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Supporting Information

Flat Conjugated Polymers Combining a Relatively Low HOMO Energy Level and Band Gap: Polyselenophenes versus Polythiophenes

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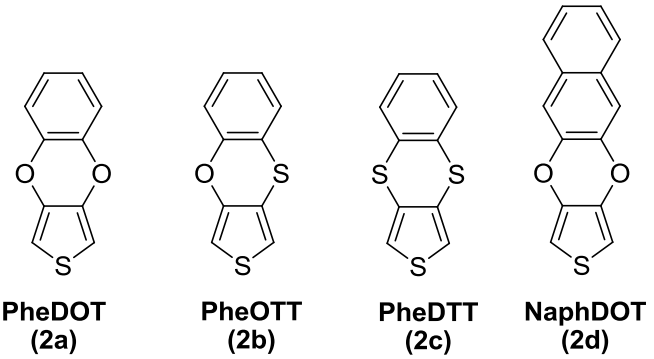
Electrochemical polymerization of phenylene-bridged thiophenes 2a–d.



Electrochemical polymerization (ECP) of phenylene-bridged thiophenes **2a**–**c** was performed at potentiodynamic conditions by repeated cyclic voltammetry (CV) in dichloromethane solution with0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as a supporting electrolyte. As previously reported,[1,2] polymerization of **PheDOT** (**2a**)is difficult, but it can be polymerized in dichloromethane solution at high concentrations. Applying a scan rate of 50 mV/s and using a potential range of –0.4 to 1.6 V, we succeed in obtaining films of proper quality (Fig. S1a). **PheOTT** (**2b**) smoothly undergoes electropolymerization to deposit insoluble film on the electrode surface (Fig. S1b). The onset potential of polymer **PPheOTT** (**P2b**) is 0.12V vs. SCE. Electrochemical polymerization of **PheDTT** (**2c**) was problematic and we did not succeed in obtaining good films. The naphthalene-bridged **PNaphDOT** (**2d**) shows very similar electrochemical properties to its phenylene-bridged analogue (Fig. S1d).

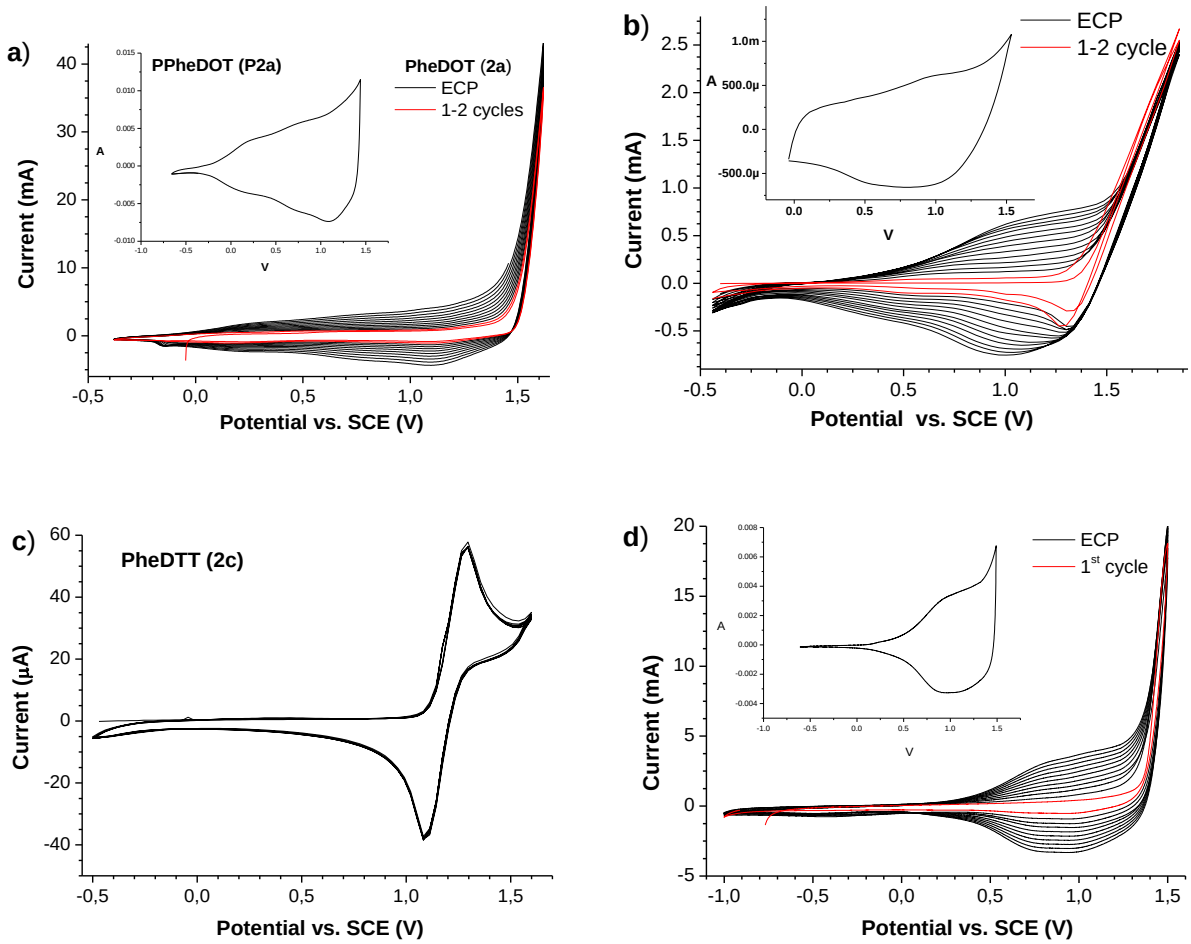


Fig. S1 Potentiodynamic electropolymerization of thiophene monomers **2a-d** on ITO electrode in CH_2Cl_2/$TBAPF_6$ (0.1M), scan rate 50 mV/s. Insets are CVs of electrodeposited polymers **P1a,b,d** in monomer free CH_2Cl_2/$TBAPF_6$ (0.1M) solutions. (a) **PheDOT** (**2a**) and **PPheDOT** (**P1a**). (b) **PheOTT** (**2b**) and **PPheOTT** (**P1b**). (c) Repeated three CV scans of **PheDTT** (**2c**) in attempts of its electropolymerization. (d) **NaphDOT** (**2d**) and **PNaphDOT** (**P1d**). All potentials are given vs. SCE and were calibrated to the Fc/Fc^+ standard, which is 0.46 V vs. SCE under these conditions.[3]

Electrochemical polymerization and spectroelectrochemistry of PEDOS.

