Supplementary Information

The crystal prediction of Polymerph Predictor mainly includes three processes:

(1) Monte Carlo simulated annealing, which includes two stages: heating and cooling.

(2) Cluster analysis: Monte Carlo simulation will obtain a large number of un-optimized structures, including results from local energy minimization and similar structures. Cluster analysis employs a method similar to energy optimization to find representatives from similar structures and remove other redundant crystal structures.

(3) Energy minimization: the "cluster representation" obtained from (2) needs to be further refined and optimized, involving all degrees of freedom.

Specific parameter setting:

(1) Two single molecules were optimised using pbe1pbe/6-311g(d), using the optimised structure as a rigid body. Calculations of electrostatic and Van der Waals interactions were carried out by the Ewald long-range summation method.

(2) The DREIDING 2.21 force field suitable for molecular crystals was selected.

(3) Select four common spatial point groups: C2/c $P\bar{1}$, $P2_1$, $P2_1/c$, and $P2_12_12_1$.

(4) The number of molecules in the asymmetric unit was chosen to be 1.

(5) The maximum temperature for simulated annealing was 10000 K and the minimum was 300 K.

By using Multiwfn software package,[1] the natural atomic orbital (NAO) can be obtained from the density matrix information of the system by analyzing the natural bond orbital (NBO). The number for NAO is the same as for the original basis function. The part of the NAO known as the minimal set corresponds to atomic orbitals in the general sense. The orbital wave functions are generally written as linear expansions of the basic functions:[2]

$$\Phi_i = \sum_a C_{a,i}\chi_a$$

.

Where a represents the ordinal number of the basis function. There is no strict standard for definition of the χ component of the orbital wave function, or the contribution η of χ to the orbital wave function. Any definition that satisfies both the following conditions meets the basic requirements:

$$\eta_a \geq 0, \sum_a \eta_a = 100\%$$

.

Here, η_a is the contribution of basis function a to the orbital wavefunction. Suppose that the orbital wave function Φ_i is an orthogonally normalized real function, written as:

$$\int \Phi_i^2(r)dr = 1$$

.

Where r represents three-dimensional space coordinates, then:

$$\sum_a C_{a,i}^2 + 2 \times \sum_a \sum_{b>a} C_{a,i} C_{b,i} S_{a,b} = 1$$

.

Thereinto:

$$S_{ab} = \int \chi_a(r)\chi_b(r)dr$$

.

The first term is treated as the sum of the independent contributions of the individual basis functions to the orbit which is called the localized term. The second term is the cross term, which embodies the joint contribution to the orbitals due to the coupling between the basis functions which satisfy the condition $S_{a,b} = \delta_{a,b}$.

References

1. Tian Lu, Feiwu Chen, Multiwfn: A multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**(5), 580-592.
2. Tian Lu, Feiwu Chen, Calculation of molecular orbital composition, *Acta Chim. Sin.*, 2011, **69**(20), 2393-2406.

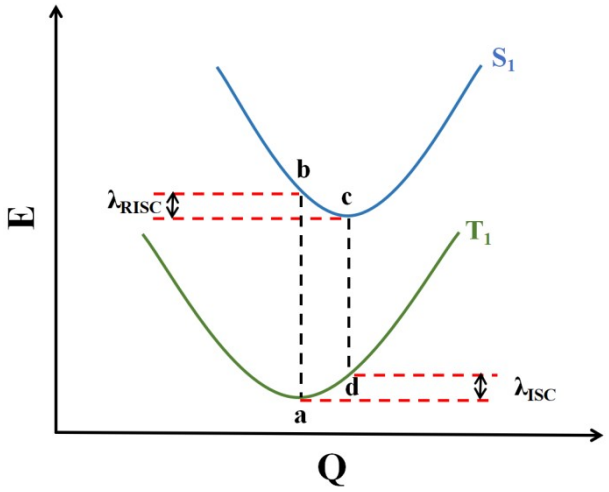

Figure S1. Schematic representation of the adiabatic potential energy surfaces for S_1 and T_1.

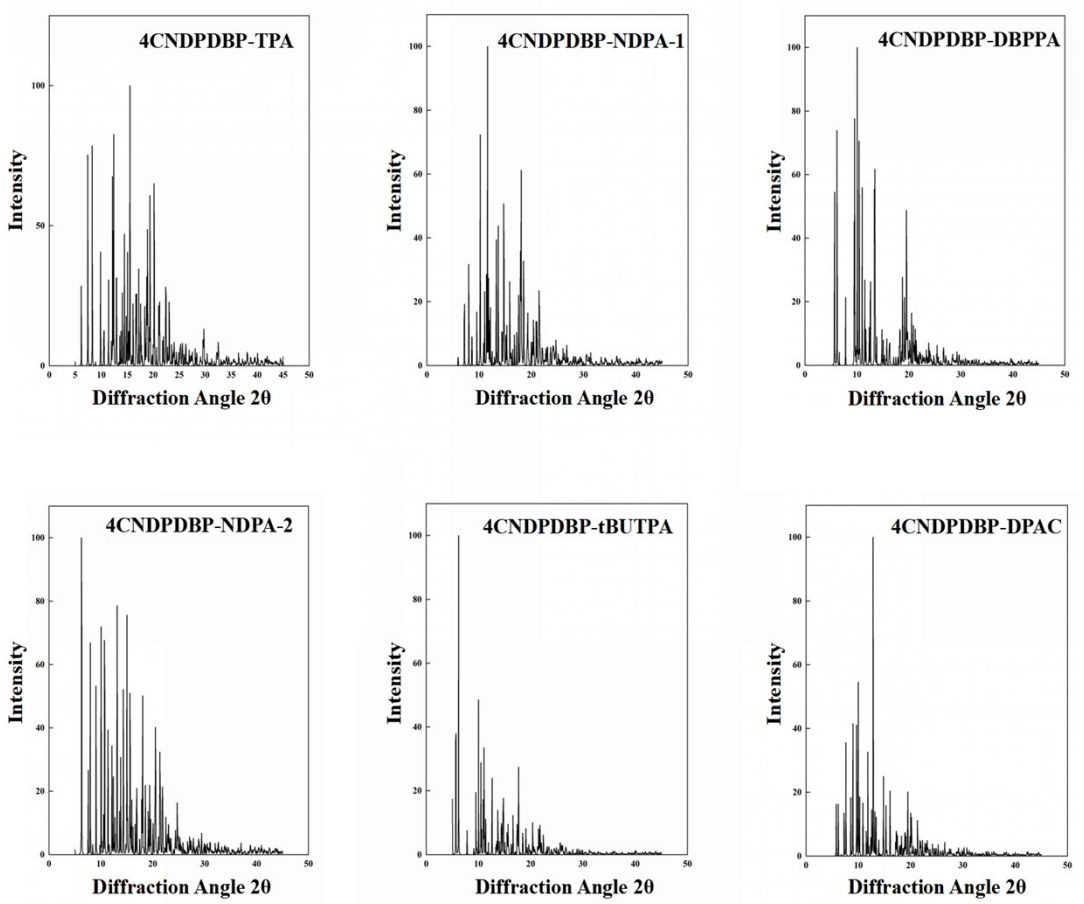

Figure S2. The simulated XRPD of chosen structures of 4CNDPDBP-TPA and the designed molecules.

