Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary data to:

π-bridge modification of thiazole-bridged DPP polymers for high performance near-IR OSCs

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Table Captions

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Table S1 The test HOMO energy levels of the monomer (**M**) and dimer (**D**) model of **P1** at the **6-31G (d)** basis set level. All energies values are in eV.

Opt test	B3LYP	PBE0	M06	BMK	Exp
M	-4.67	-4.91	-4.98	-5.38	**-5.26**
D	-4.52	-4.75	-4.82	-5.20	

Table S2 The band gaps of the oligomer models of the investigated polymers

compounds	P1	P2	P3	P4
dimer	1.40	1.35	1.33	1.22
trimer	1.23	1.22	1.20	1.13
tetramer	1.16	1.15	1.14	1.07

Table S3 The test absorption spectra of **P1** at the **6-31G (d)** and **6-311G (d)** basis set levels based on the optimization structure in dilute chloroform solvent.

Functionals	B3LYP[a]	BMK[a]	O3LYP[a]	TPSSH[a]	O3LYP[b]	TPSSH[b]	Exp
Eg	1.56	1.88	1.42	1.41	1.41	1.40	1.23
λ/nm	793	661	874	879	882	885	890~910
f	3.5010	3.8477	2.8736	2.7794	2.9266	2.8373	

a or b denotes the calculation performed at **6-31G (d)** or **6-311G (d)** basis set level, respectively.

Table S4 Characterization of the optimized solar cells adopting the experimental Polymers

Polymers	V_{OC}(V)	J_{SC}(mA/cm^2)	FF	EQE	E_{loss}(eV)	PCE(%)
P1	0.43	15.5	0.56	0.58	0.80	3.8
P2	0.69	14.9	0.54	0.52	0.59	5.6

Table S5 The different charge transfer paths and the corresponding center-of-mass distances (*r*).

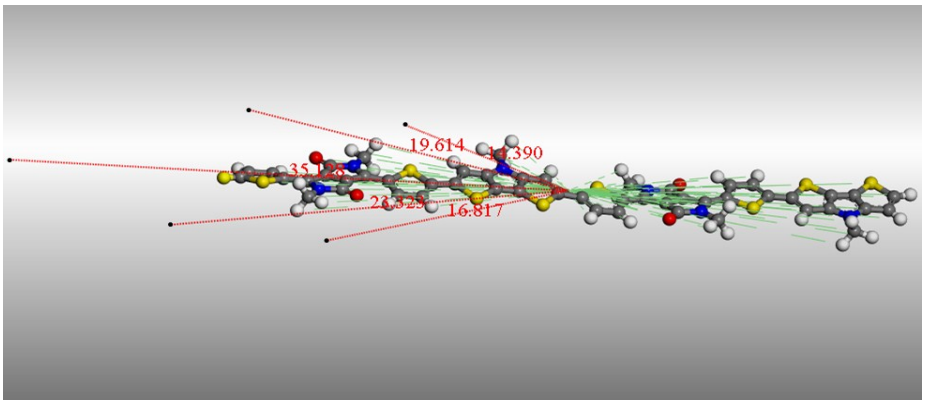
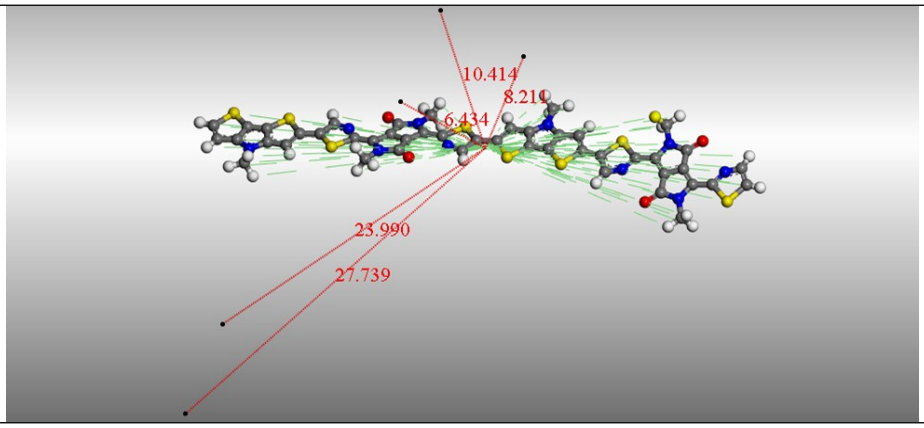
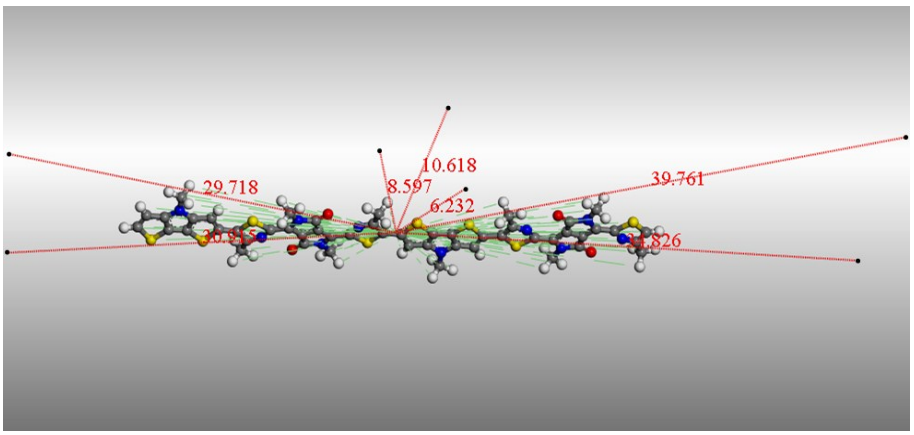
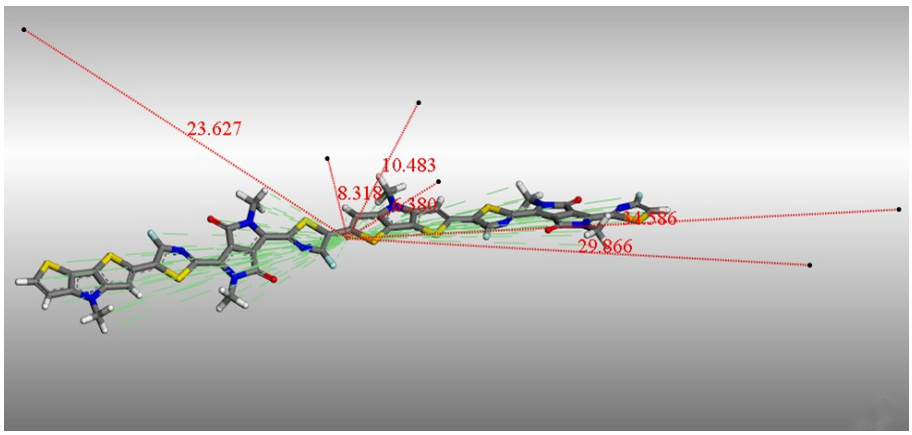
P1	
P2	
P3	
P4	

Table S6 Lattice parameters of the predicted crystal structures

Polymers	Space group	A(Å)	b(Å)	c(Å)	α (degrees)	β (degrees)	γ (degrees)
P1	P21	19.614	14.023	8.408	90.0	105.6	90.0
P2	P21	6.232	8.597	65.091	90.0	137.1	90.0
P3	P21	6.380	8.318	51.944	90.0	125.0	90.0
P4	P1	6.434	8.211	48.383	116.9	99.8	90.2