

Supplementary Information

Study on the mechanism of electrochromic change in the visible and infrared bands of D-A conjugated polymers based on PEDOT and its copolymer.

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Figure S1. The degree of polymerization of Trans-PEDOT

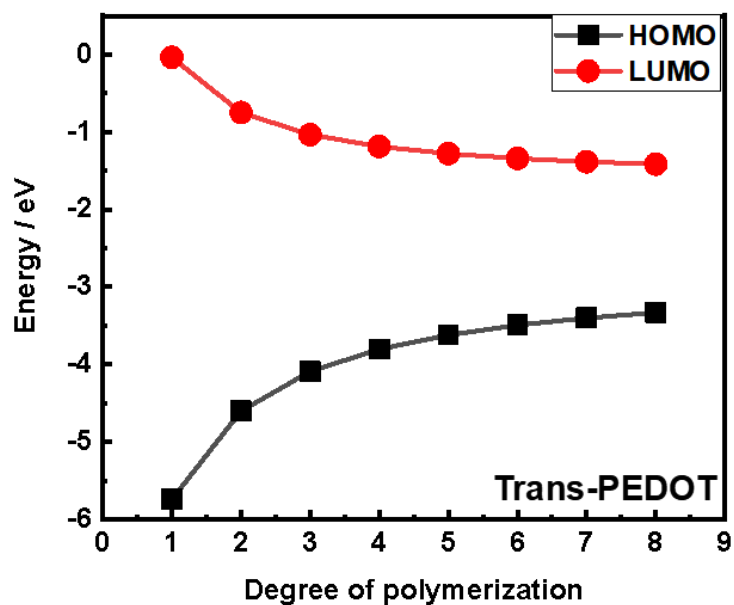


Figure S2. The degree of polymerization of Cis-PEDOT

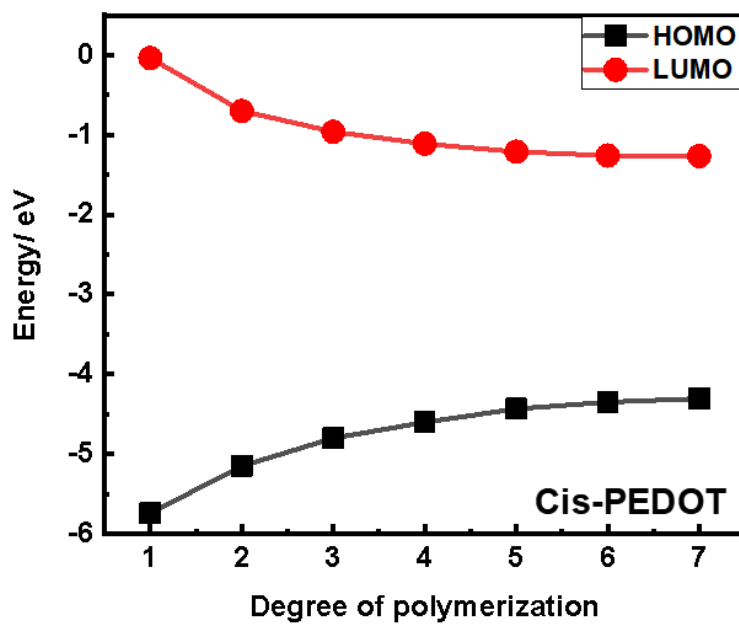


Figure S3. The degree of polymerization of PPr

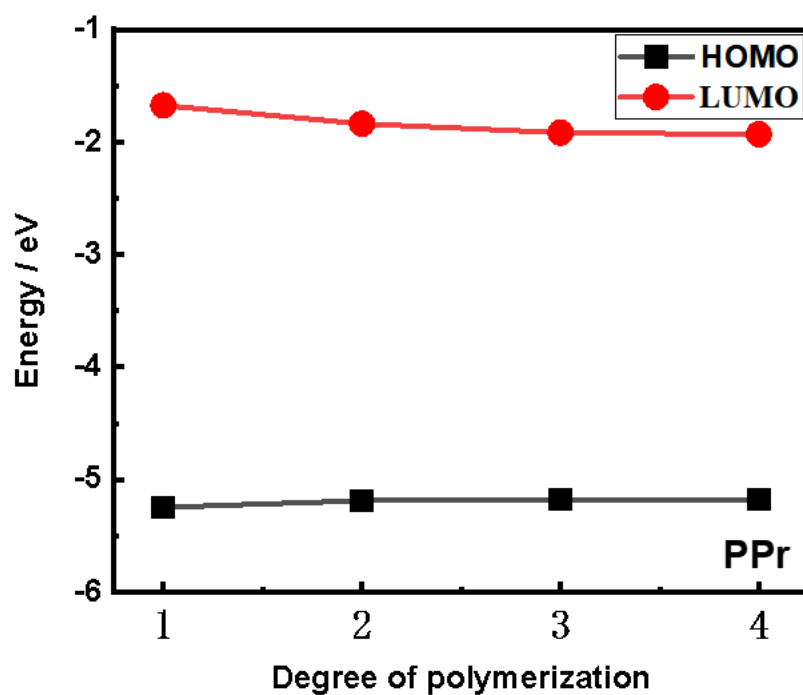


Figure S4. The degree of polymerization of PEP

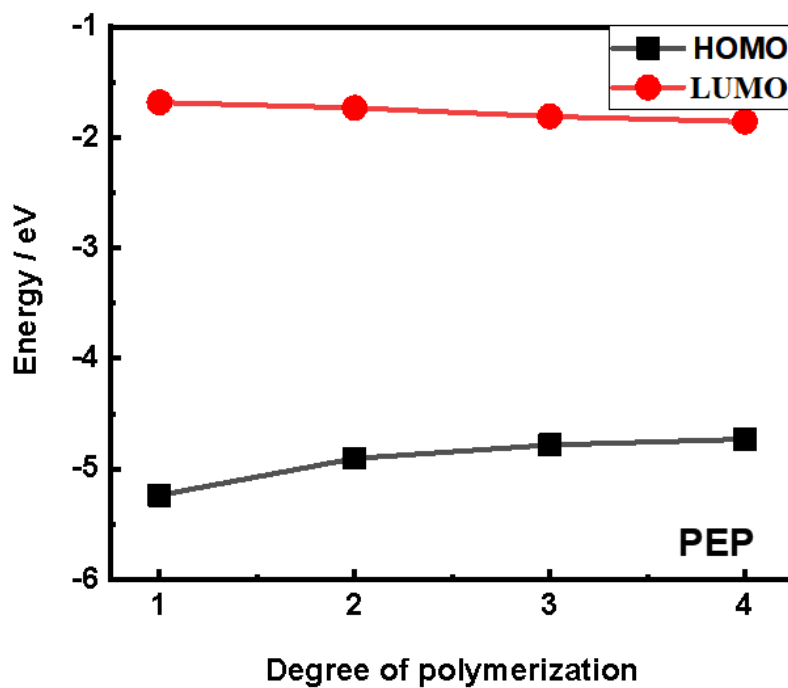
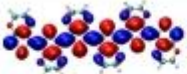
