

Supplementary Information

Small-Bandgap Quinoid-based π -Conjugated Polymers

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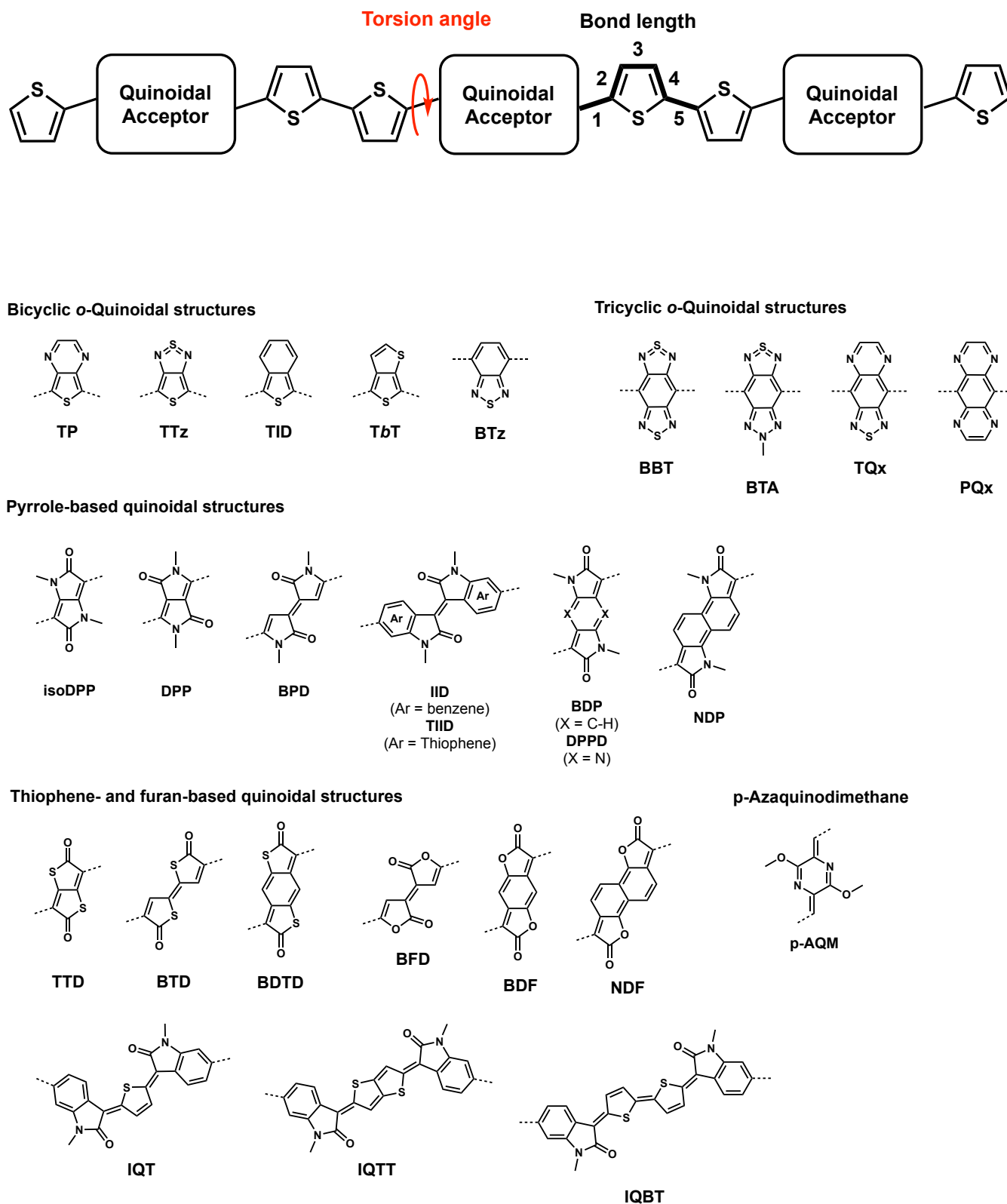


Fig S1. The trimer models of the polymer consisting of the quinoid structure and bithiophene for the computation using the DFT method at the B3LYP/6-31G(d) level.

Table S1. Calculated HOMO, LUMO, and bandgap (E_g) of the trimer models. Torsion angle between the quinoid unit and the adjacent thiophene ring, and bond length in the adjacent thiophene ring in the model compounds. Optimization of the structure and calculation were carried out by the DFT method at the B3LYP/6-31G(d) level.

Acceptor	HOMO (eV)	LUMO (eV)	E_g (eV)	Torsion ^a (°)	Bond length of each bond number ^b (Å)				
					1	2	3	4	5
Ref (Th)	-4.72	-2.32	2.39	3.709	1.44072	1.38234	1.41302	1.38221	1.44113
TP	-4.51	-2.97	1.54	0.007	1.42943	1.39014	1.40557	1.3872	1.43737
TTz	-4.43	-3.08	1.35	0.004	1.4195	1.39468	1.40149	1.39126	1.4312
TID	-4.52	-2.46	2.05	28.465	1.44126	1.38542	1.41154	1.38303	1.44082
TbT	-4.54	-2.45	2.08	6.522	1.43589	1.38604	1.40978	1.38412	1.4395
BTz	-4.89	-2.29	1.95	0.004	1.45185	1.38477	1.41145	1.38313	1.4404
BBT	-4.57	-3.83	0.74	0.001	1.43069	1.40452	1.39397	1.39604	1.42552
BTA	-4.40	-3.29	1.11	0.084	1.43653	1.39684	1.40089	1.39042	1.43318
TQx	-4.60	-3.54	1.06	0.003	1.44399	1.39937	1.39949	1.38994	1.43302
PQx	-4.57	-3.22	1.35	13.239	1.45474	1.3964	1.40209	1.38691	1.43746
isoDPP	-5.11	-2.95	2.17	19.124	1.444	1.38538	1.41138	1.38273	1.44087
DPP	-4.76	-3.02	1.74	4.11	1.43587	1.39447	1.40353	1.38768	1.44032
BPD	-4.61	-3.17	1.44	20.5	1.43656	1.38871	1.40861	1.386	1.43855
IID	-4.99	-2.96	2.04	21.265	1.45951	1.38116	1.41368	1.38228	1.44314
TIID	-4.46	-3.01	1.46	0.23	1.43543	1.38655	1.4086	1.38574	1.43708
BDP	-4.76	-3.59	1.17	1.032	1.42398	1.39694	1.40083	1.39157	1.42972
DPPD	-4.97	-3.74	1.23	0.002	1.42088	1.39606	1.40009	1.39333	1.43209
NDP	-4.52	-3.73	0.79	0.041	1.41986	1.40124	1.39686	1.39505	1.4242
TTD	-5.48	-3.74	1.74	0.029	1.43992	1.39085	1.40548	1.3871	1.43783
BTd	-5.48	-3.74	1.61	0.618	1.43894	1.38809	1.40761	1.38691	1.4375
BDTD	-5.24	-4.17	1.07	11.382	1.43226	1.39992	1.39866	1.39199	1.42967
BFD	-5.12	-3.66	1.46	0.004	1.42338	1.38853	1.40531	1.3893	1.43646
BDF	-5.22	-4.09	1.12	0.153	1.42309	1.3975	1.3997	1.39282	1.42961
NDF	-4.86	-4.14	0.73	0.578	1.41679	1.40243	1.39513	1.39708	1.42267
IQT	-4.90	-3.13	1.77	22.911	1.46046	1.38076	1.41419	1.38204	1.44312
IQTT	-4.86	-3.24	1.62	22.331	1.46	1.38119	1.41418	1.38211	1.44323
IQBT	-4.77	-3.30	1.47	21.558	1.45983	1.38142	1.41396	1.38205	1.44314
<i>p</i> -AQM	-4.35	-2.71	1.64	0.001	1.42206	1.39431	1.40264	1.39016	1.43583

^aThe torsion angle was estimated between acceptor unit and adjacent thiophene ring in the central repeat unit of the trimer model. ^bThe bond lengths were extracted from the central repeat unit of the trimer model.

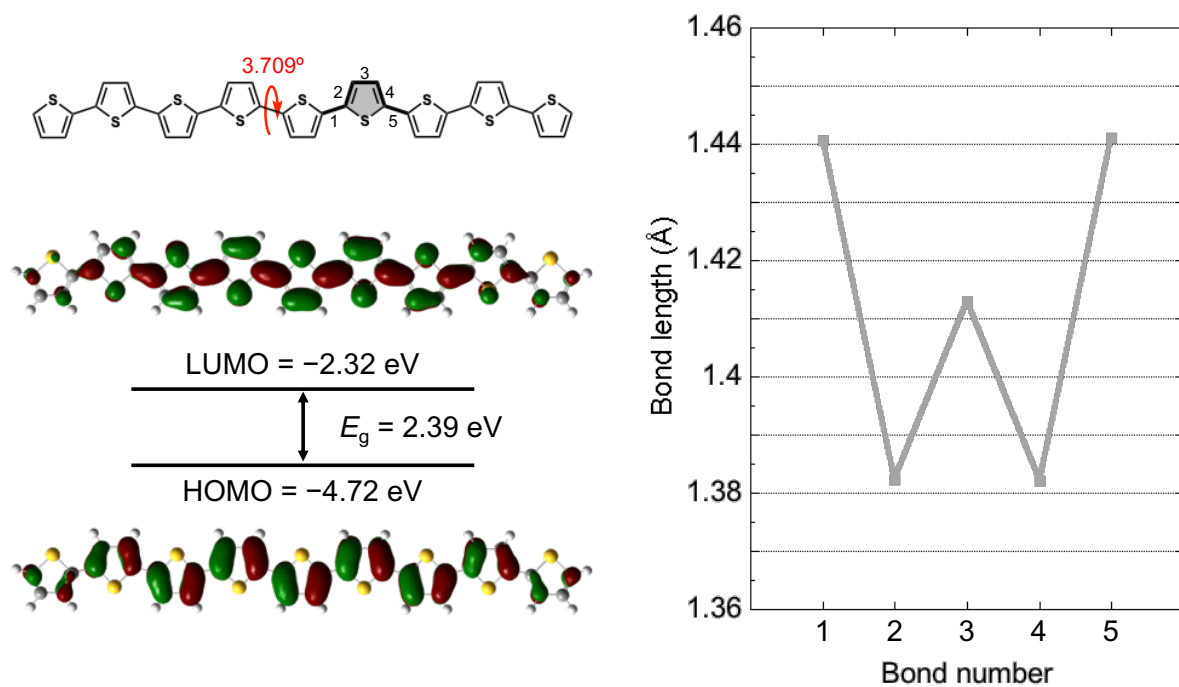


Fig S2. The model polymer of polythiophene.