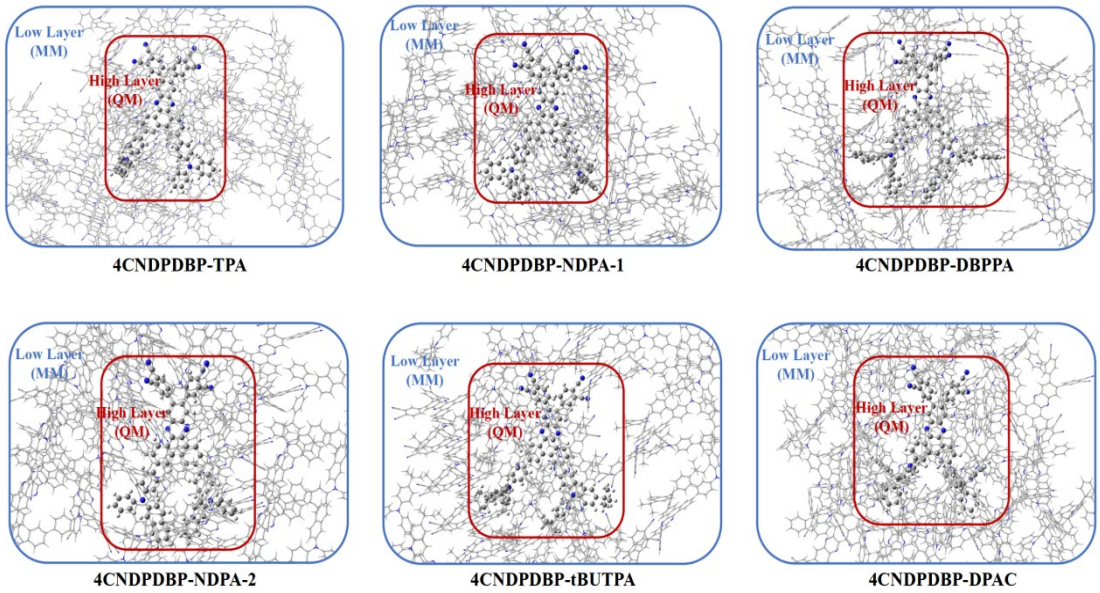

Figure S3. QM/MM models for 4CNDPDBP-TPA and the designed molecules in solid phase. Surrounding molecules are regarded as the low layer and the centered molecule is treated as the high layer

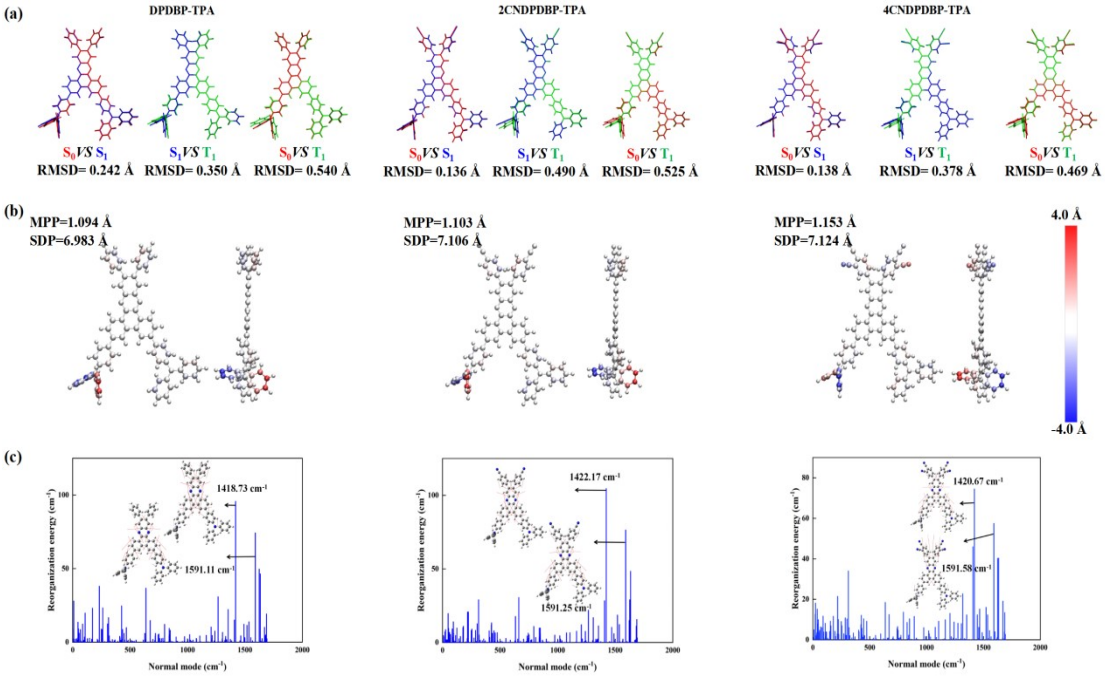

Figure S4. (a) Geometry comparisons and RMSD values of DPDBP-TPA, 2CNDPDBP-TPA and 4CNDPDBP-TPA among S_0 (red), S_1 (blue) and T_1 (green) states. (b) Molecular planarity parameters for DPDBP-TPA, 2CNDPDBP-TPA and 4CNDPDBP-TPA. (c) Calculated reorganization energies *versus* the normal-mode frequencies for DPDBP-TPA, 2CNDPDBP-TPA and 4CNDPDBP-TPA. Representative vibration modes are shown as insets.

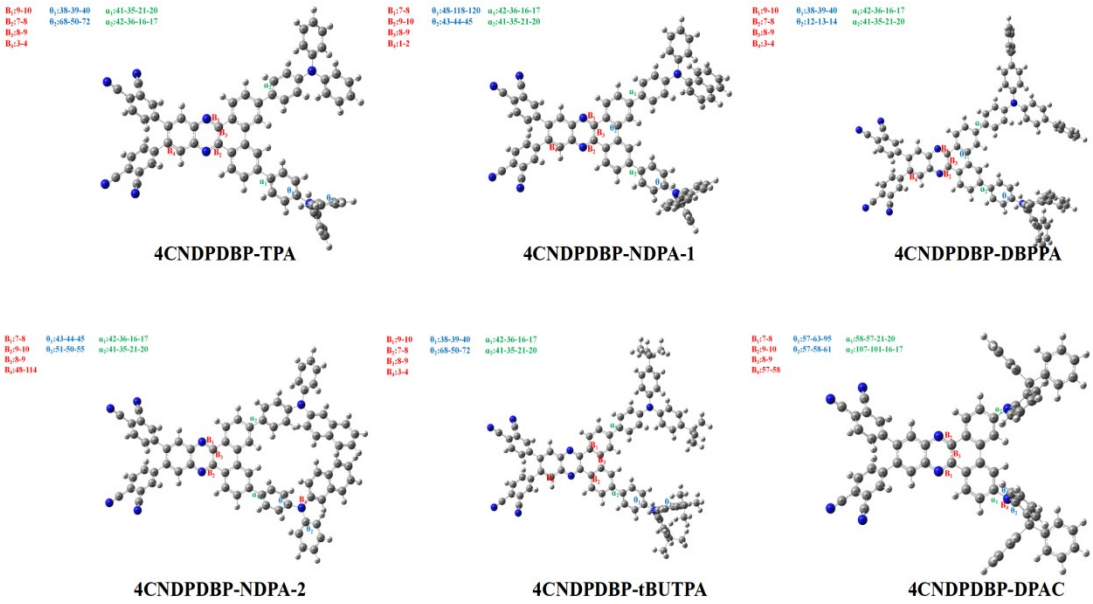

Figure S5. The atomic labels and the interesting bond lengths (B_1, B_2, B_3 and B_4), bond angles (θ_1 and θ_2) and the dihedral angles (α_1 and α_2) of 4CNDPDBP-TPA and the designed molecules.