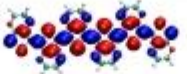






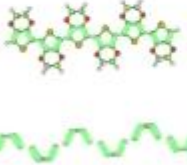
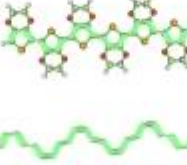
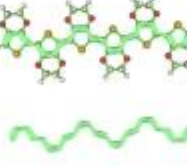
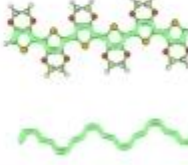
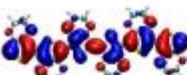

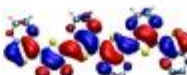



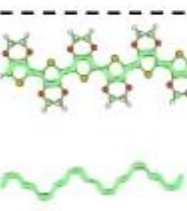
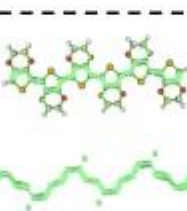
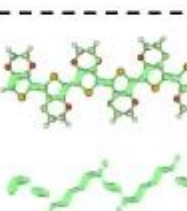


Figure S5. HOMO, LUMO, and π electron distributions of the cis and trans structures of PEDOT

PEDOT-Trans	0e	+1e	+2e	+3e
LUMO				
HOMO				
π e				
	+4e	+5e	+6e	
LUMO				
HOMO				
π e				