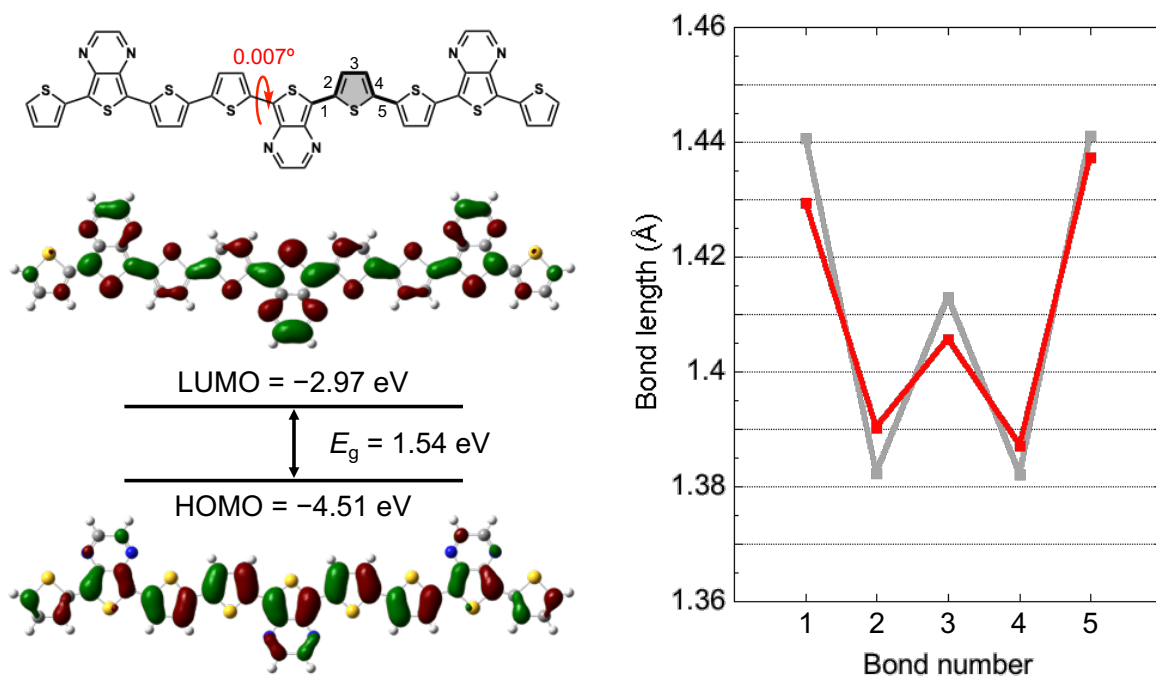


Fig S3. The model polymer based on TP.

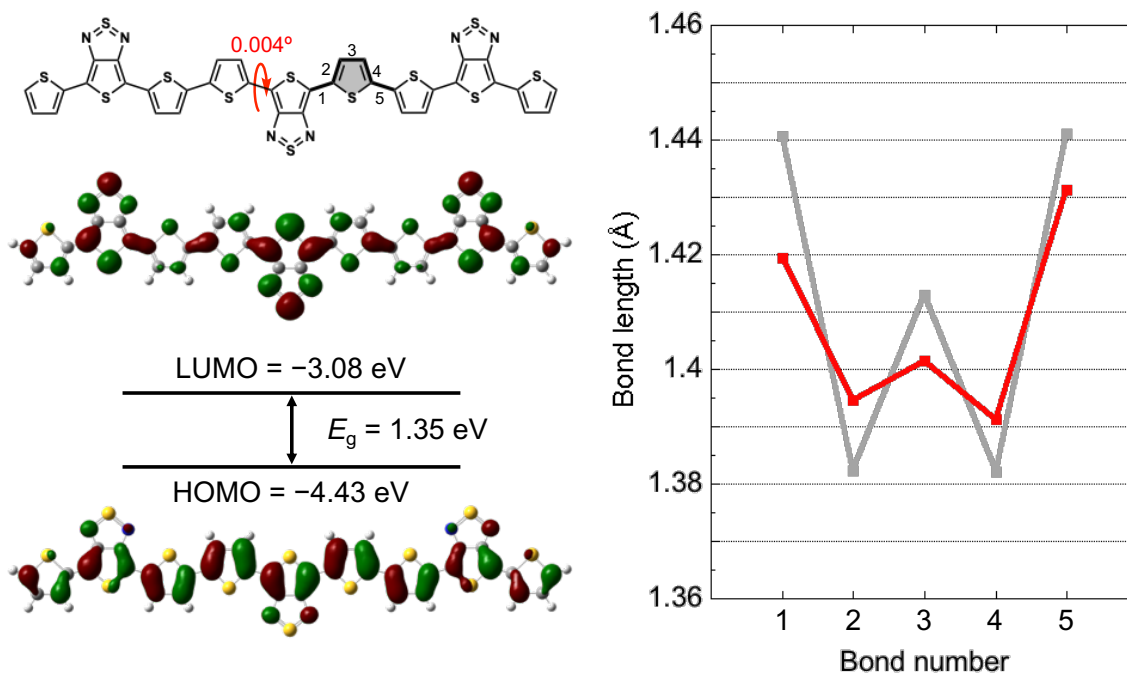


Fig S4. The model polymer based on TTz.

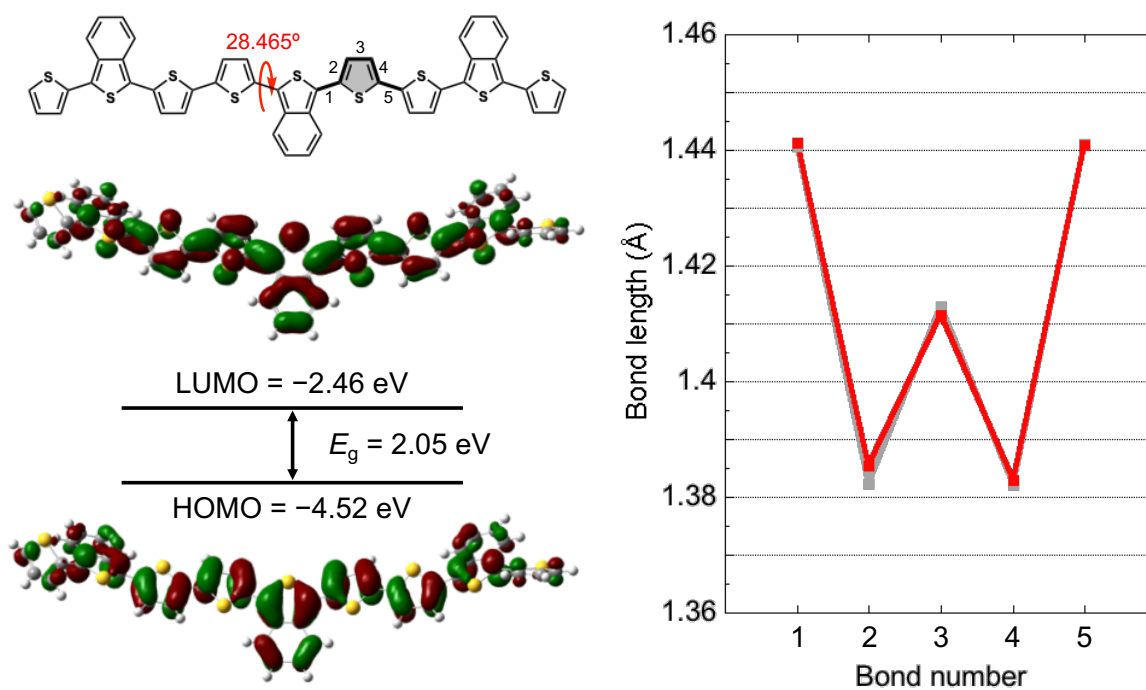


Fig S5. The model polymer based on TID.

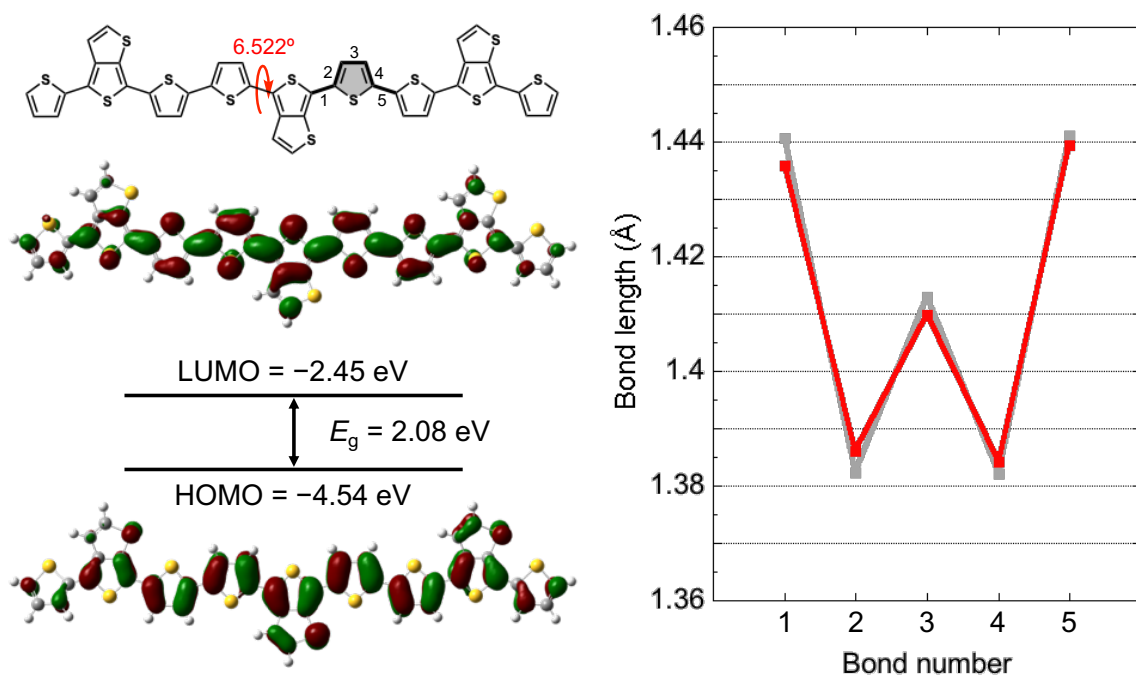


Fig S6. The model polymer based on TbT.