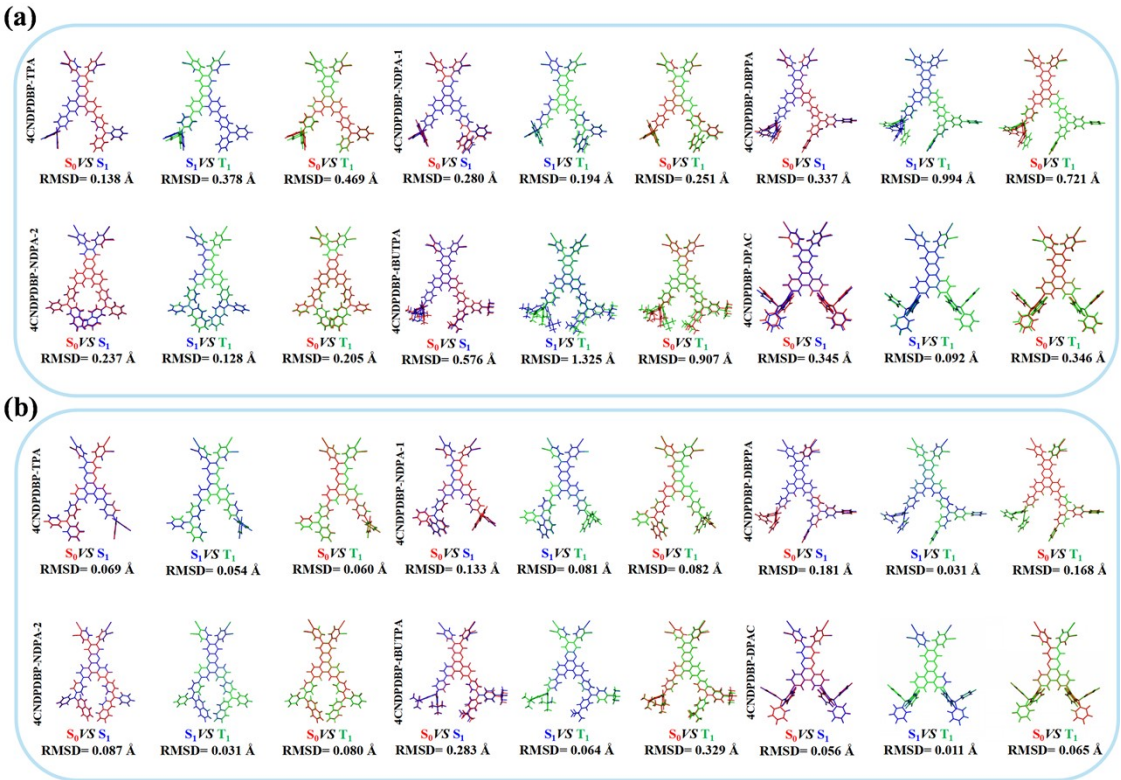

Figure S6. Geometry comparisons and RMSD values of 4CNDPDBP-TPA and the designed molecules (a) in toluene and (b) solid phase among S_0 (red), S_1 (blue) and T_1 (green) states.

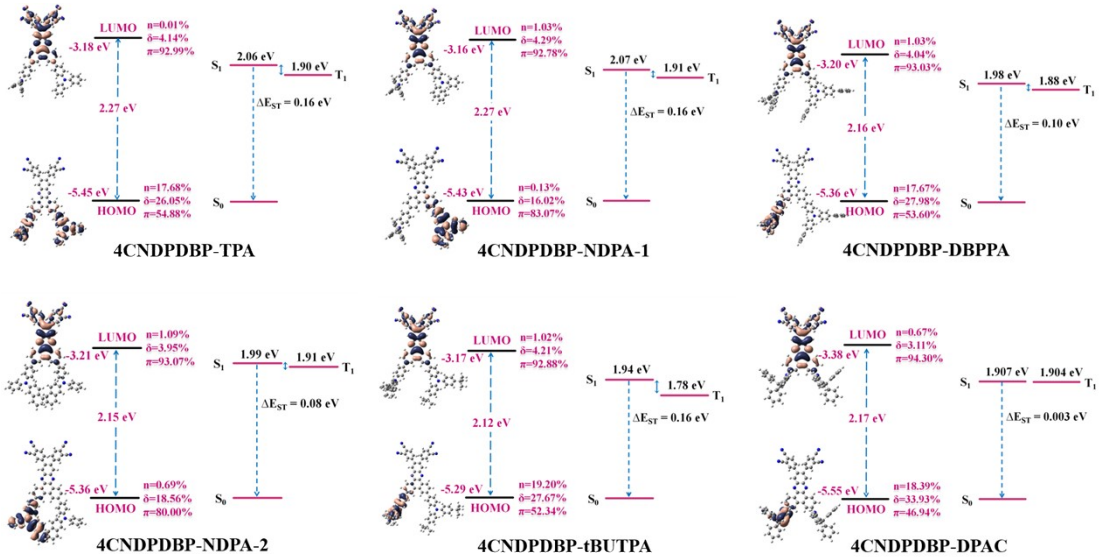

Figure S7. Adiabatic excitation energies and involved molecular orbital energies and distributions for 4CNDPDBP-TPA and the designed molecules in toluene.

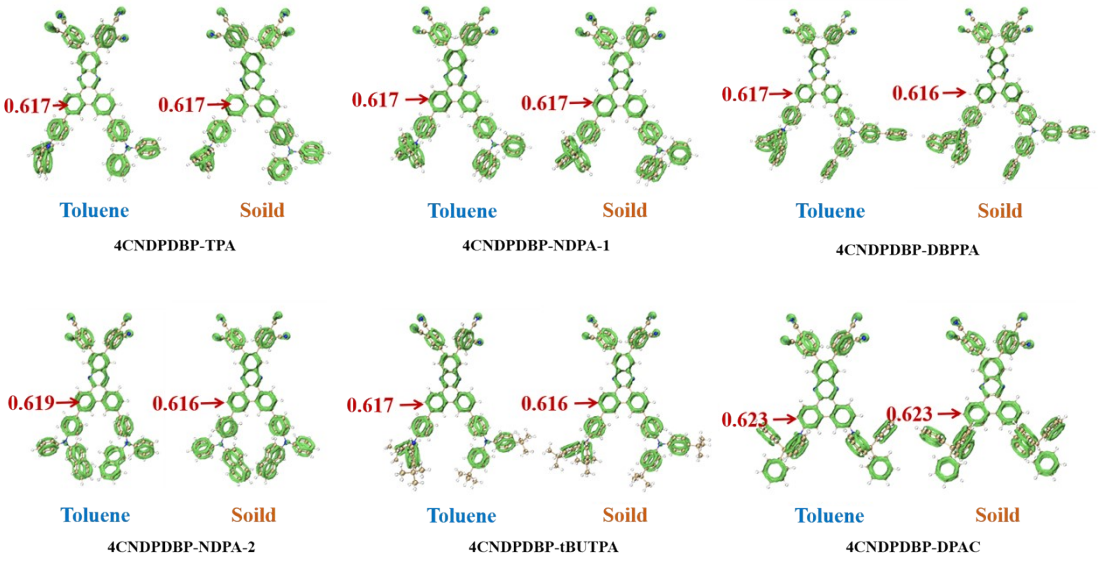

Figure S8. The localized orbital locator-π (LOL-π) isosurfaces for 4CNDPDBP-TPA and the designed molecules in toluene and solid phase.

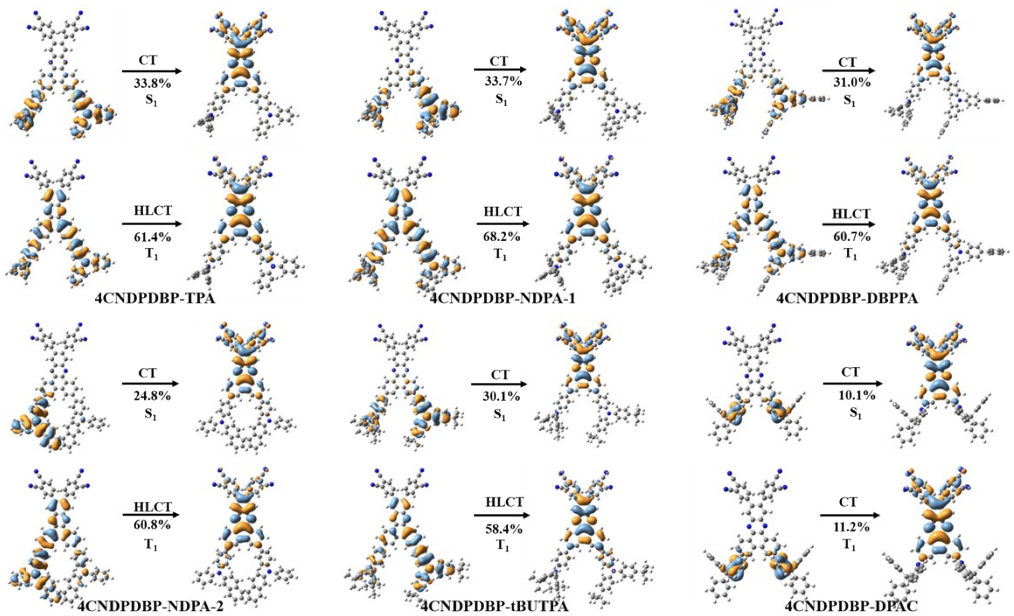

Figure S9. NTOs of the S_1 and T_1 states for 4CNDPDBP-TPA and the designed molecules in toluene. The values below the arrows are the LE proportions.

