ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Nature of Charge Carriers in a High Electron Mobility Naphthalenediimide Based Semiconducting Copolymer

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S1. Contact resistance extraction

The Differential Method assumes that the mobility is a power law of V_g

$$\mu = \mu_0 (V_g - V_T)^{\gamma}$$

and that the contact resistance is the sum of a V_g-dependent term and of a V_g-independent term:

$$R_c = \frac{\alpha}{W(V_g - V_T)^{\gamma+1}} + R_{c0}$$

R_{c0}, ɔ and V_T are extracted from each transfer curve and for each channel length L (exploiting alteration of the functional dependence of the current on V_g due to R_{c0}), whereas only the V_g-dependent term and μ_0 additionally require a transfer line approach. Once that contact resistances are extracted, the intrinsic mobility becomes accessible.[1]. The extraction procedure is reported elsewhere[2], here we report the plots and the parameters that were employed for the extraction of R_C. R_C as reported in Table 2 was calculated at V_g-V_t ~ 55 V for PS 500 nm thick devices.

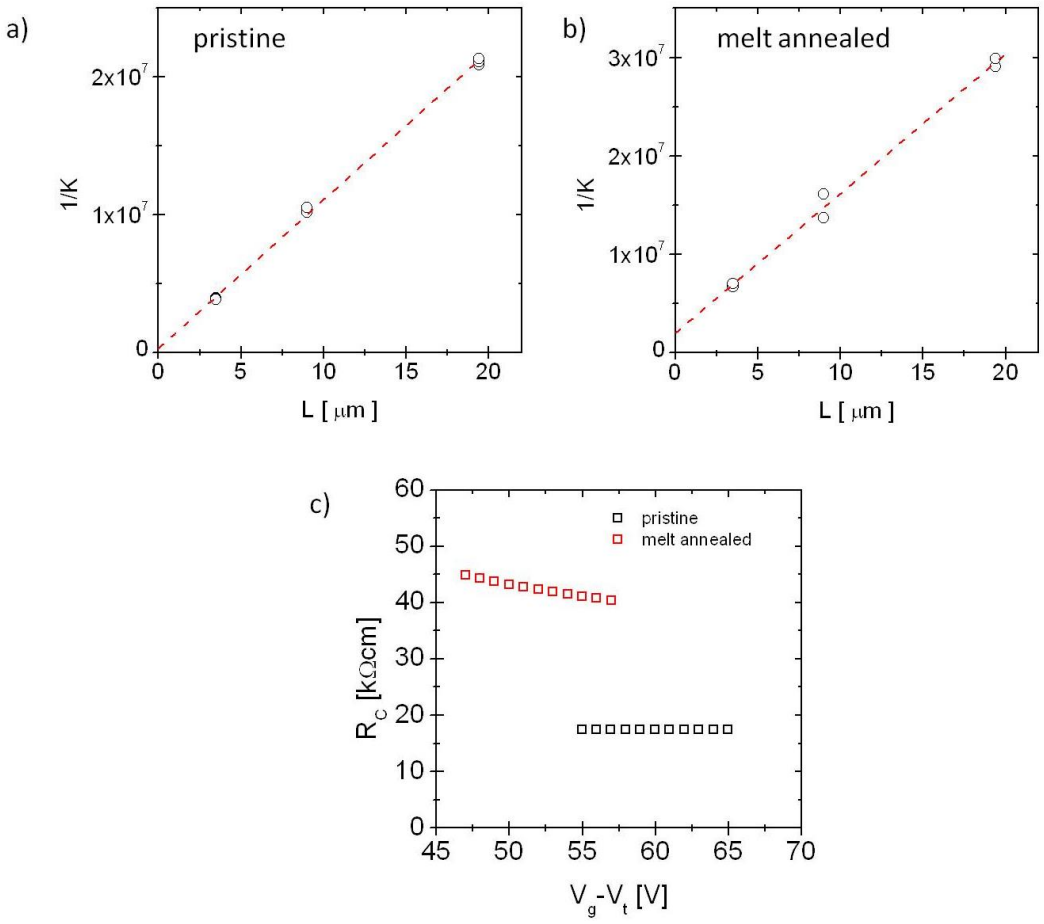


Figure S1. Plots of 1/*K* vs. *L* for the extraction of the parameters $\check{U}$ and μ_0 for OFETs using a) pristine and b) melt annealed P(NDI2OD-T2) layers; c) R_C vs. V_g - V_t, as calculated with the Differential Method (DM) for the same systems. it can be observed in (a) and (b) that: in the case of the pristine film the intersection with the y-axis of the linear interpolation of 1/*K* vs. *L* approaches 0, resulting in Vg independent R_C, as evidenced by the plot in (c); in the case of melt annealed film the intersection with the y-axis of the linear interpolation of 1/*K* vs. *L* is not negligible, resulting in not negligible Vg-dependent contribution to R_C, as evidenced by the plot in (c).

Table S1. Differential Method parameters.

Thermal treatment	μ_0 [$cm^2V^{-1}s^{-1}$]	ɔ	R_{C0} [kq cm]
Pristine	1.6×10^{-2}	0.3	17.4
Melt-annealed	1.2×10^{-2}	0.3	28.1

Summary of the main parameters extracted with the Differential Method from the measured transfer curves (*L* = 20μm).

References

(1) Natali, D.; Caironi, M. *Adv. Mater.* **2012**, *24*, 1357i 1387.

(2) Natali, D.; Fumagalli, L.; Sampietro, M. *J. Appl. Phys.* **2007**, *101*, 014501.

S2. UV-Vis Absorption

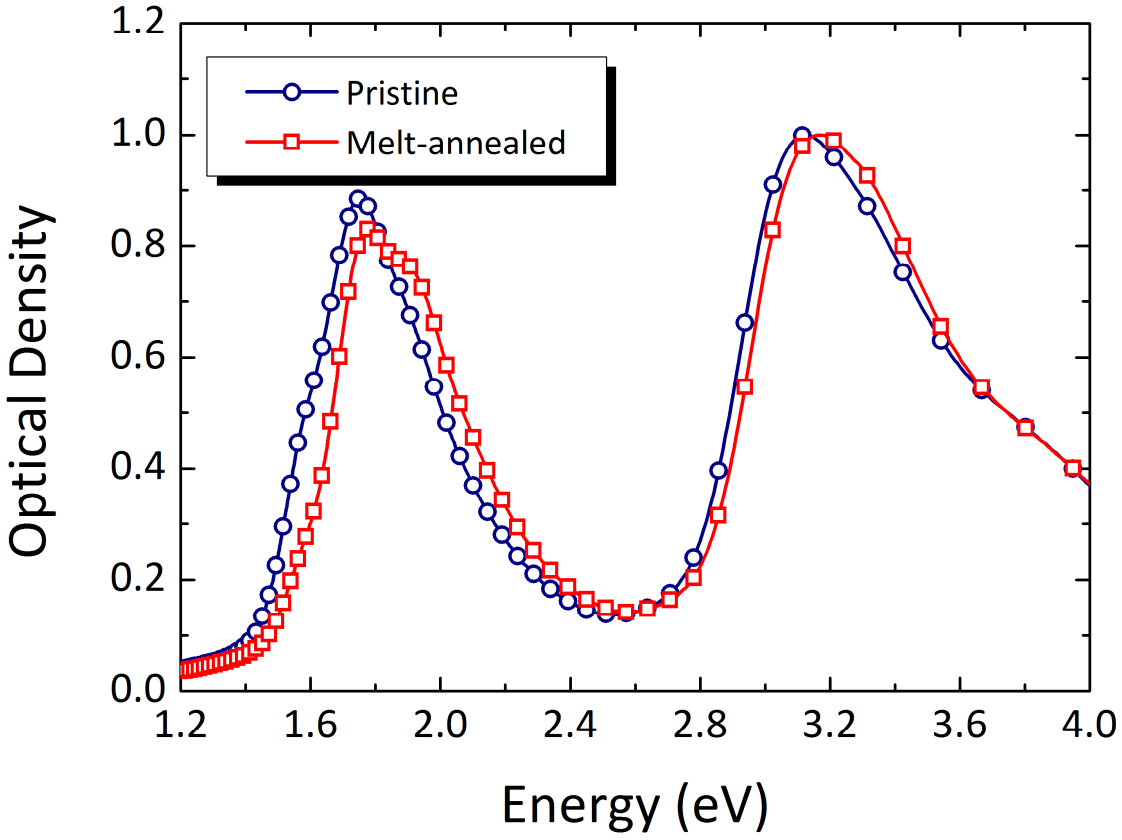


Figure S2. Absorption spectra of pristine (blue dot) and melt-annealed (red square) P(NDI2OD-T2) thin film spincoated on quartz substrate. Both spectra are normalized to the absorption peak at about 3.2 eV.

S3. Charge Modulation Spectroscopy: charge induced optical features

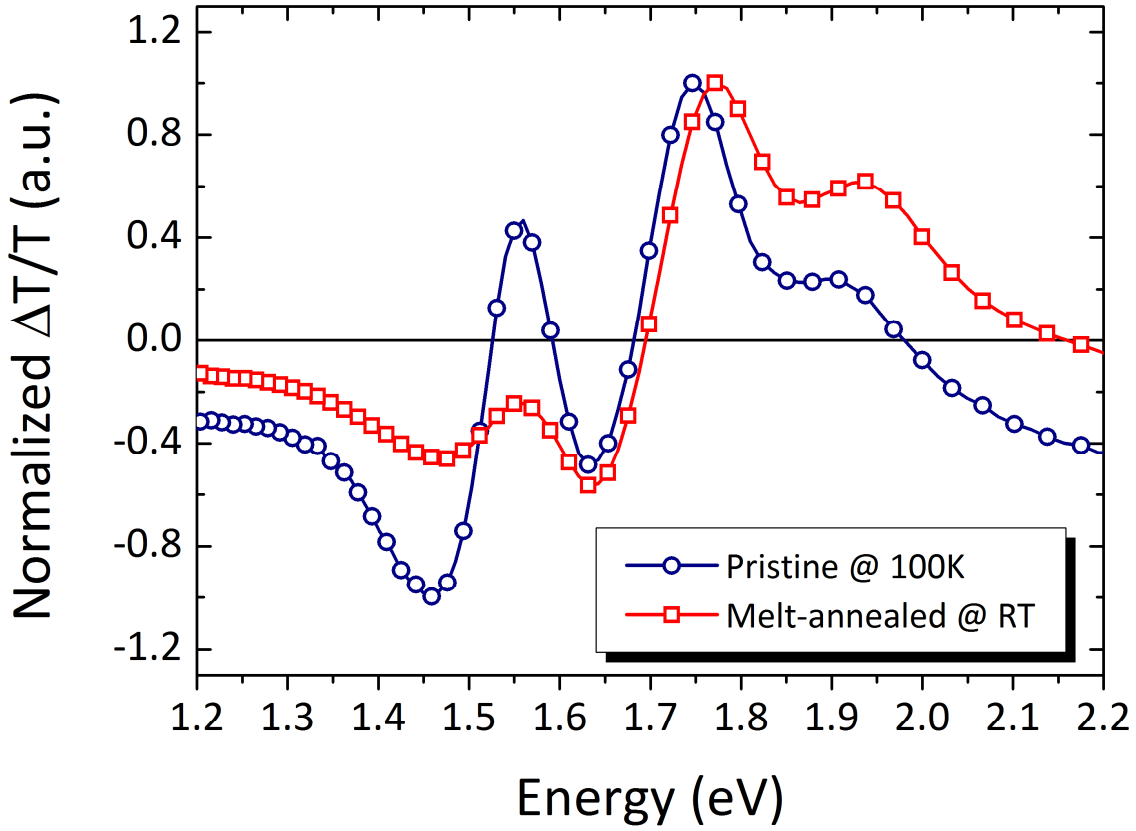


Figure S3. CMS spectra of pristine P(NDI2OD-T2) based OFET collected at 100 K (blue line) compared to the CMS spectra of a melt-annealed P(NDI2OD-T2) based OFET collected at room temperature (295 K). The measurements were taken by biasing the gate electrode at 80 V and by superimposing a 10 V ac voltage (amplitude). Each curve is normalized to its maximum (ϕT/T å 3×10^{-4} for the pristine based OFET and ϕT/T å 7×10^{-4} for the melt-annealed based OFET).