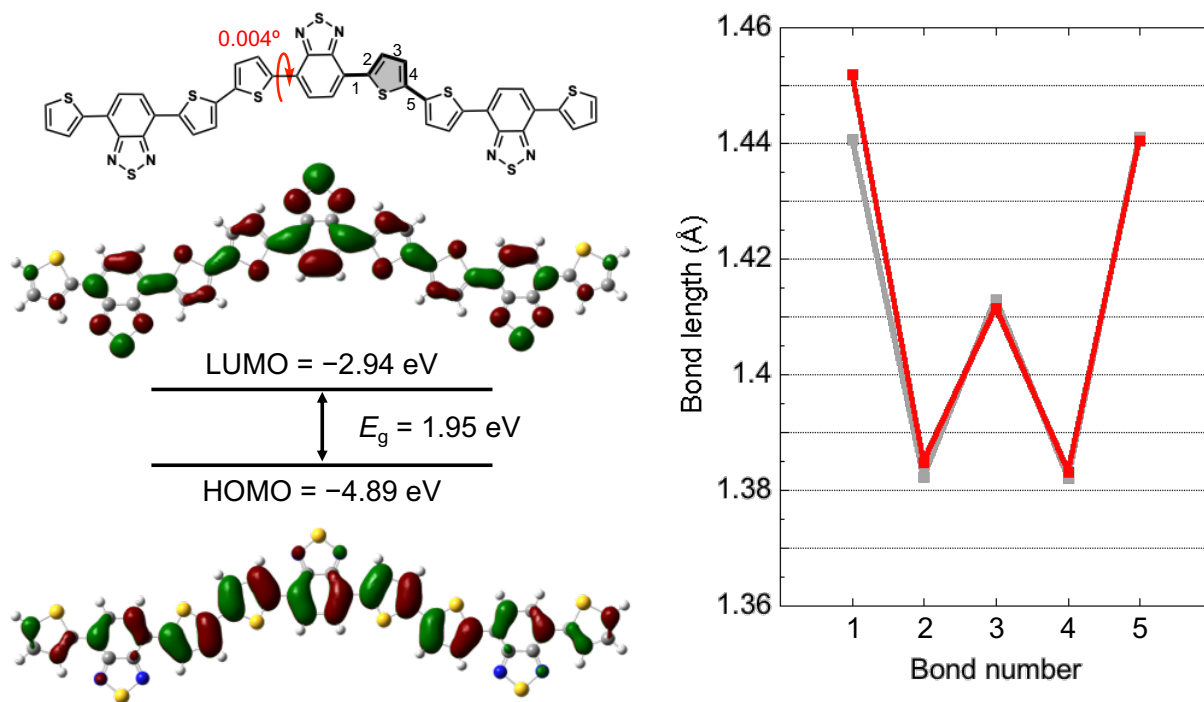


Fig S7. The model polymer based on BTz.

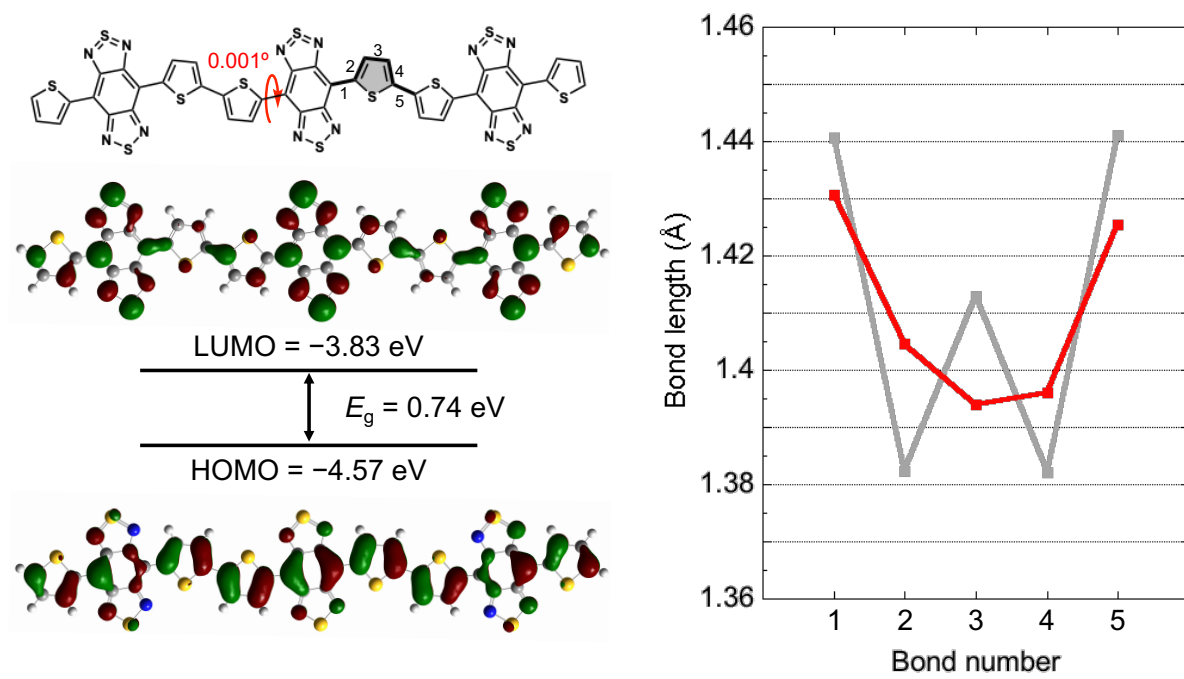


Fig S8. The model polymer based on BBT.

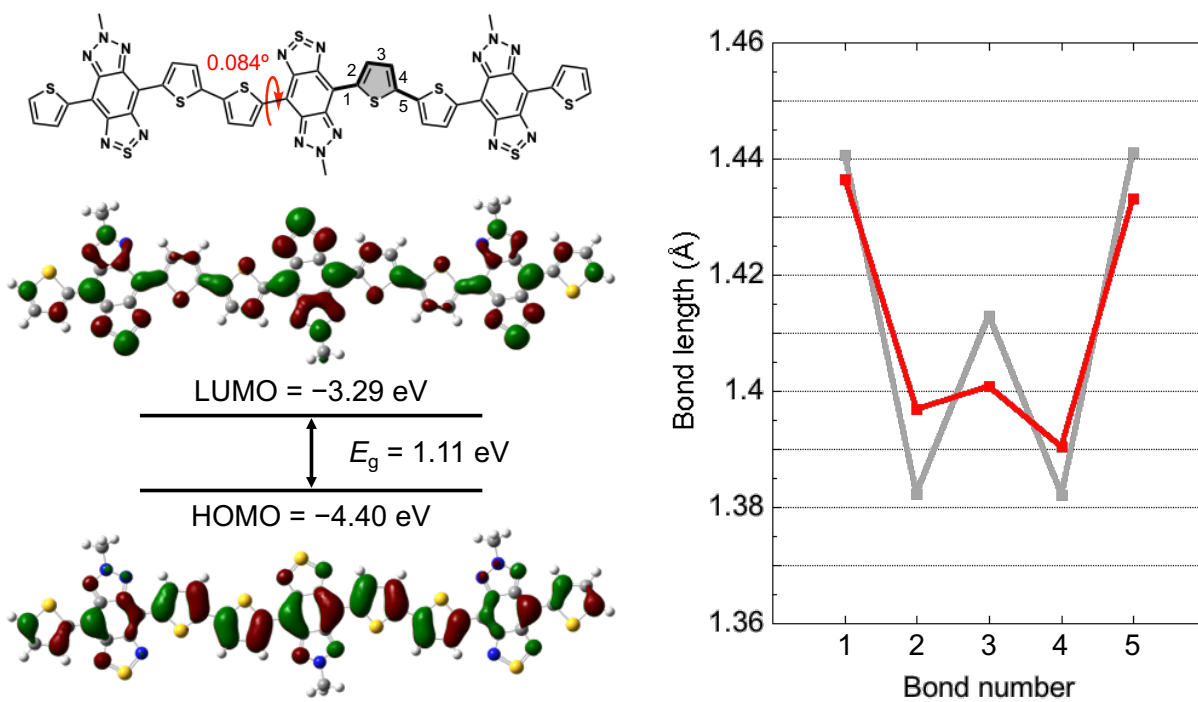


Fig S9. The model polymer based on BTA.

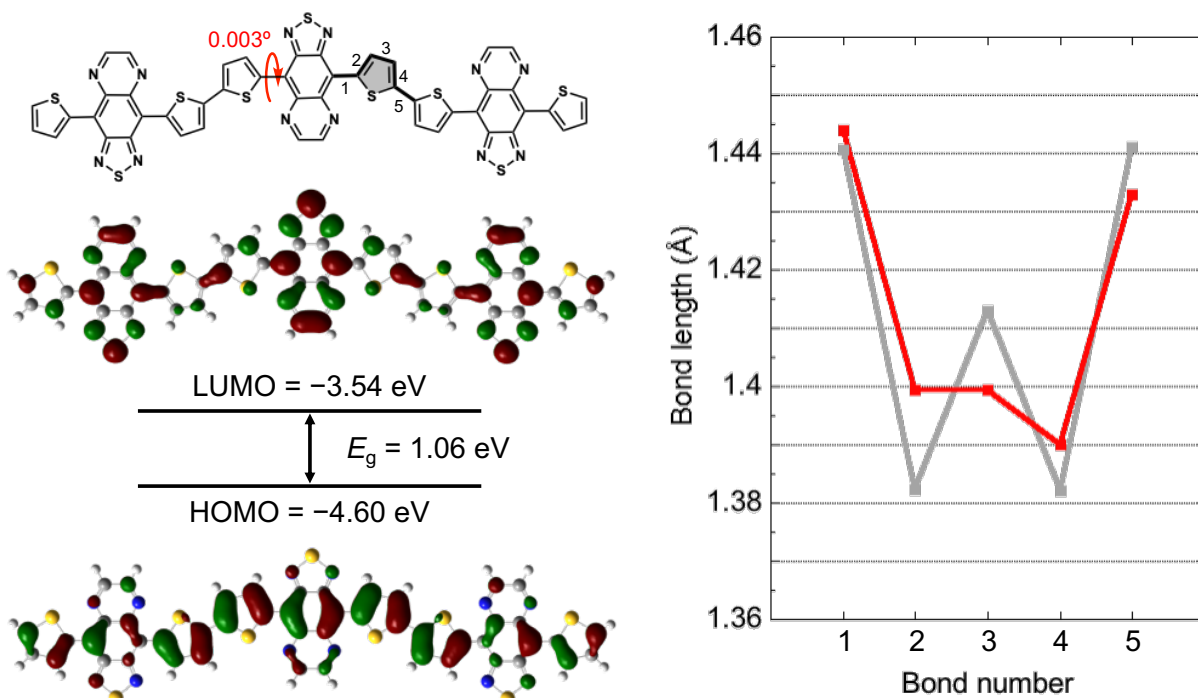


Fig S10. The model polymer based on TQx.

