Supplementary Information

Raman Spectroscopy and Microscopy of Electrochemically and Chemically Doped High-mobility Semiconducting Polymers

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Content

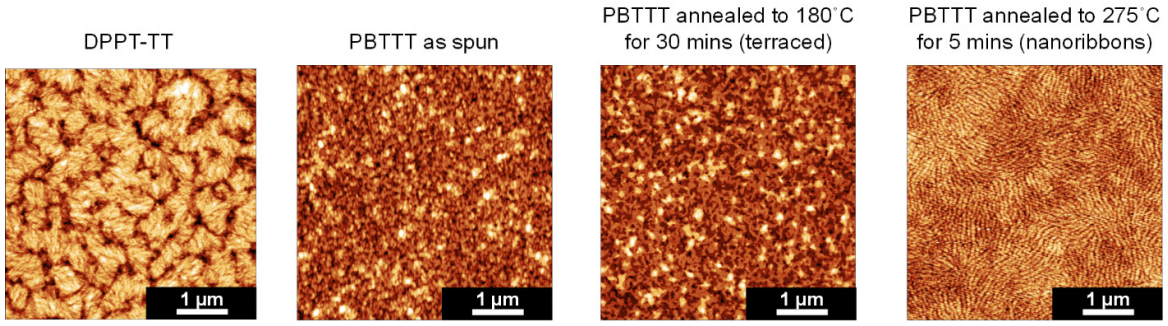

Figure S1. Atomic force microscopy (tapping-mode) images of spincoated thin films of DPPT-TT and PBTTT (Bruker Dimension Icon Atomic Force Microscope).

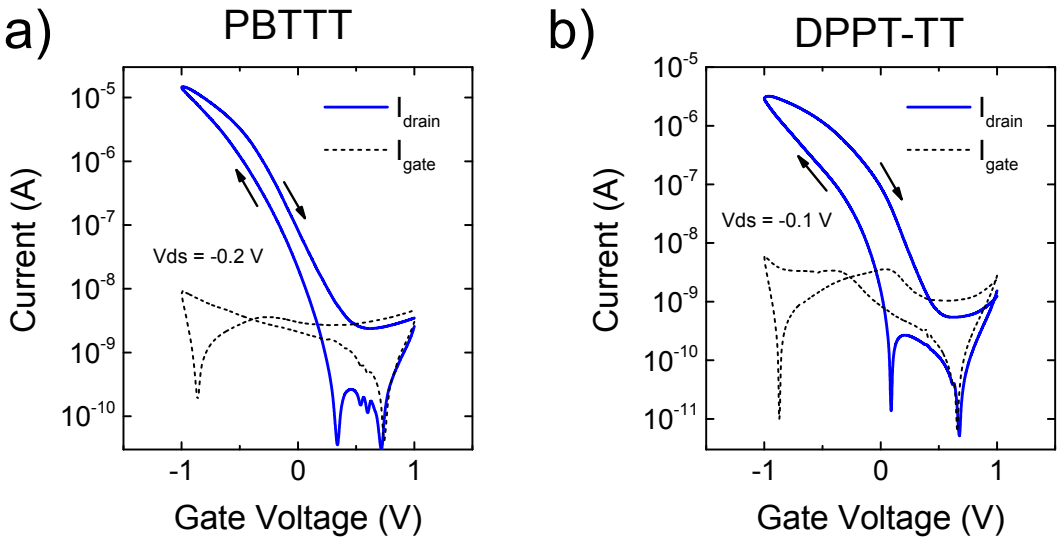

Figure S2. Transfer characteristics of electrolyte-gated PBTTT (a) and DPPT-TT (b) transistors, measured in air, indicating intrinsic hole doping.

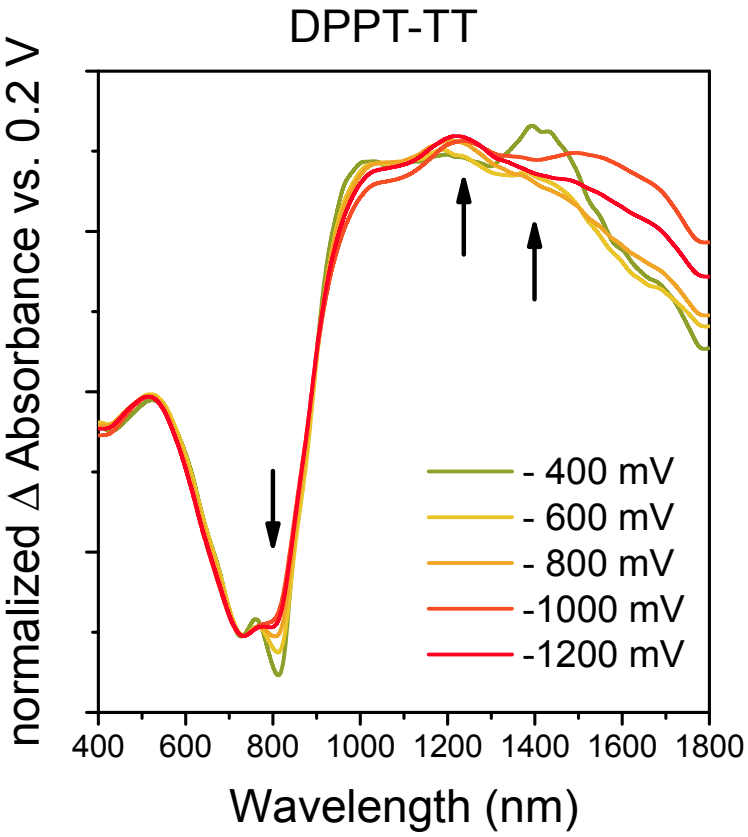

Figure S3. Normalized UV-Vis absorption spectra of electrochemically doped DPPT-TT depending on applied gate voltage.

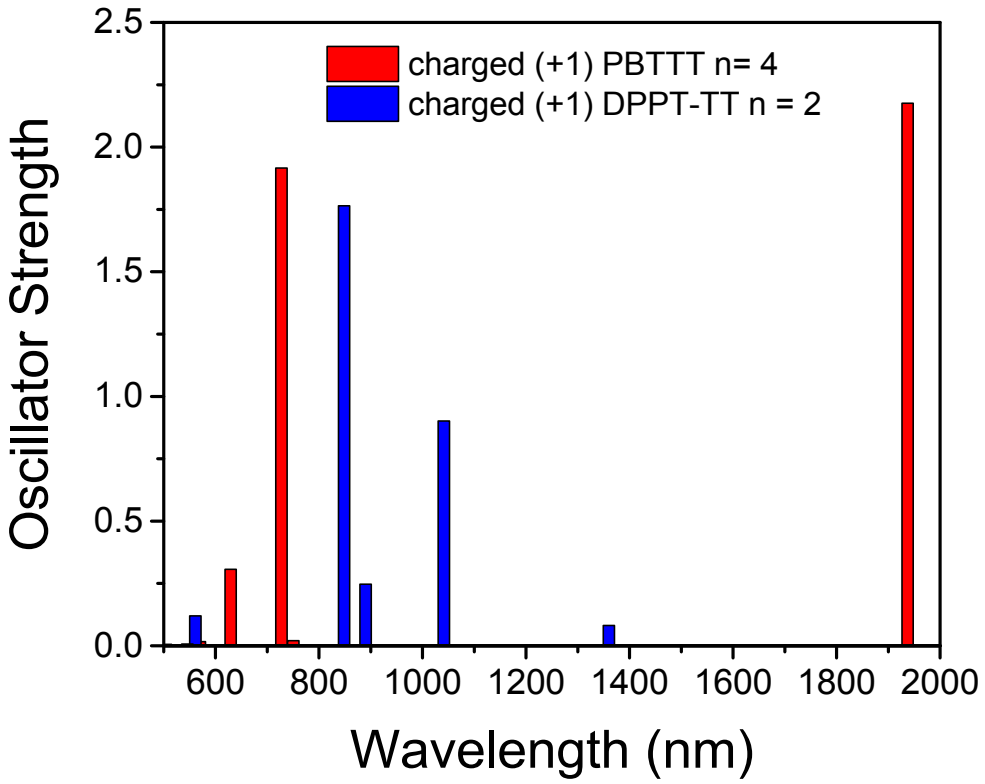

Figure S4. TD-ωB97X-D3/6-311+G* vertical transition energies for the charged (+1) species of PBTTT (n = 4, red) and DPPT-TT (n = 2, blue). n – number of monomer units.