S4. DFT and TDFT calculation

S4.1) Dihedral angles (ɤ B97XD/6-311G**) between NDI2OD-T2 units for the *segregated* dimer, the *mixed* dimer and the single chain. $S^{AB}{}_1$ and $S^{AB}{}_2$ refer to the two dihedral angles between the two NDI2OD-T2 units.

S4.2) Main molecular orbitals involved (see Table 1 in the manuscript) in the ground state to the excited states
transitions for the *segregated* dimer and the *mixed* dimer. The excited states considered are the $S^{AB}{}_1$ and $S^{AB}{}_2$.

S4.3) Supramolecular clusters (not DFT re-optimized) geometries made by replicating the optimized DFT structure of the optimized aggregates (segregated and mixed). TDDFT (ɤ B97XD/6-31G*) vertical excitation energies computed for both the supramolecular clusters. supercell

S4.4) TDUCAM-B3LYP/6-31G* electronic spectra for the charged (-1) oligomers *n* = 4, 5 of P(NDI2OD-T2). Lorentzian width = 0.07 eV

S4.5) TDUCAM-B3LYP/6-31G* single occupied and unoccupied molecular orbitals involved in the main electronic transitions for the charged (-1) oligomer n = 4 of P(NDI2OD-T2).

S4.6) ɤ B97XD/6-311G** optimized structure for the *segregated* dimer, *n* = 2 x2 P(NDI2OD-T2)

S4.7) ɤ B97XD/6-311G** optimized structure for the *mixed* dimer, *n* = 2 x2 P(NDI2OD-T2)

S4.8) ɤ B97XD/6-31G* optimized structure for the oligomer *n* = 2 P(NDI2OD-T2)

S4.9) TDDFT (ɤ B97XD/6-31G*) vertical excited state energies for the *segregated* dimer

S4.10) TDDFT (ɤ B97XD/6-31G*) vertical excited state energies for the *mixed* dimer

S4.11) TDDFT (ɤ B97XD/6-31G*) vertical excited state energies for the oligomer *n* = 2

S4.12) UCAM-B3LYP/6-31G* optimized geometry for the charged (-1) oligomer *n* = 4 of P(NDI2OD-T2)

S4.13) UCAM-B3LYP/6-31G* optimized geometry for the charged (-1) oligomer *n* = 5 of P(NDI2OD-T2)

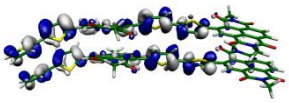
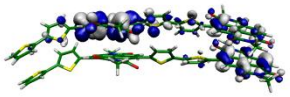
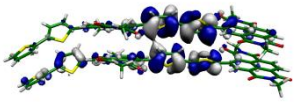
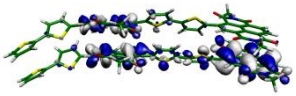
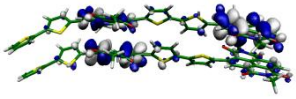
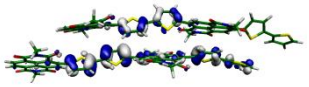
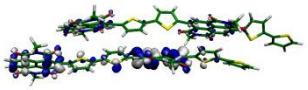
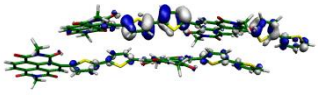
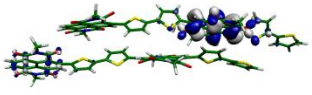
S4.14) TDUCAM-B3LYP/6-31G* vertical excited states energies for the optimized geometry for the charged (-1) oligomer *n* = 4 of P(NDI2OD-T2)

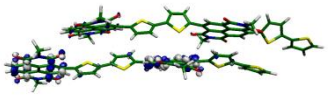
S4.15) TDUCAM-B3LYP/6-31G* vertical excited states energies for the optimized geometry for the charged (-1) oligomer *n* = 5 of P(NDI2OD-T2)

S4.1) Dihedral angles (ωB97XD/6-311G) between NDI2OD-T2 units for the *segregated* dimer, the *mixed* dimer and the single chain. τ_1 and τ_2 refer to the two dihedral angles between the two NDI2OD-T2 units.**

	τ_1	τ_2
segregated dimer		
chain 1	32°	32°
chain 2	34°	15°
mixed dimer		
chain 1	49°	36°
chain 2	42°	47°
oligomer	63°	80°

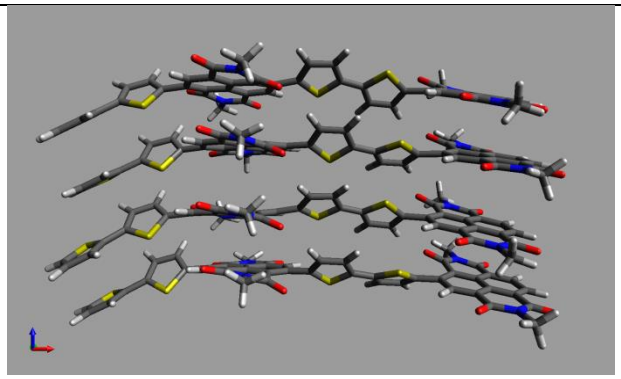
S4.2) Main molecular orbitals involved (see Table 1 in the manuscript) in the ground state to the excited states transitions for the *segregated* dimer and the *mixed* dimer. The excited states considered are the S^{AB}_1 and S^{AB}_2.

	Occupied MOs	Unoccupied MOs
segregated dimer	 HOMO	 LUMO
	 HOMO-1	 LUMO+1
		 LUMO+2
mixed dimer	 HOMO	 LUMO
	 HOMO-1	 LUMO+1

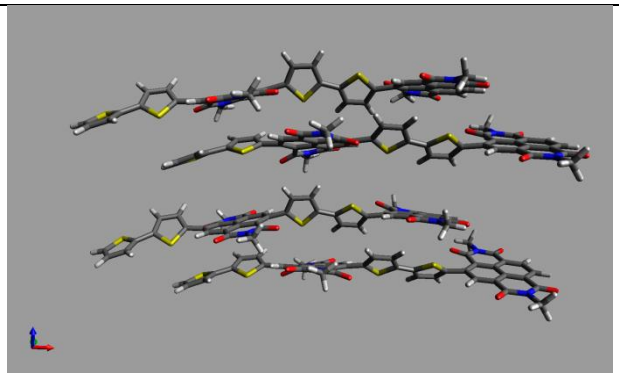
		 LUMO+2

S4.3) Supramolecular clusters (not DFT re-optimized) geometries made by replicating the optimized DFT structure of the optimized aggregates (*segregated* and *mixed*).

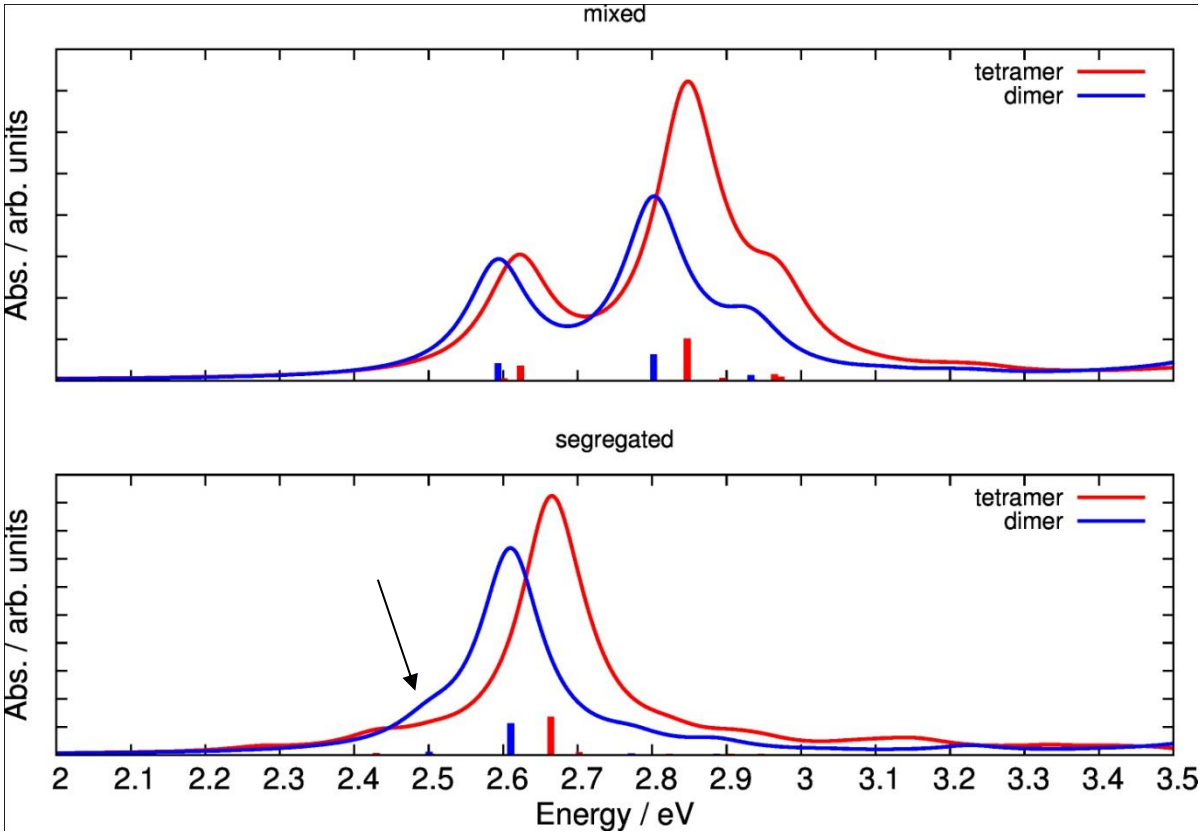
TDDFT (ωB97XD/6-31G*) vertical excitation energies computed for both the supramolecular clusters. The arrow in the bottom panel indicates the band identified as fingerprint for the local packing.