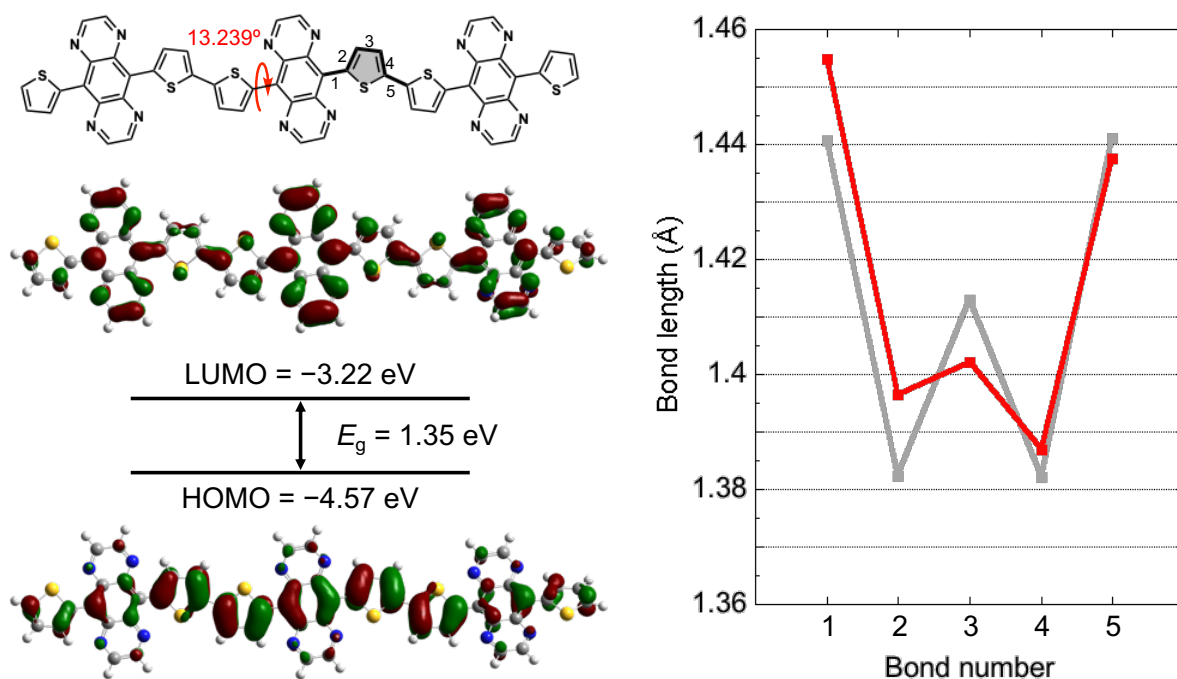


Fig S11. The model polymer based on PQx.

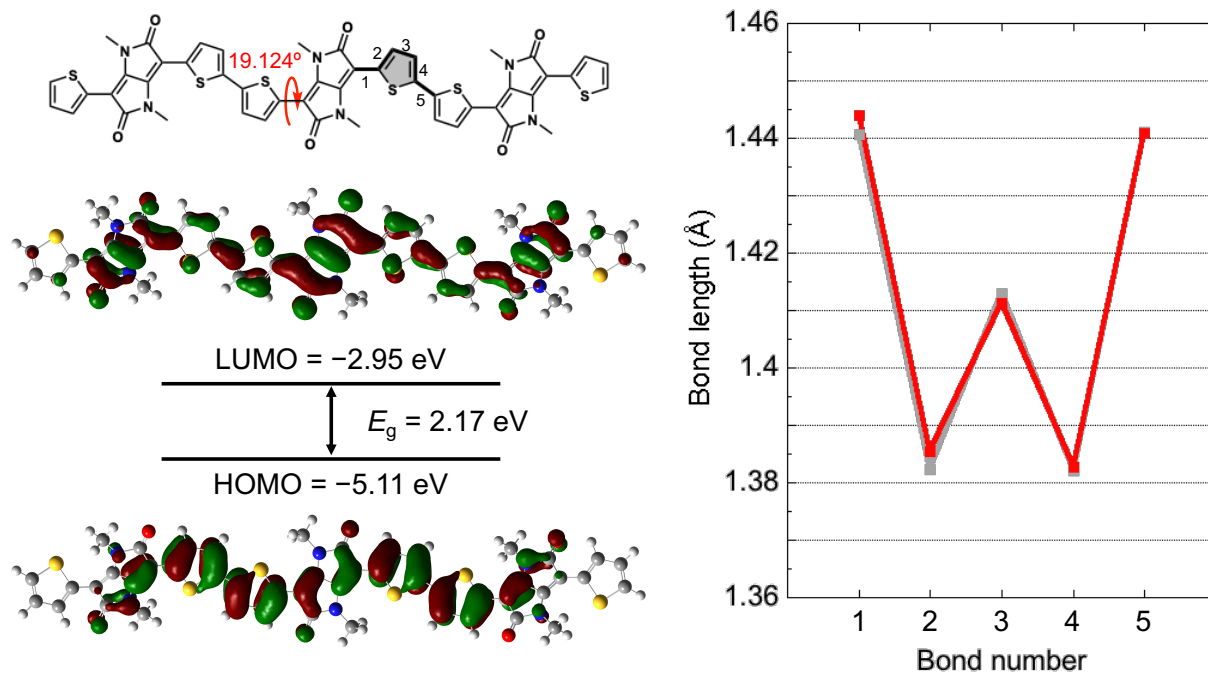


Fig S12. The model polymer based on isoDPP.

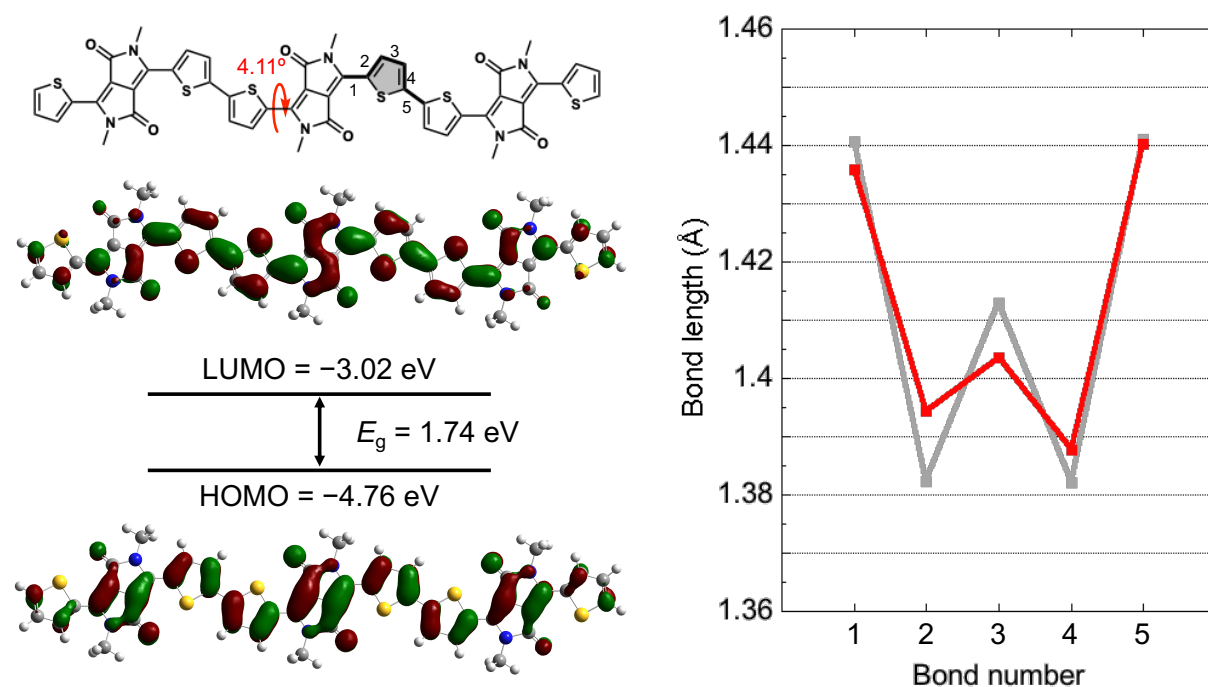


Fig S13. The model polymer based on DPP.

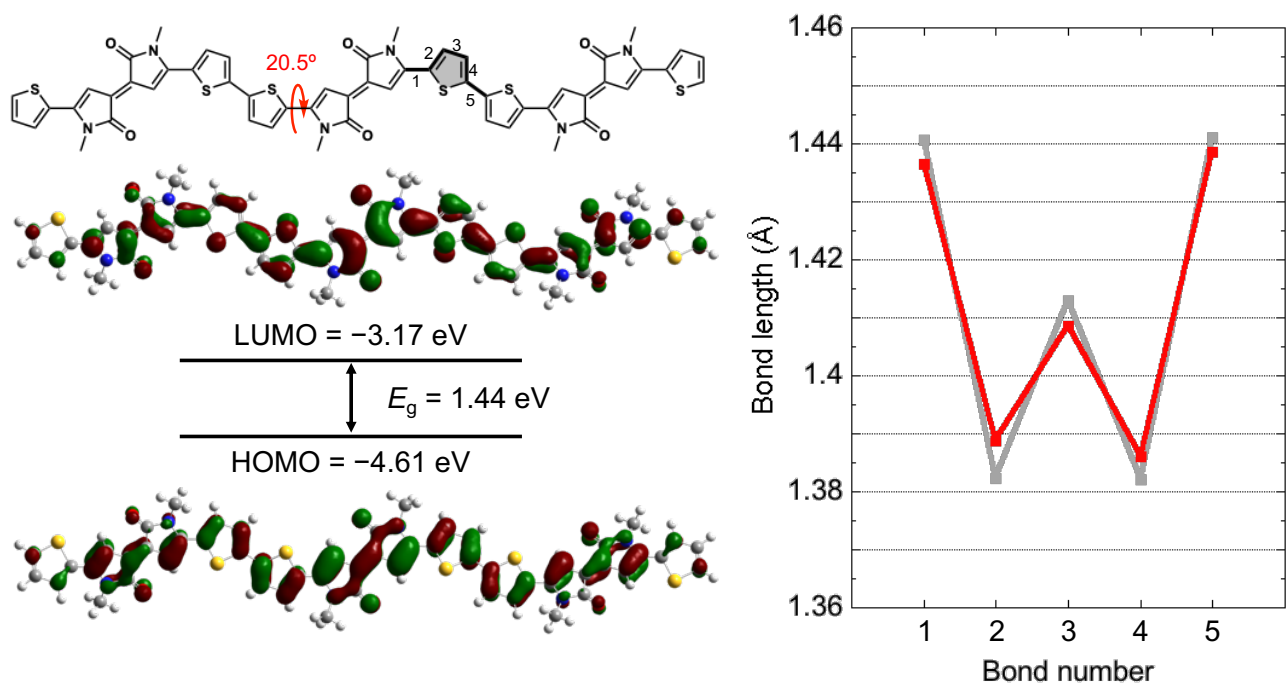


Fig S14. The model polymer based on BPD.