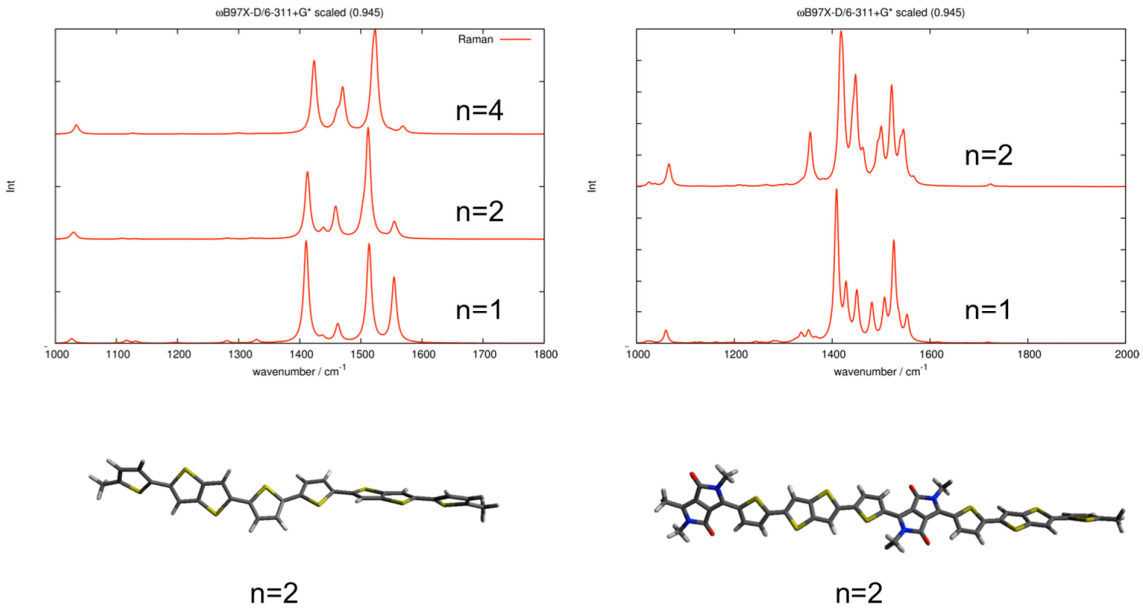

Figure S5. Evolution of DFT Raman spectra computed for PBTTT oligomers (n=1, 2, 4; left) and DPPT-TT oligomers (n=1, 2; right), together with sketches of the molecular structures of the n=2 oligomers.

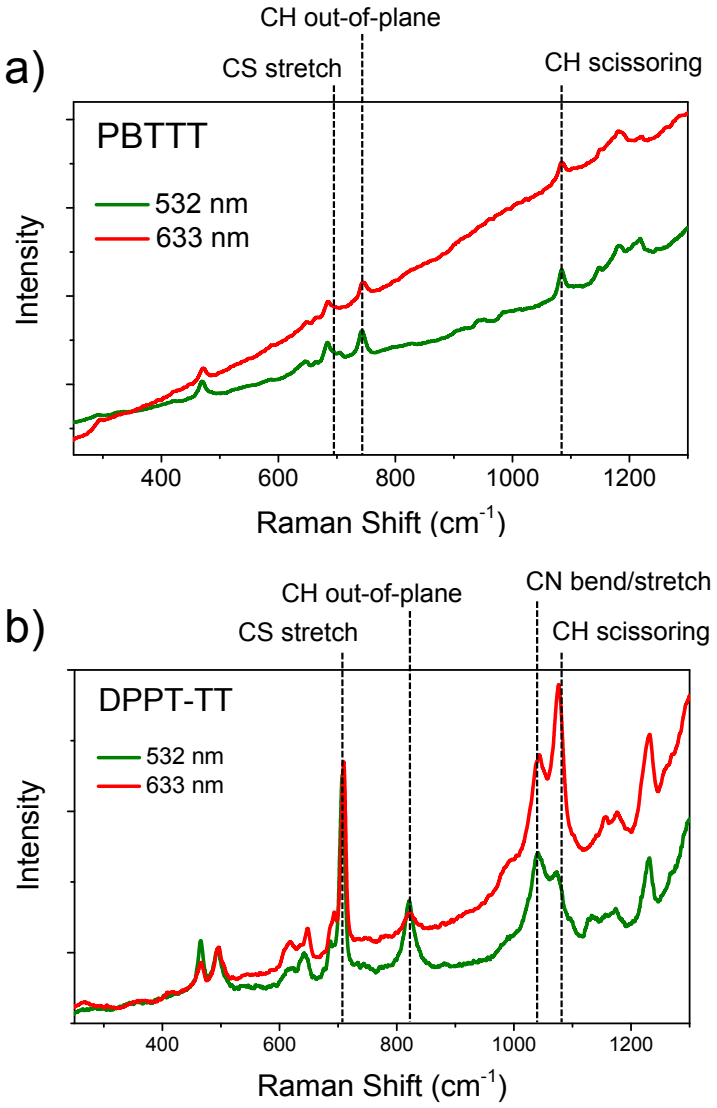

Figure S6. Raman spectra of PBTTT (a) and DPPT-TT (b) at low wavenumbers and assignment of vibrations based on DFT calculations.