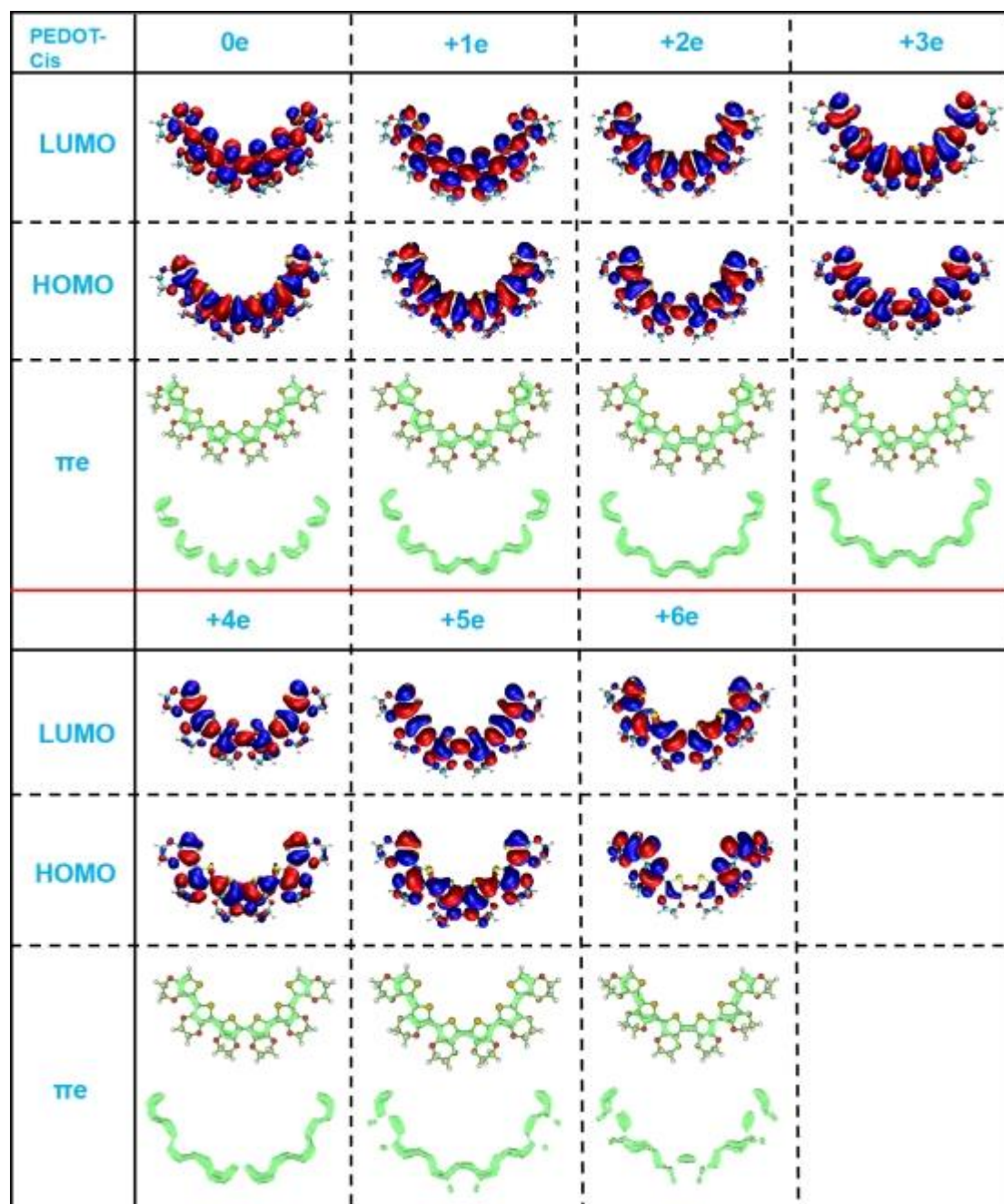


Figure S6. Schematic diagram of the cis/trans structure of PEDOT and trans- PEDOT in O-S bond length varies

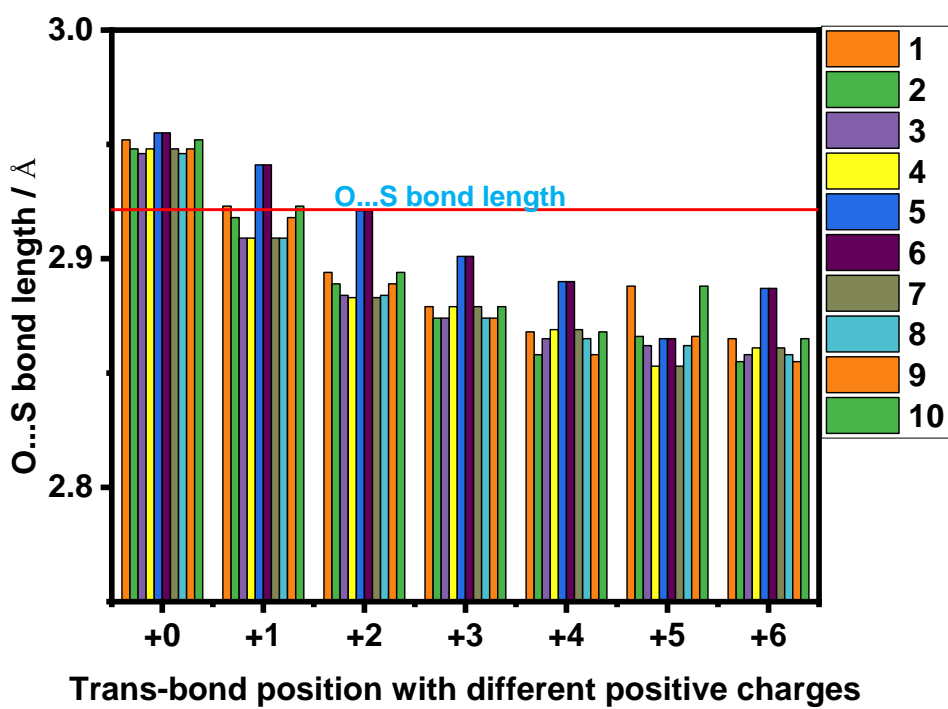
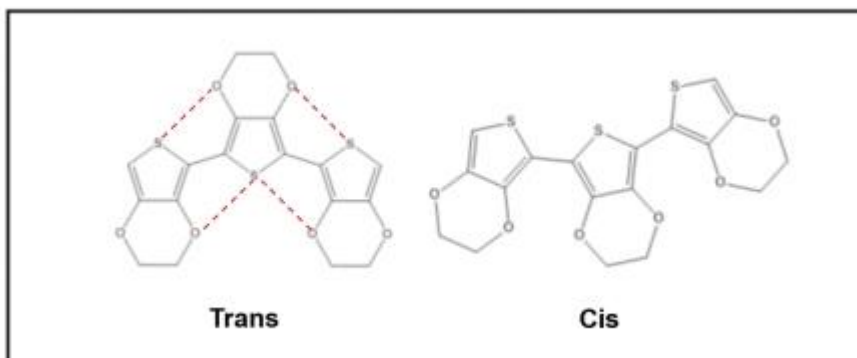