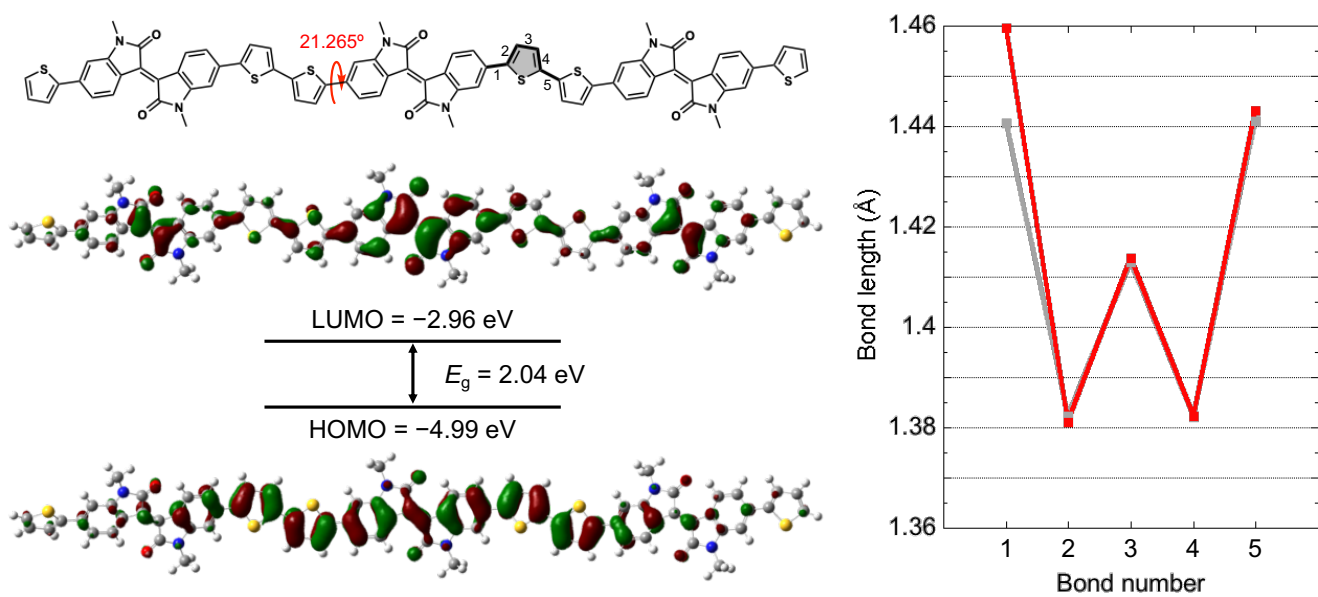


Fig S15. The model polymer based on IID.

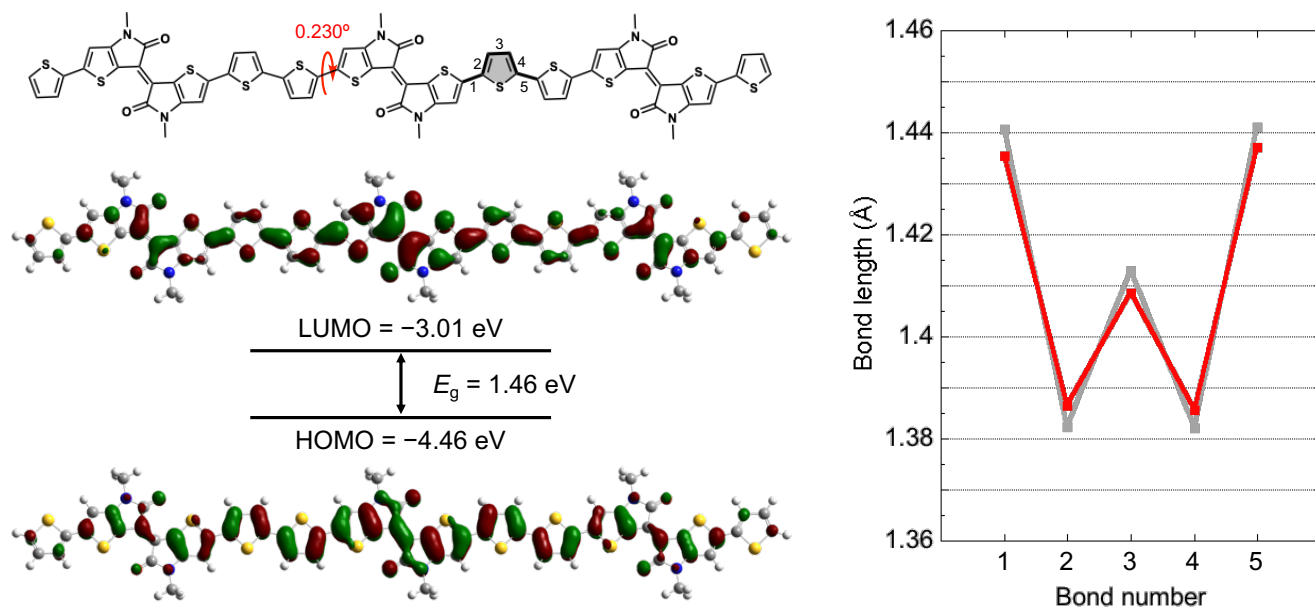


Fig S16. The model polymer based on TIID.

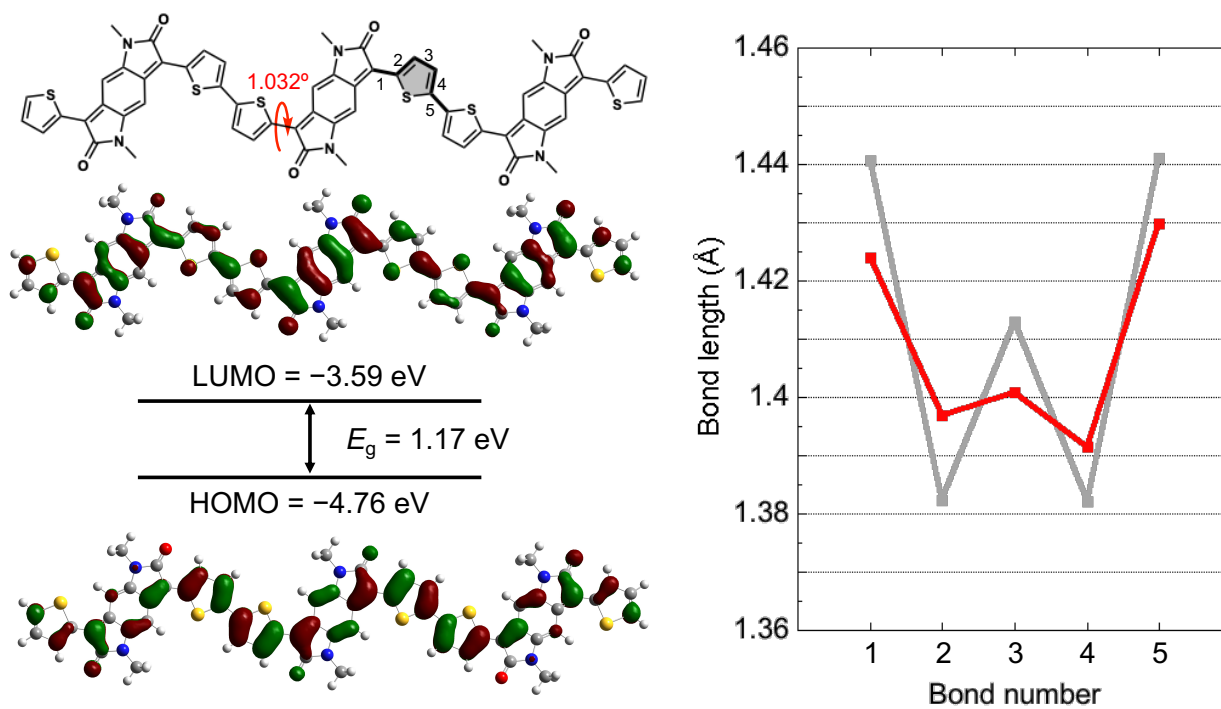


Fig S17. The model polymer based on BDP.