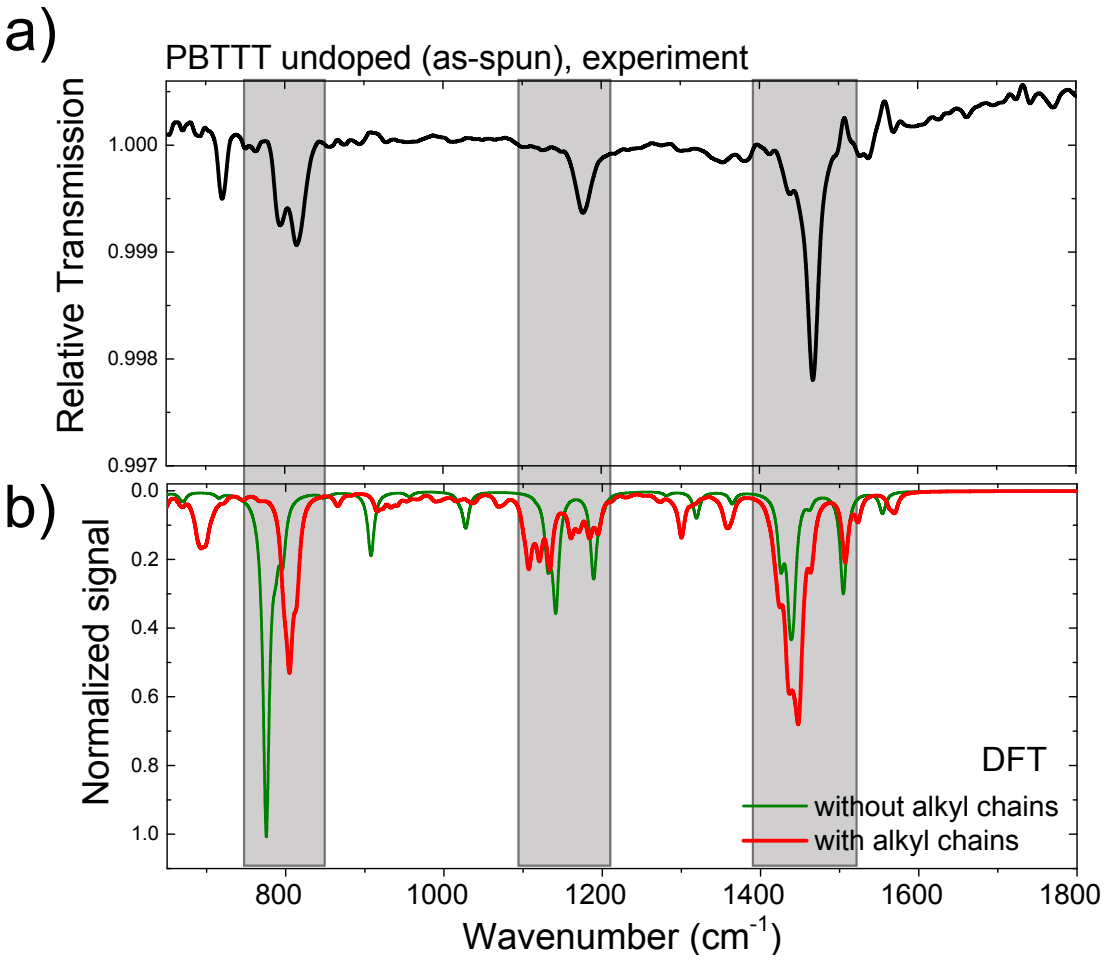

Figure S7. Experimental relative transmission spectrum of a thin layer of PBTTT on silicon (a) shown in comparison to a DFT calculated normalized absoprtion spectrum with and without alkyl side-chains (b). The experimental spectrum was measured under vacuum (3 mbar) and near normal transmission using an angle of incidence of 10°. The positions of the experimental and theoretical absorption bands, as well as the relative peak intensites are in good agreement. Minor deviations can be attributed to intermolecular interactions in the thin organic film (polarizing surrounding media) which were not taken into account for the DFT calculations of the oligomers in vacuum.

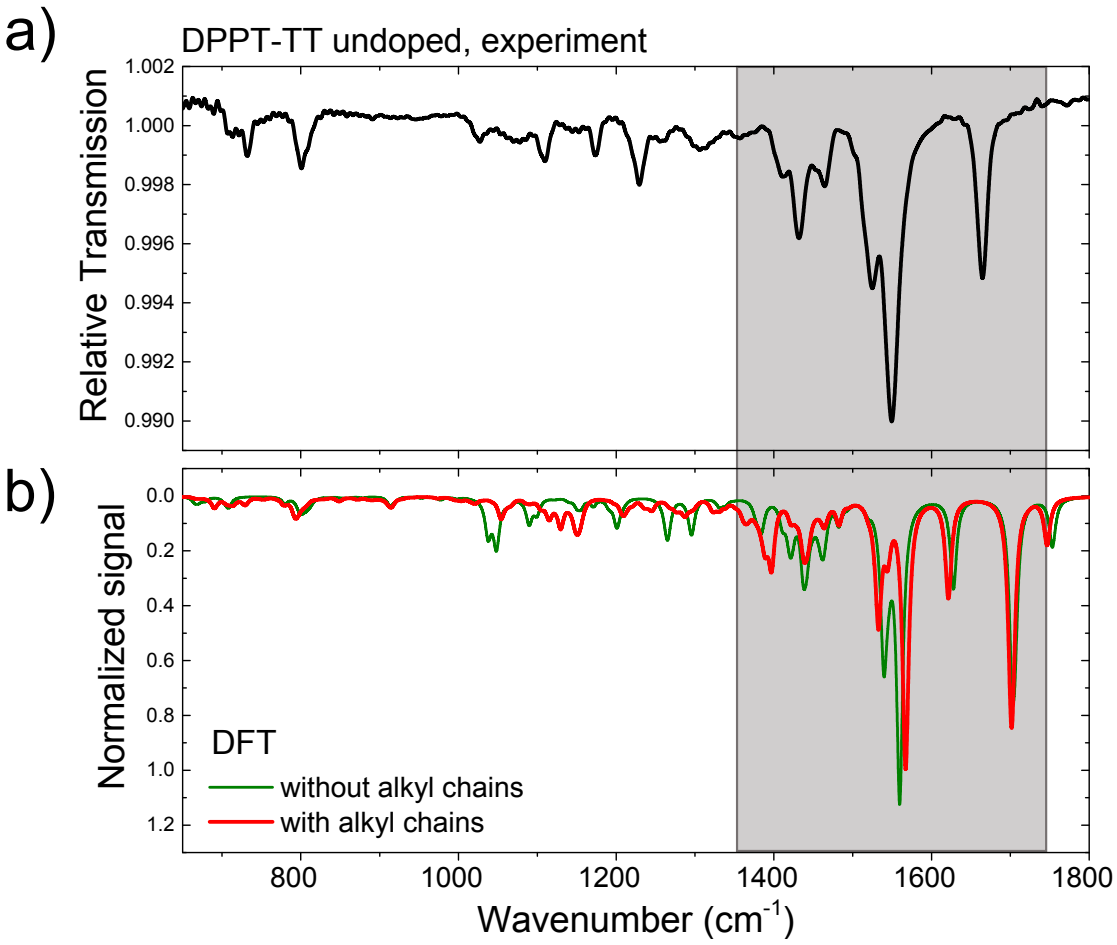

Figure S8. Experimental relative transmission spectrum of a thin layer of DPPT-TT on silicon (a) shown in comparison to a DFT calculated normalized absoprtion spectrum with and without alkyl side-chains (b). The experimental spectrum was measured under vacuum (3 mbar) and near normal transmission using an angle of incidence of 10°. The positions of the experimental and theoretical absorption bands, as well as the relative peak intensites are in good agreement. Minor deviations can be attributed to intermolecular interactions in the thin organic film (polarizing surrounding media) which were not taken into account for the DFT calculations of the oligomers in vacuum.