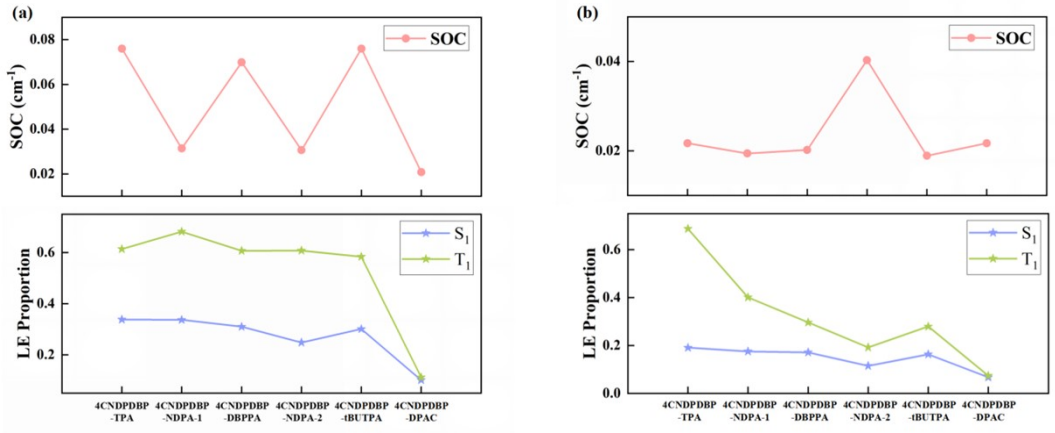

Figure S10. Qualitative correlation between LE% and SOCME for studied molecules.

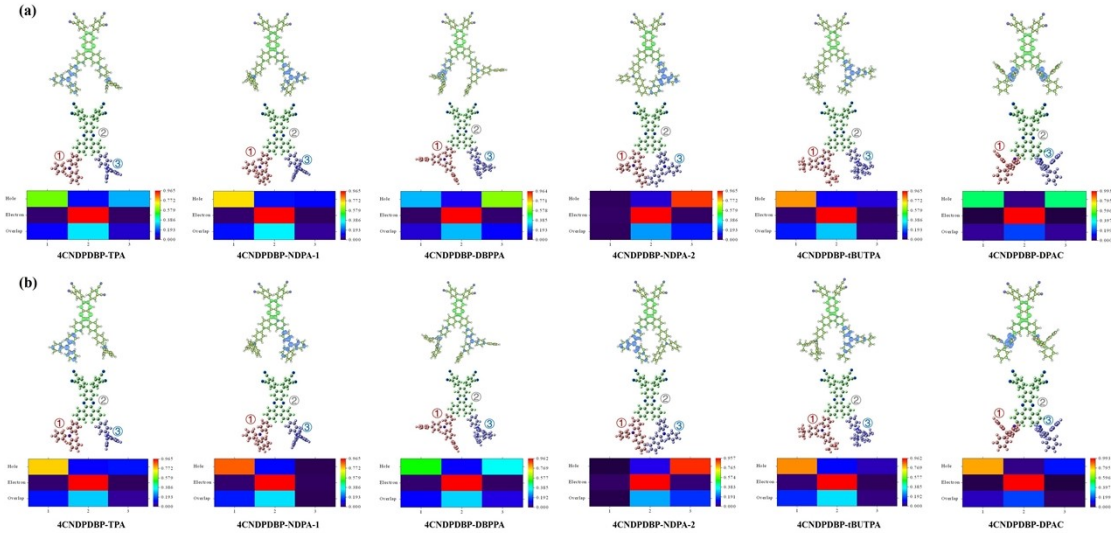

Figure S11. Distributions of holes and electrons as well as heat maps of the S_1 state for 4CNDPDBP-TPA and the designed molecules in toluene (a) and solid phase (b).

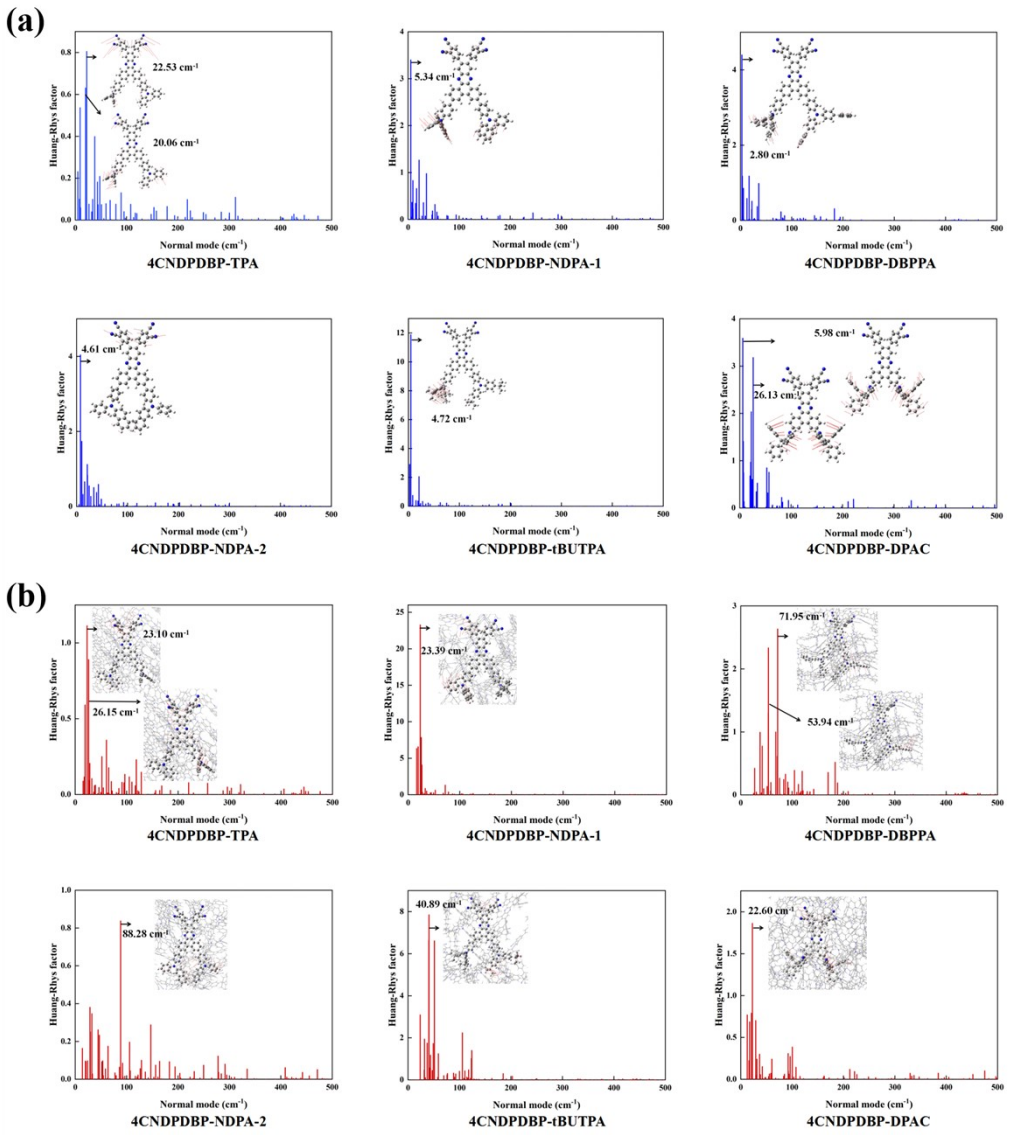

Figure S12. Calculated HR factors *versus* the normal-mode frequencies for 4CNDPDBP-TPA and the designed molecules (a) in toluene and (b) solid phase. Representative vibration modes are shown as insets.