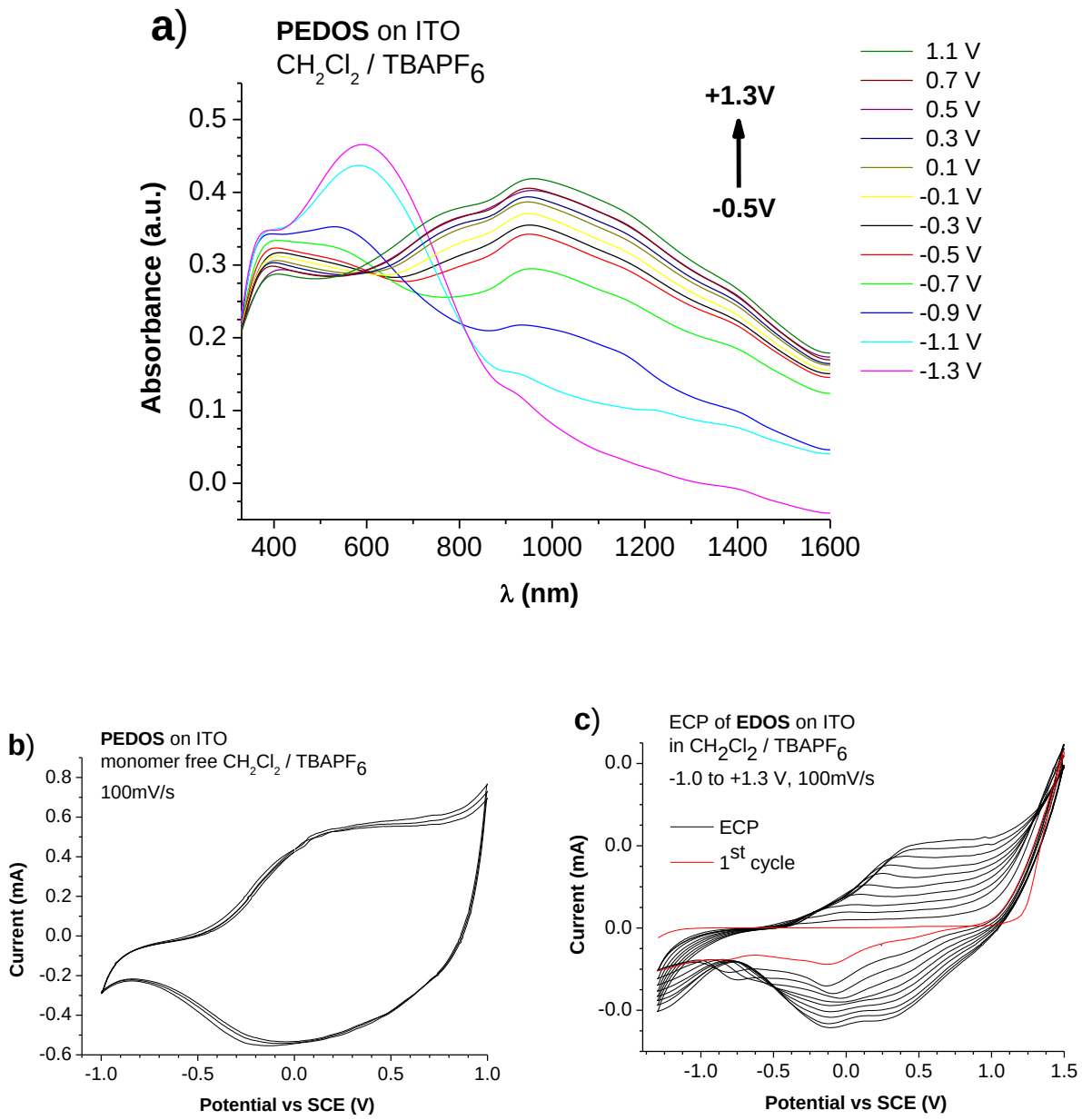


Fig. S2 (a) Spectroelectrochemical measurements of **PEDOS** on ITO performed in CH_2Cl_2/$TBAPF_6$ (0.1 M) under various potentials applied *in situ*. (b) CV measurements of the electrodeposited film of polymer **PEDOS** on ITO in monomer free CH_2Cl_2/$TBAPF_6$ (0.1 M) solution at scan rate of 100 mV/s. (c) Electrochemical polymerization of **EDOS** monomer performed in CH_2Cl_2/$TBAPF_6$ (0.1 M). All data are vs. SCE and were calibrated to the Fc/Fc^+ standard, which is 0.46 V vs. SCE under these conditions.[3]

Electrochemical polymerization and spectroelectrochemistry of phenylene-bridged polyselenophenes in acetonitrile and propylene carbonate.

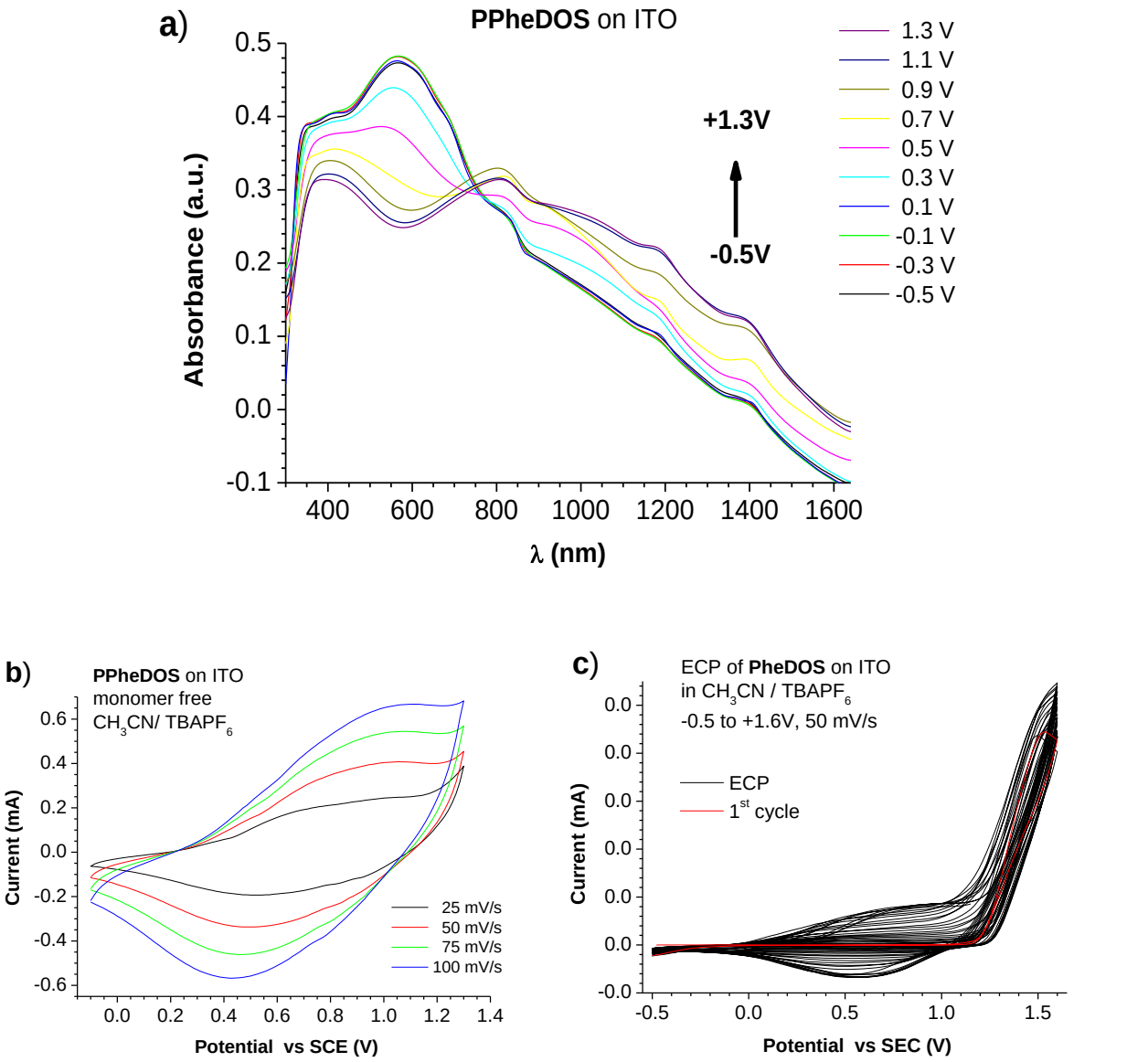


Fig. S3 (a) Spectroelectrochemical measurements for polymer **PPheDOS** (**P1a**) on ITO performed in $CH_3CN/TBAPF_6$ (0.1M) under various potentials applied *in situ*. (b) CV measurements of the electrodeposited film of polymer **PPheDOS** (**P1a**) on ITO in monomer free $CH_3CN/TBAPF_6$ (0.1 M) solution at various scan rates. (c) Electrochemical polymerization of monomer **PheDOS** (**1a**) in $CH_3CN/TBAPF_6$ (0.1 M) on ITO electrode. All data are given vs. SCE and were calibrated to the Fc/Fc^+ standard, which is 0.40 V vs. SCE under these conditions.[3]