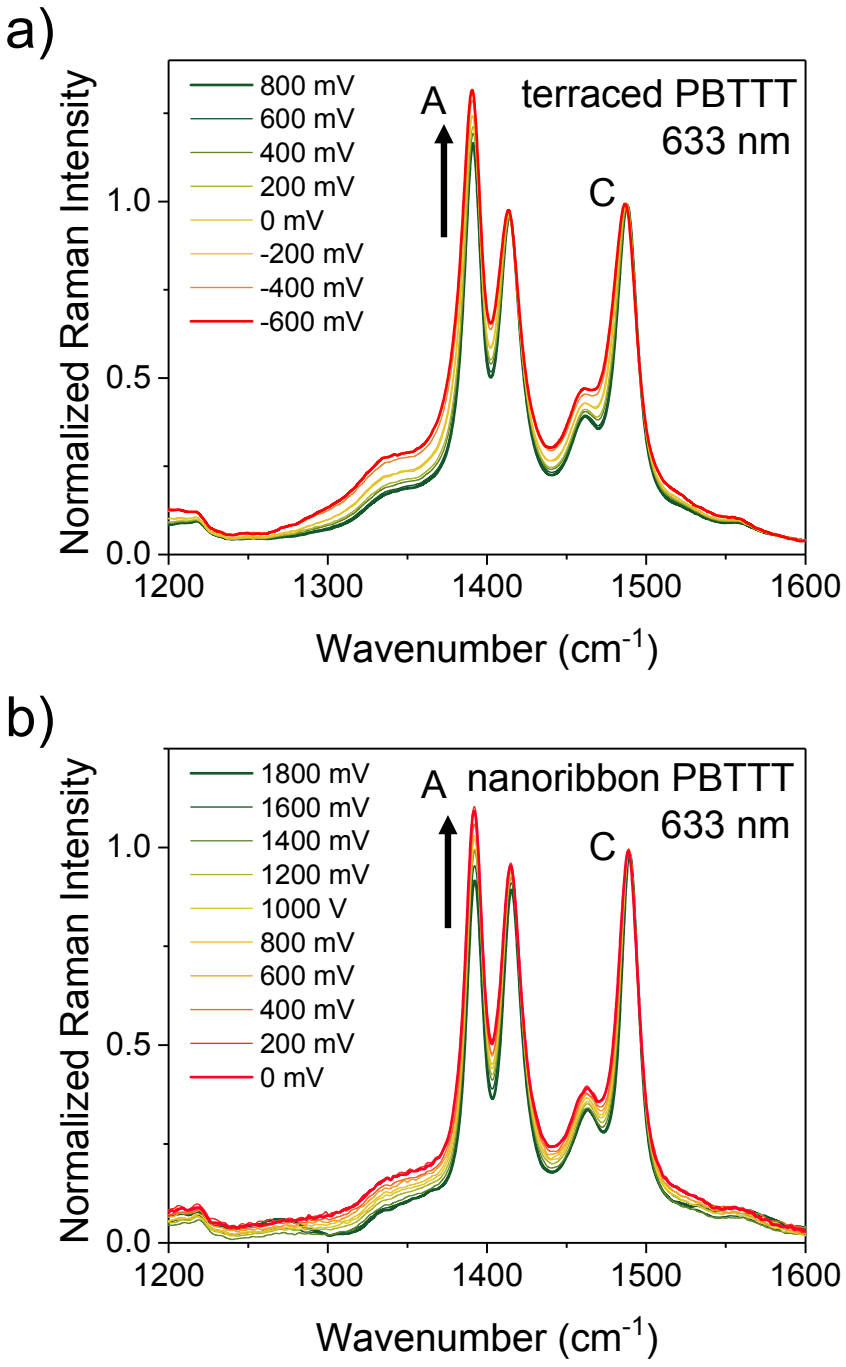

Figure S9. Raman spectra of electrochemically doped PBTTT depending on applied gate voltage, (a) terraced, (b) nanoribbon morphology. Raman intensity was normalized with respect to 1488 cm^{-1} peak (mode C). Note that the absolute gate voltage values vary due to various degrees of intrinsic p-doping in air.

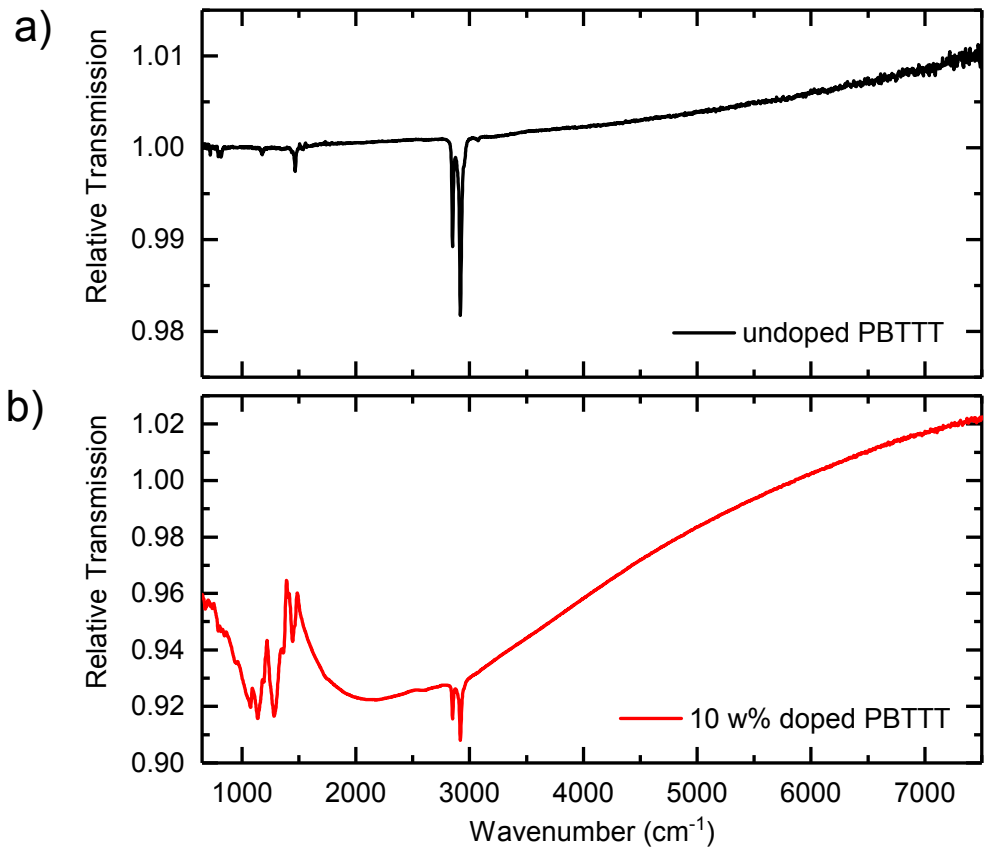

Figure S10. Experimental relative IR transmission spectra of thin layers of undoped PBTTT (a) and PBTTT doped with 10 w% Mo(tfd-$COCF_3$)$_3$ (b) on silicon. The spectra were measured under vacuum (3 mbar) and near normal transmission using an angle of incidence of 10°. The broad absorption band around 2000 cm^{-1} can be attributed to the formation of positive polarons on the polymer chain, whereas the strong increase of the vibrational modes below 1500 cm^{-1} can be ascribed to characteristic IR active vibrations (IRAV) of the charged polymer chain. Both spectral features confirm successful doping of PBTTT with Mo(tfd-$COCF_3$)$_3$.

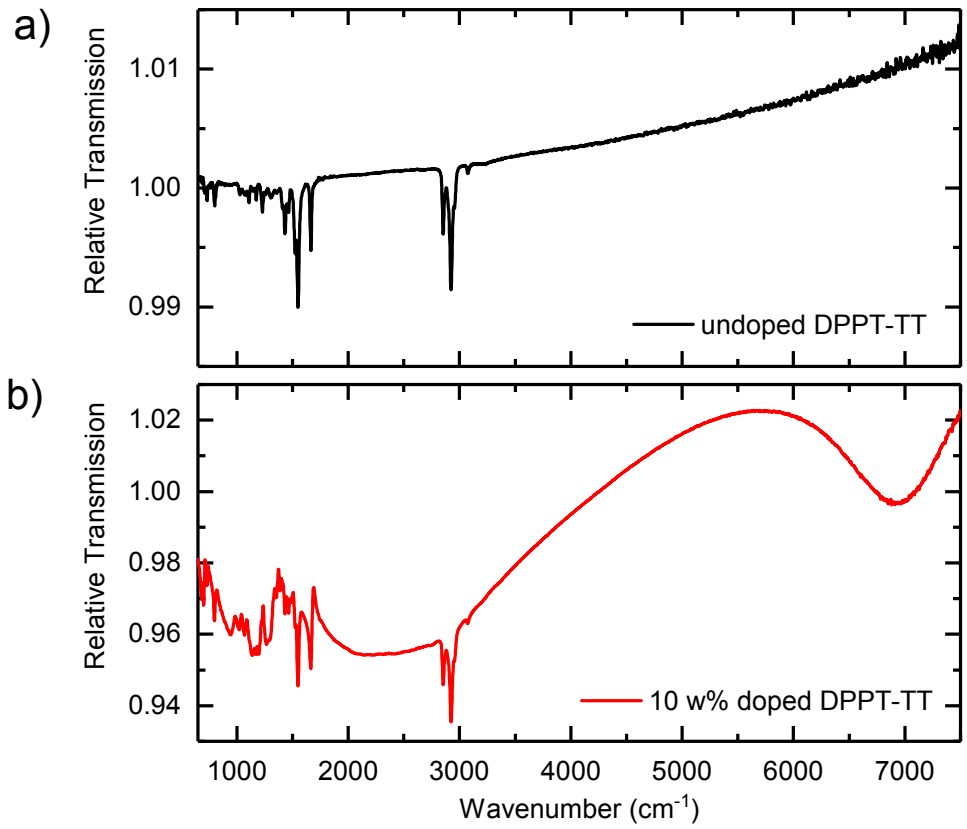

Figure S11. Experimental relative IR transmission spectra of thin layers of undoped DPPT-TT (a) and DPPT-TT doped with 10 w% $Mo(tfd\text{-}COCF_3)_3$ (b) on silicon. The spectra were measured under vacuum (3 mbar) and near normal transmission using an angle of incidence of 10°. The broad absorption band around 2000 cm^{-1} and 7000 cm^{-1} can be attributed to the formation of positive polarons on the polymer chain, whereas the strong increase of the vibrational modes below 1500 cm^{-1} can be ascribed to characteristic IR active vibrations (IRAV) of the charged polymer chain. Both spectral features confirm successful doping of DPPT-TT with $Mo(tfd\text{-}COCF_3)_3$.