Figure S7. The average dihedral angle change in the PEP

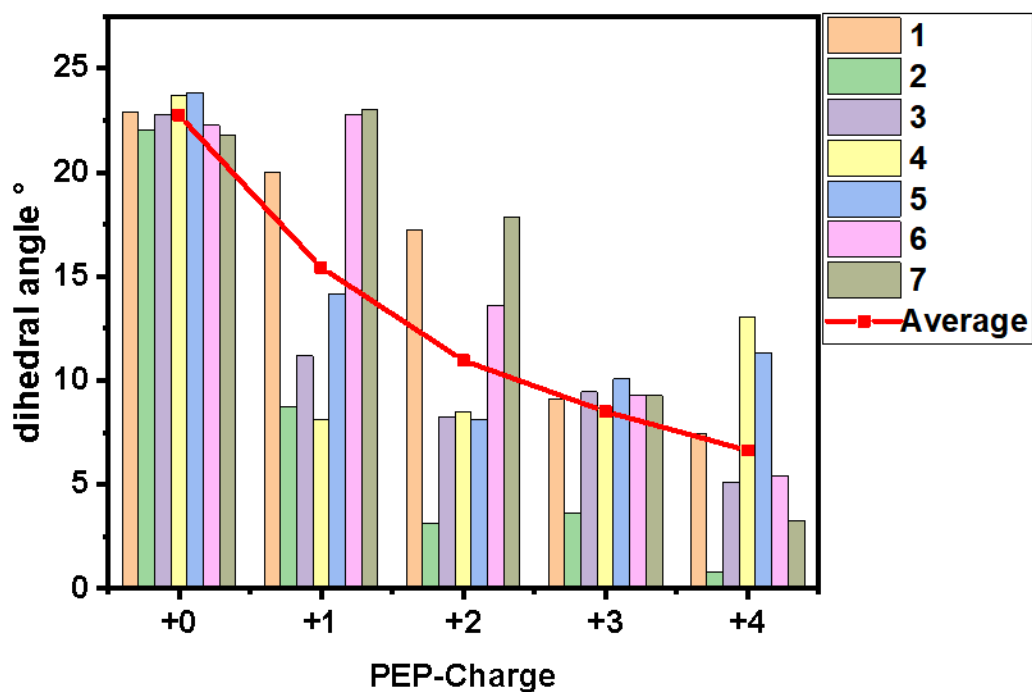


Figure S8. The PEDOT cis and trans structure with a degree of polymerization of 6 changes in the amount of charge and the average dihedral angle