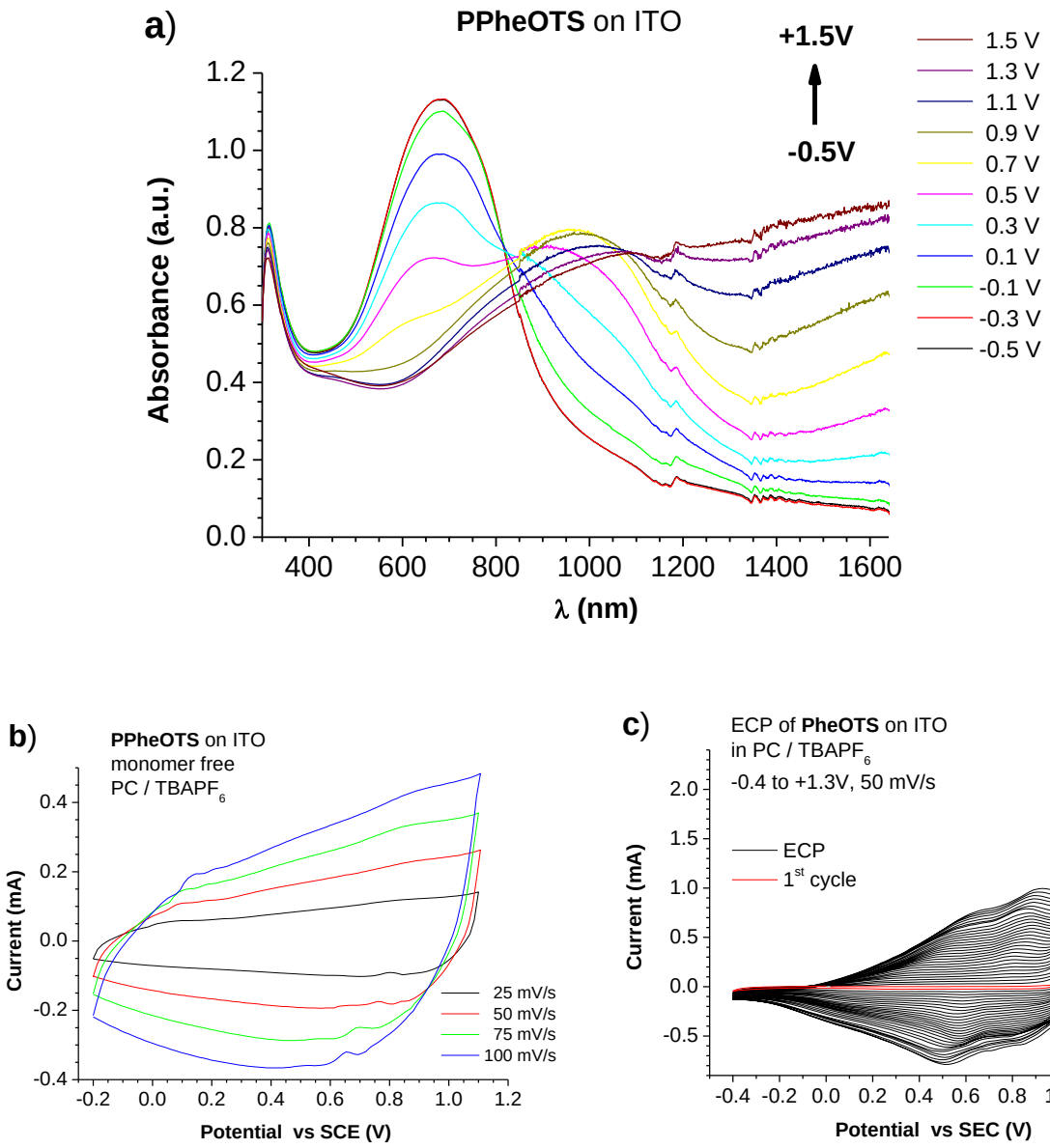


Fig. S4 (a) Spectroelectrochemical measurements for polymer **PPheOTS** (**P1b**) on ITO performed in PC/$TBAPF_6$ (0.1 M) under various potentials applied *in situ*. (b) CV measurements of the electrodeposited film of polymer **PPheOTS** (**P1b**) on ITO in monomer free PC/$TBAPF_6$ (0.1 M) solution at various scan rates. (c) Electrochemical polymerization of monomer **PheOTS** (**1b**) in PC/$TBAPF_6$ (0.1 M) on ITO electrode. All data are given vs. SCE and were calibrated to the Fc/Fc^+ standard, which is 0.38 V vs. SCE under these conditions.[3]

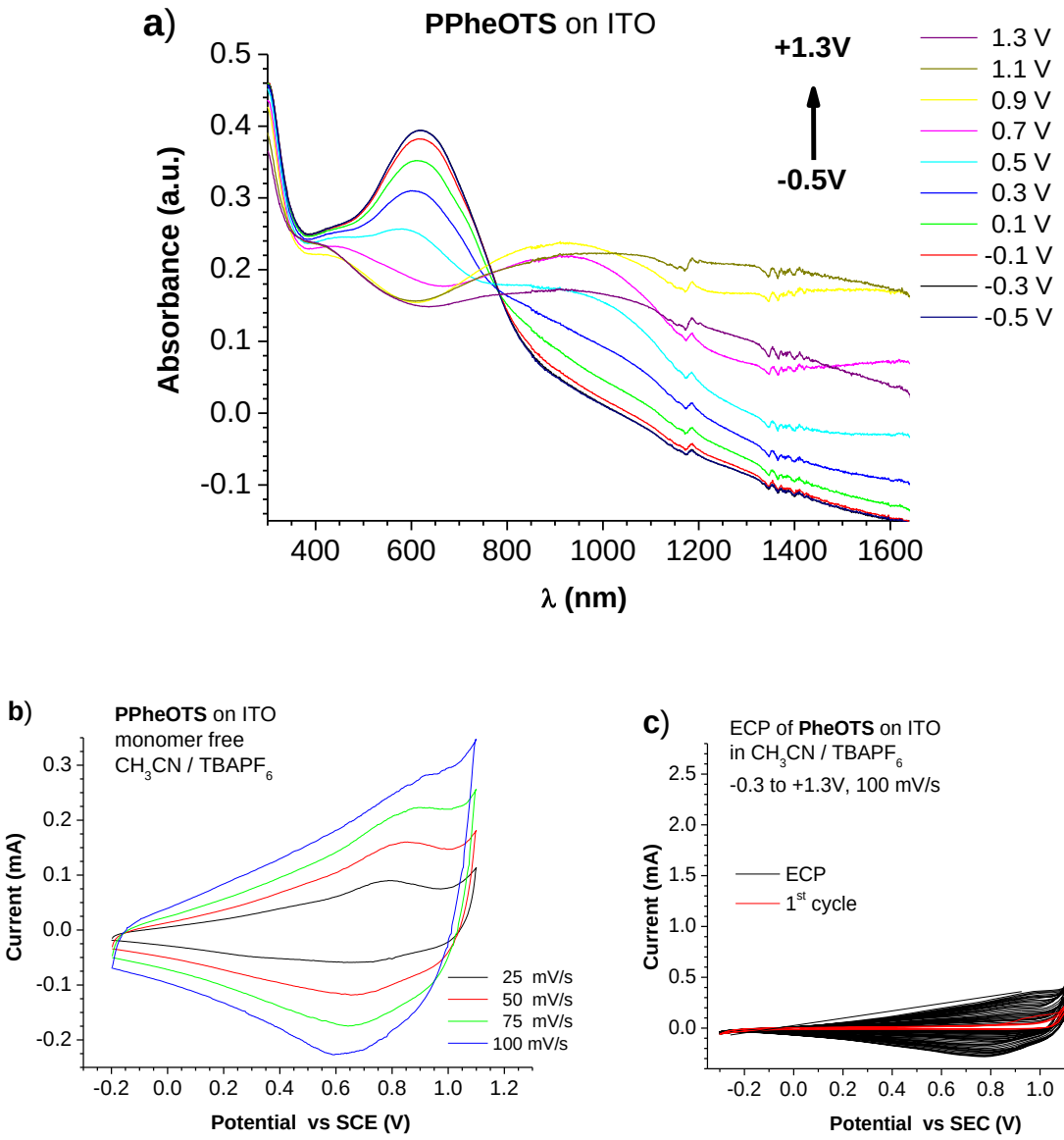


Fig. S5 (a) Spectroelectrochemical measurements for polymer **PPheOTS** (**P1b**) on ITO performed in $CH_3CN/TBAPF_6$ (0.1 M) under various potentials applied *in situ*. (b) CV measurements of the electrodeposited film of polymer **PPheOTS** (**P1b**) on ITO in monomer free $CH_3CN/TBAPF_6$ (0.1 M) solution at various scan rates. (c) Electrochemical polymerization of monomer **PheOTS** (**1b**) in $CH_3CN/TBAPF_6$ (0.1 M) on ITO electrode. All data are given vs. SCE and were calibrated to the Fc/Fc^+ standard which is 0.40 V vs. SCE under these conditions.[3]