S12. Optimized DFT (ωB97X-D3/6-311+G*) geometries.

(Atom and Cartesian Coordinates X / Y / Z)

$PBTT_1$ – Ground State (neutral)

16	-4.751664	-0.924369	-0.570124
6	-3.739203	0.295041	0.147412
6	-4.503543	1.287141	0.693235
6	-5.900836	1.062833	0.546078
6	-6.202279	-0.095139	-0.105043
6	-2.290534	0.175851	0.115958
16	-1.300441	1.623101	0.083657
6	0.147500	0.674315	0.085097
6	-0.147509	-0.674361	0.085037
6	-1.537572	-0.965002	0.107248
16	1.300459	-1.623153	0.083588
6	2.290543	-0.175853	0.116001
6	1.537559	0.964974	0.107333
6	3.739207	-0.295031	0.147464
16	4.751642	0.924339	-0.570210
6	6.202275	0.095191	-0.105036
6	5.900850	-1.062742	0.546169
6	4.503562	-1.287091	0.693327
6	7.551214	0.659278	-0.421006
6	-7.551225	-0.659238	-0.420966
1	-4.080825	2.142933	1.205968
1	-6.660401	1.738540	0.921838
1	7.690950	0.804440	-1.495763
1	7.711237	1.624519	0.067603
1	8.327212	-0.025138	-0.072516
1	6.660435	-1.738394	0.921990
1	4.080863	-2.142847	1.206133
1	-7.691011	-0.804378	-1.495719
1	-7.711198	-1.624500	0.067622
1	-8.327214	0.025154	-0.072412
1	-1.966233	-1.958364	0.142342
1	1.966204	1.958342	0.142493

$PBTT_2$ – Ground State (neutral)

C	11.191412	1.746367	0.461840
C	10.523042	0.599107	0.140453
S	11.643644	-0.710036	-0.095467
C	13.010775	0.308947	0.219655
C	12.603464	1.577020	0.507000
C	9.091714	0.388583	-0.006270
S	7.972874	1.305494	0.985316
C	6.619352	0.525432	0.238846
C	7.038708	-0.397835	-0.698344
C	8.448863	-0.477573	-0.845623
C	5.208849	0.628562	0.361730
C	4.566022	-0.230099	-0.485839
S	5.686628	-1.184619	-1.439205

C	3.134816	-0.420471	-0.652552
S	2.050908	-0.208269	0.687521
C	0.667340	-0.594784	-0.287579
C	1.045676	-0.872197	-1.573405
C	2.444217	-0.770688	-1.780991
C	-0.667325	-0.594651	0.287700
S	-2.050907	-0.208673	-0.687594
C	-3.134802	-0.420188	0.652599
C	-2.444189	-0.769804	1.781215
C	-1.045648	-0.871399	1.573673
C	-4.566012	-0.229915	0.485809
S	-5.686591	-1.183994	1.439648
C	-7.038692	-0.397547	0.698465
C	-6.619362	0.525279	-0.239170
C	-5.208862	0.628345	-0.362150
C	-8.448841	-0.477203	0.845835
C	-9.091717	0.388563	0.006101
S	-7.972906	1.305013	-0.985944
C	-10.523048	0.599031	-0.140659
S	-11.643663	-0.709956	0.096074
C	-13.010794	0.308879	-0.219532
C	-12.603476	1.576781	-0.507616
C	-11.191417	1.746125	-0.462643
C	-14.405062	-0.230304	-0.164164
C	14.405036	-0.230294	0.164684
H	-10.691500	2.691262	-0.637900
H	-13.298294	2.375881	-0.738544
H	-0.341820	-1.154315	2.347060
H	-2.924109	-0.936171	2.737965
H	-14.563789	-1.020023	-0.903937
H	-14.640744	-0.645031	0.819709
H	-15.119453	0.569060	-0.370626
H	-8.967254	-1.118469	1.547019
H	-4.689300	1.312962	-1.020395
H	2.924146	-0.937556	-2.737648
H	0.341858	-1.155534	-2.346647
H	14.563701	-1.019590	0.904921
H	14.640774	-0.645590	-0.818936
H	15.119429	0.569175	0.370733
H	13.298282	2.376235	0.737528
H	10.691499	2.691611	0.636533
H	4.689269	1.313484	1.019644
H	8.967299	-1.119169	-1.546486

$PBTT_4$ – Ground State (neutral)

C -2.519841 -1.307977 -1.674412
C -3.166320 -1.003069 -0.503824
S -2.022628 -0.759690 0.783211
C -0.678569 -1.122145 -0.258292
C -1.110143 -1.375311 -1.535161
C -4.592838 -0.873292 -0.262292
C -5.266301 -1.041618 0.919003
C -6.661915 -0.835649 0.757317
C -7.042712 -0.520398 -0.535500
S -5.666266 -0.448430 -1.585393
C -8.442575 -0.349678 -0.704322
C -9.116848 -0.532006 0.474354
S -8.037062 -0.903553 1.808156
C -10.548386 -0.451866 0.710830
S -11.563813 0.544198 -0.289296
C -12.988339 0.095593 0.601829
C -12.671936 -0.773582 1.614235
C -11.289964 -1.086543 1.674052
C -14.291020 0.625275 0.236291
S -15.740420 -0.259558 0.611128
C -16.747745 0.961314 -0.109070
C -15.984764 1.987523 -0.604483
C -14.592963 1.798204 -0.406480
C -18.193146 0.812432 -0.128616
C -18.920449 -0.348457 -0.113061
C -20.316677 -0.090278 -0.143484
C -20.642938 1.253845 -0.188889
S -19.217518 2.237989 -0.171026
C -22.038843 1.511650 -0.254203
C -22.765443 0.350685 -0.250838
S -21.743013 -1.073663 -0.155344
C -24.210226 0.196713 -0.309106
C -24.939911 -0.847519 -0.810052
C -26.345902 -0.648404 -0.705726
C -26.688114 0.541131 -0.131238
S -25.266936 1.434402 0.311646
C -28.058755 1.086937 0.126912
C 0.678603 -1.122038 0.259112
S 2.022620 -0.759791 -0.782536
C 3.166365 -1.002843 0.504528
C 2.519932 -1.307442 1.675216
C 1.110226 -1.374849 1.536030
C 4.592869 -0.873113 0.262887
C 5.266255 -1.041854 -0.918396
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C 7.042752 -0.520024 0.535786
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C 8.442612 -0.349127 0.704430
C 9.116817 -0.531859 -0.474222
S 8.036944 -0.903989 -1.807806
C 10.548325 -0.451704 -0.710840
S 11.563883 0.544210 0.289296
C 12.988294 0.095730 -0.602075
C 12.671763 -0.773313 -1.614553
C 11.289785 -1.086257 -1.674240
C 14.291012 0.625384 -0.236628
S 15.740374 -0.259493 -0.611512