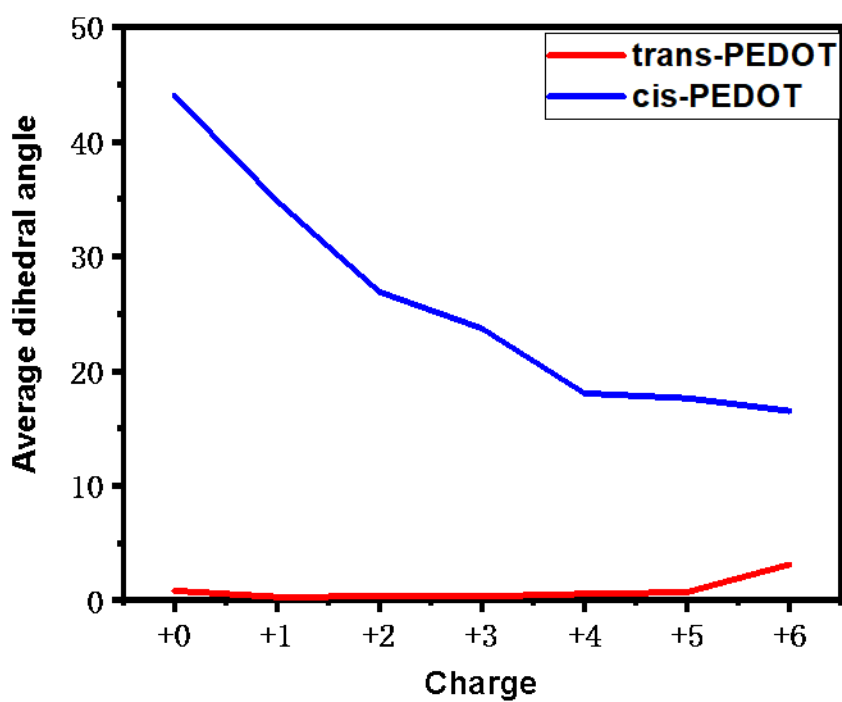


Figure S9. Electron distribution and π electrostatic potential distribution of PEP

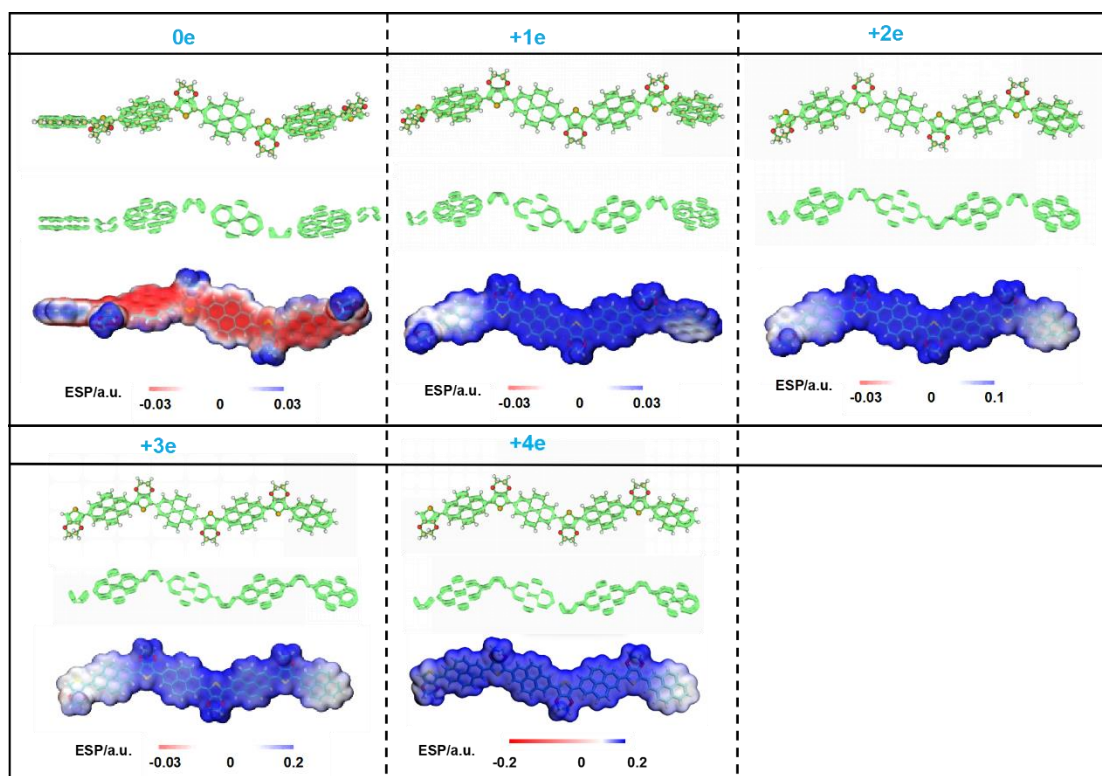


Figure S10. HOMO, LUMO, and π electronic density contour surface chart of polypyrene