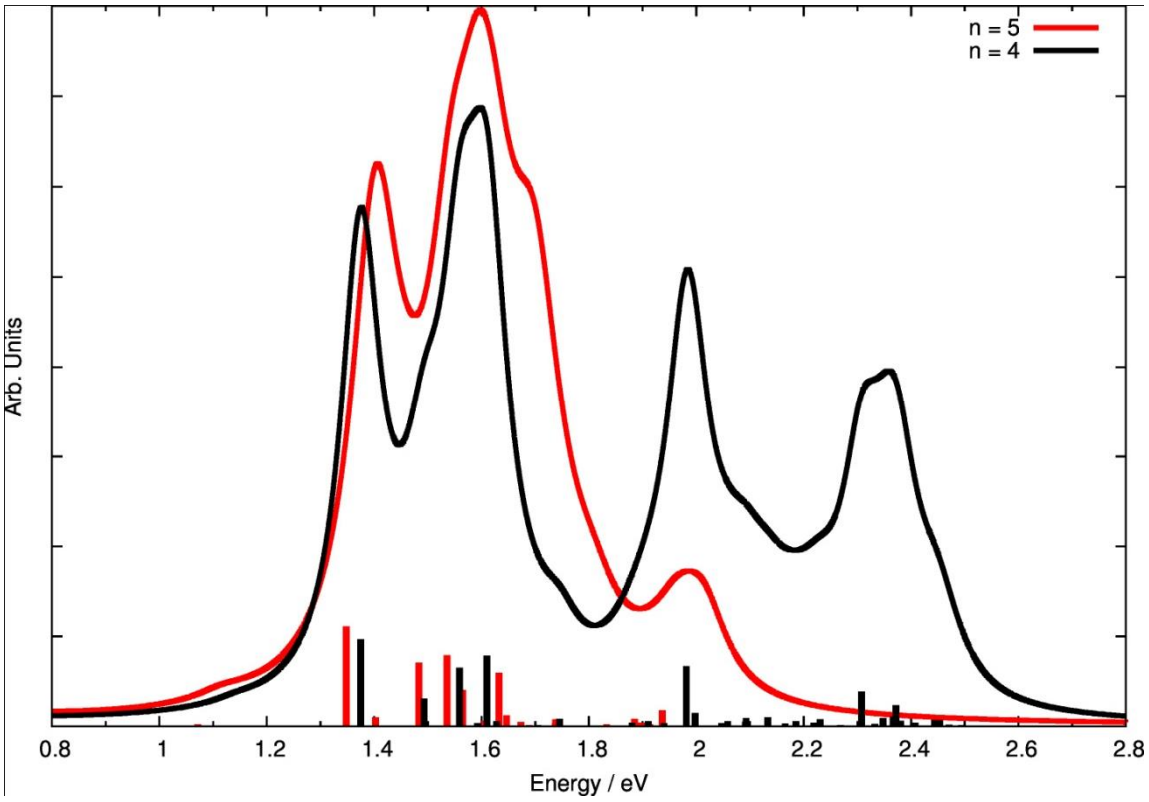
segregated



mixed



S4.4) TDUCAM-B3LYP/6-31G* electronic spectra for the charged (-1) oligomers *n* = 4, 5 of P(NDI2OD-T2). Lorentzian width = 0.07 eV



S4.5) TDUCAM-B3LYP/6-31G* single occupied and unoccupied molecular orbitals involved in the main electronic transitions for the charged (-1) oligomer n = 4 of P(NDI2OD-T2).

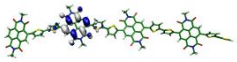
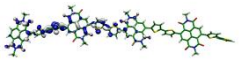
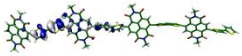
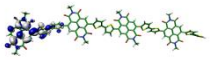
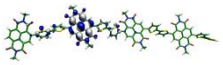
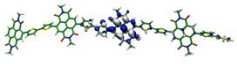
Excited State 6: E = 1.8332 eV, f= 0.4835
Main molecular orbitals contributions:
470A -> 479A -0.43336
470A -> 485A 0.51329
470A -> 488A -0.40431

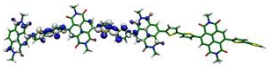
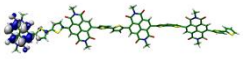
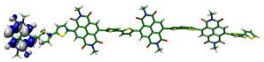
Excited State 8: E = 1.9907 eV, f= 0.1548
Main molecular orbitals contributions:
470A -> 477A -0.36102
470A -> 486A 0.38869

Excited State 9: E = 2.0790 eV, f = 0.3248
Main molecular orbitals contributions:

469A -> 473A -0.25066
469B -> 472B 0.31012

Excited State 11: E = 2.1467 eV, f= 0.3919
Main molecular orbitals contributions:
468A -> 472A -0.36694
469A -> 473A 0.37912
470A -> 488A -0.29729

Single Occupied MOs	Single Unoccupied MOs
 470A	 485A
 469A	 479 A
	 488 A
	 477 A

	 486 A
	 473A
	 472B

S4.6) ωB97XD/6-311G optimized structure for the *segregated* dimer, *n* = 2 x2 P(NDI2OD-T2)**

atom type / x / y / z coordinates

S	-16.678766	-0.222931	-0.000206
C	-15.259186	-1.169226	0.327175
C	-15.508746	-2.500335	0.126206
C	-16.845779	-2.762924	-0.279725
C	-17.593780	-1.629859	-0.381623
C	-14.014389	-0.529558	0.727560
C	-13.829538	0.599237	1.483457
C	-12.468708	0.949588	1.631994
C	-11.614481	0.095845	0.990481
S	-12.497686	-1.162008	0.189018
C	-10.145532	0.085620	1.020611
C	-9.334210	1.206197	0.861032
C	-7.946003	1.113551	1.148463
C	-7.352188	-0.119660	1.487413
C	-8.175896	-1.266299	1.516093
C	-9.521657	-1.153787	1.311599
C	-5.974379	-0.208390	1.799246
C	-5.201653	0.944375	1.837793
C	-5.796473	2.166242	1.463770
C	-7.117126	2.252685	1.107869
C	-9.845099	2.483397	0.280704
N	-8.958942	3.567117	0.218053
C	-7.639731	3.560924	0.647589
C	-7.616630	-2.604503	1.842090
N	-6.252991	-2.649742	2.095746
C	-5.380610	-1.557165	2.046622
C	-3.790077	0.988993	2.271498
C	-3.285613	0.846102	3.527960
C	-1.876788	1.005554	3.583554
C	-1.314542	1.272660	2.364893
S	-2.536338	1.329348	1.131792
C	0.080175	1.485793	2.015806
C	0.588608	2.104439	0.904610
C	2.000595	2.128724	0.873233
C	2.577188	1.554099	1.968753
S	1.362416	0.925105	3.039504
C	4.007219	1.362672	2.243949
C	4.415111	0.089898	2.713188
C	5.734325	-0.243936	2.848041
C	6.736015	0.674276	2.486391
C	6.357923	1.961987	2.058247
C	4.987329	2.320729	1.989114
C	8.097109	0.310607	2.533242
C	9.065433	1.209703	2.160211
C	8.698604	2.494856	1.732275
C	7.376771	2.865790	1.678804
C	4.667457	3.761981	1.755100
N	5.688821	4.566636	1.239240
C	7.034578	4.221969	1.188133
C	6.101034	-1.614025	3.284372
N	7.455457	-1.932559	3.299124
C	8.489592	-1.063723	2.939345
O	7.874291	4.999052	0.788718
C	5.315624	5.938050	0.898563
O	3.595705	4.259503	2.007543
O	9.645686	-1.423125	2.949287
C	7.791538	-3.298055	3.698502
O	5.269796	-2.442268	3.589228
O	-6.944621	4.550585	0.597161
C	-9.493476	4.793616	-0.371226
O	-10.954711	2.618303	-0.179666
O	-8.312602	-3.593832	1.894370
C	-5.642231	-3.944230	2.403906
O	-4.193547	-1.739080	2.191996
H	-5.196943	3.068636	1.455675
H	-9.896256	4.580909	-1.360687
H	-10.293812	5.190277	0.254676
H	-8.685216	5.515115	-0.439087
H	-6.441045	-4.663297	2.557520
H	-4.996514	-4.257094	1.584185

H	-5.041958	-3.849922	3.309221
H	-10.128128	-2.046041	1.412284
H	-12.127283	1.803440	2.201837
H	-14.647096	1.148006	1.934196
H	-14.763618	-3.270242	0.286963
H	-17.235722	-3.753770	-0.474558
H	-18.633988	-1.536447	-0.657737
H	9.451623	3.203729	1.415581
H	3.668491	-0.662932	2.936295
H	-0.030182	2.548515	0.135594
H	2.572439	2.569477	0.067583
H	-3.904634	0.622989	4.387559
H	-1.304323	0.940667	4.500851
H	7.266337	-4.006784	3.059521
H	8.863687	-3.426814	3.597375
H	7.491138	-3.466778	4.732567
H	4.383708	5.927544	0.337392
H	5.173892	6.530248	1.804127
H	6.113357	6.367642	0.301522
H	10.106634	0.912055	2.184257
C	4.464080	-1.553255	-0.026161
C	4.941906	-0.866927	-1.111426
S	3.631476	-0.301027	-2.090296
C	2.440434	-0.983102	-1.015831
C	3.054964	-1.603947	0.034766
C	6.319249	-0.586177	-1.474318
C	6.791223	0.222728	-2.475708
C	8.201199	0.303557	-2.512331
C	8.812868	-0.430990	-1.538255
S	7.635069	-1.271928	-0.577578
C	10.251834	-0.652573	-1.318271
C	10.665983	-2.005735	-1.208991
C	11.982912	-2.357656	-1.115765
C	12.979469	-1.364328	-1.147781
C	12.595870	-0.009577	-1.226098
C	11.221740	0.349224	-1.279596
C	14.343011	-1.717717	-1.106876
C	15.313589	-0.746672	-1.154631
C	14.943346	0.603809	-1.239919
C	13.616772	0.966644	-1.270214
C	10.871641	1.802696	-1.206566
N	11.923238	2.721701	-1.301951
C	13.272704	2.404238	-1.356884
C	12.348972	-3.797528	-1.019425
N	13.711039	-4.090571	-0.967673
C	14.736657	-3.147913	-1.017770
O	14.111603	3.273562	-1.447750
C	11.601440	4.149120	-1.293348
O	9.741380	2.201164	-1.049590
O	15.894447	-3.499194	-0.986758
C	14.124159	-5.489662	-0.872685
O	11.509388	-4.668043	-0.988720
C	1.015612	-0.764221	-1.303917
C	0.685912	0.479905	-1.896618
C	-0.592261	0.836408	-2.216340
C	-1.672564	-0.015833	-1.911208
C	-1.375366	-1.233955	-1.266133
C	-0.035834	-1.636365	-1.016326
C	-3.004758	0.358937	-2.222673
C	-3.181956	1.530701	-3.133556
N	-2.110966	2.426018	-3.245095
C	-0.819327	2.174571	-2.812796
C	-4.066670	-0.417381	-1.759334
C	-3.748397	-1.619261	-1.080745
C	-2.465348	-2.040358	-0.877004
C	-2.253824	-3.351883	-0.220451
N	-0.932807	-3.733637	-0.051290
C	0.174881	-3.042761	-0.555285
O	0.070789	2.989506	-2.931226
C	-2.369627	3.652982	-3.995718
O	-4.185128	1.739541	-3.773196
C	-5.493850	-0.097822	-1.898515
C	-6.145611	1.102176	-1.849768
C	-7.543032	0.992828	-2.029130
C	-7.970659	-0.297072	-2.201819
S	-6.630930	-1.389817	-2.157691

O	-3.172682	-4.066449	0.115893
C	-0.662339	-5.054822	0.511561
O	1.238333	-3.613721	-0.608806
C	-9.307818	-0.795997	-2.472645
C	-9.790700	-2.067513	-2.305794
C	-11.117801	-2.226267	-2.784121
C	-11.631990	-1.073711	-3.292758
S	-10.504477	0.221311	-3.210083
H	1.467106	1.203238	-2.094270
H	-2.490276	3.431006	-5.056553
H	-3.282927	4.116604	-3.627781
H	-1.525559	4.319806	-3.852498
H	-1.553931	-5.389344	1.031062
H	-0.409137	-5.763686	-0.277599
H	0.174296	-4.985588	1.203364
H	-4.544011	-2.252606	-0.707857
H	-5.641842	2.045653	-1.697744
H	-8.213293	1.843926	-2.031429
H	-9.215892	-2.864298	-1.849560
H	-11.672749	-3.153671	-2.727291
H	-12.620719	-0.900079	-3.690244
H	15.697877	1.379568	-1.284220
H	9.922463	-2.793419	-1.230525
H	6.146896	0.758268	-3.162249
H	8.749007	0.899481	-3.229590
H	2.519217	-2.088239	0.837236
H	5.100842	-2.016604	0.715621
H	13.231426	-6.100345	-0.788888
H	14.686816	-5.772487	-1.762518
H	14.757314	-5.626688	0.002920
H	11.961191	4.610750	-2.212329
H	10.525872	4.258998	-1.211670
H	12.088382	4.630995	-0.445977
H	16.357445	-1.034171	-1.126643