C 16.747759 0.961365 0.108636
C 15.984821 1.987609 0.604044
C 14.593008 1.798320 0.406104
C 18.193153 0.812442 0.128155
C 18.920428 -0.348464 0.112414
C 20.316661 -0.090330 0.142933
C 20.642956 1.253775 0.188551
S 19.217568 2.237963 0.170792
C 22.038868 1.511531 0.253895
C 22.765443 0.350548 0.250378
S 21.742968 -1.073758 0.154636
C 24.210214 0.196528 0.308677
C 24.939849 -0.848034 0.809013
C 26.345851 -0.648853 0.704974
C 26.688128 0.541055 0.131300
S 25.266998 1.434611 -0.311173
C 28.058802 1.087030 -0.126318
H 3.042203 -1.511477 2.603192
H 0.437097 -1.637292 2.344495
H 13.408022 -1.167095 -2.306290
H 10.858781 -1.769680 -2.397290
H 4.781952 -1.323371 -1.845778
H 8.934401 -0.131071 1.644880
H 16.409557 2.848839 1.107427
H 13.839023 2.512320 0.718021
H 28.232814 1.259355 -1.194080
H 28.221912 2.036350 0.395276
H 28.809212 0.374266 0.226665
H 27.082323 -1.364084 1.054552
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H -0.436971 -1.637929 -2.343533
H -13.408280 -1.167465 2.305823
H -10.859044 -1.770075 2.397047
H -4.782045 -1.322734 1.846533
H -8.934323 -0.132061 -1.644893
H -16.409462 2.848751 -1.107901
H -13.838951 2.512176 -0.718396
H -28.232571 1.258713 1.194793
H -28.221982 2.036523 -0.394162
H -28.809218 0.374336 -0.226292
H -27.082419 -1.363411 -1.055673
H -24.485818 -1.722684 -1.261675
H -18.469065 -1.333423 -0.104796
H -22.489401 2.494249 -0.325631

PBTT$_1$ – Charged State (+1)

S 1.574612 -2.076407 -6.741253
C 2.652483 -1.953208 -8.109736
C 3.950382 -1.710805 -7.674665
C 4.059960 -1.629594 -6.282231
C 2.859955 -1.806252 -5.627087
C 2.190595 -2.092270 -9.439581
S 3.307806 -1.958368 -10.791813
C 2.016741 -2.231316 -11.912486
C 0.784051 -2.415534 -11.235799
C 0.874571 -2.339272 -9.860750
S -0.507019 -2.688437 -12.356474
C 0.610179 -2.554490 -13.708704
C 1.926209 -2.307504 -13.287538
C 0.148283 -2.693551 -15.038549
S 1.226100 -2.570074 -16.407057
C -0.059245 -2.840351 -17.521207
C -1.259199 -3.017217 -16.866043
C -1.149584 -2.936128 -15.473599
C 0.188912 -2.864138 -18.991968
C 2.611786 -1.782345 -4.156329
H 4.792026 -1.596736 -8.347708
H 4.989321 -1.447200 -5.758121
H 0.603556 -1.915301 -19.341847
H 0.894072 -3.653607 -19.264105
H -0.745438 -3.043924 -19.524262
H -2.188558 -3.199682 -17.390132
H -1.991190 -3.050410 -14.800544
H 1.906609 -0.992874 -3.884251
H 2.197153 -2.731167 -3.806386
H 3.546130 -1.602512 -3.624042
H 0.046994 -2.452831 -9.172763
H 2.753784 -2.193960 -13.975529

PBTT$_2$ – Charged State (+1)

C 11.228330 -1.452130 0.511141
C 10.517992 -0.358016 0.086107
S 11.597966 0.900241 -0.441177
C 12.993369 -0.052908 -0.072754
C 12.629843 -1.274517 0.420038
C 9.086882 -0.176396 0.056582
S 8.035821 -1.579128 0.083037
C 6.633761 -0.561250 0.051718
C 6.999173 0.787793 -0.001555
C 8.387511 1.009679 0.002706
C 5.256913 -0.777455 0.062904
C 4.543651 0.416113 0.019367
S 5.614449 1.813765 -0.034942
C 3.138344 0.583743 0.016954
S 2.055910 -0.777569 0.019849
C 0.652261 0.260453 0.020476
C 1.046723 1.606200 0.016216
C 2.415470 1.784607 0.013281
C -0.652261 -0.260453 0.020476
S -2.055910 0.777568 0.019845

C -3.138344 -0.583743 0.016953
C -2.415470 -1.784608 0.013284
C -1.046723 -1.606200 0.016219
C -4.543651 -0.416113 0.019366
S -5.614449 -1.813766 -0.034945
C -6.999173 -0.787793 -0.001556
C -6.633761 0.561250 0.051716
C -5.256913 0.777455 0.062903
C -8.387512 -1.009679 0.002704
C -9.086882 0.176396 0.056581
S -8.035821 1.579128 0.083034
C -10.517992 0.358017 0.086106
S -11.597967 -0.900236 -0.441187
C -12.993369 0.052906 -0.072748
C -12.629843 1.274516 0.420043
C -11.228329 1.452131 0.511140
C -14.370973 -0.475585 -0.311964
C 14.370972 0.475581 -0.311978
H -10.763541 2.349837 0.901730
H -13.352587 2.024794 0.715849
H -0.337093 -2.424560 0.015777
H -2.893036 -2.756226 0.011741
H -14.545991 -0.673088 -1.372827
H -14.547778 -1.405911 0.233466
H -15.109928 0.255293 0.019747
H -8.863753 -1.980877 -0.006486
H -4.785994 1.751797 0.105660
H 2.893036 2.756225 0.011736
H 0.337093 2.424559 0.015771
H 14.545982 0.673092 -1.372841
H 14.547785 1.405902 0.233458
H 15.109928 -0.255301 0.019721
H 13.352588 -2.024796 0.715839
H 10.763542 -2.349838 0.901729
H 4.785995 -1.751798 0.105661
H 8.863753 1.980877 -0.006484

$PBTT_4$ – Charged State (+1)

C -2.431675 0.353996 -1.768035
C -3.146575 0.352733 -0.561033
S -2.052590 0.347744 0.794848
C -0.655425 0.348108 -0.254364
C -1.058638 0.351349 -1.598534
C -4.551448 0.355838 -0.383228
C -5.256880 0.355670 0.819101
C -6.635839 0.359846 0.612396
C -7.013223 0.363662 -0.737812
S -5.633427 0.362107 -1.775630
C -8.401757 0.374885 -0.949405
C -9.096922 0.378098 0.246522
S -8.030453 0.359139 1.643414
C -10.522420 0.391077 0.435298
S -11.612115 0.210977 -0.912113
C -13.003774 0.365866 0.114249
C -12.625750 0.523019 1.430435
C -11.228327 0.536566 1.610559
C -14.338792 0.317102 -0.440934

S -15.717236 0.012827 0.576265
C -16.809975 0.113951 -0.770289
C -16.127361 0.379311 -1.933183
C -14.730222 0.496447 -1.745626
C -18.237275 -0.063917 -0.578774
C -18.874309 -0.741982 0.428580
C -20.283872 -0.693983 0.279476
C -20.710702 0.009485 -0.834583
S -19.366096 0.646605 -1.720091
C -22.120821 0.038954 -1.000741
C -22.757796 -0.644177 0.001727
S -21.633569 -1.321087 1.167740
C -24.186970 -0.837543 0.184070
C -24.839141 -1.872386 0.799166
C -26.255044 -1.729475 0.779748
C -26.681166 -0.594200 0.152354
S -25.327877 0.333001 -0.414510
C -28.086307 -0.121746 -0.060338
C 0.655201 0.346554 0.258573
S 2.052283 0.347054 -0.790670
C 3.146395 0.347175 0.565250
C 2.431386 0.346152 1.772320
C 1.058438 0.345732 1.602835
C 4.551028 0.349095 0.387487
C 5.256467 0.351866 -0.815067
C 6.635249 0.353938 -0.608530
C 7.012896 0.353209 0.741801
S 5.633218 0.349932 1.779817
C 8.401279 0.362257 0.953196
C 9.096415 0.368507 -0.242940
S 8.029704 0.355117 -1.639773
C 10.521693 0.380715 -0.431785
S 11.611594 0.200212 0.915481
C 13.003139 0.354108 -0.111180
C 12.624883 0.511515 -1.427386
C 11.227575 0.525838 -1.607238
C 14.338220 0.304743 0.443515
S 15.716996 0.007137 -0.575305
C 16.809772 0.103814 0.771499
C 16.127001 0.363074 1.935720
C 14.729712 0.478929 1.748945
C 18.237266 -0.070999 0.578831
C 18.875010 -0.744097 -0.431425
C 20.284536 -0.694099 -0.282858
C 20.710676 0.005962 0.833635
S 19.365365 0.637123 1.722327
C 22.120828 0.037498 0.999110
C 22.758507 -0.640649 -0.006298
S 21.634919 -1.315206 -1.174272
C 24.187927 -0.830710 -0.190192
C 24.841621 -1.862595 -0.808647
C 26.257260 -1.717072 -0.789786
C 26.681653 -0.582757 -0.159487
S 25.327013 0.340320 0.410867
C 28.086040 -0.108103 0.053313
H 2.916666 0.345946 2.741296
H 0.352715 0.345258 2.425885
H 13.336626 0.637858 -2.234720
H 10.754569 0.661171 -2.573909
H 4.776854 0.352824 -1.787119