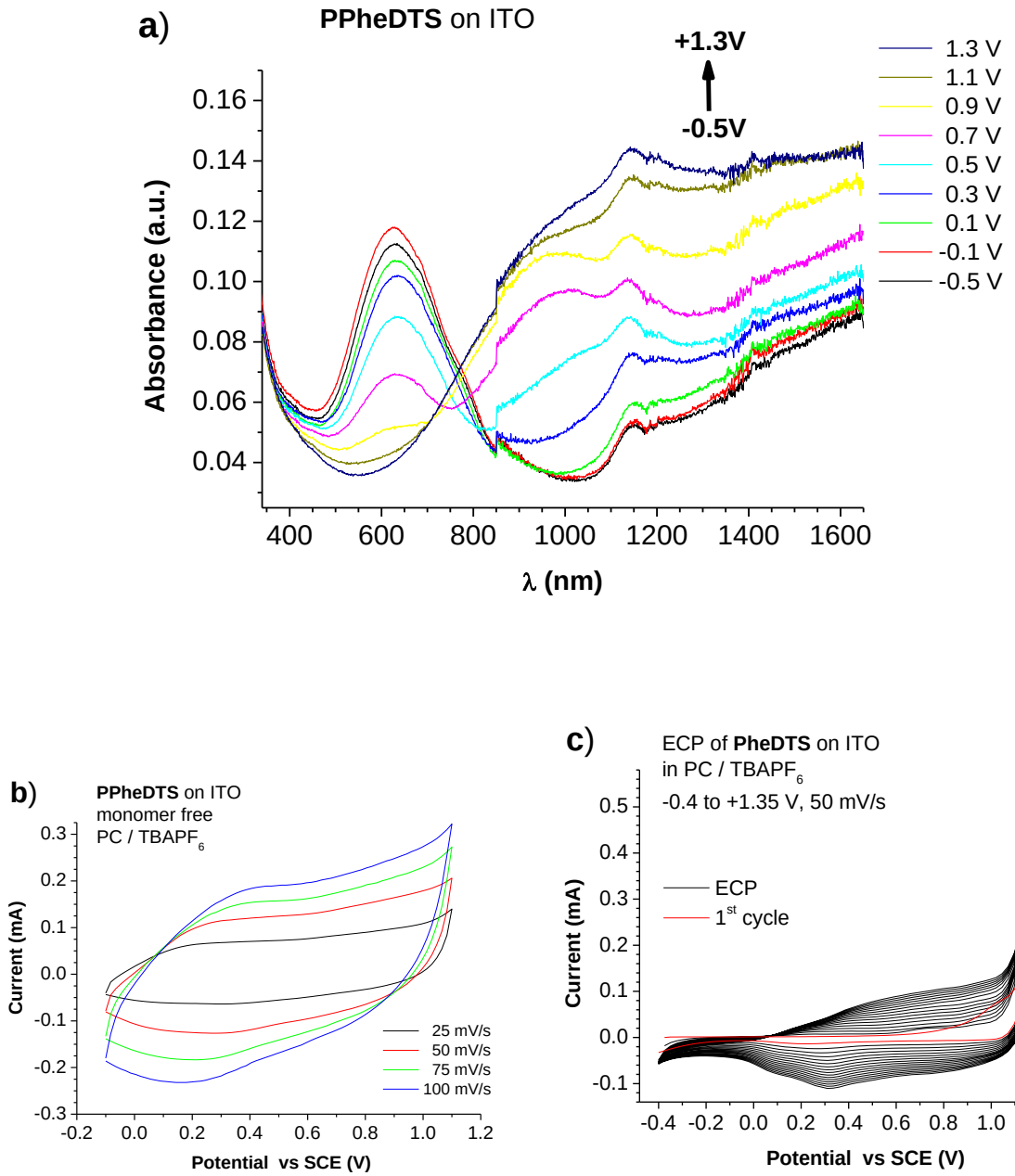


Fig. S6 (a) Spectroelectrochemical measurements for polymer **PPheDTS** (**P1c**) on ITO performed in PC/$TBAPF_6$ (0.1 M) under various potentials applied *in situ*. (b) CV measurements of the electrodeposited film of polymer **PPheDTS** (**P1c**) on ITO in monomer free PC/$TBAPF_6$ (0.1 M) solution at various scan rates. (c) Electrochemical polymerization of monomer **PheDTS** (**1c**) in PC/$TBAPF_6$ (0.1 M) on ITO electrode. All data are given vs. SCE and were calibrated to the Fc/Fc^+ standard, which is 0.38 V vs. SCE under these conditions.[3]

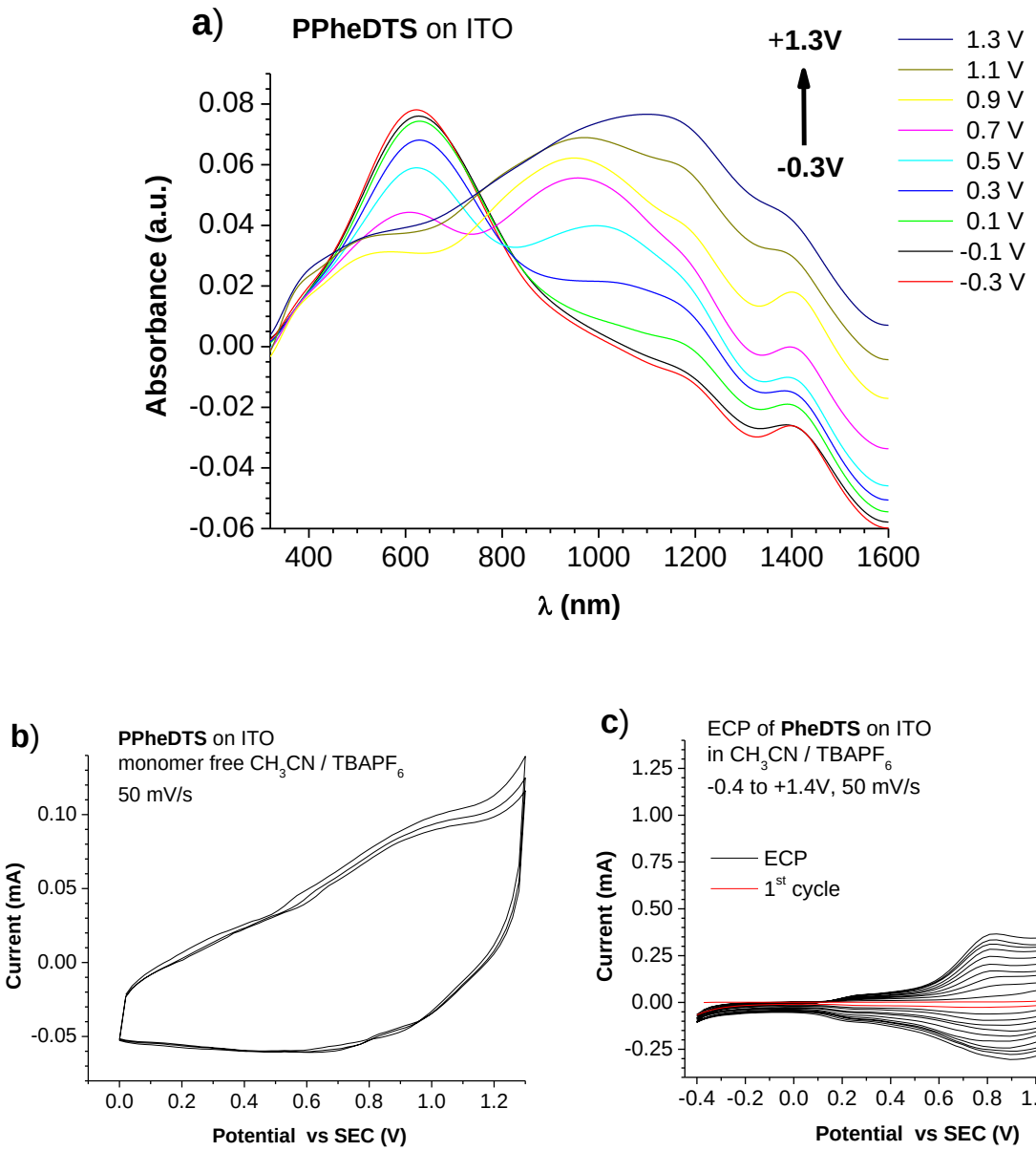
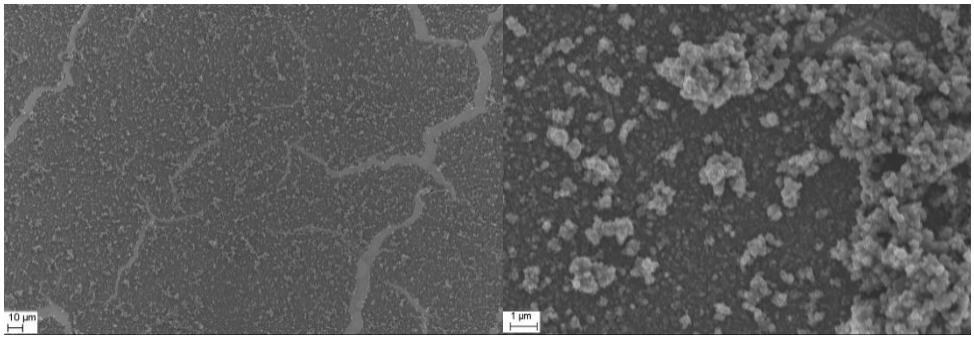


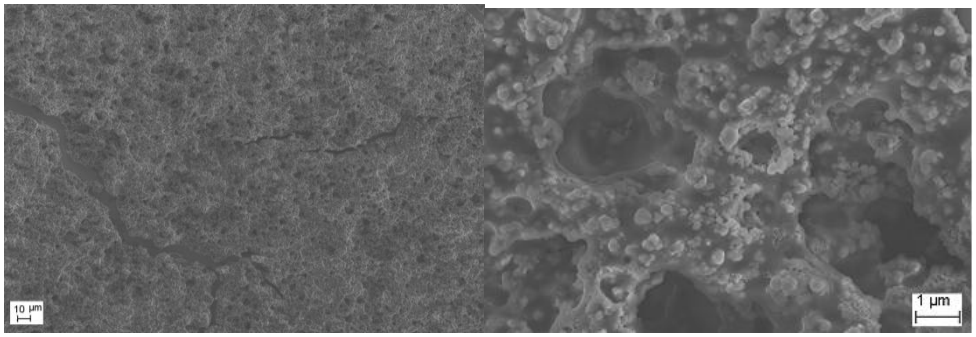
Fig. S7 (a) Spectroelectrochemical measurements for polymer **PPheDTS** (**P1c**) on ITO performed in $CH_3CN/TBAPF_6$ (0.1 M) under various potentials applied *in situ*. (b) CV measurements of the electrodeposited film of polymer **PPheDTS** (**P1c**) on ITO in monomer free $CH_3CN/TBAPF_6$ (0.1 M) solution at scan rate of 50 mV/s. (c) Electrochemical polymerization of monomer **PheDTS** (**1c**) in $CH_3CN/TBAPF_6$ (0.1 M) on ITO electrode. All data are given vs. SCE and were calibrated to the Fc/Fc^+ standard, which is 0.40 V vs. SCE under these conditions.[3]