Energy = -8515.24608706 Hartree

S4.7) ωB97XD/6-311G** optimized structure for the *mixed* dimer, *n* = 2 x2 P(NDI2OD-T2)

S	-16.678766	-0.222931	-0.000206
C	-15.259186	-1.169226	0.327175
C	-15.508746	-2.500335	0.126206
C	-16.845779	-2.762924	-0.279725
C	-17.593780	-1.629859	-0.381623
C	-14.014389	-0.529558	0.727560
C	-13.829538	0.599237	1.483457
C	-12.468708	0.949588	1.631994
C	-11.614481	0.095845	0.990481
S	-12.497686	-1.162008	0.189018
C	-10.145532	0.085620	1.020611
C	-9.334210	1.206197	0.861032
C	-7.946003	1.113551	1.148463
C	-7.352188	-0.119660	1.487413
C	-8.175896	-1.266299	1.516093
C	-9.521657	-1.153787	1.311599
C	-5.974379	-0.208390	1.799246
C	-5.201653	0.944375	1.837793
C	-5.796473	2.166242	1.463770
C	-7.117126	2.252685	1.107869
C	-9.845099	2.483397	0.280704
N	-8.958942	3.567117	0.218053
C	-7.639731	3.560924	0.647589
C	-7.616630	-2.604503	1.842090
N	-6.252991	-2.649742	2.095746
C	-5.380610	-1.557165	2.046622
C	-3.790077	0.988993	2.271498
C	-3.285613	0.846102	3.527960
C	-1.876788	1.005554	3.583554
C	-1.314542	1.272660	2.364893
S	-2.536338	1.329348	1.131792
C	0.080175	1.485793	2.015806
C	0.588608	2.104439	0.904610
C	2.000595	2.128724	0.873233
C	2.577188	1.554099	1.968753
S	1.362416	0.925105	3.039504
C	4.007219	1.362672	2.243949
C	4.415111	0.089898	2.713188
C	5.734325	-0.243936	2.848041
C	6.736015	0.674276	2.486391
C	6.357923	1.961987	2.058247
C	4.987329	2.320729	1.989114
C	8.097109	0.310607	2.533242
C	9.065433	1.209703	2.160211
C	8.698604	2.494856	1.732275
C	7.376771	2.865790	1.678804
C	4.667457	3.761981	1.755100
N	5.688821	4.566636	1.239240
C	7.034578	4.221969	1.188133
C	6.101034	-1.614025	3.284372
N	7.455457	-1.932559	3.299124
C	8.489592	-1.063723	2.939345
O	7.874291	4.999052	0.788718
C	5.315624	5.938050	0.898563
O	3.595705	4.259503	2.007543
O	9.645686	-1.423125	2.949287
C	7.791538	-3.298055	3.698502
O	5.269796	-2.442268	3.589228
O	-6.944621	4.550585	0.597161
C	-9.493476	4.793616	-0.371226
O	-10.954711	2.618303	-0.179666
O	-8.312602	-3.593832	1.894370
C	-5.642231	-3.944230	2.403906
O	-4.193547	-1.739080	2.191996
H	-5.196943	3.068636	1.455675
H	-9.896256	4.580909	-1.360687
H	-10.293812	5.190277	0.254676
H	-8.685216	5.515115	-0.439087
H	-6.441045	-4.663297	2.557520
H	-4.996514	-4.257094	1.584185
H	-5.041958	-3.849922	3.309221
H	-10.128128	-2.046041	1.412284
H	-12.127283	1.803440	2.201837
H	-14.647096	1.148006	1.934196

H	-14.763618	-3.270242	0.286963
H	-17.235722	-3.753770	-0.474558
H	-18.633988	-1.536447	-0.657737
H	9.451623	3.203729	1.415581
H	3.668491	-0.662932	2.936295
H	-0.030182	2.548515	0.135594
H	2.572439	2.569477	0.067583
H	-3.904634	0.622989	4.387559
H	-1.304323	0.940667	4.500851
H	7.266337	-4.006784	3.059521
H	8.863687	-3.426814	3.597375
H	7.491138	-3.466778	4.732567
H	4.383708	5.927544	0.337392
H	5.173892	6.530248	1.804127
H	6.113357	6.367642	0.301522
H	10.106634	0.912055	2.184257
C	4.464080	-1.553255	-0.026161
C	4.941906	-0.866927	-1.111426
S	3.631476	-0.301027	-2.090296
C	2.440434	-0.983102	-1.015831
C	3.054964	-1.603947	0.034766
C	6.319249	-0.586177	-1.474318
C	6.791223	0.222728	-2.475708
C	8.201199	0.303557	-2.512331
C	8.812868	-0.430990	-1.538255
S	7.635069	-1.271928	-0.577578
C	10.251834	-0.652573	-1.318271
C	10.665983	-2.005735	-1.208991
C	11.982912	-2.357656	-1.115765
C	12.979469	-1.364328	-1.147781
C	12.595870	-0.009577	-1.226098
C	11.221740	0.349224	-1.279596
C	14.343011	-1.717717	-1.106876
C	15.313589	-0.746672	-1.154631
C	14.943346	0.603809	-1.239919
C	13.616772	0.966644	-1.270214
C	10.871641	1.802696	-1.206566
N	11.923238	2.721701	-1.301951
C	13.272704	2.404238	-1.356884
C	12.348972	-3.797528	-1.019425
N	13.711039	-4.090571	-0.967673
C	14.736657	-3.147913	-1.017770
O	14.111603	3.273562	-1.447750
C	11.601440	4.149120	-1.293348
O	9.741380	2.201164	-1.049590
O	15.894447	-3.499194	-0.986758
C	14.124159	-5.489662	-0.872685
O	11.509388	-4.668043	-0.988720
C	1.015612	-0.764221	-1.303917
C	0.685912	0.479905	-1.896618
C	-0.592261	0.836408	-2.216340
C	-1.672564	-0.015833	-1.911208
C	-1.375366	-1.233955	-1.266133
C	-0.035834	-1.636365	-1.016326
C	-3.004758	0.358937	-2.222673
C	-3.181956	1.530701	-3.133556
N	-2.110966	2.426018	-3.245095
C	-0.819327	2.174571	-2.812796
C	-4.066670	-0.417381	-1.759334
C	-3.748397	-1.619261	-1.080745
C	-2.465348	-2.040358	-0.877004
C	-2.253824	-3.351883	-0.220451
N	-0.932807	-3.733637	-0.051290
C	0.174881	-3.042761	-0.555285
O	0.070789	2.989506	-2.931226
C	-2.369627	3.652982	-3.995718
O	-4.185128	1.739541	-3.773196
C	-5.493850	-0.097822	-1.898515
C	-6.145611	1.102176	-1.849768
C	-7.543032	0.992828	-2.029130
C	-7.970659	-0.297072	-2.201819
S	-6.630930	-1.389817	-2.157691
O	-3.172682	-4.066449	0.115893
C	-0.662339	-5.054822	0.511561
O	1.238333	-3.613721	-0.608806
C	-9.307818	-0.795997	-2.472645

C	-9.790700	-2.067513	-2.305794
C	-11.117801	-2.226267	-2.784121
C	-11.631990	-1.073711	-3.292758
S	-10.504477	0.221311	-3.210083
H	1.467106	1.203238	-2.094270
H	-2.490276	3.431006	-5.056553
H	-3.282927	4.116604	-3.627781
H	-1.525559	4.319806	-3.852498
H	-1.553931	-5.389344	1.031062
H	-0.409137	-5.763686	-0.277599
H	0.174296	-4.985588	1.203364
H	-4.544011	-2.252606	-0.707857
H	-5.641842	2.045653	-1.697744
H	-8.213293	1.843926	-2.031429
H	-9.215892	-2.864298	-1.849560
H	-11.672749	-3.153671	-2.727291
H	-12.620719	-0.900079	-3.690244
H	15.697877	1.379568	-1.284220
H	9.922463	-2.793419	-1.230525
H	6.146896	0.758268	-3.162249
H	8.749007	0.899481	-3.229590
H	2.519217	-2.088239	0.837236
H	5.100842	-2.016604	0.715621
H	13.231426	-6.100345	-0.788888
H	14.686816	-5.772487	-1.762518
H	14.757314	-5.626688	0.002920
H	11.961191	4.610750	-2.212329
H	10.525872	4.258998	-1.211670
H	12.088382	4.630995	-0.445977
H	16.357445	-1.034171	-1.126643

Energy = -8515.19541376 Hartree

S4.8) ωB97XD/6-311G* optimized structure for the oligomer *n* = 2 P(NDI2OD-T2)

S	-13.589104	-0.275079	-0.539190
C	-12.137316	-1.228022	-0.536518
C	-12.362159	-2.454347	-1.100529
C	-13.706973	-2.634951	-1.526335
C	-14.484981	-1.546050	-1.278364
C	-10.897144	-0.692600	0.007332
C	-10.720844	0.168997	1.054143
C	-9.358150	0.481449	1.298724
C	-8.506516	-0.138590	0.436301
S	-9.368441	-1.121011	-0.697563
C	-7.028753	-0.111496	0.448591
C	-6.259586	0.973965	0.057519
C	-4.850341	0.926890	0.210186
C	-4.214179	-0.225612	0.719213
C	-5.016734	-1.331514	1.069790
C	-6.377774	-1.265917	0.939826
C	-2.805557	-0.273281	0.869836
C	-2.037704	0.823223	0.508018
C	-2.688510	1.976651	0.016213
C	-4.048958	2.036534	-0.128576
C	-6.869878	2.180766	-0.580669
N	-6.030647	3.269996	-0.833303
C	-4.654751	3.289541	-0.647112
C	-4.412287	-2.579504	1.601917
N	-3.032396	-2.570401	1.759342
C	-2.188244	-1.496763	1.465408
C	-0.561826	0.897544	0.593227
C	0.173328	1.590342	1.506167
C	1.568898	1.546083	1.244532
C	1.882175	0.834972	0.120236
S	0.449099	0.190862	-0.620064
C	3.192827	0.593478	-0.465080
C	3.529758	0.445526	-1.781799
C	4.916867	0.213818	-1.979324
C	5.628667	0.214569	-0.817200
S	4.591506	0.437026	0.550698
C	7.072055	-0.056034	-0.652094
C	7.492894	-1.376907	-0.940710
C	8.795347	-1.767081	-0.781664
C	9.750874	-0.852328	-0.300526
C	9.356230	0.472078	-0.021060
C	8.010452	0.871560	-0.219323
C	11.088935	-1.249832	-0.101185
C	12.012484	-0.350737	0.374422
C	11.625672	0.968106	0.661370
C	10.326730	1.375296	0.466692
C	7.663289	2.311045	-0.026445
N	8.645514	3.143693	0.516817
C	9.960465	2.778687	0.782997
C	9.189895	-3.164757	-1.096616
N	10.522762	-3.508123	-0.883234
C	11.509019	-2.645038	-0.402189
O	10.762659	3.565445	1.234673
C	8.248988	4.532330	0.744836
O	6.590549	2.779948	-0.326149
O	12.649359	-3.016219	-0.240081
C	10.889632	-4.888472	-1.194804
O	8.403092	-3.981453	-1.519250
O	-3.987003	4.266458	-0.903079
C	-6.675087	4.453077	-1.401297
O	-8.034631	2.251097	-0.892125
O	-5.083361	-3.545625	1.887932
C	-2.383110	-3.761000	2.305821
O	-1.007436	-1.592407	1.702713
H	-2.093671	2.839353	-0.258554
H	-7.102200	4.214793	-2.375134
H	-7.473847	4.788036	-0.740747
H	-5.923554	5.228634	-1.503542
H	-3.141809	-4.523425	2.446473
H	-1.619744	-4.113085	1.613153
H	-1.910144	-3.523865	3.258510
H	-6.972412	-2.121257	1.237995
H	-9.019033	1.142558	2.086128