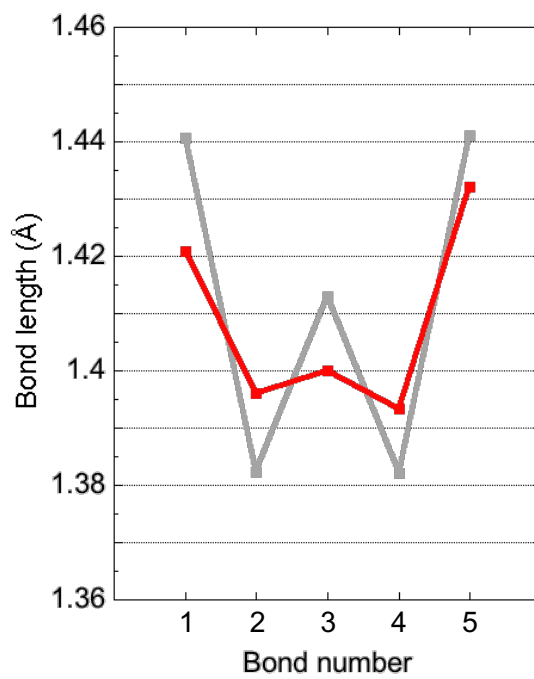
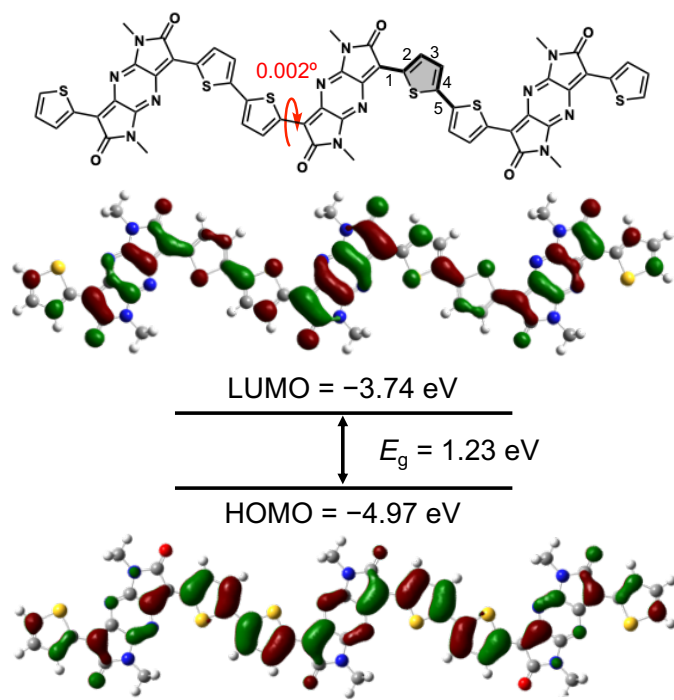


Fig S18. The model polymer based on PDDP.

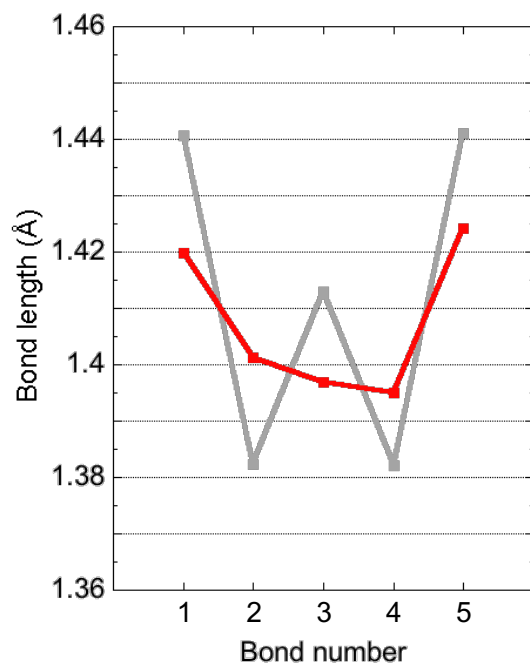
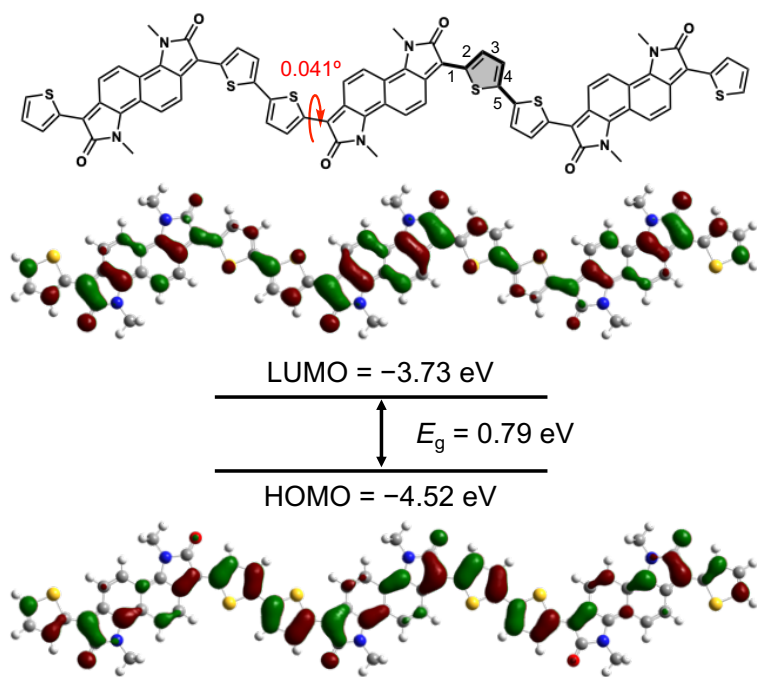


Fig S19. The model polymer based on NDP.

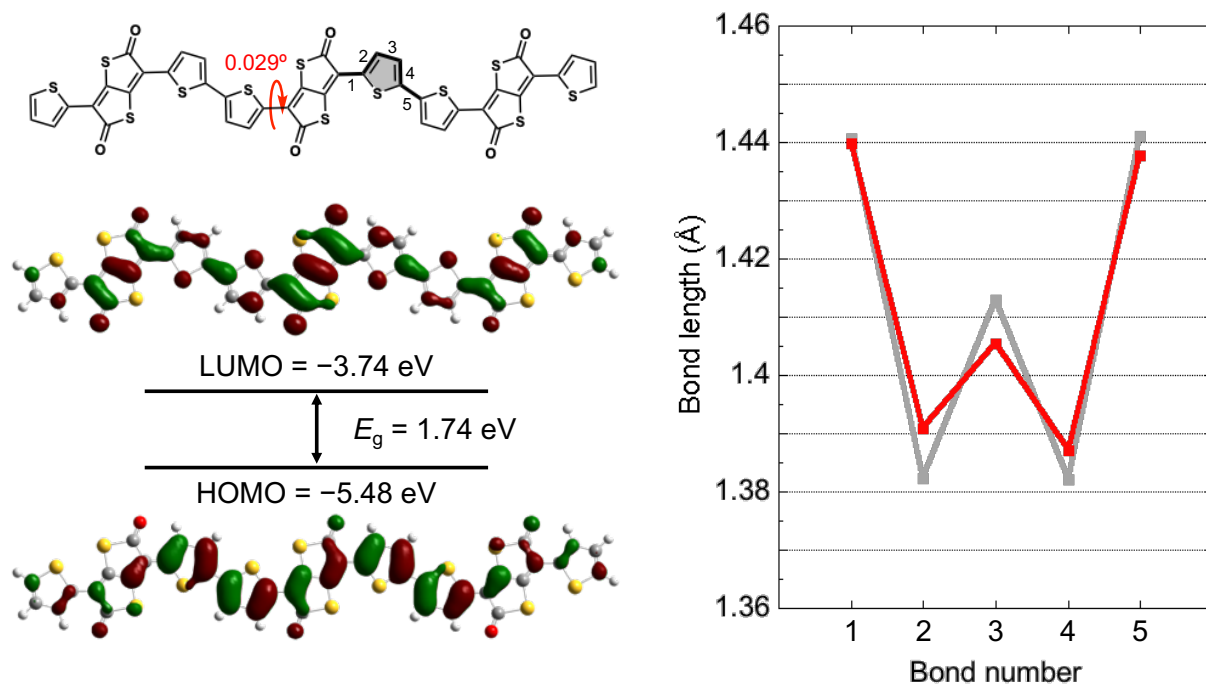


Fig S20. The model polymer based on TTD.

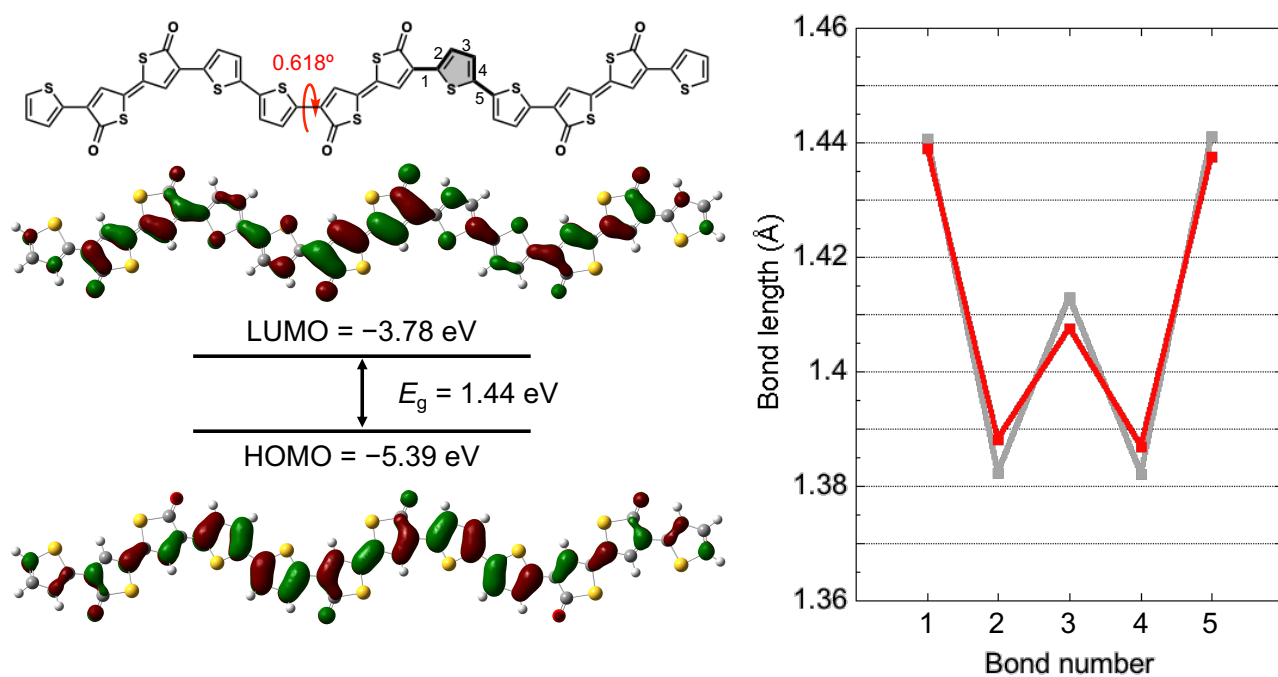


Fig S21. The model polymer based on BTD.