H 8.882397 0.375985 1.923162
H 16.615135 0.454008 2.899005
H 14.034991 0.694890 2.553374
H 28.268100 0.851325 -0.442901
H 28.313140 0.018243 1.117222
H 28.787549 -0.839395 -0.357245
H 26.942778 -2.437640 -1.221933
H 24.328606 -2.713550 -1.243267
H 18.353320 -1.264429 -1.226272
H 22.641968 0.510016 1.822723
H -2.916963 0.356987 -2.736994
H -0.352952 0.352088 -2.421625
H -13.337618 0.649968 2.237566
H -10.755378 0.671904 2.577258
H -4.777422 0.352926 1.791230
H -8.882717 0.392470 -1.919387
H -16.615422 0.473777 -2.896171
H -14.035643 0.717242 -2.548858
H -28.270171 0.836865 0.436778
H -28.313306 0.005284 -1.124193
H -28.786686 -0.854651 0.349270
H -26.939511 -2.452522 1.209416
H -24.324835 -2.723567 1.231812
H -18.352060 -1.264430 1.221670
H -22.642384 0.513602 -1.822865

DPPT-TT$_2$ – Ground State (neutral)

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.368962
S	1.631772	0.000000	1.977532
C	2.302382	-0.019924	0.376126
C	1.308887	-0.009365	-0.559463
C	-1.136212	0.002829	2.275726
S	-2.670674	0.668077	1.740226
C	-3.402799	0.297086	3.266636
C	-2.485715	-0.285561	4.124754
C	-1.191978	-0.458848	3.564213
C	-4.702381	0.441628	3.817519
C	-4.759984	-0.031126	5.103216
S	-3.212611	-0.652556	5.652705
C	-5.904866	-0.064761	5.994893
C	-6.131879	-0.898464	7.064009
C	-7.361721	-0.658346	7.711024
C	-8.089953	0.365207	7.138907
S	-7.216308	1.048542	5.788954
C	-9.383555	0.796686	7.609765
C	-10.091496	0.281350	8.679106
C	-11.318865	0.989076	8.810126
C	-11.373945	1.992381	7.771770
N	-10.149442	1.819574	7.065202
C	-10.037405	-0.723661	9.714877
N	-11.263911	-0.553269	10.419344
C	-12.028204	0.471666	9.876441
C	-13.320372	0.907118	10.351353
S	-14.199521	0.209146	11.689002
C	-15.521970	1.306439	11.471433
C	-15.276849	2.173072	10.433894
C	-14.036465	1.949868	9.799364
C	-16.684949	1.238408	12.339177
S	-17.604482	2.695096	12.673906
C	-18.700735	1.808280	13.679162
C	-18.344911	0.471110	13.743967
C	-17.195462	0.139475	12.979832
C	-19.863599	2.135833	14.424354
C	-20.381481	1.034786	15.054914
S	-19.441822	-0.415240	14.749419
C	-21.559989	0.965453	15.902234
C	-22.423949	-0.086886	16.085016
C	-23.478081	0.204534	16.977527
C	-23.422971	1.485327	17.487398
S	-22.031026	2.329741	16.859107
C	-24.399448	2.030370	18.403026
C	-25.533441	1.398291	18.867084
C	-26.222584	2.288251	19.746010
C	-25.478869	3.525555	19.834446
N	-24.358571	3.298900	18.974632
C	-26.300383	0.169948	18.786777
N	-27.415030	0.420866	19.636662
C	-27.355832	1.683322	20.199645
C	-28.401814	2.190663	21.125855
O	-26.142200	-0.884118	18.187305
C	-28.453790	-0.559829	19.849928
O	-25.658647	4.559861	20.448706
C	-23.353455	4.327206	18.822611

O	-9.210103	-1.569792	10.022386
C	-11.559186	-1.396729	11.557156
O	-12.200733	2.839383	7.466231
C	-9.849415	2.668757	5.932808
C	3.783575	-0.048118	0.156193
H	-5.441301	-1.679255	7.361403
H	-7.724903	-1.216834	8.568390
H	-10.705165	3.336461	5.819496
H	-8.951664	3.268517	6.109055
H	-9.731304	2.083753	5.016134
H	-10.697130	-2.054927	11.678123
H	-11.686355	-0.806232	12.469100
H	-12.449745	-2.007711	11.382753
H	4.282502	0.802831	0.632189
H	4.233302	-0.964200	0.554685
H	3.994964	-0.007616	-0.915897
H	1.507279	-0.017157	-1.625548
H	-0.909201	-0.014003	-0.591054
H	-5.558177	0.848116	3.291604
H	-0.351322	-0.918734	4.069590
H	-22.319440	-1.034300	15.568690
H	-24.274827	-0.486746	17.236581
H	-23.670464	5.155665	19.459326
H	-22.370819	3.978792	19.154604
H	-23.291212	4.680102	17.788748
H	-28.192042	-1.433964	19.251492
H	-28.514529	-0.851152	20.903579
H	-29.427923	-0.180378	19.524764
H	-29.383733	2.210468	20.638857
H	-28.486126	1.550848	22.011980
H	-28.142920	3.202259	21.443012
H	-13.668122	2.518463	8.950914
H	-15.982923	2.933359	10.120091
H	-20.315908	3.118917	14.475186
H	-16.776421	-0.854853	12.882788

DPPT-TT$_2$ – Charged State (+1)

C	-16.941751	-0.172546	0.447601
C	-15.803803	0.579478	0.435018
C	-14.684541	-0.268673	0.187124
C	-15.181963	-1.626779	0.033268
N	-16.585573	-1.487258	0.207634
C	-15.334081	1.937134	0.603593
N	-13.915280	1.815531	0.448054
C	-13.541365	0.497927	0.202775
C	-12.188461	0.019884	0.012405
C	-11.865173	-1.293311	-0.264225
C	-10.477583	-1.508142	-0.385141
C	-9.730357	-0.367799	-0.200716
S	-10.749929	0.994022	0.133380
C	-8.291036	-0.219112	-0.244875
S	-7.270059	-1.641346	-0.124814
C	-5.845842	-0.660542	-0.239721
C	-6.176806	0.689514	-0.348633
C	-7.566482	0.945335	-0.356418
S	-4.766136	1.677993	-0.447585
C	-3.731236	0.259440	-0.336715
C	-4.464340	-0.910002	-0.233810
C	-2.308569	0.401770	-0.346123
S	-1.267716	-0.979983	-0.263634
C	0.169829	0.024978	-0.304236
C	-0.195871	1.377594	-0.385375
C	-1.566550	1.582978	-0.410064
C	1.497803	-0.433267	-0.253613
C	2.677018	0.368862	-0.260028
C	3.790350	-0.445252	-0.186522
C	3.343965	-1.831532	-0.134590
N	1.923052	-1.738333	-0.180248
C	3.123412	1.755906	-0.308438
N	4.543820	1.663435	-0.256570
C	4.970291	0.358248	-0.181270
C	6.295205	-0.098169	-0.110889
C	6.662878	-1.452919	-0.036455
C	8.030445	-1.655877	0.025432
C	8.773432	-0.470722	-0.000176
S	7.731793	0.910254	-0.097837
C	10.191641	-0.326117	0.043061
S	11.229116	-1.740798	0.189048
C	12.637029	-0.744888	0.163396
C	12.303896	0.605660	0.047230
C	10.925456	0.848179	-0.021510
S	13.727863	1.594625	0.024891
C	14.749950	0.172634	0.141933
C	14.026220	-0.995701	0.216248
C	16.188837	0.328082	0.154497
S	17.227333	-0.933720	0.756016
C	18.654636	-0.014962	0.407590
C	18.330022	1.198777	-0.132396
C	16.932630	1.397414	-0.277843
C	20.016830	-0.561355	0.702823
O	2.529508	2.812229	-0.377884
C	5.346433	2.873110	-0.279817
O	3.937898	-2.888447	-0.068747
C	1.119988	-2.947843	-0.157755