Film Morphology

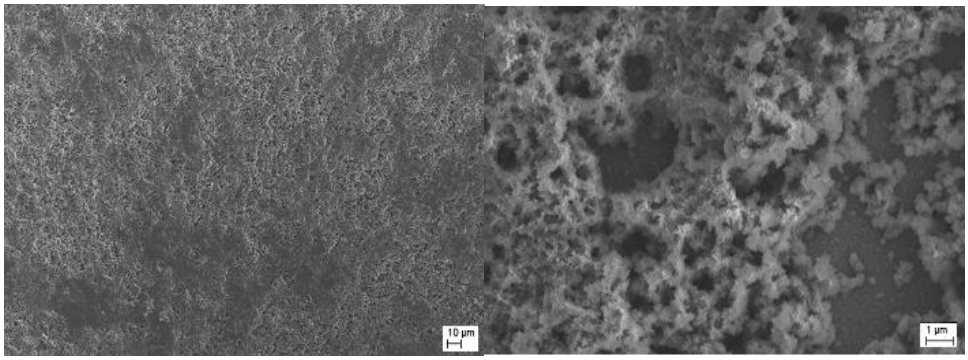
SEM measurements were performed on all poly[3,4-(phenylene-X,Y)selenophene] films (Fig. S8). The films were prepared on ITO in the CV mode in CH_2Cl_2 using $TBAPF_6$ as the supporting electrolyte and operating at 5 keV power. At a magnification of 1000, it can be observed that **PPheDOS** (**P1a**), has a smoother structure than **PPheOTS** (**P1b**) and **PPheDTS** (**P1c**). At high magnification (20,000), all poly[3,4-(phenylene-X,Y)selenophene] films show a globular coral-shaped morphology. Polymers that bear sulfur substituents at the 3,4-positions of the selenophene ring (**P1b** and **P1c**) form the films with a rough and bumpy surface with large pores that can achieve a diameter of 1 μm, while the film of only oxygen-substituted **PPheDOS** (**P1a**) is thinner and less porous. Also, in thiophene-based polymer films, sulfur-substituted polymer **PPheOTT** (**P2b**) has a rougher structure than oxygen-substituted **PPheDOT** (**P2a**).



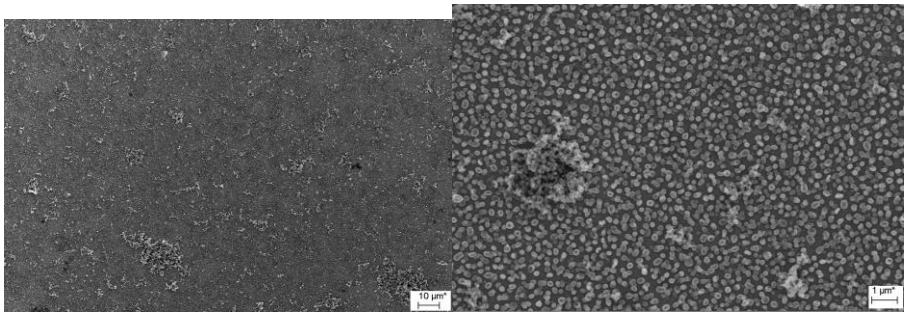
(a) **PPheDOS**(**P1a**)



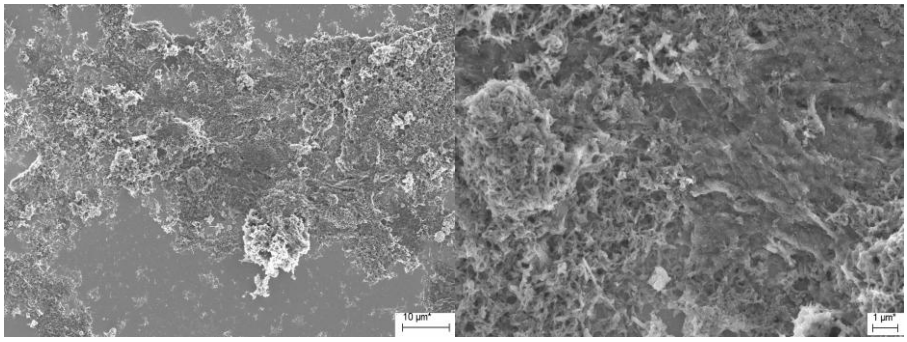
(b) **PPheOTS**(**P1b**)



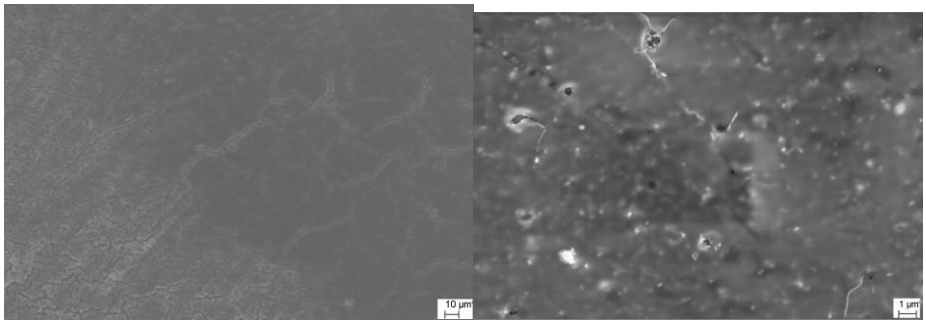
(c) **PPheDTS**, **P1c**



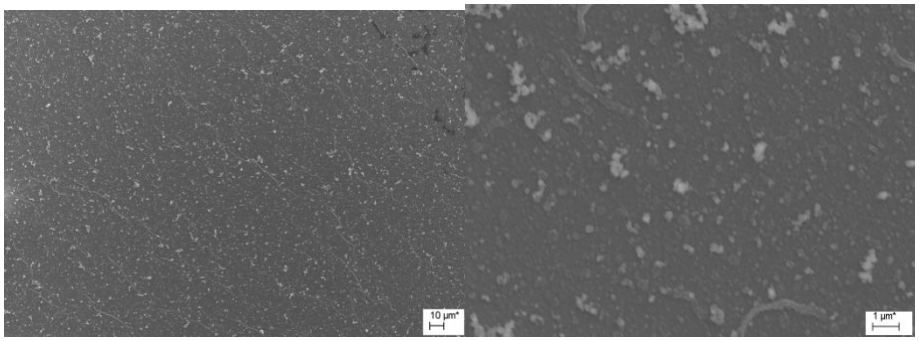
(d) **PPheDOT, P2a**



(e) **PPheOTT**, **P2b**



(f) **PNaphDOS**, **P1d**



(g) **PNaphDOT**, **P2d**

Fig. S8. SEM images of polymer films prepared in CH_2Cl_2/$TBAPF_6$. (a) **PPheDOS** (**P1a**). (b) **PPheOTS** (**P1b**). (c) **PPheDTS** (**P1c**). (d) **PPheDOT** (**P2a**), (e) **PPheOTT** (**P2b**). (f) **PNaphDOS** (**P1d**). (g) **PNaphDOT** (**P2d**). Magnification is ~1000 (left images) and ~20000 (right images), working distance is 3 mm, EHT is 5 keV.

X-ray structural analysis of PheDOS (1a)

PheDOS (**1a**) was crystallized from ethyl acetate/hexane solution to give colorless crystals suitable for single crystal X-ray analysis.

Crystal Data: $C_{10}H_6O_2Se$, colorless, plates, 0.40×0.30×0.05 mm^3, monoclinic, P2(1)/n, a = 5.820(1) Å, b = 14.522(3) Å, c = 10.036(2)Å, β= 93.12(3)°, from 20 degrees of data, T = 120(2) K, V= 847.0(3) $Å^3$, Z = 4, Fw = 237.11, Dc = 1.859 g/cm^3, μ = 4.389 mm^{-1}.

Data Collection and Treatment: Nonius Kappa CCD diffractometer, MoKα (g = 0.71073 Å), graphite monochromator, 11446 reflections collected, $-7 \le h \le 7$, $0 \le k \le 18$, $0 \le l \le 13$, frame scan width 1.0°, scan speed 1° per 120 sec, typical peak mosaicity of 0.612° , 2164 independent reflections (R-int = 0.056). The data were processed with Denzo-Scale pack.

Solution and Refinement: The structure was solved by direct methods with SHELXS. Full-matrix least-squares refinement based on F^2 with SHELXL-97. 146 parameters with 0 restraints, final R_1 = 0.0303 (based on F^2) for data with $I > 2\sigma(I)$ and R_1 =0.0404 on 1939 reflections, goodness-of -fit on F^2 =1.019, largest electron density peak =0.247e/$Å^3$, deepest hole = -0.253 e/$Å^3$.

The structure is refined as disordered; the molecules $C_{10}H_6O_2Se$ in the crystal have two mutually inverted orientations with occupancies of approximately 55% and 45%. This result can be described either as statistical disordering of the molecules in the crystal or as presence of racemic twining such as each twin domain contains molecules of only orientation. The analysis of molecule packing makes us to suggest the presence of twining in the crystal with domains volume ratio close to 1:1.