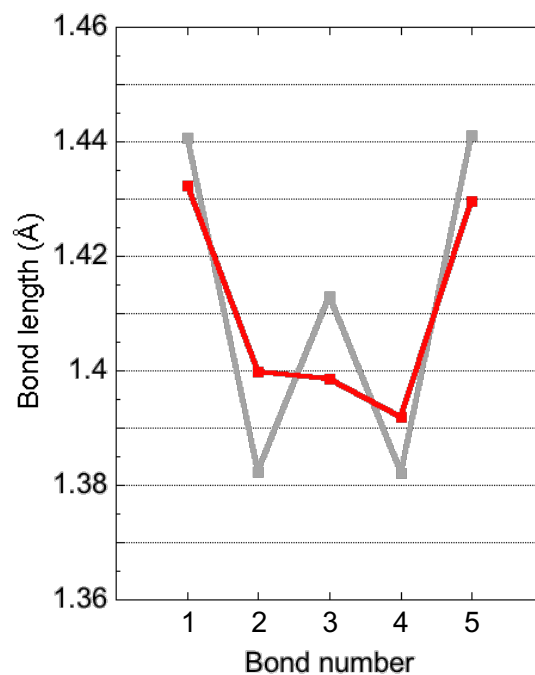
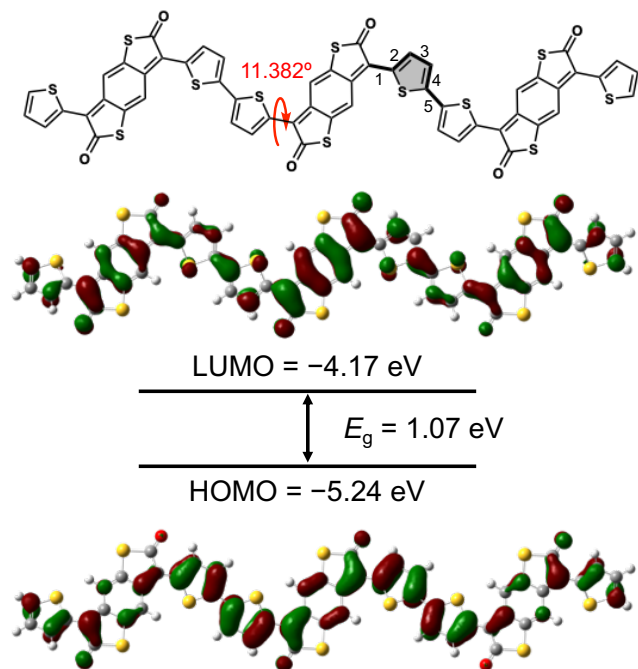


Fig S22. The model polymer based on BDTD.

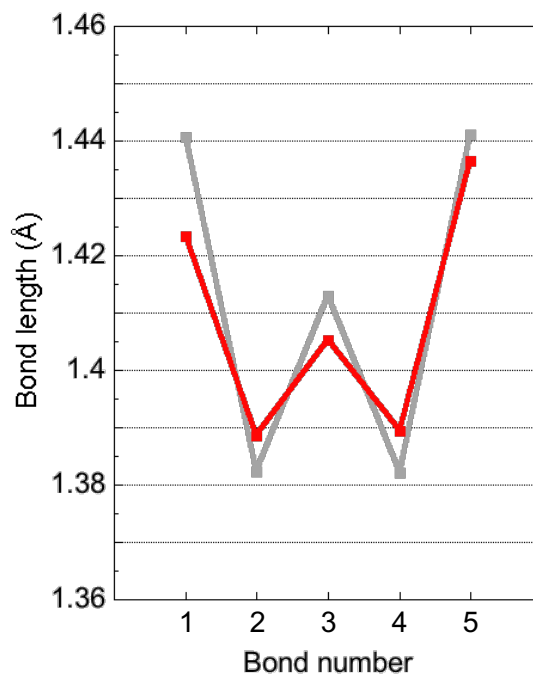
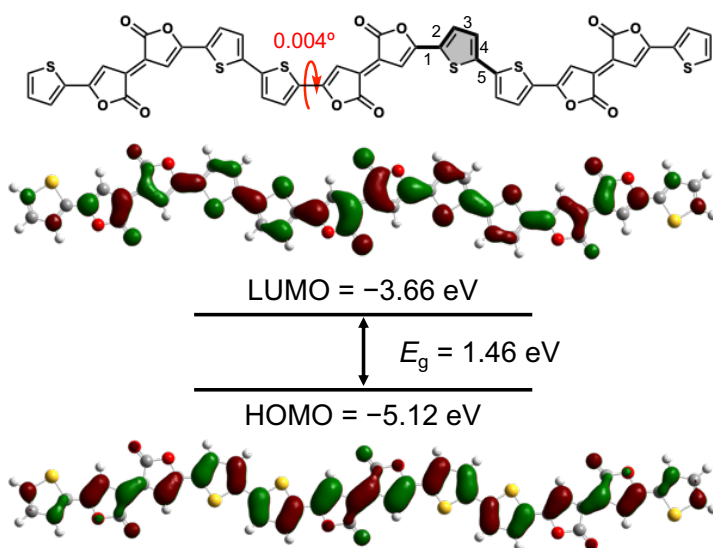


Fig S23. The model polymer based on BFD.

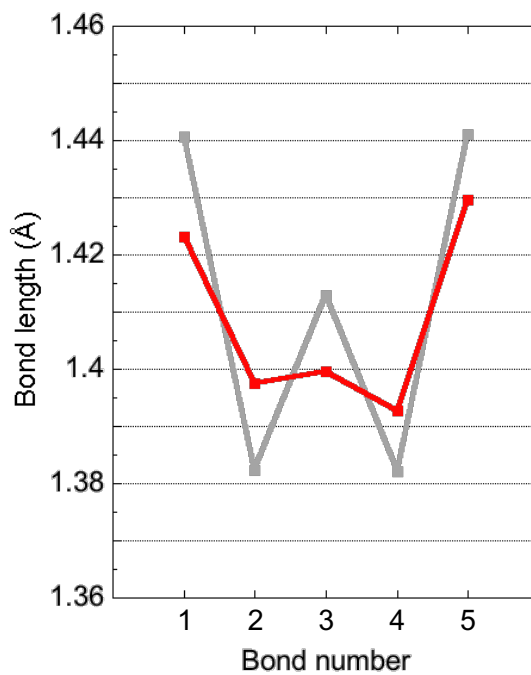
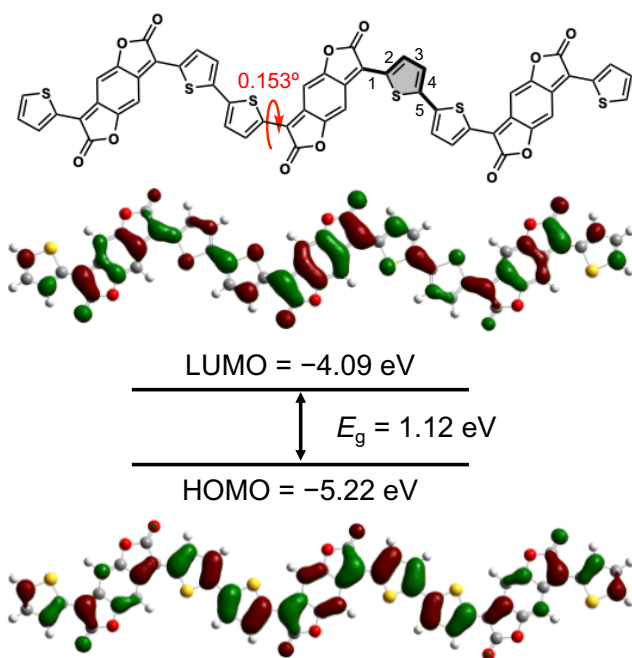


Fig S24. The model polymer based on BDF.

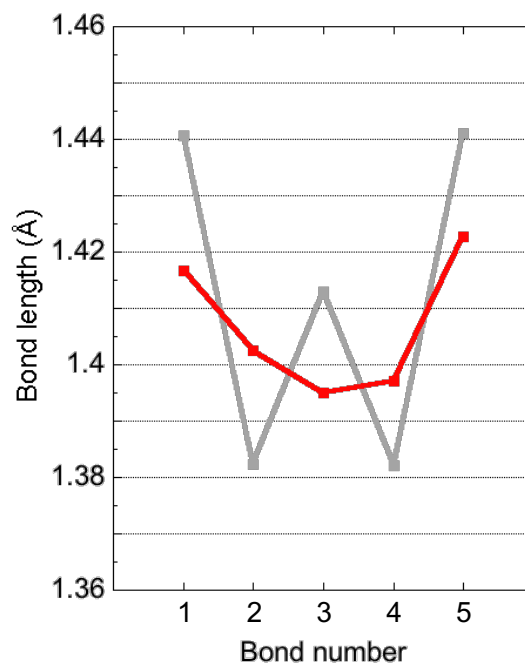
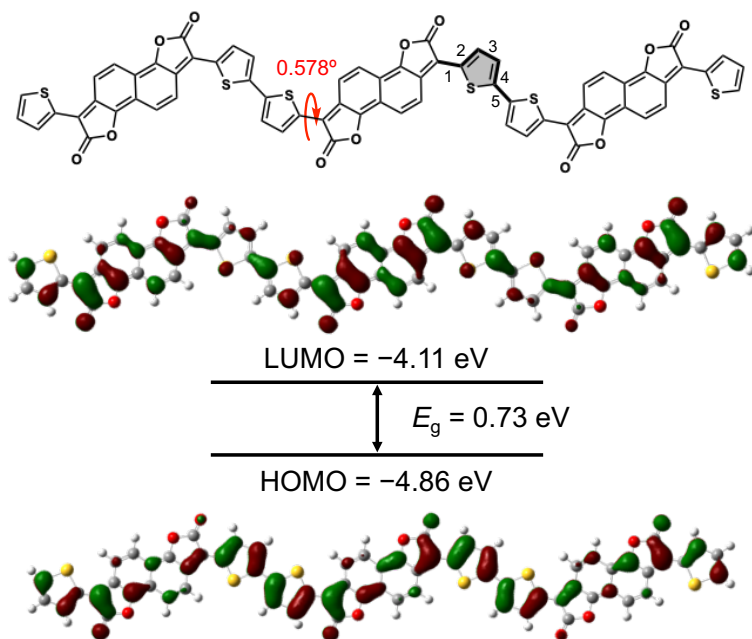


Fig S25. The model polymer based on NDF.

