## 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 S2. The degree of polymerization of Cis-PEDOT

Figure S3. The degree of polymerization of PPr

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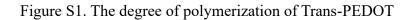
Figure S15. Open or shell state and closed-shell state energy level distribution of bipolarizing PEP molecules and HOMO-LUMO

Figure S16. Energy level distribution of the open-shell state of the polarizing-PEP molecules and HOMO-LUMO

Table S1. The degree of polymerization of  $PE_mP_n$ 

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

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



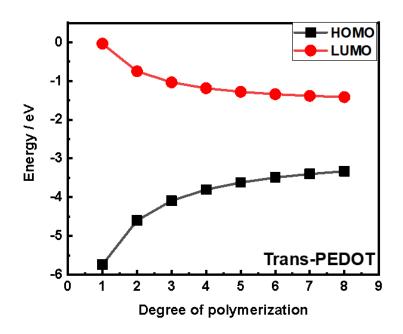


Figure S2. The degree of polymerization of Cis-PEDOT

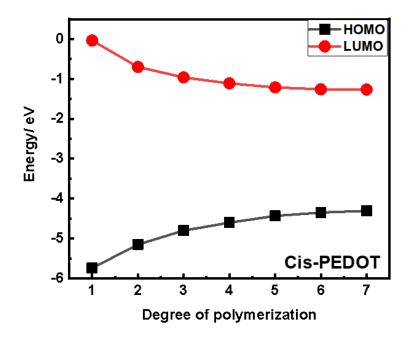


Figure S3. The degree of polymerization of PPr

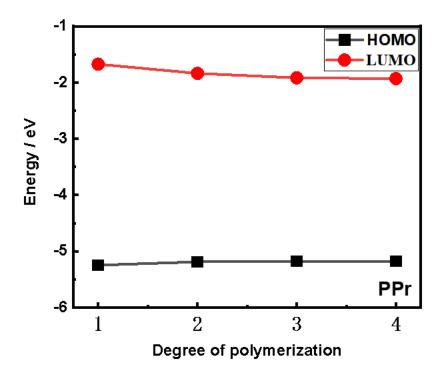


Figure S4. The degree of polymerization of PEP

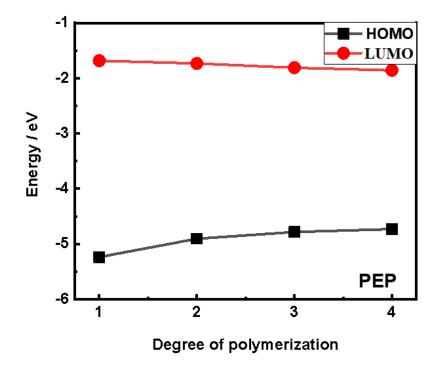


Figure S5. HOMO, LUMO, and  $\pi$  electron distributions of the cis and trans structures of PEDOT

PEDOT- Trans	0e	+1e	+2e	+3e
LUMO	2 <b>428</b> 22	3 <b>38</b> 82	30 Builde	Sold Barloto
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πе	\$ <sup>\$\$</sup> 8 <sup>\$</sup> 8 <sup>\$</sup> 8	\$ <sup>8</sup> 8888	S <sup>S</sup> S <sup>S</sup> S <sup>S</sup> S	S <sup>SS</sup> SSS
	nununu	$\sim\sim\sim$	~~~	$\sim$
	+4e	+5e	+6e	
LUMO	ઌૢૢૢૡૢૢૢૡૢૢૡૢૢૡૢ ૡૢૡૢૢૡૢૢૡૢૡૢૡૢૡૢ		Contesting to	
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πе	8 <sup>8</sup> 8 <sup>8</sup> 8 <sup>8</sup> 8	\$ <sup>8</sup> 8 <sup>8</sup> 8 <sup>8</sup> 8	88888	       
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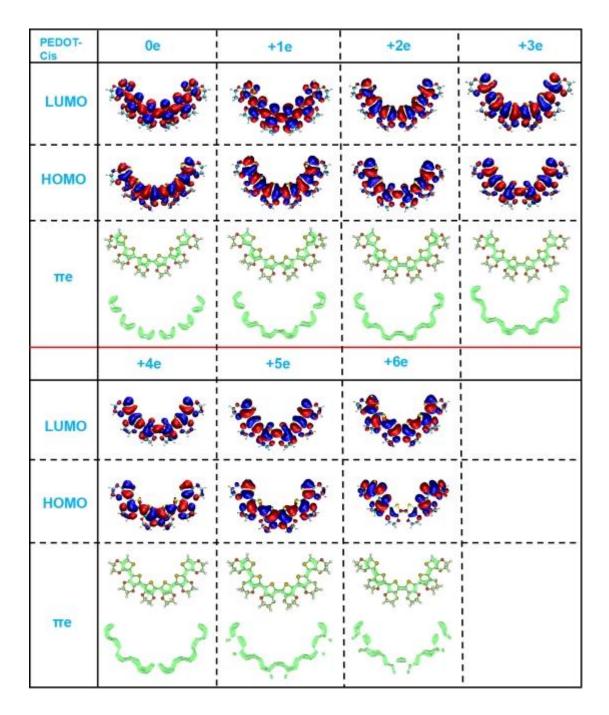
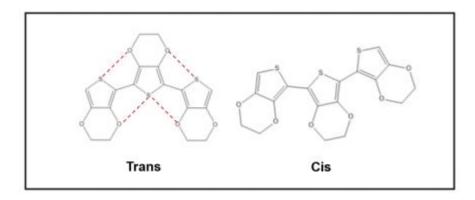