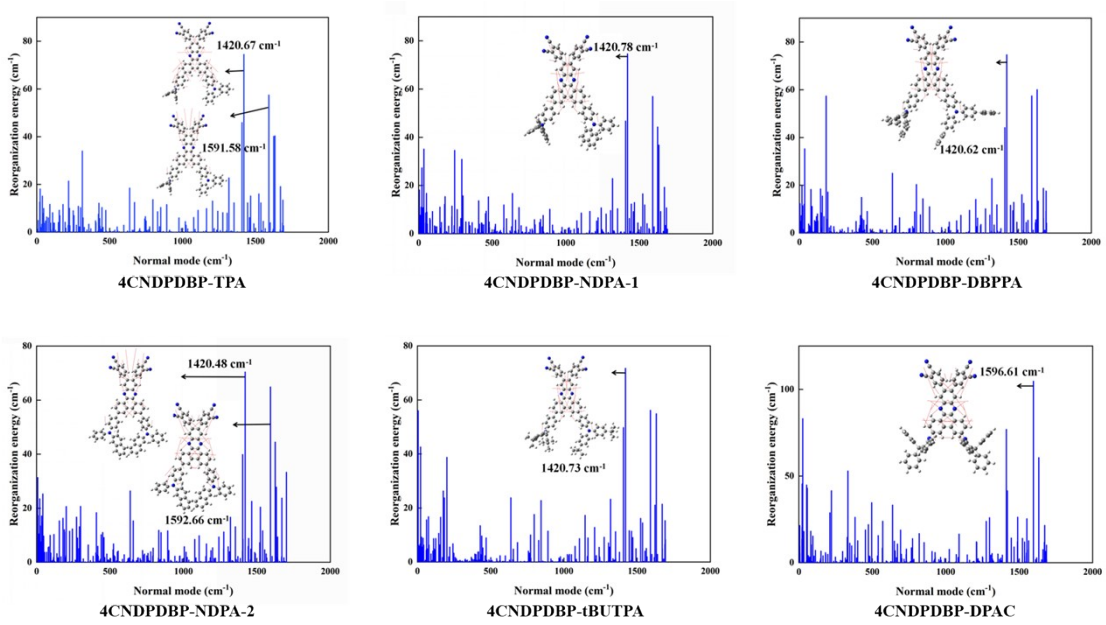

Figure S13. Calculated reorganization energies *versus* the normal-mode frequencies for 4CNDPDBP-TPA and the designed molecules in toluene. Representative vibration modes are shown as insets。

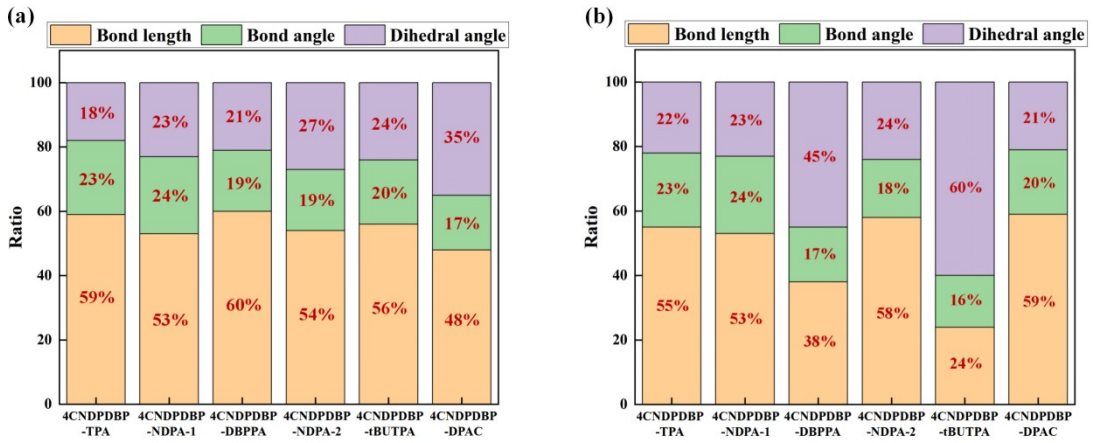

Figure S14. Contributions of the reorganization energies from bond lengths (orange), bond angles (green) and dihedral angles (purple) for 4CNDPDBP-TPA and the designed molecules.

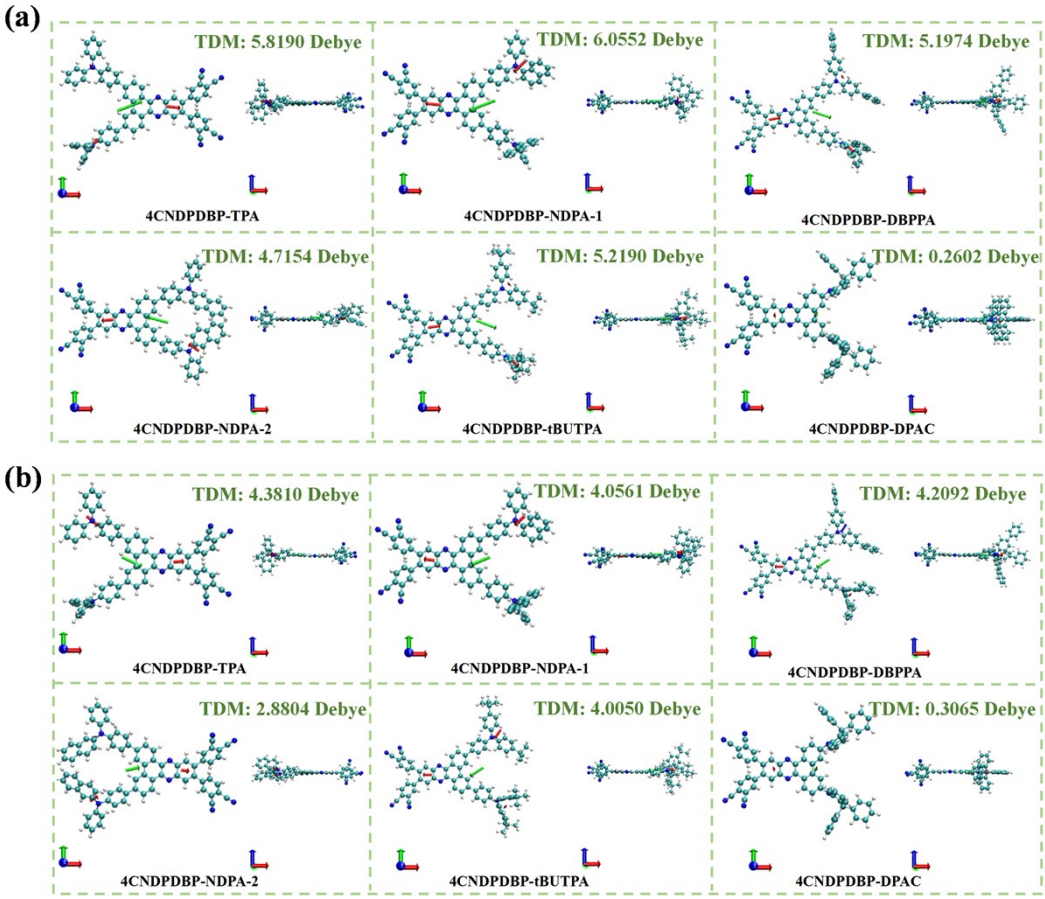

Figure S15. Fragment transition dipole moment vector (red) and the whole transition dipole moment vector (green) of 4CNDPDBP-TPA and the designed molecules (a) in toluene and (b) solid phase.