H	-11.541814	0.549812	1.649086
H	-11.594118	-3.213302	-1.186903
H	-14.079336	-3.541197	-1.986377
H	-15.536285	-1.411965	-1.486696
H	12.346573	1.682190	1.040113
H	6.761933	-2.099016	-1.284346
H	2.810579	0.521224	-2.587962
H	5.377494	0.082836	-2.950472
H	-0.270517	2.113061	2.344045
H	2.311212	2.049695	1.851363
H	10.694194	-5.093714	-2.246970
H	11.945463	-5.014798	-0.980390
H	10.298702	-5.572888	-0.586839
H	8.039980	5.023033	-0.206024
H	7.350020	4.559645	1.358711
H	9.065843	5.036489	1.250146
H	13.036380	-0.669876	0.525291

Energy = -4258.22507139 Hartree

S4.9) TDDFT (ωB97XD/6-31G*) vertical excited state energies for the *segregated* dimer

Excited State 1:	Singlet-A	2.5007 eV	495.81 nm	f= 0.2202	<S**2>=0.000
Excited State 2:	Singlet-A	2.6100 eV	475.03 nm	f= 2.2623	<S**2>=0.000
Excited State 3:	Singlet-A	2.7722 eV	447.25 nm	f= 0.1105	<S**2>=0.000
Excited State 4:	Singlet-A	2.8866 eV	429.51 nm	f= 0.0884	<S**2>=0.000
Excited State 5:	Singlet-A	3.0343 eV	408.60 nm	f= 0.0103	<S**2>=0.000
Excited State 6:	Singlet-A	3.1256 eV	396.67 nm	f= 0.0027	<S**2>=0.000
Excited State 7:	Singlet-A	3.2151 eV	385.63 nm	f= 0.0033	<S**2>=0.000
Excited State 8:	Singlet-A	3.2270 eV	384.21 nm	f= 0.0588	<S**2>=0.000
Excited State 9:	Singlet-A	3.3177 eV	373.71 nm	f= 0.0008	<S**2>=0.000
Excited State 10:	Singlet-A	3.4134 eV	363.23 nm	f= 0.0033	<S**2>=0.000
Excited State 11:	Singlet-A	3.5593 eV	348.34 nm	f= 0.0088	<S**2>=0.000
Excited State 12:	Singlet-A	3.6135 eV	343.11 nm	f= 0.0461	<S**2>=0.000
Excited State 13:	Singlet-A	3.6247 eV	342.06 nm	f= 0.0060	<S**2>=0.000
Excited State 14:	Singlet-A	3.6908 eV	335.93 nm	f= 0.5739	<S**2>=0.000
Excited State 15:	Singlet-A	3.7561 eV	330.08 nm	f= 0.4405	<S**2>=0.000
Excited State 16:	Singlet-A	3.7638 eV	329.41 nm	f= 0.0580	<S**2>=0.000
Excited State 17:	Singlet-A	3.7779 eV	328.19 nm	f= 0.5199	<S**2>=0.000
Excited State 18:	Singlet-A	3.8235 eV	324.27 nm	f= 0.9771	<S**2>=0.000
Excited State 19:	Singlet-A	3.9218 eV	316.14 nm	f= 0.0467	<S**2>=0.000
Excited State 20:	Singlet-A	3.9590 eV	313.17 nm	f= 0.0618	<S**2>=0.000
Excited State 21:	Singlet-A	3.9737 eV	312.01 nm	f= 0.1413	<S**2>=0.000
Excited State 22:	Singlet-A	3.9978 eV	310.13 nm	f= 0.0598	<S**2>=0.000
Excited State 23:	Singlet-A	4.0376 eV	307.07 nm	f= 0.0239	<S**2>=0.000
Excited State 24:	Singlet-A	4.0760 eV	304.18 nm	f= 0.0545	<S**2>=0.000
Excited State 25:	Singlet-A	4.1109 eV	301.60 nm	f= 0.0510	<S**2>=0.000
Excited State 26:	Singlet-A	4.1258 eV	300.51 nm	f= 0.0500	<S**2>=0.000
Excited State 27:	Singlet-A	4.1449 eV	299.12 nm	f= 0.0744	<S**2>=0.000
Excited State 28:	Singlet-A	4.1686 eV	297.42 nm	f= 0.0223	<S**2>=0.000
Excited State 29:	Singlet-A	4.1725 eV	297.14 nm	f= 0.0014	<S**2>=0.000
Excited State 30:	Singlet-A	4.2094 eV	294.54 nm	f= 0.2155	<S**2>=0.000
Excited State 31:	Singlet-A	4.2339 eV	292.84 nm	f= 0.0058	<S**2>=0.000
Excited State 32:	Singlet-A	4.2677 eV	290.52 nm	f= 0.0145	<S**2>=0.000
Excited State 33:	Singlet-A	4.2823 eV	289.53 nm	f= 0.0073	<S**2>=0.000
Excited State 34:	Singlet-A	4.2889 eV	289.08 nm	f= 0.0153	<S**2>=0.000
Excited State 35:	Singlet-A	4.2971 eV	288.53 nm	f= 0.0181	<S**2>=0.000
Excited State 36:	Singlet-A	4.3179 eV	287.14 nm	f= 0.0006	<S**2>=0.000
Excited State 37:	Singlet-A	4.3281 eV	286.47 nm	f= 0.2517	<S**2>=0.000
Excited State 38:	Singlet-A	4.3325 eV	286.18 nm	f= 0.0719	<S**2>=0.000
Excited State 39:	Singlet-A	4.3408 eV	285.62 nm	f= 0.1099	<S**2>=0.000
Excited State 40:	Singlet-A	4.3513 eV	284.94 nm	f= 0.0119	<S**2>=0.000
Excited State 41:	Singlet-A	4.3715 eV	283.62 nm	f= 0.1060	<S**2>=0.000
Excited State 42:	Singlet-A	4.3937 eV	282.19 nm	f= 0.0266	<S**2>=0.000
Excited State 43:	Singlet-A	4.4160 eV	280.76 nm	f= 0.1565	<S**2>=0.000
Excited State 44:	Singlet-A	4.4212 eV	280.43 nm	f= 0.0189	<S**2>=0.000
Excited State 45:	Singlet-A	4.4621 eV	277.86 nm	f= 0.0029	<S**2>=0.000
Excited State 46:	Singlet-A	4.4787 eV	276.83 nm	f= 0.0096	<S**2>=0.000
Excited State 47:	Singlet-A	4.4926 eV	275.98 nm	f= 0.0063	<S**2>=0.000
Excited State 48:	Singlet-A	4.5059 eV	275.16 nm	f= 0.0004	<S**2>=0.000
Excited State 49:	Singlet-A	4.5190 eV	274.36 nm	f= 0.0087	<S**2>=0.000
Excited State 50:	Singlet-A	4.5229 eV	274.13 nm	f= 0.0074	<S**2>=0.000

S4.10) TDDFT (ωB97XD/6-31G*) vertical excited state energies for the *mixed* dimer

Excited State 1:	Singlet-A	2.5929 eV	478.16 nm	f= 0.8382	<S**2>=0.000
Excited State 2:	Singlet-A	2.8020 eV	442.49 nm	f= 1.2820	<S**2>=0.000
Excited State 3:	Singlet-A	2.8648 eV	432.78 nm	f= 0.0454	<S**2>=0.000
Excited State 4:	Singlet-A	2.9328 eV	422.75 nm	f= 0.2750	<S**2>=0.000
Excited State 5:	Singlet-A	2.9350 eV	422.43 nm	f= 0.0646	<S**2>=0.000
Excited State 6:	Singlet-A	3.1117 eV	398.44 nm	f= 0.0183	<S**2>=0.000
Excited State 7:	Singlet-A	3.1638 eV	391.88 nm	f= 0.0013	<S**2>=0.000
Excited State 8:	Singlet-A	3.1987 eV	387.61 nm	f= 0.0125	<S**2>=0.000
Excited State 9:	Singlet-A	3.2317 eV	383.65 nm	f= 0.0150	<S**2>=0.000
Excited State 10:	Singlet-A	3.6716 eV	337.69 nm	f= 0.0169	<S**2>=0.000
Excited State 11:	Singlet-A	3.6843 eV	336.52 nm	f= 0.5290	<S**2>=0.000
Excited State 12:	Singlet-A	3.7199 eV	333.30 nm	f= 0.2592	<S**2>=0.000
Excited State 13:	Singlet-A	3.7236 eV	332.97 nm	f= 0.8676	<S**2>=0.000
Excited State 14:	Singlet-A	3.8282 eV	323.87 nm	f= 0.9858	<S**2>=0.000
Excited State 15:	Singlet-A	3.9176 eV	316.48 nm	f= 0.0940	<S**2>=0.000
Excited State 16:	Singlet-A	3.9437 eV	314.39 nm	f= 0.0091	<S**2>=0.000
Excited State 17:	Singlet-A	3.9540 eV	313.57 nm	f= 0.0447	<S**2>=0.000
Excited State 18:	Singlet-A	3.9793 eV	311.57 nm	f= 0.0577	<S**2>=0.000
Excited State 19:	Singlet-A	3.9910 eV	310.66 nm	f= 0.4095	<S**2>=0.000
Excited State 20:	Singlet-A	4.0429 eV	306.67 nm	f= 0.1557	<S**2>=0.000
Excited State 21:	Singlet-A	4.1228 eV	300.73 nm	f= 0.0587	<S**2>=0.000
Excited State 22:	Singlet-A	4.1311 eV	300.13 nm	f= 0.1991	<S**2>=0.000
Excited State 23:	Singlet-A	4.1539 eV	298.48 nm	f= 0.0692	<S**2>=0.000
Excited State 24:	Singlet-A	4.1641 eV	297.75 nm	f= 0.0268	<S**2>=0.000
Excited State 25:	Singlet-A	4.1876 eV	296.07 nm	f= 0.1185	<S**2>=0.000
Excited State 26:	Singlet-A	4.2314 eV	293.01 nm	f= 0.0027	<S**2>=0.000
Excited State 27:	Singlet-A	4.2584 eV	291.15 nm	f= 0.2162	<S**2>=0.000
Excited State 28:	Singlet-A	4.2841 eV	289.40 nm	f= 0.0330	<S**2>=0.000
Excited State 29:	Singlet-A	4.3187 eV	287.08 nm	f= 0.0039	<S**2>=0.000
Excited State 30:	Singlet-A	4.3226 eV	286.83 nm	f= 0.0919	<S**2>=0.000
Excited State 31:	Singlet-A	4.3374 eV	285.85 nm	f= 0.0106	<S**2>=0.000
Excited State 32:	Singlet-A	4.3589 eV	284.44 nm	f= 0.0746	<S**2>=0.000
Excited State 33:	Singlet-A	4.3795 eV	283.10 nm	f= 0.0392	<S**2>=0.000
Excited State 34:	Singlet-A	4.3826 eV	282.90 nm	f= 0.0556	<S**2>=0.000
Excited State 35:	Singlet-A	4.3933 eV	282.21 nm	f= 0.0158	<S**2>=0.000
Excited State 36:	Singlet-A	4.4027 eV	281.61 nm	f= 0.0320	<S**2>=0.000
Excited State 37:	Singlet-A	4.4310 eV	279.81 nm	f= 0.0158	<S**2>=0.000
Excited State 38:	Singlet-A	4.4490 eV	278.68 nm	f= 0.0051	<S**2>=0.000
Excited State 39:	Singlet-A	4.4783 eV	276.85 nm	f= 0.0253	<S**2>=0.000
Excited State 40:	Singlet-A	4.4888 eV	276.20 nm	f= 0.0144	<S**2>=0.000
Excited State 41:	Singlet-A	4.5227 eV	274.14 nm	f= 0.0077	<S**2>=0.000
Excited State 42:	Singlet-A	4.5326 eV	273.54 nm	f= 0.0108	<S**2>=0.000
Excited State 43:	Singlet-A	4.5479 eV	272.62 nm	f= 0.0171	<S**2>=0.000
Excited State 44:	Singlet-A	4.5612 eV	271.82 nm	f= 0.0268	<S**2>=0.000
Excited State 45:	Singlet-A	4.5679 eV	271.42 nm	f= 0.0042	<S**2>=0.000
Excited State 46:	Singlet-A	4.5815 eV	270.62 nm	f= 0.0012	<S**2>=0.000
Excited State 47:	Singlet-A	4.5877 eV	270.25 nm	f= 0.0017	<S**2>=0.000
Excited State 48:	Singlet-A	4.6020 eV	269.41 nm	f= 0.0041	<S**2>=0.000
Excited State 49:	Singlet-A	4.6093 eV	268.98 nm	f= 0.0210	<S**2>=0.000
Excited State 50:	Singlet-A	4.6313 eV	267.71 nm	f= 0.0030	<S**2>=0.000