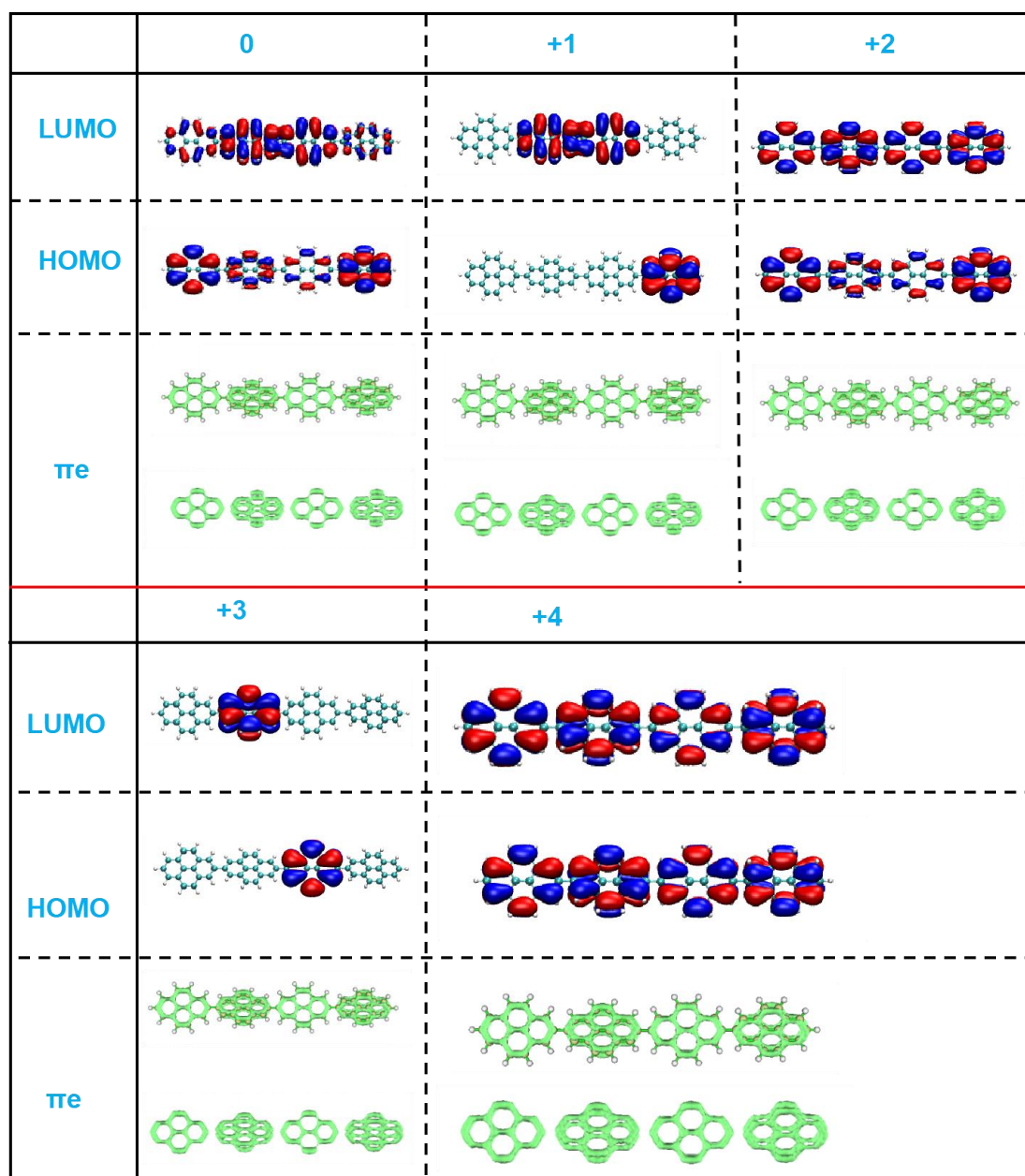


Figure S11. HOMO, LUMO, and π electronic density contour surface chart of PE_mP_n