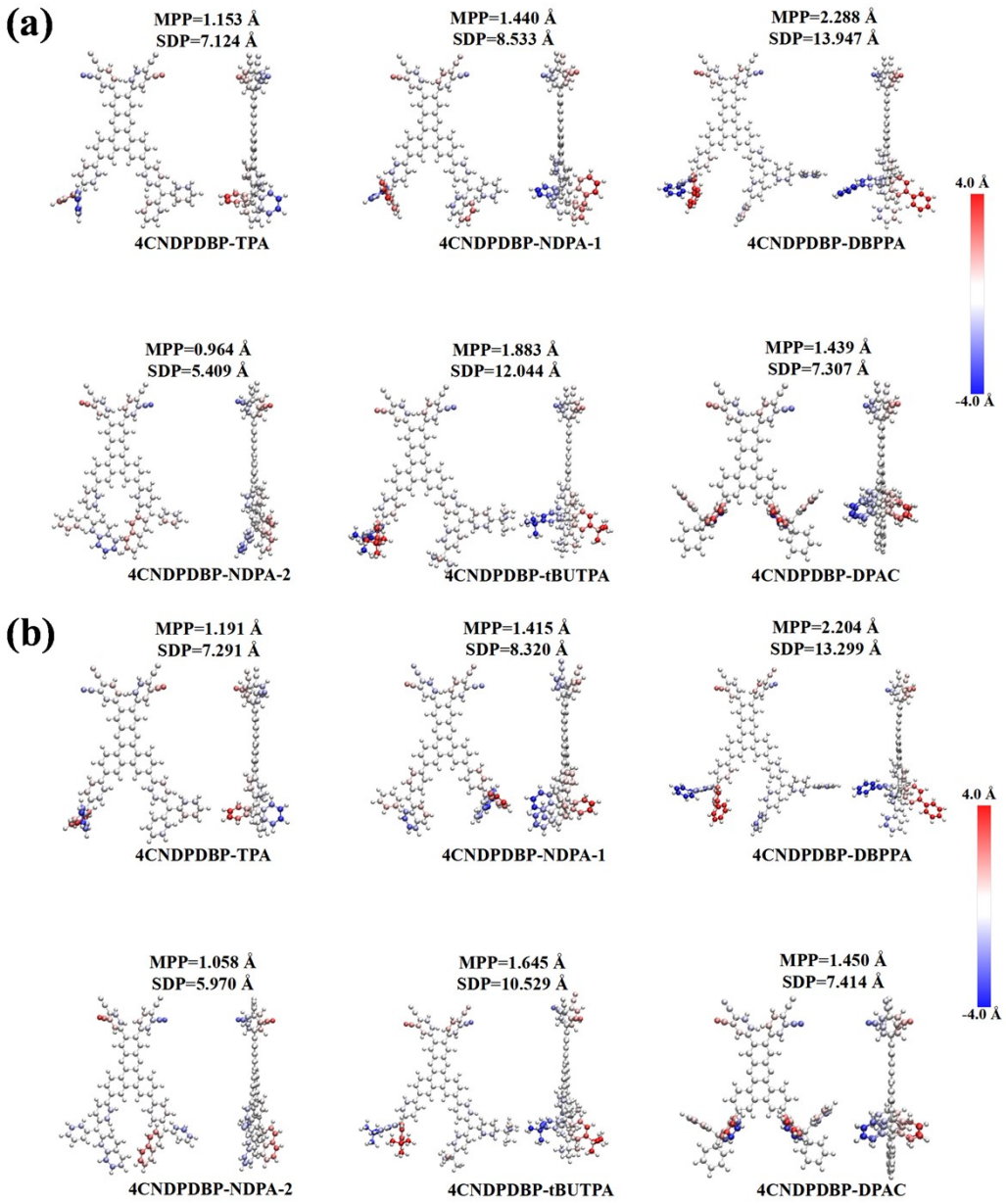

Figure S16. Molecular planarity parameters for 4CNDPDBP-TPA and the designed molecules (a) in toluene and (b) solid phase.

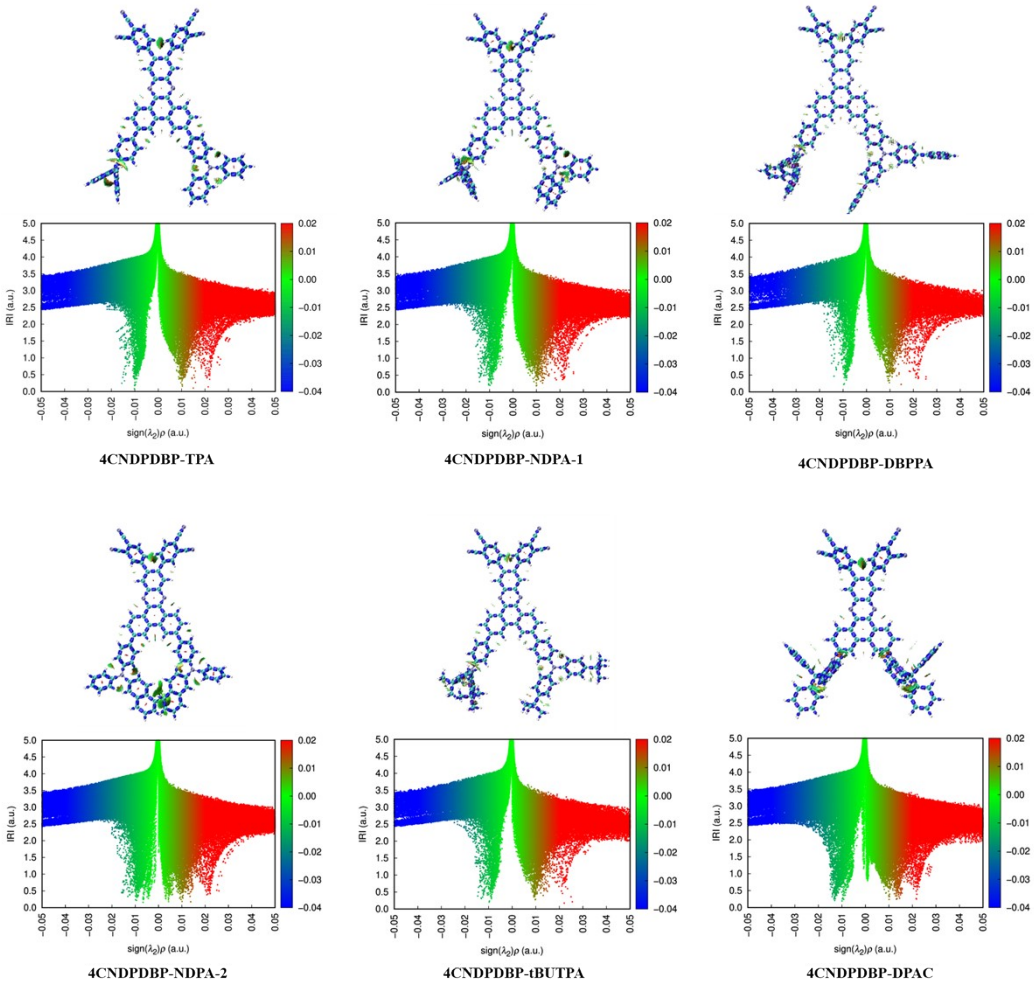

Figure S17. IRI graphical analyses of weak interactions of 4CNDPDBP-TPA and the designed molecules in toluene.

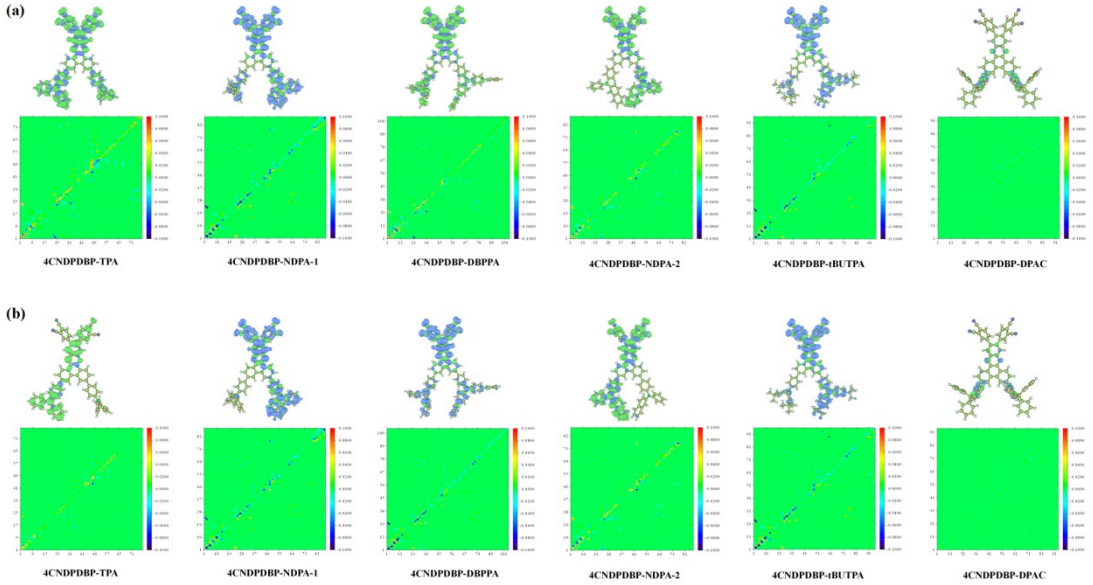

Figure S18. The X component of the transition dipole moment matrix and the sosurface of the X component of the transition dipole moment density (Tx(r)) for 4CNDPDBP-TPA and the designed molecules (a) in toluene and (b) solid phase.