S4.11)TDDFT (ωB97XD/6-311G*) vertical excited state energies for the oligomer *n* = 2

Excited State	1:	Singlet-A	3.0710 eV	403.72 nm	f= 0.2811	<S**2>=0.000
Excited State	2:	Singlet-A	3.1441 eV	394.33 nm	f= 0.1314	<S**2>=0.000
Excited State	3:	Singlet-A	3.1870 eV	389.03 nm	f= 0.0075	<S**2>=0.000
Excited State	4:	Singlet-A	3.7152 eV	333.72 nm	f= 0.5284	<S**2>=0.000
Excited State	5:	Singlet-A	3.7185 eV	333.42 nm	f= 0.4032	<S**2>=0.000
Excited State	6:	Singlet-A	3.9280 eV	315.64 nm	f= 0.3318	<S**2>=0.000
Excited State	7:	Singlet-A	3.9704 eV	312.27 nm	f= 0.0909	<S**2>=0.000
Excited State	8:	Singlet-A	4.0828 eV	303.67 nm	f= 0.0449	<S**2>=0.000
Excited State	9:	Singlet-A	4.0961 eV	302.69 nm	f= 0.0062	<S**2>=0.000
Excited State	10:	Singlet-A	4.1993 eV	295.25 nm	f= 0.3452	<S**2>=0.000
Excited State	11:	Singlet-A	4.2184 eV	293.91 nm	f= 0.1070	<S**2>=0.000
Excited State	12:	Singlet-A	4.2621 eV	290.90 nm	f= 0.6635	<S**2>=0.000
Excited State	13:	Singlet-A	4.3535 eV	284.79 nm	f= 0.3667	<S**2>=0.000
Excited State	14:	Singlet-A	4.3755 eV	283.36 nm	f= 0.0083	<S**2>=0.000
Excited State	15:	Singlet-A	4.4011 eV	281.71 nm	f= 0.0510	<S**2>=0.000
Excited State	16:	Singlet-A	4.4132 eV	280.94 nm	f= 0.1143	<S**2>=0.000
Excited State	17:	Singlet-A	4.5012 eV	275.44 nm	f= 0.0091	<S**2>=0.000
Excited State	18:	Singlet-A	4.5067 eV	275.11 nm	f= 0.0025	<S**2>=0.000
Excited State	19:	Singlet-A	4.5887 eV	270.19 nm	f= 0.0001	<S**2>=0.000
Excited State	20:	Singlet-A	4.5959 eV	269.77 nm	f= 0.0016	<S**2>=0.000

TDDFT (ωB97XD/6-31G*) vertical excited state energies for the oligomer *n* = 2

Excited State	1:	Singlet-A	2.9827 eV	415.68 nm	f= 0.5280	<S**2>=0.000
Excited State	2:	Singlet-A	3.0982 eV	400.18 nm	f= 0.0109	<S**2>=0.000
Excited State	3:	Singlet-A	3.1279 eV	396.38 nm	f= 0.0352	<S**2>=0.000
Excited State	4:	Singlet-A	3.7191 eV	333.37 nm	f= 0.6641	<S**2>=0.000
Excited State	5:	Singlet-A	3.7251 eV	332.84 nm	f= 0.2967	<S**2>=0.000
Excited State	6:	Singlet-A	3.9197 eV	316.31 nm	f= 0.3118	<S**2>=0.000
Excited State	7:	Singlet-A	3.9603 eV	313.07 nm	f= 0.0993	<S**2>=0.000
Excited State	8:	Singlet-A	4.0464 eV	306.40 nm	f= 0.0372	<S**2>=0.000
Excited State	9:	Singlet-A	4.0981 eV	302.54 nm	f= 0.0574	<S**2>=0.000
Excited State	10:	Singlet-A	4.1282 eV	300.34 nm	f= 0.3019	<S**2>=0.000

S4.12) UCAM-B3LYP/6-31G* optimized geometry for the charged (-1) oligomer *n* = 4 of P(NDI2OD-T2)

C	-18.893853	-0.950800	0.483448
C	-17.935167	-1.846318	1.008100
C	-16.633780	-1.453394	1.173929
C	-16.187467	-0.148154	0.848139
C	-17.127014	0.767501	0.382064
C	-18.473171	0.363177	0.180553
C	-19.431619	1.258486	-0.342519
C	-20.732445	0.863156	-0.515668
C	-21.174950	-0.442616	-0.196424
C	-20.238438	-1.355379	0.279625
C	-16.787447	2.205115	0.176425
N	-17.756173	3.025079	-0.412002
C	-19.063654	2.651670	-0.695973
C	-20.585547	-2.788889	0.503760
N	-19.616054	-3.609532	1.085717
C	-18.305494	-3.237475	1.366025
O	-19.861308	3.425688	-1.189596
O	-15.725830	2.693094	0.503919
O	-21.657661	-3.269387	0.198079
O	-17.511023	-4.012356	1.861877
C	-17.357023	4.410158	-0.655293
C	-20.018625	-4.991460	1.340351
H	-15.920413	-2.178660	1.547118
H	-20.916918	-5.002306	1.958726
H	-20.244070	-5.494567	0.398214
H	-19.194878	-5.486321	1.847398
H	-18.172455	4.900876	-1.179521
H	-17.155258	4.913692	0.292054
H	-16.445448	4.427055	-1.253486
H	-21.444006	1.587164	-0.894648
C	-22.618904	-0.693770	-0.383793
C	-23.322053	-0.527008	-1.542409
C	-24.721213	-0.707777	-1.382807
C	-25.083668	-0.984815	-0.092858
S	-23.685674	-1.054830	0.936143
C	-26.415371	-1.205274	0.447931
C	-26.853239	-1.044955	1.734585
C	-28.233663	-1.348537	1.900475
C	-28.829128	-1.733632	0.739596
S	-27.713750	-1.748880	-0.575217
H	-22.849217	-0.286160	-2.487509
H	-25.436906	-0.610915	-2.190805
H	-26.210663	-0.700073	2.536524
H	-28.757390	-1.273428	2.845911
H	-29.860608	-2.013609	0.578334
C	-14.741726	0.091298	1.009849
C	-14.007019	-0.144319	2.138368
C	-12.616571	0.072010	1.960561
C	-12.288666	0.438728	0.682596
S	-13.707937	0.525295	-0.314660
C	-10.977970	0.727608	0.127518
C	-10.668460	1.462032	-0.984950
C	-9.271809	1.553210	-1.221959
C	-8.521954	0.871082	-0.307370
S	-9.535636	0.121141	0.883643
C	-7.046586	0.882039	-0.203735
C	-6.211919	-0.230811	-0.280908
C	-4.815188	-0.081819	-0.103186
C	-4.235094	1.185519	0.127602
C	-5.098729	2.301263	0.165451
C	-6.453733	2.144656	0.009394
C	-3.950796	-1.201610	-0.141216
C	-2.600317	-1.041287	-0.010290
C	-1.986660	0.227796	0.186696
C	-2.830755	1.335636	0.301220
C	-4.482464	-2.567403	-0.360925
C	-6.741130	-1.580459	-0.628856
N	-5.853659	-2.657333	-0.588058
C	-4.573197	3.668764	0.393768
C	-2.328013	2.671862	0.718859

N	-3.214202	3.756513	0.651214
C	-6.426527	-3.968538	-0.883088
C	-2.649529	5.061635	0.988077
O	-5.293074	4.650685	0.375961
O	-1.202530	2.867627	1.128308
O	-7.896216	-1.780595	-0.948575
O	-3.771403	-3.553493	-0.355729
H	-1.975101	-1.921267	-0.097829
H	-7.081047	3.026255	0.067826
H	-11.416757	1.945366	-1.602323
H	-8.833761	2.103805	-2.046173
H	-14.454735	-0.438920	3.080659
H	-11.885143	-0.025177	2.754095
H	-3.413443	5.810246	0.796385
H	-2.351207	5.082790	2.038172
H	-1.764432	5.243138	0.377864
H	-7.256195	-4.167033	-0.203379
H	-6.808547	-3.988264	-1.905545
H	-5.639414	-4.706955	-0.757428
C	-0.520855	0.212920	0.190008
C	0.254676	-0.776829	0.746271
C	1.631207	-0.654189	0.463258
C	1.920312	0.415806	-0.350653
S	0.479063	1.312295	-0.714190
C	3.204423	0.828421	-0.873869
C	3.465426	1.653566	-1.937593
C	4.849152	1.820918	-2.185565
C	5.651285	1.111583	-1.330819
S	4.687023	0.254327	-0.170766
H	-0.158822	-1.574037	1.353913
H	2.386614	-1.344736	0.817593
H	2.686620	2.107527	-2.540701
H	5.253222	2.430652	-2.984504
C	7.122241	1.192232	-1.246070
C	8.014699	0.086327	-1.278420
C	9.399120	0.293775	-1.076309
C	9.931503	1.608196	-0.877639
C	9.020014	2.686996	-0.918301
C	7.653061	2.461984	-1.083111
C	10.306715	-0.787983	-1.076514
C	11.661541	-0.572507	-0.841726
C	12.198590	0.689866	-0.618339
C	11.319521	1.815618	-0.666418
C	9.474523	4.062930	-0.768711
C	11.804629	3.195925	-0.584251
N	10.850070	4.223194	-0.617299
C	7.550530	-1.261058	-1.613553
C	9.851266	-2.154926	-1.299265
N	8.487669	-2.298853	-1.560863
O	6.399873	-1.534706	-1.941623
O	10.596437	-3.130613	-1.278979
O	8.720558	5.032720	-0.782863
O	12.983825	3.524444	-0.494395
C	7.977578	-3.629045	-1.859535
C	11.377491	5.575915	-0.510872
H	6.999461	3.325562	-1.049952
H	12.293943	-1.451634	-0.801062
H	7.582575	-3.660767	-2.877531
H	8.803212	-4.326878	-1.746139
H	7.162081	-3.875943	-1.176839
H	10.530787	6.257053	-0.533902
H	11.939056	5.685326	0.419238
H	12.060715	5.778511	-1.338447
C	13.634522	0.736814	-0.294398
C	14.302901	1.386542	0.711189
C	15.677335	1.076240	0.772066
C	16.087383	0.188342	-0.193512
S	14.740688	-0.264091	-1.195475
C	17.407280	-0.350178	-0.420730
C	17.787885	-1.353905	-1.282707
C	19.164659	-1.648798	-1.215707
C	19.865261	-0.856880	-0.336143
S	18.785180	0.265838	0.439071
H	13.813903	2.080838	1.378867
H	16.348570	1.489376	1.517534
H	17.090315	-1.872411	-1.929182