Computational Studies

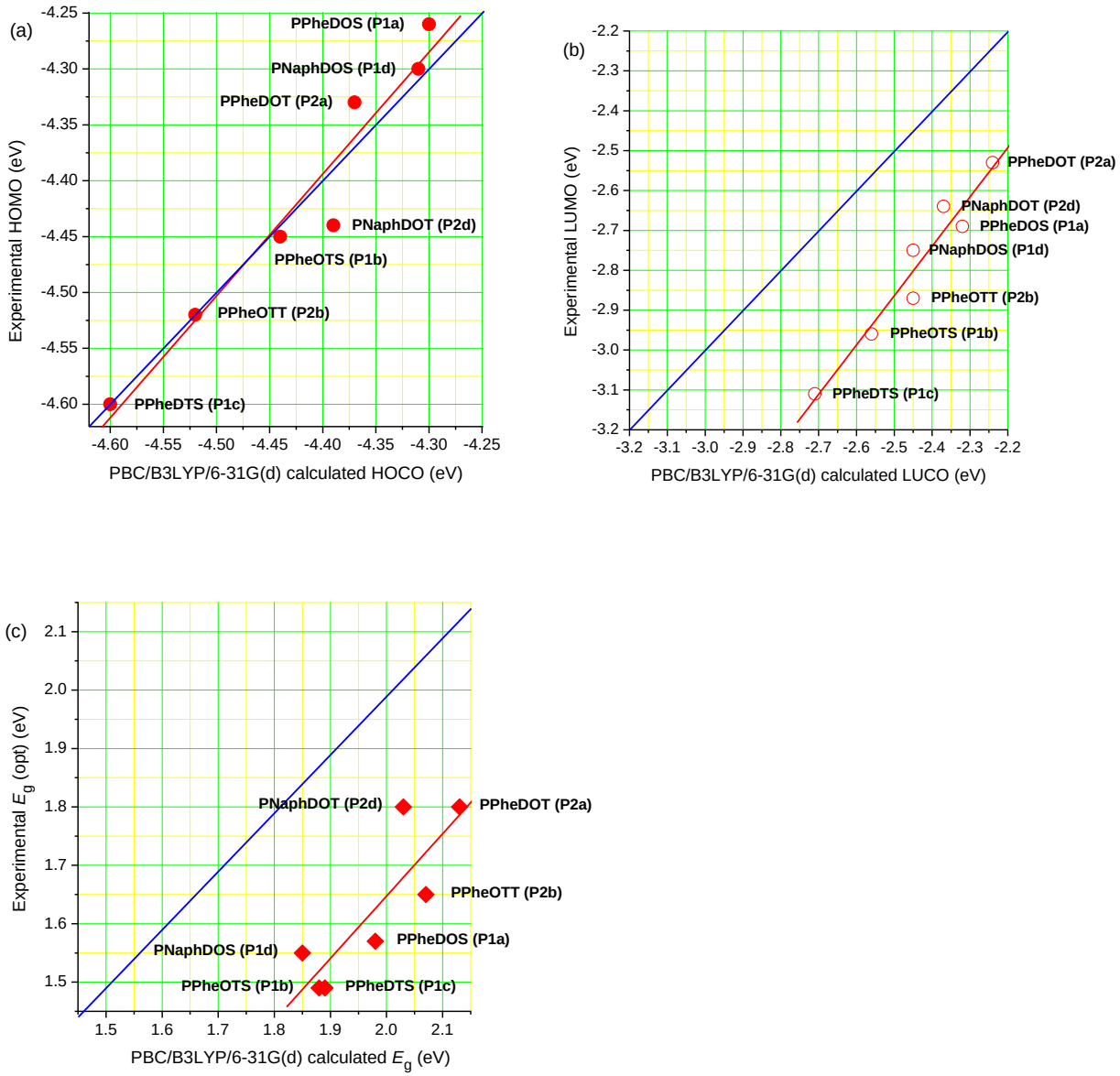


Fig. S9 Correlation between calculated [PBC/B3LYP/6-31G(d)] and experimental energy levels for polymers **P1a-d, P2a,b,d**: a) HOMO vs. HOCO, b) LUMO vs. LUCO, c) E_g(opt) vs. E_g(calc). Data have taken from Table 1. Straight blue lines correspond to bissectrices of equal E(calc) = E(exp) energies. Red lines are linear fits between the experimental and calculated energies.

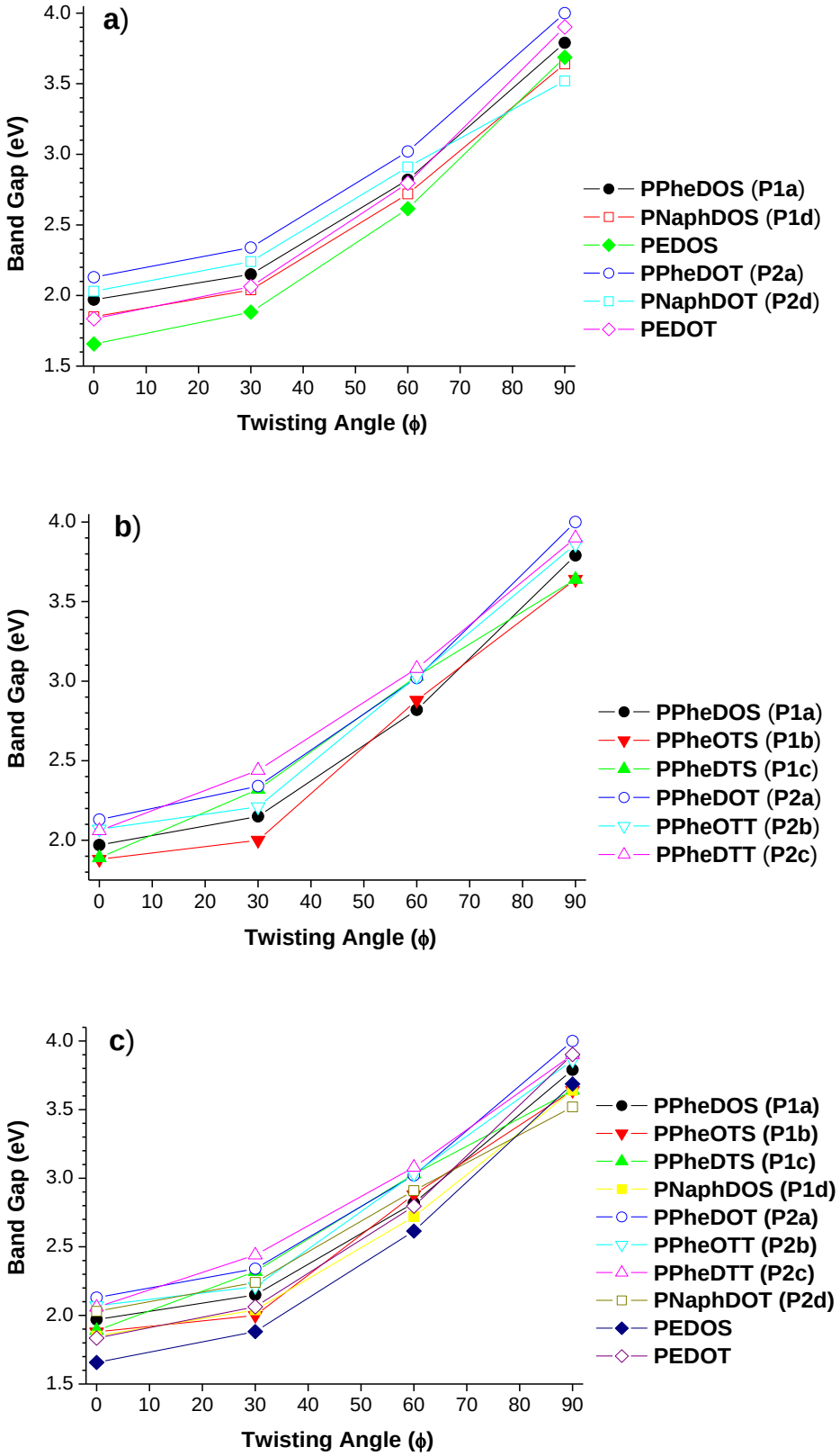


Fig. S10 Band gap of polymers as a function of interring twist angle (φ) calculated at the PBC/B3LYP/6-31G(d) level of theory. **PPheOTS** (**P1b**) and **PPheOTT** (**P2b**) are shown as head-to-tail polymers. Numerical values are given in Table S2.

Table S1. Relative energies (kcal/mol)[a] of polymers as a function of interring twist angle (φ) calculated at the PBC/B3LYP/6-31G(d) level of theory.

Dihedral angle (φ)	PPheDOS	PPheOTS	PPheDTS	PPheDOT	PPheOTT	PPheDTT	PNaphDOS	PNaphDOT	PEDOS	PEDOT
0	0	0	0	0	0	0.04	0	0	0	0
30	2.01	1.75	1.38	1.27	0.94	0	2.04	1.28	2.19	1.45
60	5.41	4.34	0.49	3.50	2.03	0.01	5.49	3.52	6.02	4.08
90	8.16	6.49	1.65	5.47	3.78	1.19	8.28	5.52	8.98	6.24

[a] Relative to the minimum energy conformer.

Table S2. Energy gap (eV) of polymers as a function of interring twist angle (φ) calculated at the PBC/B3LYP/6-31G(d) level of theory.