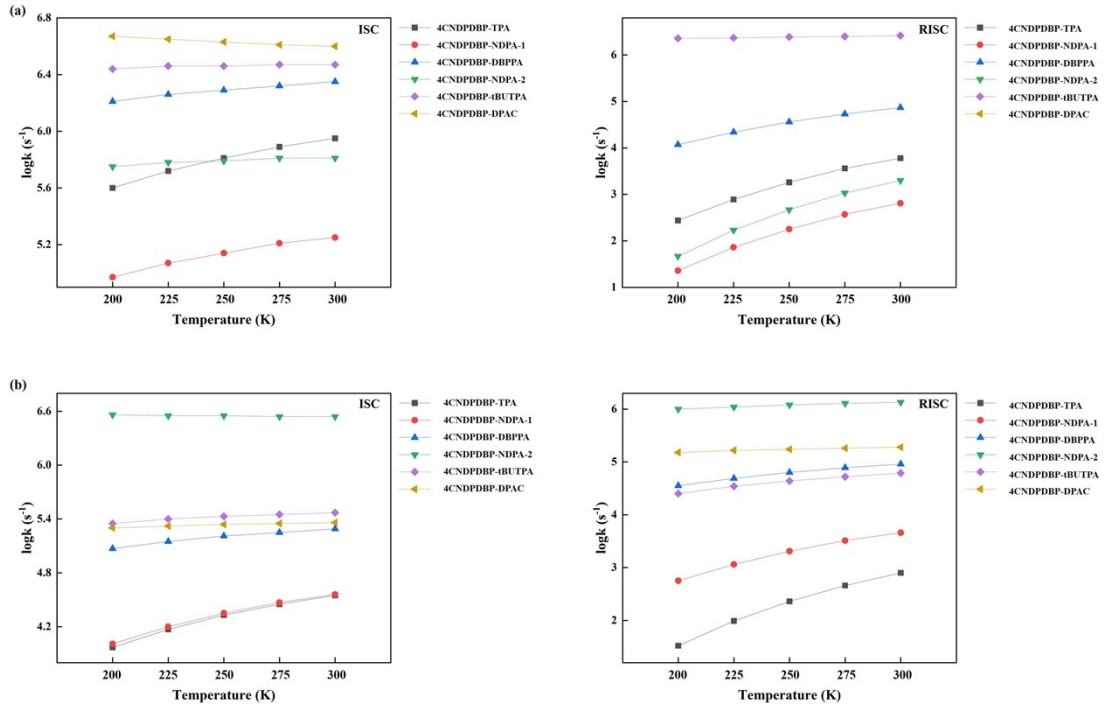

Figure S19. Variations of the ISC and RISC rates with temperature for 4CNDPDBP-TPA and the designed molecules in toluene (a) and solid phase (b).

Table S1. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-TPA in toluene as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\lvert S_0\text{-}S_1\rvert$	$\Delta\lvert S_1\text{-}T_1\rvert$
Bond length	B_1	9-10	1.319	1.347	1.332	0.028	0.015
	B_2	7-8	1.319	1.343	1.356	0.024	0.013
	B_3	8-9	1.439	1.409	1.419	0.030	0.010
	B_4	3-4	1.375	1.391	1.386	0.016	0.005
Bond angle	θ_1	38-39-40	118.4	119.6	118.4	1.2	1.2
	θ_2	68-50-72	119.2	120.3	120.2	1.1	0.1
Dihedral angle	α_1	41-35-21-20	37.09	35.86	21.96	1.23	13.9
	α_2	42-36-16-17	-36.42	-37.38	-37.26	0.96	0.12

Table S2. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-TPA in solid phase as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\lvert S_0\text{-}S_1\rvert$	$\Delta\lvert S_1\text{-}T_1\rvert$
Bond length	B_1	9-10	1.321	1.343	1.350	0.022	0.007
	B_2	7-8	1.318	1.345	1.337	0.027	0.008
	B_3	8-9	1.441	1.405	1.410	0.036	0.005
	B_4	3-4	1.377	1.390	1.395	0.013	0.005

Bond angle	θ_1	38-39-40	118.8	118.8	118.8	0	0
	θ_2	68-50-72	118.9	118.7	118.8	0.2	0.1
Dihedral angle	α_1	41-35-21-20	37.64	37.35	37.82	0.29	0.47
	α_2	42-36-16-17	-39.26	-44.16	-36.66	4.90	7.50

Table S3. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-NDPA-1 in toluene as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	7-8	1.319	1.347	1.332	0.028	0.015
	B_2	9-10	1.319	1.343	1.356	0.024	0.013
	B_3	8-9	1.439	1.409	1.419	0.030	0.010
	B_4	1-2	1.375	1.391	1.386	0.016	0.005
Bond angle	θ_1	48-118-120	119.7	117.8	118.5	1.9	0.7
	θ_2	43-44-45	118.4	119.6	118.5	1.2	1.1
Dihedral angle	α_1	42-36-16-17	-36.88	-35.52	-22.94	1.36	12.58
	α_2	41-35-21-20	36.68	38.09	37.69	1.41	0.40

Table S4. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-NDPA-1 in solid phase as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	7-8	1.317	1.347	1.340	0.030	0.007
	B_2	9-10	1.321	1.338	1.350	0.017	0.012
	B_3	8-9	1.442	1.407	1.410	0.035	0.003
	B_4	1-2	1.377	1.394	1.390	0.017	0.004
Bond angle	θ_1	48-118-120	120.0	118.2	118.4	1.8	0.2
	θ_2	43-44-45	118.6	120.2	119.3	1.6	0.9
Dihedral angle	α_1	42-36-16-17	-39.93	-44.75	-37.02	4.82	7.73
	α_2	41-35-21-20	35.79	36.25	36.66	0.46	0.41

Table S5. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-DBPPA in toluene as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	9-10	1.319	1.346	1.334	0.027	0.012
	B_2	7-8	1.319	1.344	1.354	0.025	0.010
	B_3	8-9	1.439	1.410	1.418	0.029	0.008
	B_4	3-4	1.375	1.391	1.387	0.016	0.004

Bond angle	θ_1	38-39-40	118.5	120.0	118.7	1.5	1.3
	θ_2	12-13-14	120.0	119.2	119.3	0.8	0.1
Dihedral angle	α_1	42-36-16-17	-36.70	-37.94	-38.15	1.24	0.21
	α_2	41-35-21-20	37.36	37.40	23.93	0.04	13.47

Table S6. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-DBPPA in solid phase as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	9-10	1.320	1.340	1.346	0.020	0.006
	B_2	7-8	1.320	1.350	1.345	0.030	0.005
	B_3	8-9	1.443	1.406	1.408	0.037	0.002
	B_4	3-4	1.376	1.387	1.391	0.011	0.004
Bond angle	θ_1	38-39-40	117.9	118.0	118.0	0.1	0
	θ_2	12-13-14	120.3	120.0	119.9	0.3	0.1
Dihedral angle	α_1	42-36-16-17	-33.00	-39.19	-34.38	6.19	4.81
	α_2	41-35-21-20	37.76	39.36	39.45	1.6	0.09