H	19.636661	-2.421038	-1.812900
C	21.265747	-1.057936	0.044998
C	21.657132	-2.421255	0.190022
C	22.894510	-2.789959	0.636312
C	23.838458	-1.804034	0.999764
C	23.496453	-0.444349	0.838964
C	22.220264	-0.074790	0.328325
C	24.456924	0.525838	1.208088
C	25.684472	0.152599	1.714244
C	26.013729	-1.200006	1.866134
C	25.099398	-2.167052	1.509621
C	25.448815	-3.599995	1.664004
C	23.221368	-4.231661	0.773798
C	24.166436	1.970474	1.056466
C	22.002389	1.359546	0.005356
N	24.487726	-4.535711	1.284079
N	22.950577	2.284908	0.466761
O	21.064686	1.767974	-0.648628
O	24.954098	2.830789	1.408189
O	22.439273	-5.108137	0.461696
O	26.523490	-3.969498	2.099080
H	20.937191	-3.201345	-0.024846
H	26.976104	-1.507451	2.258457
H	26.382769	0.934976	1.988190
C	22.650114	3.688894	0.195302
C	24.857720	-5.939298	1.443409
H	21.657148	3.928887	0.576434
H	23.410342	4.289228	0.687560
H	22.656729	3.873990	-0.880769
H	24.016876	-6.542440	1.111939
H	25.745624	-6.157993	0.847568
H	25.088160	-6.144299	2.490286

Energy = -8513.18755722 Hartree

S4.13) UCAM-B3LYP/6-31G* optimized geometry for the charged (-1) oligomer *n* = 5 of P(NDI2OD-T2)

6	25.922931	-0.885530	-0.654966
6	24.918676	-1.779466	-1.091964
6	23.627601	-1.354698	-1.264489
6	23.232414	-0.012201	-1.051701
6	24.219074	0.904913	-0.697634
6	25.550519	0.466111	-0.475532
6	26.550715	1.372200	-0.061359
6	27.825262	0.938797	0.177068
6	28.219452	-0.415641	0.022846
6	27.254854	-1.327531	-0.416706
6	23.943048	2.369485	-0.644773
7	24.953516	3.207157	-0.161295
6	26.248193	2.810420	0.144452
6	27.578815	-2.755146	-0.714615
7	26.546941	-3.582156	-1.170194
6	25.224749	-3.202914	-1.361852
8	27.086483	3.597750	0.540239
8	22.897992	2.864512	-1.012865
8	28.687347	-3.237160	-0.595939
8	24.378099	-3.990627	-1.737966
6	24.616188	4.626175	-0.066178
6	26.919730	-4.967669	-1.449394
1	22.883707	-2.086256	-1.556998
1	27.698358	-4.994019	-2.213029
1	27.310844	-5.436145	-0.544819
1	26.027733	-5.484789	-1.791874
1	25.460500	5.135454	0.390266
1	24.418425	5.031646	-1.060255
1	23.717068	4.747411	0.538784
1	28.545934	1.669470	0.524603
6	29.620979	-0.710890	0.369658
6	30.144916	-1.667207	1.193726
6	31.539177	-1.537419	1.397483
6	32.093361	-0.482718	0.720145
16	30.878565	0.366707	-0.179443
6	33.482782	-0.061177	0.674363
6	33.990311	1.180442	0.399730
6	35.411132	1.229654	0.449708
6	35.966737	0.027860	0.763752
16	34.768630	-1.190938	0.988175
1	29.545906	-2.444624	1.646866
1	32.115399	-2.194643	2.038297
1	33.363483	2.039350	0.189247
1	35.989442	2.127481	0.267668
1	37.014121	-0.215030	0.874966
6	21.792544	0.262467	-1.201542
6	21.012206	-0.094868	-2.266546
6	19.636768	0.195643	-2.080766
6	19.364781	0.744594	-0.855958
16	20.817668	0.909800	0.080041
6	18.084631	1.160866	-0.310053
6	17.836967	2.095022	0.658534
6	16.453374	2.263850	0.929678
6	15.653335	1.444475	0.187156
16	16.600315	0.462101	-0.883477
6	14.174838	1.463369	0.142786
6	13.332731	0.414181	0.504075
6	11.931779	0.544842	0.352101
6	11.346562	1.735006	-0.139006
6	12.222332	2.800469	-0.442595
6	13.582702	2.656494	-0.315454
6	11.063902	-0.518666	0.694702
6	9.716360	-0.394572	0.528708
6	9.095232	0.779229	0.007579
6	9.934700	1.860280	-0.306309
6	11.592482	-1.799738	1.222742
6	13.869369	-0.828127	1.130716
7	12.971666	-1.861051	1.402304
6	11.708362	4.109165	-0.903584
6	9.409064	3.185871	-0.733628
7	10.330616	4.213838	-0.988286

6	13.547224	-3.074662	1.976951
6	9.753770	5.491749	-1.399789
8	12.447005	5.038366	-1.177744
8	8.229767	3.445929	-0.864810
8	15.040513	-0.973856	1.420199
8	10.871987	-2.739762	1.495559
1	9.104171	-1.253215	0.776646
1	14.211566	3.495676	-0.588403
1	18.620541	2.665670	1.143357
1	16.061060	2.966850	1.655049
1	21.418190	-0.529634	-3.172823
1	18.876157	0.022457	-2.832780
1	10.574766	6.183909	-1.565148
1	9.172427	5.359854	-2.313779
1	9.085443	5.863141	-0.621662
1	14.333381	-3.452764	1.322194
1	13.988373	-2.854096	2.950855
1	12.746372	-3.801920	2.078494
6	7.643818	0.698319	-0.153661
6	6.830853	1.104408	-1.183160
6	5.487703	0.701699	-1.046146
6	5.240471	-0.010540	0.104747
16	6.698674	-0.191117	1.025663
6	3.987318	-0.545180	0.586000
6	3.784791	-1.550953	1.497021
6	2.415625	-1.827960	1.723374
6	1.567036	-1.055398	0.974215
16	2.467382	0.066592	0.005310
1	7.195190	1.665767	-2.030655
1	4.718493	0.911102	-1.779623
1	4.596182	-2.093689	1.969698
1	2.054634	-2.591532	2.401535
6	0.096199	-1.014188	1.085379
6	-0.817704	-1.181197	0.010247
6	-2.203737	-1.012356	0.232991
6	-2.714562	-0.709847	1.535919
6	-1.778991	-0.614917	2.590291
6	-0.412183	-0.752338	2.347832
6	-3.133917	-1.149591	-0.820769
6	-4.491858	-0.950449	-0.593103
6	-5.010186	-0.628640	0.656402
6	-4.105024	-0.532016	1.758038
6	-2.209143	-0.352555	3.957590
6	-4.562445	-0.334293	3.136017
7	-3.585504	-0.236106	4.137578
6	-0.369162	-1.622232	-1.312164
6	-2.699398	-1.482025	-2.172419
7	-1.329655	-1.703272	-2.326163
8	0.787937	-1.928905	-1.582624
8	-3.465810	-1.581973	-3.126272
8	-1.433973	-0.247873	4.904544
8	-5.736842	-0.253418	3.483462
6	-0.836844	-2.105436	-3.635522
6	-4.087059	-0.019297	5.487112
1	0.258377	-0.617042	3.188169
1	-5.144755	-1.020026	-1.455263
1	-0.405123	-3.107596	-3.583660
1	-1.680594	-2.086370	-4.320499
1	-0.052792	-1.420071	-3.963355
1	-3.225599	0.051403	6.146110
1	-4.679153	0.897540	5.522415
1	-4.735265	-0.846610	5.783768
6	-6.457629	-0.365666	0.709344
6	-7.159464	0.668017	1.277085
6	-8.539864	0.638967	0.994464
6	-8.921301	-0.426321	0.212427
16	-7.540070	-1.409419	-0.170576
6	-10.237761	-0.765180	-0.266165
6	-10.590180	-1.628118	-1.280967
6	-11.980324	-1.752641	-1.459505
6	-12.727354	-0.979480	-0.603183
16	-11.658160	-0.092280	0.468563
1	-6.687221	1.422420	1.889184
1	-9.236914	1.395074	1.339937
1	-9.857845	-2.145740	-1.888877
1	-12.423432	-2.384260	-2.214893

6	-14.162848	-0.712053	-0.565323
6	-14.526179	0.641829	-0.309438
6	-15.814813	1.088407	-0.308551
6	-16.890397	0.202945	-0.562220
6	-16.564472	-1.158455	-0.771764
6	-15.214709	-1.621109	-0.770702
6	-17.643174	-2.046792	-0.970740
6	-18.936201	-1.591716	-1.002360
6	-19.274565	-0.231845	-0.833261
6	-18.231074	0.667560	-0.586991
6	-18.482089	2.107066	-0.278209
6	-16.048494	2.526428	-0.045813
6	-17.423990	-3.499557	-1.147276
6	-14.989392	-3.085812	-0.900247
7	-17.379274	2.928651	-0.033885
7	-16.107828	-3.917842	-1.067840
8	-13.898232	-3.618728	-0.856614
8	-18.341960	-4.278486	-1.335947
8	-15.142313	3.311568	0.156840
8	-19.590626	2.602094	-0.218500
1	-13.749447	1.377697	-0.139913
1	-19.715378	-2.321787	-1.186965
6	-15.822091	-5.345550	-1.187778
6	-17.679768	4.328283	0.256943
1	-15.303992	-5.694750	-0.293580
1	-16.771071	-5.860385	-1.309671
1	-15.174933	-5.524473	-2.048055
1	-16.734668	4.839809	0.416892
1	-18.220787	4.773196	-0.579842
1	-18.309338	4.395114	1.145613
6	-20.709929	0.091830	-0.950556
6	-21.346517	1.008511	-1.738750
6	-22.758075	0.920744	-1.681523
6	-23.208259	-0.063345	-0.840494
16	-21.873146	-0.894097	-0.108323
6	-24.576055	-0.432522	-0.525078
6	-25.056106	-1.639940	-0.090801
6	-26.455536	-1.632282	0.133725
6	-27.048024	-0.435152	-0.162014
16	-25.861612	0.726109	-0.666438
1	-23.423242	1.551075	-2.260460
1	-20.816185	1.729673	-2.345405
1	-24.426908	-2.511467	0.045396
1	-27.014349	-2.495127	0.477828
6	-28.462065	-0.092732	0.078912
6	-29.348462	0.455111	-0.846391
6	-30.661056	0.818995	-0.441603
6	-31.089264	0.585490	0.882450
6	-30.198525	-0.018001	1.793725
6	-28.926204	-0.333533	1.399776
1	-28.247347	-0.761310	2.127983
6	-29.003074	0.586313	-2.290742
6	-31.571054	1.424411	-1.339512
6	-32.837240	1.778343	-0.929652
6	-33.255361	1.538280	0.388438
6	-32.392349	0.947633	1.281807
6	-31.179812	1.689224	-2.744730
6	-30.620851	-0.292488	3.192308
6	-32.837224	0.689505	2.674250
7	-31.921561	0.085738	3.534934
7	-29.913585	1.252843	-3.118283
8	-27.987770	0.135056	-2.779120
8	-31.926294	2.241203	-3.530783
8	-29.879117	-0.818265	3.997921
8	-33.949366	0.982050	3.068655
6	-29.505643	1.412377	-4.512989
6	-32.385150	-0.159498	4.898915
1	-34.250524	1.808755	0.722139
1	-33.498361	2.244353	-1.651156
1	-29.417149	0.435287	-4.991859
1	-30.262706	2.011471	-5.011416
1	-28.533010	1.903597	-4.554128
1	-31.570919	-0.625656	5.446907
1	-32.671667	0.783993	5.366275
1	-33.258633	-0.813388	4.880171