Dihedral angle (φ)	PPheDOS	PPheOTS	PPheDTS	PPheDOT	PPheOTT	PPheDTT	PNaphDOS	PNaphDOT	PEDOS	PEDOT
0	1.97	1.88	1.89	2.13	2.07	2.06	1.85	2.03	1.68	1.84
30	2.15	2.00	2.32	2.34	2.21	2.44	2.04	2.24	1.88	2.06
60	2.82	2.88	3.03	3.02	3.03	3.08	2.72	2.91	2.62	2.80
90	3.79	3.64	3.64	4.00	3.86	3.90	3.64	3.52	3.69	3.90

Table S3. Calculated total energies (hartree) of polymers as a function of interring twist angle (φ) calculated at the PBC/B3LYP/6-31G(d) level of theory.

Dihedral angle (φ)	PPheDOS	PPheOTS	PPheDTS	PPheDOT	PPheOTT	PPheDTT	PNaphDOS	PNaphDOT
0	-5866.565807	-6512.515710	-7158.450310	-1864.173098	-2510.119497	-3156.058644	-6173.854124	-2171.461188
30	-5866.559390	-6512.510132	-7158.445927	-1864.169047	-2510.116492	-3156.058785	-6173.847606	-2171.457119
60	-5866.548551	-6512.501886	-7158.448760	-1864.161956	-2510.113038	-3156.058760	-6173.836621	-2171.449982
90	-5866.539811	-6512.495023	-7158.445041	-1864.155661	-2510.107452	-3156.054985	-6173.827720	-2171.443594

Coordinates of compounds with planar geometry calculated at PBC/B3LYP/6-31G(d)

PPheDOS, P1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.707142	0.098208	-0.000041
2	6	0	-1.380296	1.298353	0.015073
3	6	0	-2.792802	1.236427	0.014303
4	6	0	-3.358840	-0.017629	-0.001298
5	6	0	-2.888705	3.576641	0.043938
6	6	0	-1.490474	3.638123	0.045011
7	6	0	-0.847578	4.871114	0.061310
8	1	0	0.237790	4.883426	0.061843
9	6	0	-1.598997	6.046881	0.076372
10	6	0	-2.993784	5.985388	0.075108
11	6	0	-3.638218	4.747817	0.058904
12	1	0	-1.091843	7.006680	0.089085
13	1	0	-3.583723	6.896665	0.086763
14	1	0	-4.720354	4.663392	0.057523
15	8	0	-0.708086	2.499250	0.030138
16	8	0	-3.567738	2.373462	0.028295
17	34	0	-1.973536	-1.322436	-0.017995
18	6	0	0.707149	-0.098165	-0.002693
19	6	0	1.380301	-1.298310	-0.017808
20	34	0	1.973544	1.322483	0.014848
21	6	0	2.792807	-1.236387	-0.017068
22	8	0	0.708088	-2.499207	-0.032847
23	6	0	3.358846	0.017670	-0.001615
24	8	0	3.567740	-2.373423	-0.031096
25	6	0	1.490473	-3.638104	-0.045889
26	6	0	2.888705	-3.576624	-0.044865
27	6	0	0.847574	-4.871115	-0.060391
28	6	0	3.638215	-4.747822	-0.058113
29	1	0	-0.237794	-4.883425	-0.060893
30	6	0	1.598990	-6.046904	-0.073790
31	6	0	2.993777	-5.985413	-0.072597
32	1	0	4.720351	-4.663399	-0.056808
33	1	0	1.091833	-7.006718	-0.085136
34	1	0	3.583713	-6.896708	-0.082946
35	-2	0	8.109755	0.352463	0.003383

PPheOTS, P1b.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.225478	0.089380	0.056964
2	6	0	-1.826565	1.277390	-0.306233

3	6	0	-3.240897	1.355506	-0.248293
4	6	0	-3.880470	0.210335	0.197015
5	8	0	-1.050803	2.334513	-0.729074
6	16	0	-4.035514	2.846949	-0.809615
7	34	0	-2.582527	-1.148044	0.538824
8	6	0	-2.764169	4.007841	-0.336167
9	6	0	-1.422305	3.617879	-0.358064
10	6	0	-3.082962	5.327606	-0.004354
11	6	0	-0.406321	4.516330	-0.045648
12	6	0	-2.069500	6.242525	0.283328
13	1	0	-4.125038	5.632698	0.025182
14	6	0	-0.733565	5.836145	0.264566
15	1	0	0.618399	4.159606	-0.047122
16	1	0	-2.326399	7.267705	0.532792
17	1	0	0.056358	6.542212	0.503069
18	6	0	0.179995	-0.181878	0.066383
19	6	0	0.854276	-1.340398	0.415457
20	34	0	1.442930	1.159702	-0.435678
21	6	0	2.265272	-1.282968	0.289824
22	16	0	0.117023	-2.824314	1.067759
23	6	0	2.832401	-0.100086	-0.138526
24	8	0	3.073086	-2.354599	0.601085
25	6	0	1.297789	-3.999962	0.426580
26	6	0	2.636718	-3.629603	0.274784
27	6	0	0.918506	-5.312764	0.132981
28	6	0	3.589485	-4.540216	-0.172419
29	6	0	1.871810	-6.240162	-0.288995
30	1	0	-0.123063	-5.602591	0.238036
31	6	0	3.204708	-5.853183	-0.443409
32	1	0	4.610782	-4.197813	-0.302892
33	1	0	1.568991	-7.259870	-0.507478
34	1	0	3.945874	-6.568885	-0.786665
35	-2	0	8.109090	-0.059967	-0.527423

PPheDTS, P1c.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.713633	0.166686	-1.230462
2	6	0	-1.367760	1.394442	-1.213312
3	6	0	-2.797879	1.363991	-1.194448
4	6	0	-3.397739	0.108705	-1.186105
5	6	0	-2.815174	3.845411	0.005116
6	6	0	-1.414411	3.875368	-0.017847
7	6	0	-0.716587	4.654747	0.909132
8	1	0	0.369283	4.653079	0.899352
9	6	0	-1.419069	5.428356	1.833783
10	6	0	-2.815024	5.398598	1.856831
11	6	0	-3.514241	4.595227	0.955341
12	1	0	-0.874567	6.042202	2.545595
13	1	0	-3.361364	5.989156	2.586710
14	1	0	-4.598819	4.548153	0.981654
15	34	0	-2.026768	-1.211544	-1.215775

16	6	0	0.699290	-0.129766	-1.241872
17	6	0	1.353419	-1.357510	-1.259022
18	34	0	2.012701	1.247979	-1.212888
19	6	0	2.783658	-1.327350	-1.256036
20	6	0	3.383747	-0.072443	-1.228076
21	6	0	1.412662	-3.862873	-0.116856
22	6	0	2.813596	-3.833253	-0.108595
23	6	0	0.724845	-4.661557	0.801091
24	6	0	3.522897	-4.602759	0.818021
25	1	0	-0.361059	-4.659826	0.803067
26	6	0	1.437277	-5.454260	1.701645
27	6	0	2.833403	-5.424843	1.710086
28	1	0	4.607705	-4.556194	0.833495
29	1	0	0.900526	-6.082991	2.406320
30	1	0	3.387555	-6.030525	2.421450
31	16	0	-3.698072	2.908051	-1.233299
32	16	0	-0.534852	2.973926	-1.284494
33	16	0	0.519550	-2.935167	-1.354747
34	16	0	3.683105	-2.870230	-1.336837
35	-2	0	8.179853	0.177684	-0.046405

PPheDOT, P2a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.691026	0.195963	0.000726
2	6	0	-1.218780	1.469492	0.010075
3	6	0	-2.630398	1.519290	0.010246
4	6	0	-3.246482	0.286092	0.001028
5	6	0	-2.542083	3.850573	0.027891
6	6	0	-1.142156	3.801282	0.027707
7	6	0	-0.404179	4.980092	0.036963
8	1	0	0.678966	4.909531	0.036588
9	6	0	-1.059578	6.211940	0.046425
10	6	0	-2.454488	6.261065	0.046629
11	6	0	-3.195062	5.078475	0.037360
12	1	0	-0.477588	7.128384	0.053651
13	1	0	-2.970394	7.216266	0.054023
14	1	0	-4.280492	5.084058	0.037292
15	8	0	-0.447422	2.604132	0.018536
16	8	0	-3.319735	2.705599	0.018850
17	6	0	0.691025	-0.195955	-0.001912
18	6	0	1.218780	-1.469485	-0.011261
19	6	0	2.630398	-1.519283	-0.011410
20	8	0	0.447422	-2.604124	-0.019813
21	6	0	3.246481	-0.286084	-0.002172
22	8	0	3.319735	-2.705590	-0.020072
23	6	0	1.142156	-3.801280	-0.028260
24	6	0	2.542084	-3.850570	-0.028411
25	6	0	0.404180	-4.980094	-0.036873
26	6	0	3.195064	-5.078477	-0.037196
27	1	0	-0.678965	-4.909534	-0.036540
28	6	0	1.059580	-6.211948	-0.045682

29	6	0	2.454490	-6.261072	-0.045846
30	1	0	4.280493	-5.084059	-0.037110
31	1	0	0.477590	-7.128396	-0.052422
32	1	0	2.970397	-7.216276	-0.052720
33	16	0	-2.011754	-0.980375	-0.008120
34	16	0	2.011753	0.980383	0.006931
35	-2	0	7.899234	-0.277580	-0.000832