Figure S6. Schematic diagram of the cis/trans structure of PEDOT and trans- PEDOT in O-S bond length varies



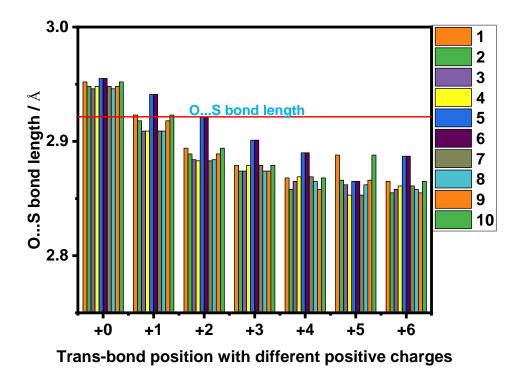


Figure S7. The average dihedral angle change in the PEP

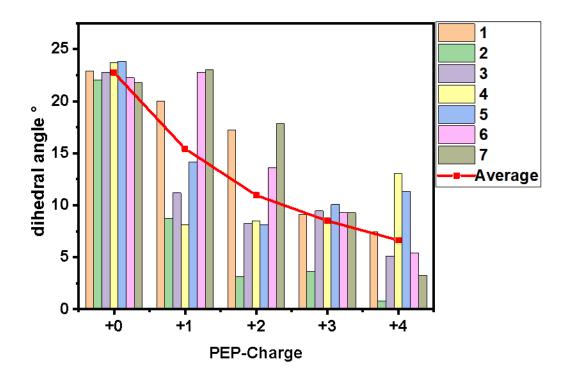


Figure S8. The PEDOT cis and trans structure with a degree of polymerization of 6 changes in the amount of charge and the average dihedral angle

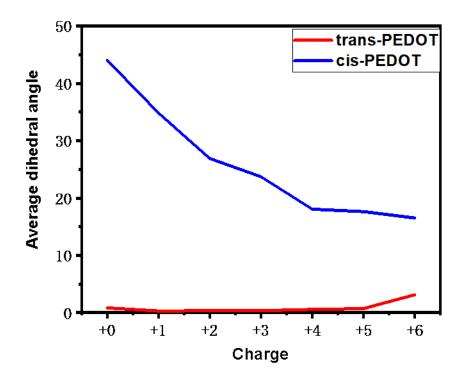


Figure S9. Electron distribution and  $\pi$  electrostatic potential distribution of PEP

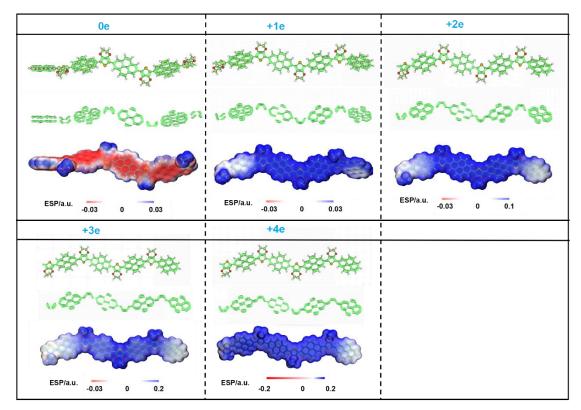


Figure S10. HOMO, LUMO, and  $\pi$  electronic density contour surface chart of polypyrene

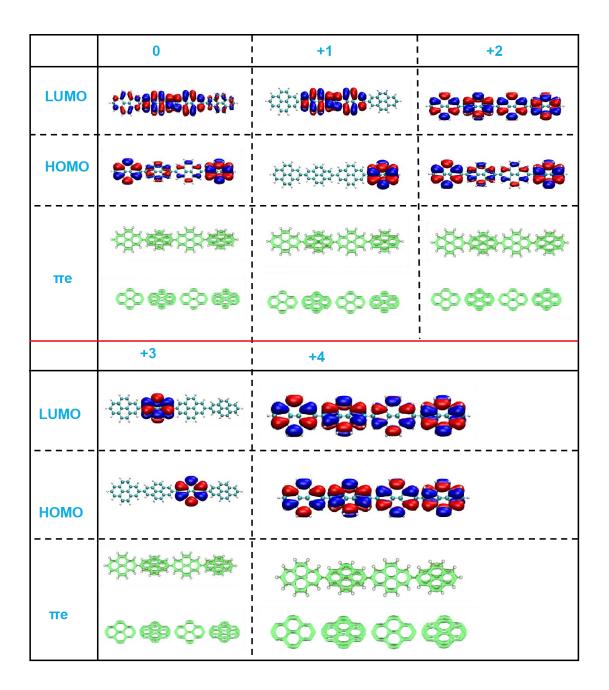


Figure S11. HOMO, LUMO, and  $\pi$  electronic density contour surface chart of  $PE_mP_n$ 