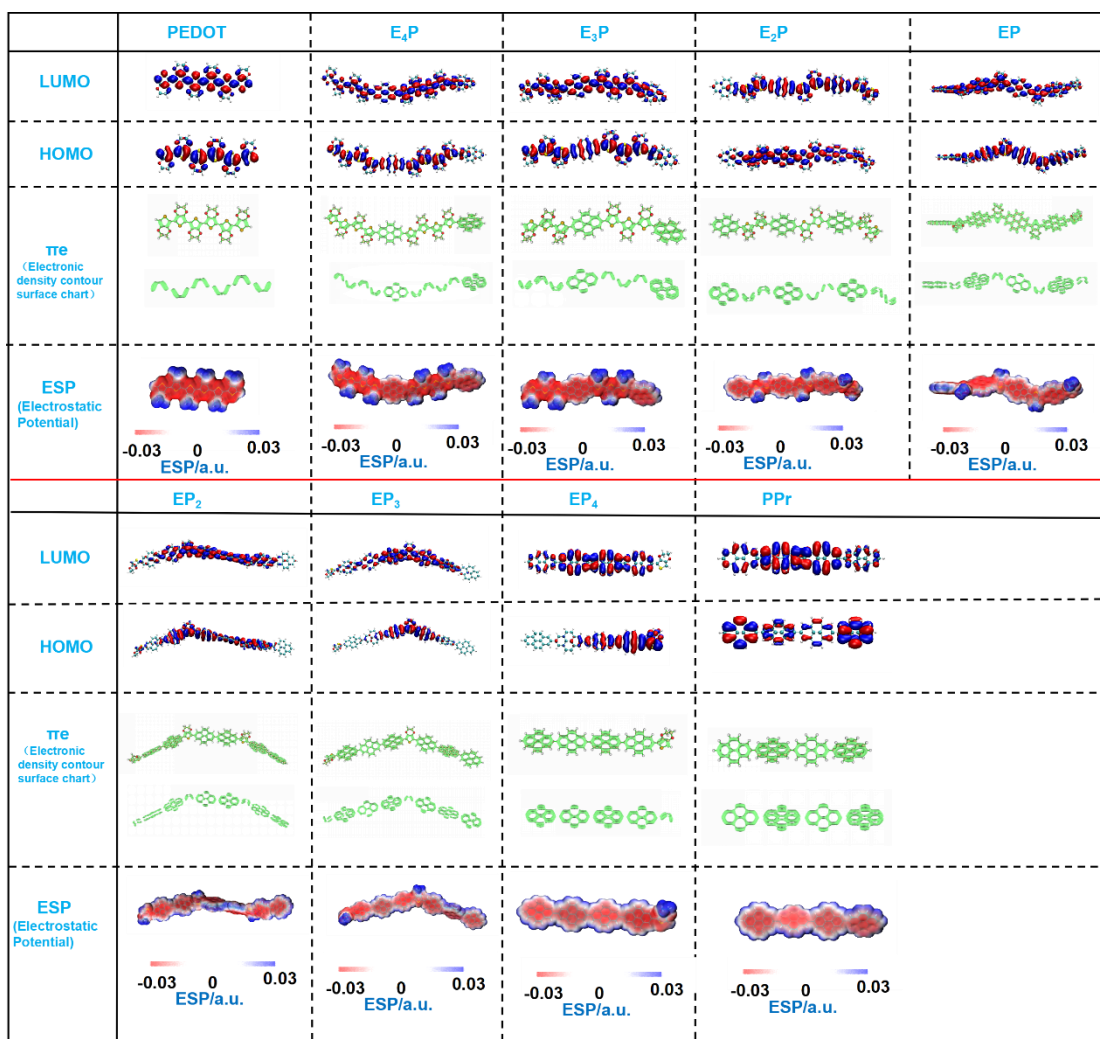


Figure S12. NTO of PEP

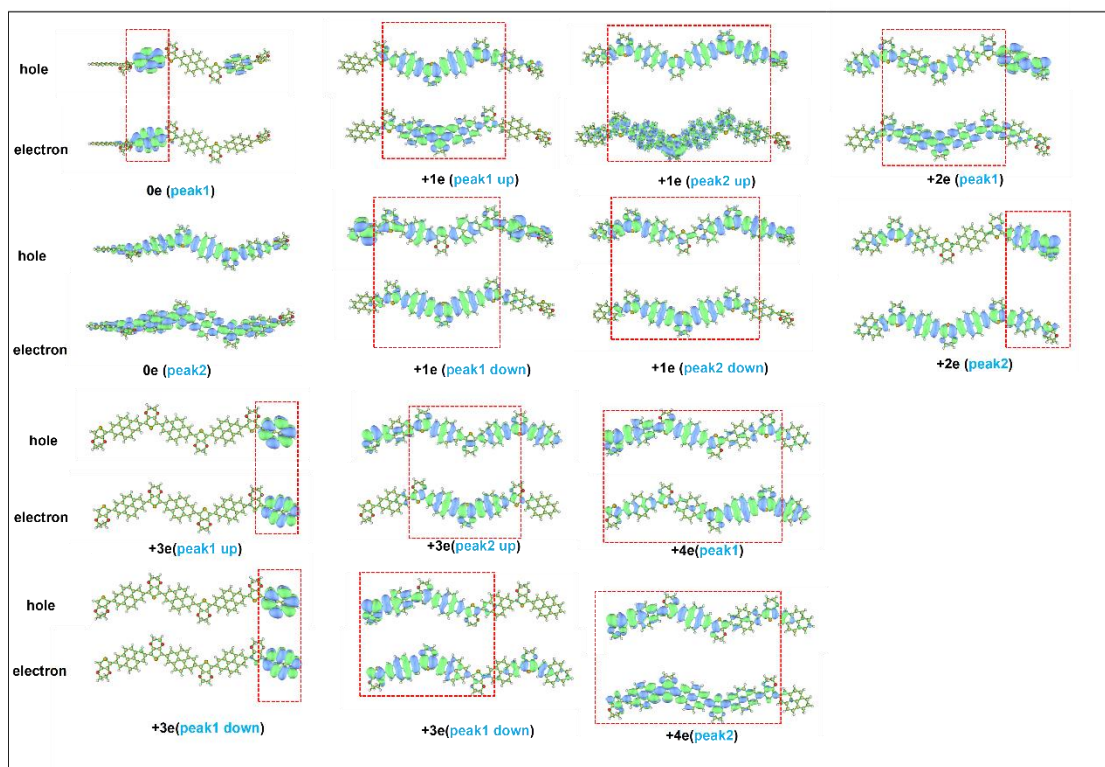


Figure S13. Vertical ionization potential

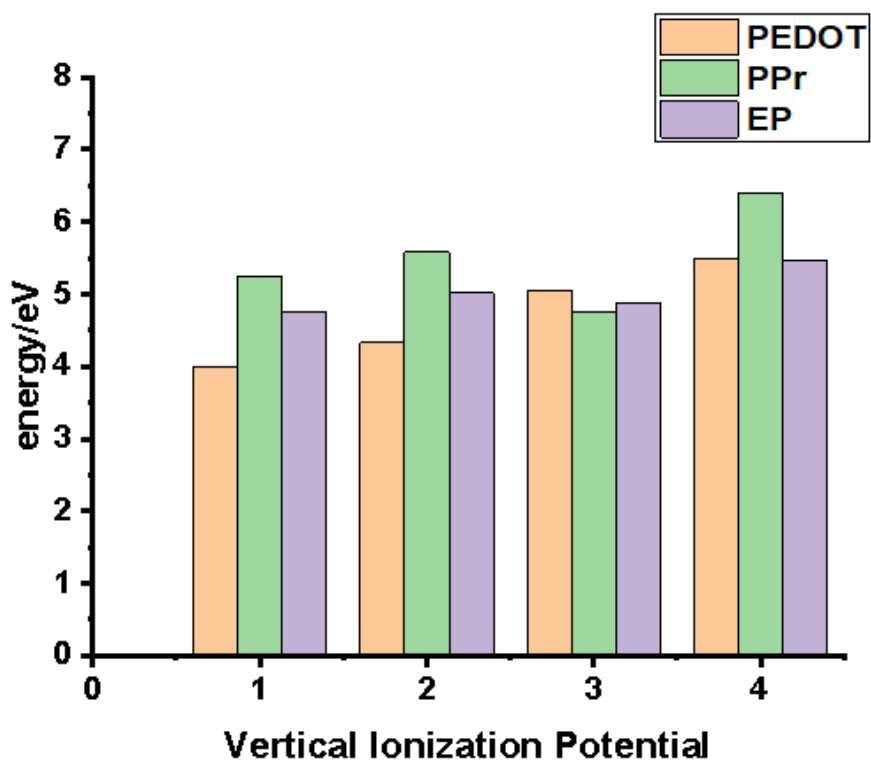


Table S1. The degree of polymerization of PE_mP_n

structure	Degree of aggregation	HOMO	LUMO	gap/eV
E4P	1	-4.33	-1.69	2.64
	2	-4.08	-1.90	2.18
	3	-4.46	-1.87	2.59
E3P	1	-4.51	-1.68	2.83
	2	-4.24	-1.87	2.37
	3	-4.63	-1.76	2.87
E2P	1	-4.68	-1.67	3.01
	2	-4.47	-1.78	2.70
	3	-4.40	-1.88	2.57
EP2	1	-5.19	-1.87	3.34
	2	-4.92	-1.86	3.06
	3	-4.88	-1.88	3.00
EP3	1	-5.19	-1.89	3.31
	2	-4.95	-1.91	3.03
	3	-5.19	-1.88	3.31
EP4	1	-5.18	-1.91	3.28
	2	-5.39	-1.67	3.73

Table S2. MPI index, polar and non-polar surface area, and molecular dipole moments of PEP formed by different link structures

Structure	1	2	3	4	5
MPI / kcal/mol	12.75	12.70	12.73	12.73	12.67
Nonpolar surface area / Angstrom ²	127	123	125	125	124
	(37%)	(36%)	(37%)	(37%)	(36%)
Polar surface area / Angstrom ²	214	216	213	214	215
