50,51,53)	-179.9169	-179.9222
D(49,50,51,52)	-179.9896	-179.9907
D(49,50,51,53)	0.0362	0.0368
D(50,51,53,54)	-0.0371	-0.0308
D(50,51,53,62)	179.9525	179.9564
D(52,51,53,54)	179.9887	179.9967
D(52,51,53,62)	-0.0217	-0.016
D(51,53,54,55)	0.0051	-0.0019
D(51,53,54,59)	179.9704	179.9696

D(62,53,54,55)	-179.9848	-179.9895
D(62,53,54,59)	-0.0196	-0.018
D(51,53,62,61)	-179.9664	-179.9665
D(51,53,62,64)	0.0261	0.0241
D(54,53,62,61)	0.0232	0.0207
D(54,53,62,64)	-179.9843	-179.9888
D(53,54,55,49)	0.0276	0.0283
D(53,54,55,58)	179.9743	179.9812
D(59,54,55,49)	-179.9368	-179.9422
D(59,54,55,58)	0.0099	0.0106
D(53,54,59,60)	0.0023	0.004
D(53,54,59,63)	-179.974	-179.9749
D(55,54,59,60)	179.9666	179.9746
D(55,54,59,63)	-0.0097	-0.0043
D(54,59,60,61)	0.0119	0.0078
D(54,59,60,65)	-179.9826	-179.9814
D(63,59,60,61)	179.9876	179.9861
D(63,59,60,65)	-0.0069	-0.0031
D(59,60,61,62)	-0.0085	-0.0055
D(59,60,61,67)	179.9932	-179.9994
D(65,60,61,62)	179.9868	179.9854
D(65,60,61,67)	-0.0116	-0.0085
D(59,60,65,66)	-179.9942	179.999
D(61,60,65,66)	0.0108	0.0088
D(60,61,62,53)	-0.0095	-0.0091
D(60,61,62,64)	179.9981	-179.9996
D(67,61,62,53)	179.9885	179.9835
D(67,61,62,64)	-0.004	-0.0069
D(60,61,67,66)	0.0061	0.0034
D(60,61,67,69)	179.9978	179.9951
D(62,61,67,66)	-179.992	-179.9897
D(62,61,67,69)	-0.0003	0.002
D(60,65,66,67)	-0.0077	-0.0071
D(60,65,66,68)	179.9879	-179.9942
D(65,66,67,61)	0.0023	0.0035
D(65,66,67,69)	-179.9894	-179.9881
D(68,66,67,61)	180.0072	179.9892
D(68,66,67,69)	0.0155	-0.0024
D(46,70,72,27)	-179.7652	-179.7957
D(46,70,72,71)	-0.1929	-0.1816
D(73,70,72,27)	0.2102	0.2023
D(73,70,72,71)	179.7825	179.8165
D(45,71,72,70)	0.1783	0.1572