	PEDOT	E₄P	E <sub>3</sub> P	E <sub>2</sub> P	EP
LUMO	9 <b>399</b> 99	Stand and a second s	SAN CARGE	Stanging (1) an (1) the	
номо	ġŵ <u>ġ</u> ŵ <sub>ŵ</sub> ŵ	and the constant of the consta	egages (1) and the second	~ <b>****</b> ****	**************************************
πе	\$ <sup>8</sup> 8888	<sup>€</sup> ¢€¢¢¢¢¢¢¢¢¢	***	\$\$\$	
(Electronic density contour surface chart)	~~~~	moournes	<u>~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~</u>	<i>ড়৾৶৸ড়৾৶৸ড়৾৶ঀ</i> ৢ	<sup>∞∞</sup> ੪ੴ^ੴvੴ
ESP (Electrostatic Potential)			<b>ANN</b>		
	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.
	EP <sub>2</sub>	EP <sub>3</sub>	EP <sub>4</sub>	PPr	
LUMO	A MARCANIC	······································	-;;;= <b>2();23();2</b> ;;}; čž	-:{}: <b>::::::::::::::::::::::::::::::::::</b>	
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TTE (Electronic density contour surface chart)	******	A CONTRACTOR OF	Å	<b>發鐵磁線</b>	
surface chart)	10	<sup>ඳේ ො</sup> ස් කොස	<b>\$\$\$\$</b> \$	ර <b>ි දේ</b> ෂ රට <b>දේ</b> ෂ	
ESP (Electrostatic Potential)	<i></i>	<i></i>			
	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.	-0.03 0 0.03 ESP/a.u.	

Figure S12. NTO of PEP

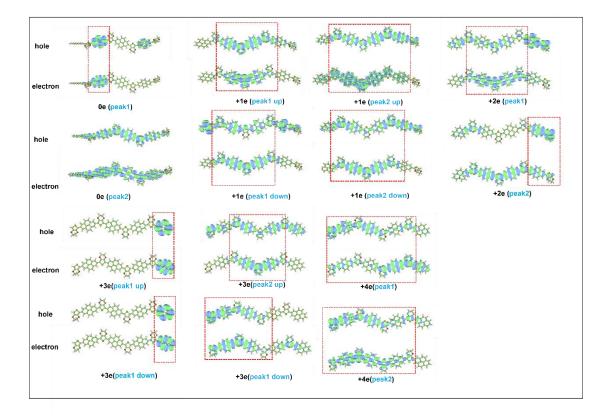
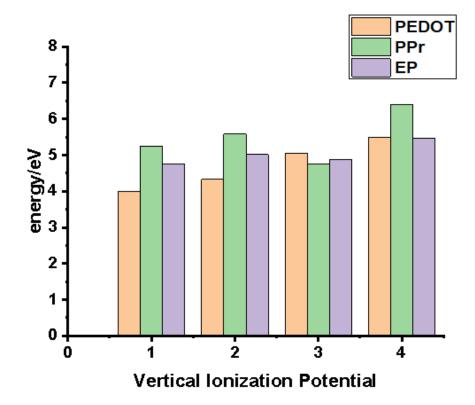


Figure S13. Vertical ionization potential



structure	Degree of aggregation	HOMO	LUMO	gap/eV
	1	-4.33	-1.69	2.64
E4P	2	-4.08	-1.90	2.18
	3	-4.46	-1.87	2.59
	1	-4.51	-1.68	2.83
E3P	2	-4.24	-1.87	2.37
	3	-4.63	-1.76	2.87
	1	-4.68	-1.67	3.01
E2P	2	-4.47	-1.78	2.70
	3	-4.40	-1.88	2.57
	1	-5.19	-1.87	3.34
EP2	2	-4.92	-1.86	3.06
	3	-4.88	-1.88	3.00
	1	-5.19	-1.89	3.31
EP3	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 S1. The degree of polymerization of  $PE_mP_n$ 

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 <sup>2</sup>	127	123	125	125	124
	(37%)	(36 %)	(37%)	(37%)	(36%)
Polar surface area / Angstrom <sup>2</sup>	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	19	44	92	140	189	238	287
dex / kcal/mol							
Nonpolar surface area	146	4.15	0.00	0.00	0.00	0.00	0.00
/ Angstrom <sup>2</sup>							
	(21	(1%	(0%)	(0%)	(0 %)	(0%)	(0%)
	%)	)					

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