O	-15.898856	2.990873	0.820684
C	-13.085535	2.997777	0.516303
O	-14.635606	-2.695314	-0.194397
C	-17.486580	-2.616421	0.142228
C	-18.351078	0.240529	0.670781
H	8.488305	-2.635900	0.085220
H	5.926168	-2.250018	-0.030706
H	4.648692	3.706755	-0.367195
H	5.914731	2.983304	0.647418
H	6.018592	2.880237	-1.141537
H	1.818949	-3.783522	-0.107737
H	0.473994	-2.972995	0.723497
H	0.524547	-3.037761	-1.069852
H	20.154893	-0.741603	1.774129
H	20.195302	-1.505819	0.178617
H	20.776491	0.154866	0.379774
H	19.076101	1.928531	-0.424789
H	16.495830	2.291505	-0.709711
H	10.476951	1.830440	-0.118782
H	14.481565	-1.975955	0.280218
H	-10.043422	-2.474711	-0.615880
H	-12.621304	-2.066064	-0.369007
H	-13.767937	3.834179	0.680987
H	-12.380872	2.951025	1.352287
H	-12.543787	3.161710	-0.420234
H	-16.881420	-3.495640	-0.083902
H	-17.996875	-2.768525	1.098393
H	-18.231706	-2.480620	-0.647561
H	-18.975116	-0.009627	-0.194986
H	-18.776934	-0.270302	1.542008
H	-18.391443	1.318268	0.837035
H	0.541338	2.173404	-0.420120
H	-2.023541	2.563524	-0.468140
H	-8.018655	1.924305	-0.455426
H	-4.016531	-1.893783	-0.150536

PBTT$_1$ – Electric field 0.007 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366444
S	1.635432	0.000000	1.971741
C	2.304810	-0.037245	0.367533
C	1.309304	-0.020461	-0.560735
C	-1.145909	0.024884	2.258521
S	-2.598807	0.866758	1.754691
C	-3.425529	0.374104	3.190831
C	-2.597582	-0.374728	4.008012
C	-1.298886	-0.578962	3.478397
C	-4.750608	0.526147	3.672848
C	-4.928009	-0.113805	4.869646
S	-3.451046	-0.888596	5.428666
C	-6.141662	-0.216976	5.655197
S	-7.377573	1.002348	5.558457
C	-8.421244	0.128380	6.630810
C	-7.823916	-1.028560	7.042927
C	-6.532906	-1.229071	6.490498
C	-9.777827	0.650153	6.980639
C	3.782840	-0.087796	0.139909
H	-5.934647	-2.114555	6.673071
H	-8.312515	-1.729102	7.708926
H	4.294440	0.781414	0.567975
H	4.233829	-0.986103	0.575801
H	3.987195	-0.099687	-0.934076
H	1.499859	-0.039264	-1.628485
H	-0.911023	-0.013625	-0.584973
H	-9.726577	1.638076	7.444685
H	-10.416511	0.730372	6.097769
H	-10.266458	-0.026588	7.682674
H	-5.550356	1.036129	3.152361
H	-0.525143	-1.175850	3.946413

DPPT-TT$_2$ – Electric field 0.005 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.395423
C	1.343905	0.000000	1.881720
C	2.277670	0.084056	0.727821
N	1.431483	0.108849	-0.448172
C	-0.977925	-0.047225	2.484640
N	-0.220170	-0.171694	3.724569
C	1.180824	-0.188834	3.546855
C	2.229407	-0.219605	4.571551
C	3.590142	-0.188950	4.324997
C	4.373712	-0.222308	5.496008
C	3.624141	-0.271816	6.652023
S	1.924536	-0.296728	6.283458
C	4.034437	-0.273537	8.035816
C	3.285931	0.162941	9.112111
C	3.957870	-0.055699	10.328788
C	5.218797	-0.642859	10.199712
S	5.580744	-0.945775	8.525986
C	5.862798	-0.878031	11.427116

C	5.101000	-0.452982	12.502754
S	3.569615	0.243985	11.982618
C	5.380569	-0.562286	13.899907
S	6.629634	-1.596991	14.512806
C	6.259106	-1.164610	16.176571
C	5.194044	-0.262018	16.202333
C	4.708883	0.065367	14.940366
C	6.891663	-1.657728	17.341209
C	6.531595	-1.407999	18.677259
C	7.406029	-2.116432	19.528753
C	8.376827	-2.816657	18.701579
N	7.999318	-2.498424	17.376744
C	5.537776	-0.754577	19.481697
N	5.905689	-1.103321	20.814812
C	7.031212	-1.925109	20.841901
C	7.653951	-2.483801	22.014665
C	8.749530	-3.330583	22.008695
C	9.138835	-3.748973	23.295371
C	8.362132	-3.230636	24.306456
S	7.108071	-2.218003	23.653580
C	8.487704	-3.423649	25.731958
C	8.068670	-2.594104	26.745629
C	8.365317	-3.137819	28.021261
C	8.996203	-4.371146	27.990204
S	9.236316	-4.891442	26.350053
C	9.273360	-4.916307	29.268918
C	8.839480	-4.093874	30.278529
S	8.108342	-2.620272	29.657769
C	8.920664	-4.316271	31.709911
C	8.249107	-3.688511	32.726616
C	8.591521	-4.175615	34.020586
C	9.528307	-5.166453	34.001677
S	10.016828	-5.506910	32.368137
C	10.092073	-5.939449	35.154606
O	4.564141	-0.047086	19.235712
C	5.150194	-0.562825	21.917179
O	9.323893	-3.535227	18.978052
C	8.818548	-2.940439	16.262505
O	-2.194481	-0.045922	2.518982
C	-0.988225	-0.288243	4.936262
O	3.489573	0.020782	0.654112
C	1.982364	0.186250	-1.788338
C	-1.141153	-0.006094	-0.943399
H	9.997581	-4.384312	23.481887
H	9.251471	-3.604569	21.083921
H	4.340929	0.007406	21.460412
H	4.726835	-1.353842	22.543158
H	5.755905	0.108766	22.538443
H	9.678049	-3.450299	16.696600
H	8.270570	-3.637644	15.623584
H	9.161107	-2.084329	15.675283
H	9.782283	-6.991063	35.113173
H	11.187216	-5.916359	35.161084
H	9.735193	-5.512848	36.097596
H	8.146762	-3.799822	34.935122
H	7.504077	-2.927336	32.539814
H	7.599070	-1.632006	26.585340
H	9.757822	-5.871341	29.440938
H	5.456768	-0.180935	5.479801
H	3.999910	-0.114831	3.322133

H	-2.038120	-0.295425	4.632313
H	-0.768664	-1.215098	5.476294
H	-0.839248	0.569563	5.602074
H	3.068558	0.169369	-1.684521
H	1.665364	-0.663938	-2.397199
H	1.688226	1.118387	-2.282432
H	-1.129839	0.889759	-1.575814
H	-1.095726	-0.869780	-1.613683
H	-2.079917	-0.032728	-0.388701
H	4.796096	0.123765	17.136460
H	3.896325	0.761254	14.770163
H	2.312613	0.623638	9.005914
H	6.841214	-1.334486	11.528221