	(63%)	(64%)	(63%)	(63%)	(64%)
Molecular dipole moment / D	3.46	3.13	3.25	3.16	3.20
dihedral angle	21.3	54.4	52.8	55.5	49.5

Table S3. MPI index, polar and non-polar surface area and energy difference of cis-PEDOT (Cis) and trans-PEDOT (Trans) structures

Trans	0	+1	+2	+3	+4	+5	+6
Molecular polarity in dex / kcal/mol	19	44	92	140	189	238	287
Nonpolar surface area / Angstrom ²	146	4.15	0.00	0.00	0.00	0.00	0.00
	(21%)	(1%)	(0%)	(0%)	(0%)	(0%)	(0%)

Polar surface area / Angstrom ²	564 (79 %)	701 (99%)	702 (100 %)	699 (100 %)	696 (100 %)	694 (100 %)	693 (100 %)
Cis	0	+1	+2	+3	+4	+5	+6
Molecular polarity in dex / kcal/mol	20	43	91	139	187	236	285
Nonpolar surface area / Angstrom ²	138 (19%)	8 (1%)	0.00 (0%)	0.00 (0%)	0.00 (0. %)	0.00 (0%)	0.00 (0 %)
Polar surface area / Angstrom ²	590 (81%)	711 (99 %)	712 (100 %)	708 (100 %)	704 (100 %)	702 (100 %)	700 (100%)
Cis-Trans	0	+1	+2	+3	+4	+5	+6
Poor energy / eV	0.53	0.91	1.19	1.28	1.29	1.24	1.10