Energy = -10641.1659602 Hartree

S4.14) TDUCAM-B3LYP/6-31G* vertical excited states energies for the optimized geometry for the charged (-1) oligomer *n* = 4 of P(NDI2OD-T2)

Excited State 1: 2.035-?Sym 0.3711 eV 3341.21 nm f= 0.0035 <S**2>=0.785
Excited State 2: 2.055-?Sym 0.5364 eV 2311.62 nm f= 0.0971 <S**2>=0.806
Excited State 3: 2.092-?Sym 0.6254 eV 1982.62 nm f= 0.1210 <S**2>=0.844
Excited State 4: 3.362-?Sym 1.5169 eV 817.33 nm f= 0.0035 <S**2>=2.576
Excited State 5: 3.439-?Sym 1.5518 eV 798.98 nm f= 0.0013 <S**2>=2.707
Excited State 6: 2.233-?Sym 1.8332 eV 676.34 nm f= 0.4835 <S2>=0.997**
Excited State 7: 3.478-?Sym 1.8575 eV 667.47 nm f= 0.0004 <S**2>=2.775
Excited State 8: 2.505-?Sym 1.9907 eV 622.81 nm f= 0.1548 <S2>=1.319**
Excited State 9: 2.997-?Sym 2.0790 eV 596.37 nm f= 0.3248 <S2>=1.995**
Excited State 10: 2.995-?Sym 2.1230 eV 584.02 nm f= 0.0159 <S**2>=1.992
Excited State 11: 2.619-?Sym 2.1467 eV 577.56 nm f= 0.3919 <S2>=1.464**
Excited State 12: 2.448-?Sym 2.1708 eV 571.16 nm f= 0.0278 <S**2>=1.248
Excited State 13: 3.386-?Sym 2.2212 eV 558.19 nm f= 0.0031 <S**2>=2.617
Excited State 14: 2.162-?Sym 2.2401 eV 553.47 nm f= 0.0044 <S**2>=0.919
Excited State 15: 2.609-?Sym 2.2734 eV 545.38 nm f= 0.0059 <S**2>=1.452
Excited State 16: 2.841-?Sym 2.2906 eV 541.28 nm f= 0.0008 <S**2>=1.768
Excited State 17: 2.038-?Sym 2.3100 eV 536.73 nm f= 0.0007 <S**2>=0.788
Excited State 18: 2.468-?Sym 2.3272 eV 532.77 nm f= 0.0405 <S**2>=1.273
Excited State 19: 3.479-?Sym 2.3521 eV 527.13 nm f= 0.0000 <S**2>=2.776
Excited State 20: 3.209-?Sym 2.4586 eV 504.30 nm f= 0.0040 <S**2>=2.324
Excited State 21: 2.615-?Sym 2.5071 eV 494.54 nm f= 0.0201 <S**2>=1.460
Excited State 22: 2.838-?Sym 2.5160 eV 492.79 nm f= 0.0022 <S**2>=1.763
Excited State 23: 2.264-?Sym 2.5473 eV 486.72 nm f= 0.0292 <S**2>=1.032
Excited State 24: 2.120-?Sym 2.5866 eV 479.33 nm f= 0.0176 <S**2>=0.873
Excited State 25: 3.452-?Sym 2.6409 eV 469.48 nm f= 0.0007 <S**2>=2.728
Excited State 26: 2.356-?Sym 2.6421 eV 469.27 nm f= 0.3344 <S2>=1.138**
Excited State 27: 2.683-?Sym 2.6632 eV 465.55 nm f= 0.0734 <S**2>=1.550
Excited State 28: 2.137-?Sym 2.7292 eV 454.30 nm f= 0.0180 <S**2>=0.892
Excited State 29: 2.918-?Sym 2.7444 eV 451.78 nm f= 0.0282 <S**2>=1.879
Excited State 30: 2.732-?Sym 2.7890 eV 444.54 nm f= 0.0258 <S**2>=1.616
Excited State 31: 2.206-?Sym 2.7901 eV 444.37 nm f= 0.0445 <S**2>=0.966
Excited State 32: 2.423-?Sym 2.8439 eV 435.96 nm f= 0.0510 <S**2>=1.218
Excited State 33: 2.853-?Sym 2.8557 eV 434.17 nm f= 0.0015 <S**2>=1.785
Excited State 34: 3.370-?Sym 2.8782 eV 430.77 nm f= 0.0003 <S**2>=2.589
Excited State 35: 3.041-?Sym 2.8871 eV 429.44 nm f= 0.0151 <S**2>=2.062
Excited State 36: 2.779-?Sym 2.9141 eV 425.47 nm f= 0.0274 <S**2>=1.680
Excited State 37: 2.115-?Sym 2.9583 eV 419.11 nm f= 0.0200 <S**2>=0.868
Excited State 38: 2.028-?Sym 2.9739 eV 416.91 nm f= 0.0383 <S**2>=0.778
Excited State 39: 3.433-?Sym 3.0248 eV 409.89 nm f= 0.0072 <S**2>=2.696
Excited State 40: 2.447-?Sym 3.0768 eV 402.97 nm f= 0.1928 <S**2>=1.247
Excited State 41: 2.239-?Sym 3.1102 eV 398.64 nm f= 0.0120 <S**2>=1.003
Excited State 42: 2.885-?Sym 3.1308 eV 396.01 nm f= 0.0446 <S**2>=1.831
Excited State 43: 2.217-?Sym 3.1556 eV 392.91 nm f= 0.0555 <S**2>=0.979
Excited State 44: 2.968-?Sym 3.1625 eV 392.05 nm f= 0.1172 <S**2>=1.952
Excited State 45: 3.122-?Sym 3.1738 eV 390.65 nm f= 0.0308 <S**2>=2.186
Excited State 46: 2.484-?Sym 3.2100 eV 386.25 nm f= 0.0198 <S**2>=1.293
Excited State 47: 2.421-?Sym 3.2583 eV 380.52 nm f= 0.0353 <S**2>=1.215
Excited State 48: 2.976-?Sym 3.2707 eV 379.07 nm f= 0.0348 <S**2>=1.964
Excited State 49: 3.199-?Sym 3.2942 eV 376.37 nm f= 0.0084 <S**2>=2.309
Excited State 50: 3.113-?Sym 3.3253 eV 372.85 nm f= 0.0056 <S**2>=2.172

S4.15) TDUCAM-B3LYP/6-31G* vertical excited states energies for the optimized geometry for the charged (-1) oligomer *n* = 5 of P(NDI2OD-T2)

Excited State	1:	2.036-?Sym	0.4410 eV	2811.25 nm	f= 0.0045	<S**2>=0.786
Excited State	2:	2.044-?Sym	0.4528 eV	2737.98 nm	f= 0.0489	<S**2>=0.795
Excited State	3:	2.090-?Sym	0.5617 eV	2207.27 nm	f= 0.2142	<S**2>=0.842
Excited State	4:	2.063-?Sym	0.5915 eV	2096.14 nm	f= 0.0365	<S**2>=0.814
Excited State	5:	3.376-?Sym	1.4284 eV	867.98 nm	f= 0.0097	<S**2>=2.599
Excited State	6:	3.440-?Sym	1.4943 eV	829.70 nm	f= 0.0025	<S**2>=2.709
Excited State	7:	3.480-?Sym	1.7658 eV	702.15 nm	f= 0.0000	<S**2>=2.777
Excited State	8:	2.267-?Sym	1.7976 eV	689.74 nm	f= 0.5559	<S**2>=1.035
Excited State	9:	3.429-?Sym	1.8699 eV	663.04 nm	f= 0.0500	<S**2>=2.690
Excited State	10:	2.506-?Sym	1.9776 eV	626.96 nm	f= 0.3548	<S**2>=1.320
Excited State	11:	2.509-?Sym	2.0472 eV	605.63 nm	f= 0.3941	<S**2>=1.324
Excited State	12:	3.002-?Sym	2.0864 eV	594.24 nm	f= 0.2012	<S**2>=2.002
Excited State	13:	3.274-?Sym	2.1409 eV	579.13 nm	f= 0.0305	<S**2>=2.429
Excited State	14:	2.471-?Sym	2.1768 eV	569.57 nm	f= 0.2978	<S**2>=1.276
Excited State	15:	3.273-?Sym	2.1956 eV	564.71 nm	f= 0.0616	<S**2>=2.428
Excited State	16:	2.815-?Sym	2.2310 eV	555.73 nm	f= 0.0228	<S**2>=1.731
Excited State	17:	2.038-?Sym	2.2380 eV	554.01 nm	f= 0.0001	<S**2>=0.788
Excited State	18:	2.803-?Sym	2.2520 eV	550.56 nm	f= 0.0074	<S**2>=1.714
Excited State	19:	2.681-?Sym	2.2621 eV	548.10 nm	f= 0.0033	<S**2>=1.546
Excited State	20:	3.443-?Sym	2.2990 eV	539.29 nm	f= 0.0006	<S**2>=2.714
Excited State	21:	2.160-?Sym	2.3166 eV	535.19 nm	f= 0.0164	<S**2>=0.916
Excited State	22:	2.482-?Sym	2.3169 eV	535.12 nm	f= 0.0397	<S**2>=1.290
Excited State	23:	2.806-?Sym	2.3591 eV	525.56 nm	f= 0.0037	<S**2>=1.718
Excited State	24:	2.844-?Sym	2.3747 eV	522.11 nm	f= 0.0003	<S**2>=1.772
Excited State	25:	3.170-?Sym	2.4440 eV	507.30 nm	f= 0.0109	<S**2>=2.263
Excited State	26:	2.874-?Sym	2.5102 eV	493.92 nm	f= 0.0126	<S**2>=1.816
Excited State	27:	2.762-?Sym	2.5134 eV	493.29 nm	f= 0.0408	<S**2>=1.658
Excited State	28:	2.196-?Sym	2.5305 eV	489.95 nm	f= 0.0188	<S**2>=0.955
Excited State	29:	2.136-?Sym	2.5511 eV	486.00 nm	f= 0.0102	<S**2>=0.891
Excited State	30:	2.738-?Sym	2.5820 eV	480.18 nm	f= 0.0897	<S**2>=1.625