PPheOTT, P2b.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.201639	0.130274	0.037439
2	6	0	-1.779983	1.344948	-0.283792
3	6	0	-3.195183	1.383238	-0.215116
4	6	0	-3.755981	0.175876	0.180103
5	8	0	-1.011228	2.416033	-0.662423
6	16	0	-4.051122	2.863073	-0.698510
7	6	0	-2.780647	4.045377	-0.278203
8	6	0	-1.427910	3.695092	-0.327938
9	6	0	-3.129872	5.363141	0.032861
10	6	0	-0.434661	4.638277	-0.076645
11	6	0	-2.140825	6.318042	0.267318
12	1	0	-4.180085	5.636086	0.084498
13	6	0	-0.794018	5.954608	0.211277
14	1	0	0.603631	4.324458	-0.115642
15	1	0	-2.424380	7.339944	0.500673
16	1	0	-0.019903	6.692093	0.401798
17	6	0	0.198433	-0.210360	0.058374
18	6	0	0.825909	-1.408762	0.372126
19	6	0	2.238196	-1.342069	0.270984
20	16	0	0.062953	-2.908930	0.940792
21	6	0	2.750108	-0.113738	-0.105864
22	8	0	3.067369	-2.399968	0.544674
23	6	0	1.296660	-4.062273	0.361140
24	6	0	2.638398	-3.684891	0.250644
25	6	0	0.938343	-5.384955	0.083000
26	6	0	3.612345	-4.605711	-0.127297
27	6	0	1.910373	-6.317825	-0.277484
28	1	0	-0.104891	-5.679140	0.155701
29	6	0	3.246713	-5.927309	-0.381386
30	1	0	4.641349	-4.270586	-0.210944
31	1	0	1.620676	-7.343812	-0.483834
32	1	0	4.006372	-6.647547	-0.670496
33	16	0	-2.476273	-1.019499	0.428158
34	16	0	1.415574	1.012350	-0.331229
35	-2	0	7.886402	0.078401	-0.475405

PPheDTT, P2c.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.704659	0.201946	-1.169720
2	6	0	-1.318373	1.452710	-1.152745
3	6	0	-2.744556	1.405370	-1.154518
4	6	0	-3.274306	0.116855	-1.174521
5	6	0	-2.817642	3.868901	0.061751
6	6	0	-1.416952	3.915044	0.066228
7	6	0	-0.749273	4.714240	0.999400
8	1	0	0.336636	4.725843	1.011562
9	6	0	-1.477662	5.491175	1.900495
10	6	0	-2.873064	5.445209	1.895931
11	6	0	-3.542726	4.622230	0.990211
12	1	0	-0.953970	6.119576	2.615199
13	1	0	-3.441680	6.037543	2.607097
14	1	0	-4.627122	4.562326	0.994776
15	6	0	0.700045	-0.160629	-1.177826
16	6	0	1.313800	-1.411362	-1.194802
17	6	0	2.739960	-1.363907	-1.201886
18	6	0	3.269622	-0.075205	-1.193385
19	6	0	1.416160	-3.903017	-0.037514
20	6	0	2.816816	-3.856313	-0.045448
21	6	0	0.751708	-4.725632	0.877384
22	6	0	3.545110	-4.632215	0.861698
23	1	0	-0.334145	-4.738249	0.892463
24	6	0	1.483226	-5.524501	1.756497
25	6	0	2.878582	-5.477750	1.748757
26	1	0	4.629492	-4.572011	0.864331
27	1	0	0.962041	-6.170921	2.456818
28	1	0	3.449622	-6.087437	2.443118
29	16	0	-3.688028	2.915415	-1.174328
30	16	0	-0.476978	3.022255	-1.164495
31	16	0	0.472108	-2.980020	-1.242563
32	16	0	3.683273	-2.873032	-1.260800
33	16	0	-1.949535	-1.044396	-1.217829
34	16	0	1.944674	1.086637	-1.201881
35	-2	0	7.921691	0.262257	-0.016719

PNaphDOT, P2d.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.255680	0.168128	-0.000015
2	6	0	2.683261	1.423263	-0.001285
3	6	0	1.272356	1.424697	-0.001308
4	6	0	0.697390	0.170723	-0.000026
5	6	0	1.268564	3.762840	-0.003669
6	6	0	2.691819	3.761399	-0.003625
7	6	0	3.383936	4.945594	-0.004809
8	1	0	4.469407	4.914393	-0.004742
9	6	0	2.699446	6.188931	-0.006099
10	6	0	1.265867	6.190381	-0.006160
11	6	0	0.578853	4.948437	-0.004913

12	1	0	-0.506679	4.919420	-0.004925
13	8	0	3.413655	2.583136	-0.002401
14	8	0	0.544325	2.586054	-0.002461
15	16	0	1.975300	-1.051583	0.000999
16	6	0	3.386647	7.430775	-0.007332
17	6	0	0.581197	7.433622	-0.007461
18	6	0	1.277339	8.622173	-0.008641
19	6	0	2.692925	8.620739	-0.008574
20	1	0	4.474141	7.427472	-0.007280
21	1	0	-0.506302	7.432539	-0.007511
22	6	0	-0.697390	-0.170723	0.000356
23	6	0	-1.272356	-1.424697	0.001523
24	16	0	-1.975300	1.051584	-0.000638
25	6	0	-2.683261	-1.423263	0.001477
26	8	0	-0.544325	-2.586054	0.002619
27	6	0	-3.255680	-0.168128	0.000273
28	8	0	-3.413655	-2.583136	0.002506
29	6	0	-1.268564	-3.762840	0.003749
30	6	0	-2.691819	-3.761399	0.003676
31	6	0	-0.578853	-4.948437	0.004942
32	6	0	-3.383936	-4.945594	0.004776
33	6	0	-1.265867	-6.190381	0.006105
34	1	0	0.506679	-4.919420	0.004980
35	1	0	-4.469407	-4.914393	0.004686
36	6	0	-2.699446	-6.188931	0.006010
37	6	0	-0.581197	-7.433623	0.007355
38	6	0	-3.386647	-7.430775	0.007159
39	6	0	-1.277339	-8.622174	0.008456
40	1	0	0.506302	-7.432539	0.007433
41	6	0	-2.692925	-8.620739	0.008353
42	1	0	-4.474142	-7.427473	0.007079
43	1	0	3.231198	9.564374	-0.009512
44	1	0	0.740984	9.566900	-0.009636
45	1	0	-0.740984	-9.566901	0.009414
46	1	0	-3.231198	-9.564375	0.009227
47	-2	0	7.905439	-0.007988	0.000139

PNaphtDOS, P1d.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.356975	0.125213	0.000037
2	6	0	2.736714	1.354633	-0.000069
3	6	0	1.324552	1.356003	-0.000071
4	6	0	0.701922	0.127777	0.000031
5	6	0	1.322041	3.703628	-0.000322
6	6	0	2.743815	3.702243	-0.000319
7	6	0	3.437122	4.885735	-0.000445
8	1	0	4.522439	4.850590	-0.000444
9	6	0	2.752334	6.128903	-0.000579
10	6	0	1.318315	6.130305	-0.000581
11	6	0	0.631073	4.888489	-0.000451
12	1	0	-0.454312	4.855508	-0.000453

13	8	0	3.460654	2.523561	-0.000208
14	8	0	0.602894	2.526349	-0.000213
15	6	0	3.439259	7.371156	-0.000714
16	6	0	0.633840	7.373910	-0.000718
17	6	0	1.329832	8.562408	-0.000847
18	6	0	2.745609	8.561021	-0.000844
19	1	0	4.526750	7.367086	-0.000712
20	1	0	-0.453657	7.371989	-0.000721
21	6	0	-0.701922	-0.127777	-0.000045
22	6	0	-1.324552	-1.356003	0.000062
23	6	0	-2.736714	-1.354633	0.000061
24	8	0	-0.602894	-2.526349	0.000206
25	6	0	-3.356975	-0.125213	-0.000047
26	8	0	-3.460654	-2.523561	0.000203
27	6	0	-1.322041	-3.703628	0.000318
28	6	0	-2.743815	-3.702243	0.000316
29	6	0	-0.631073	-4.888489	0.000450
30	6	0	-3.437122	-4.885735	0.000446
31	6	0	-1.318315	-6.130305	0.000584
32	1	0	0.454312	-4.855508	0.000452
33	1	0	-4.522439	-4.850590	0.000444
34	6	0	-2.752334	-6.128903	0.000582
35	6	0	-0.633840	-7.373910	0.000724
36	6	0	-3.439259	-7.371156	0.000721
37	6	0	-1.329832	-8.562408	0.000856
38	1	0	0.453657	-7.371989	0.000726
39	6	0	-2.745609	-8.561021	0.000854
40	1	0	-4.526750	-7.367086	0.000720
41	34	0	-2.028135	1.236527	-0.000514
42	34	0	2.028135	-1.236527	0.000499
43	1	0	-3.284126	-9.504611	0.000959
44	1	0	-0.793171	-9.507055	0.000963
45	1	0	3.284126	9.504611	-0.000947
46	1	0	0.793171	9.507055	-0.000952
47	-2	0	8.117306	-0.007786	0.000013

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