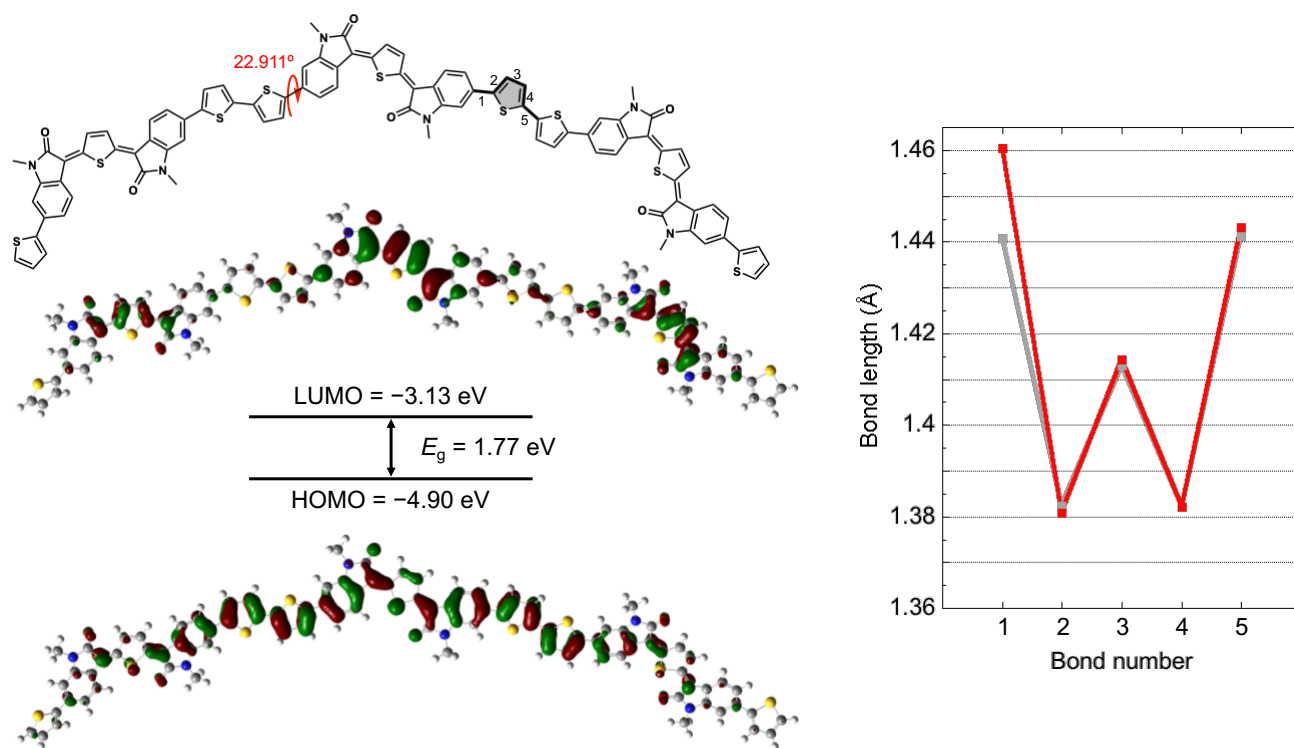


Fig S26. The model polymer based on IQT.

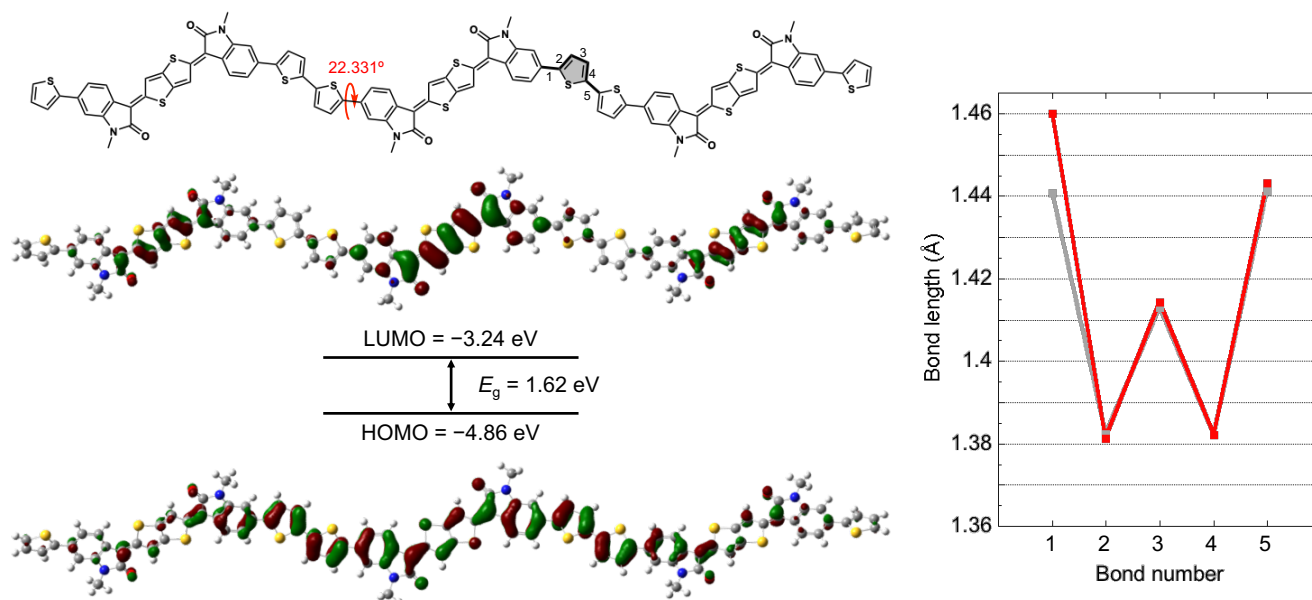


Fig S27. The model polymer based on IQTT.

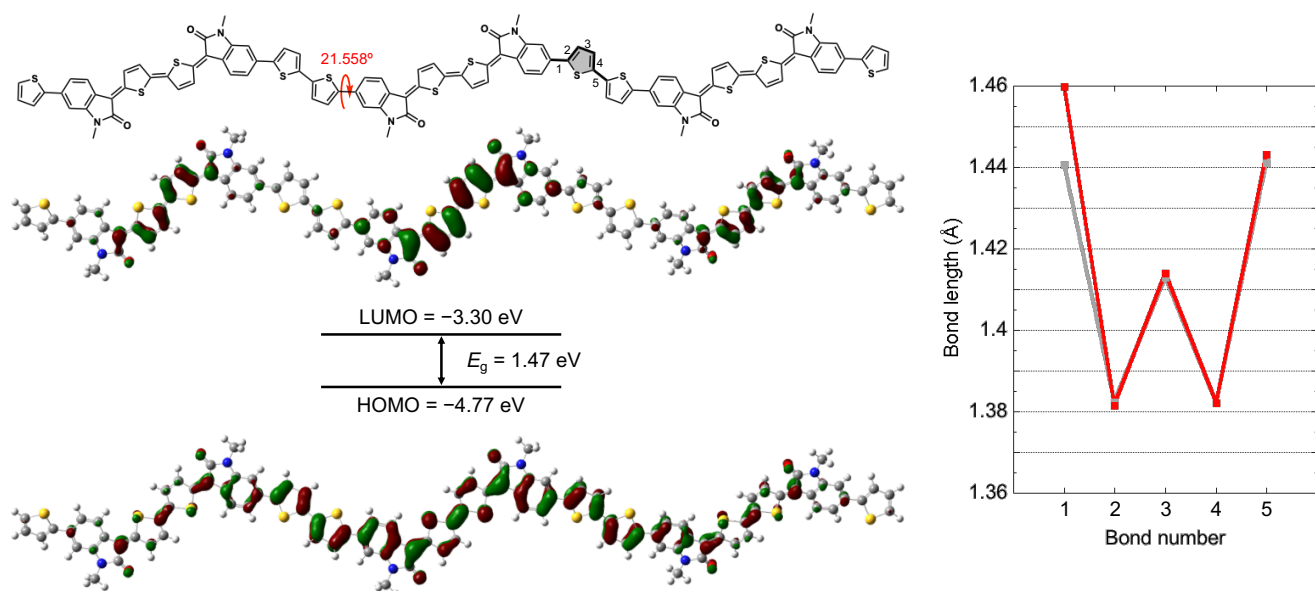


Fig S28. The model polymer based on IQBT.

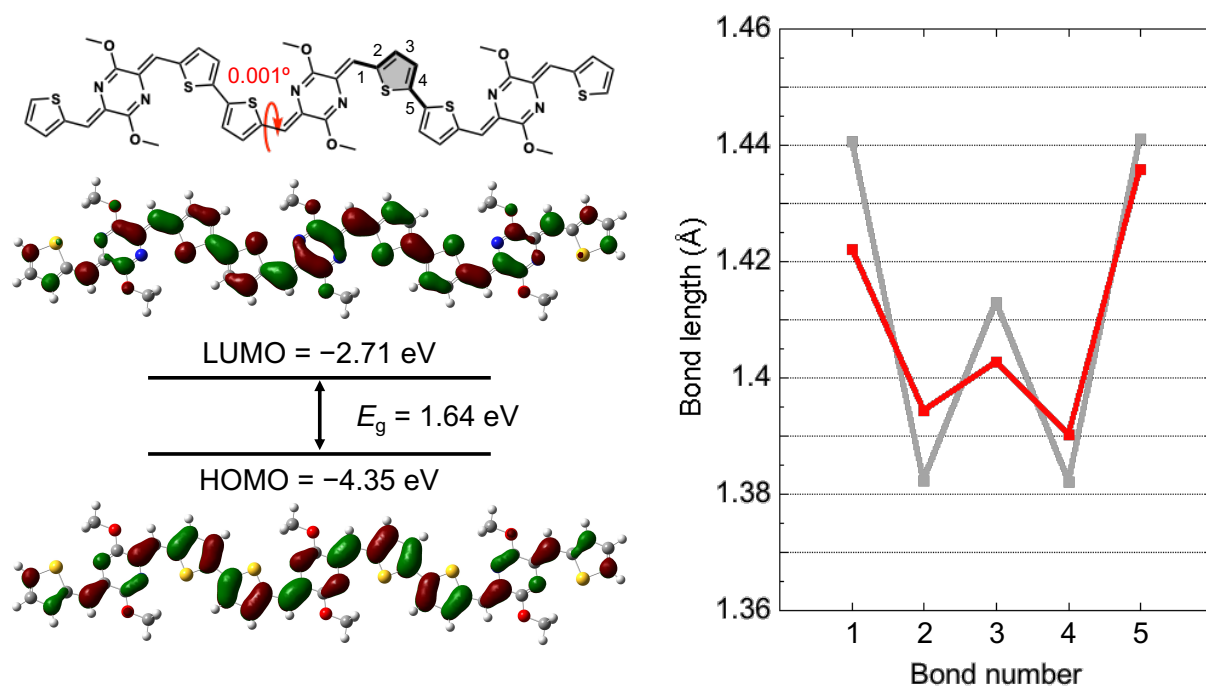


Fig S29. The model polymer based on *p*-AQM.