Electronic Supplementary Material (ESI) for RSC Advances.

Tunable spectra and charge transfer process of benzodifurandione-based polymer by sulfur substitution

Supporting materials

Table S1. Energy levels of HOMO, LUMO and energy gap Δ_{H-L} of the original and the designed tri-polymers (in unit: eV).

	B	Su1	Su2	Su3	Su4	Su5	Su6	Su
H	-5.44	-5.39	-5.38	-5.37	-5.29	-5.28	-5.26	-5.16
L	-3.67	-4.04	-3.97	-3.71	-4.31	-4.07	-4.04	-4.40
Δ_{H-L}	1.77	1.35	1.41	1.66	0.98	1.21	1.22	0.76

Table S2. Percentage composition of several frontier molecular orbitals of BDPPV and designed molecules.

	HOMO			**LUMO**		
Subunit	**1**	**2**	**3**	**1**	**2**	**3**
B	37	43	20	20	59	21
Su1	33	33	34	19	49	32
Su2	36	34	31	20	48	32
Su3	41	39	20	26	54	20
Su4	29	29	42	19	39	42
Su5	35	31	33	23	48	49
Su6	35	30	35	23	45	32
Su	28	28	44	24	35	42

Table S3. Calculated absorption peak and oscillator strength for original and designed molecules along with the increasing number of N.

	N=1		N=2		N=3		N=∞	
	Ab(nm)	*f*	Ab(nm)	*f*	Ab(nm)	*f*	Ab(nm)	*f*
B	511.34	1.1381	566.75	3.3932	592.86	5.4408	630.09	6.99403
Su1	691.08	0.4906	737.97	1.8770	768.85	3.1040	800.70	4.05767
Su2	642.22	0.4274	706.38	1.9509	736.81	3.3903	779.93	4.44178
Su3	552.13	0.8904	615.24	2.8308	639.49	4.7047	681.69	6.04548
Su4	849.47	0.4347	941.55	1.4708	996.01	2.3817	1058.31	3.09418
Su5	786.92	0.3521	844.85	1.3298	877.93	2.2637	917.08	2.93888
Su6	769.92	0.2114	851.07	1.0836	879.65	2.1670	933.81	2.77895
Su	1027.54	0.2760	1171.07	1.0154	1252.37	1.7196	1349.34	2.23013

*Ab and *f* is Absorption peak and oscillator strength, respectively.

Table S4. Energy levels (H and L) and energy gaps under the field.

	1×10^{-3}			2×10^{-3}			3×10^{-3}		
	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}
B	-5.456	-3.325	2.131	-5.335	-3.359	1.976	-5.195	-3.405	1.790
Su1	-5.407	-3.725	1.682	-5.365	-3.739	1.626	-5.302	-3.758	1.544
Su2	-5.373	-3.608	1.765	-5.283	-3.66	1.623	-5.178	-3.722	1.456
Su3	-5.441	-3.365	2.076	-5.383	-3.404	1.979	-5.284	-3.456	1.828
Su4	-5.287	-3.967	1.32	-5.246	-3.984	1.262	-5.195	-4.004	1.191
Su5	-5.292	-3.746	1.546	-5.264	-3.759	1.505	-5.219	-3.778	1.441
Su6	-5.284	-3.66	1.624	-5.238	-3.716	1.522	-5.172	-3.78	1.392

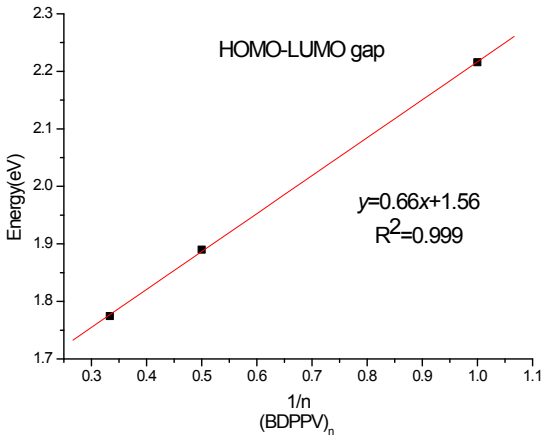
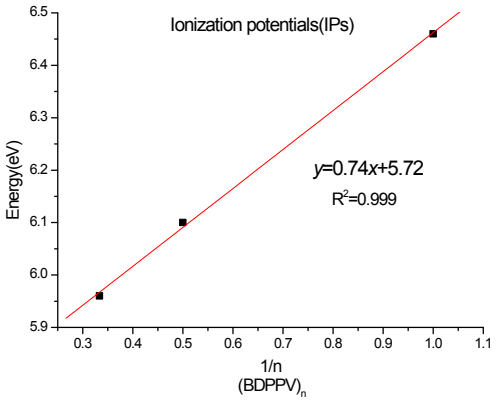
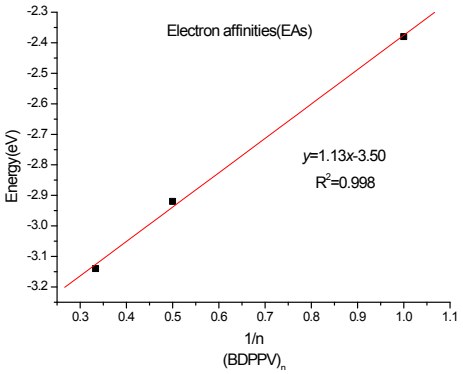


Fig. S1. HOMO-LUMO gaps ($\Delta H-L$) as a function of reciprocal chain length n in oligomers of BDPPV.



(a)



(b)

Fig S2. The IP (a) and EA (b) as a function of reciprocal chain length *n* in oligomers of BDPPV.