Table S7. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-NDPA-2 in toluene as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	7-8	1.319	1.346	1.335	0.027	0.011
	B_2	9-10	1.319	1.343	1.352	0.024	0.009
	B_3	8-9	1.444	1.414	1.421	0.030	0.007
	B_4	48-114	1.415	1.392	1.410	0.023	0.018
Bond angle	θ_1	43-44-45	118.6	120.1	119.0	1.5	1.1
	θ_2	51-50-55	119.1	120.3	120.2	1.2	0.1
Dihedral angle	α_1	42-36-16-17	-47.63	-48.59	-35.81	0.96	12.78
	α_2	41-35-21-20	35.50	37.73	36.89	2.23	0.84

Table S8. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-NDPA-2 in solid phase as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	7-8	1.319	1.339	1.342	0.020	0.003
	B_2	9-10	1.319	1.347	1.346	0.028	0.001
	B_3	8-9	1.448	1.410	1.342	0.038	0.068
	B_4	48-114	1.415	1.407	1.407	0.008	0

Bond angle	θ_1	43-44-45	118.5	118.7	118.7	0.2	0
	θ_2	51-50-55	119.0	118.9	118.9	0.1	0
Dihedral angle	α_1	42-36-16-17	-35.70	-39.26	-39.35	3.56	0.09
	α_2	41-35-21-20	30.00	33.80	30.68	3.80	3.12

Table S9. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-tBUTPA in toluene as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\lvert S_0\text{-}S_1\rvert$	$\Delta\lvert S_1\text{-}T_1\rvert$
Bond length	B_1	9-10	1.319	1.347	1.333	0.028	0.014
	B_2	7-8	1.319	1.343	1.354	0.024	0.011
	B_3	8-9	1.440	1.409	1.420	0.031	0.011
	B_4	3-4	1.375	1.391	1.420	0.016	0.029
Bond angle	θ_1	38-39-40	118.2	120.6	118.3	2.4	2.3
	θ_2	68-50-72	118.5	119.3	119.5	0.8	0.2
Dihedral angle	α_1	42-36-16-17	-36.58	-37.83	-42.35	1.25	4.52
	α_2	41-35-21-20	35.87	38.53	17.25	2.66	21.28

Table S10. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-tBUTPA in solid phase as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\lvert S_0\text{-}S_1\rvert$	$\Delta\lvert S_1\text{-}T_1\rvert$
Bond length	B_1	9-10	1.321	1.341	1.347	0.020	0.006
	B_2	7-8	1.374	1.347	1.341	0.027	0.006
	B_3	8-9	1.443	1.406	1.408	0.037	0.002
	B_4	3-4	1.374	1.383	1.388	0.009	0.005
Bond angle	θ_1	38-39-40	117.6	117.5	117.5	0.1	0
	θ_2	68-50-72	118.7	118.5	118.5	0.2	0
Dihedral angle	α_1	42-36-16-17	-33.99	-41.09	-37.11	7.10	3.98
	α_2	41-35-21-20	35.01	35.73	35.52	0.72	0.21

Table S11. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-DPAC in toluene as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\lvert S_0\text{-}S_1\rvert$	$\Delta\lvert S_1\text{-}T_1\rvert$
Bond length	B_1	7-8	1.319	1.346	1.347	0.027	0.001
	B_2	9-10	1.319	1.341	1.340	0.022	0.001
	B_3	8-9	1.436	1.411	1.411	0.025	0
	B_4	57-58	1.400	1.377	1.377	0.023	0

Bond angle	θ_1	57-63-95	121.7	119.7	119.7	2.0	0
	θ_2	57-58-61	121.6	119.8	119.9	1.8	-0.1
Dihedral angle	α_1	58-57-21-20	96.30	93.95	97.49	2.35	-3.54
	α_2	107-101-16-17	-97.93	-97.96	-97.90	0.03	-0.06

Table S12. Geometry parameters of S_0, S_1 and T_1 states for 4CNDPDBP-DPAC in solid phase as well as their differences (Δ). (Bond length: Å. Bond angle: °. Dihedral angle: °)

	Geometry	Atomic number	S_0	S_1	T_1	$\Delta\|S_0-S_1\|$	$\Delta\|S_1-T_1\|$
Bond length	B_1	7-8	1.319	1.345	1.345	0.026	0
	B_2	9-10	1.320	1.346	1.346	0.026	0
	B_3	8-9	1.440	1.406	1.406	0.034	0
	B_4	57-58	1.400	1.398	1.398	0.002	0
Bond angle	θ_1	57-63-95	121.3	121.3	121.3	0	0
	θ_2	57-58-61	121.4	121.4	121.4	0	0
Dihedral angle	α_1	58-57-21-20	92.83	95.15	95.11	2.32	0.04
	α_2	107-101-16-17	-100.8	-94.40	-94.86	6.40	0.46

Table S13. Reorganization energies (meV) for 4CNDPDBP-TPA and the designed molecules in toluene and solid phase contributed from low frequency regions (<500 cm^{-1}), middle frequency regions (500-1500 cm^{-1}) and high frequency regions (>1500 cm^{-1}).

		Reorganization energies (meV)			
		Low frequency	Middle frequency	High frequency	Total
Toluene	4CNDPDBP-TPA	46.0	53.1	28.1	127.2
	4CNDPDBP-NDPA-1	60.2	56.5	29.6	146.3
	4CNDPDBP-DBPPA	53.5	55.3	30.8	139.6
	4CNDPDBP-NDPA-2	64.1	61.5	34.3	159.9
	4CNDPDBP-tBUTPA	60.0	58.4	31.0	149.4
	4CNDPDBP-DPAC	98.1	77.7	42.5	218.3
Solid	4CNDPDBP-TPA	58.1	56.9	26.8	141.8
	4CNDPDBP-NDPA-1	62.9	102.3	30.3	195.5
	4CNDPDBP-DBPPA	154.5	71.0	38.8	264.3
	4CNDPDBP-NDPA-2	72.8	74.1	43.9	190.8
	4CNDPDBP-tBUTPA	332.9	77.0	43.8	453.7
	4CNDPDBP-DPAC	80.5	88.0	47.5	216.0

Table S14. Transition dipole moment vector contributions from fragment 1, fragment 2 and fragment 3 of 4CNDPDBP-TPA and the designed molecules in toluene.

Transition dipole moment					
	Fragment	X	Y	Z	Total (Debye)
4CNDPDBP-TPA	1	-0.0096	-0.0062	0.0007	0.0291
	2	1.0933	-0.1100	-0.0079	2.7929
	3	1.0493	0.9479	-0.0023	3.5941
	All	2.1330	0.8316	-0.0095	5.8190
4CNDPDBP-NDPA-1	1	-1.0102	-0.9763	0.0240	3.5713
	2	-1.2275	0.1198	0.0069	3.1348
	3	0.0148	0.0002	-0.0003	0.0376
	All	-2.2229	-0.8563	0.0306	6.0552
4CNDPDBP-DBPPA	1	-0.0245	-0.0148	0.0017	0.0729
	2	1.1650	0.1980	-0.0136	3.0037
	3	0.8005	-0.8263	0.0390	2.9258
	All	1.9409	-0.6431	0.0271	5.1974
4CNDPDBP-NDPA-2	1	-0.0118	-0.0334	0.0013	0.0901
	2	-0.9497	-0.0717	-0.0029	2.4207
	3	-0.8311	0.5784	0.0702	2.5798
	All	-1.7925	0.4733	0.0685	4.7154
4CNDPDBP-tBUTPA	1	-0.0271	-0.02334	0.0004	0.0909
	2	1.1465	0.1544	-0.0125	2.9405
	3	0.7975	-0.8671	0.0078	2.9944
	All	1.9169	-0.7360	-0.0043	5.2190
4CNDPDBP-DPAC	1	-0.0001	-0.0002	-0.0002	0.0008
	2	-0.0532	-0.0067	0.0005	0.1363
	3	-0.0396	0.0465	-0.0170	0.1611
	All	-0.0929	0.0396	-0.0167	0.2602

Table S15. Transition dipole moment vector contributions from fragment 1, fragment 2 and fragment 3 of 4CNDPDBP-TPA and the designed molecules in solid phase.

Transition dipole moment					
	Fragment	X	Y	Z	Total (Debye)
4CNDPDBP-TPA	1	0.8633	-0.7510	0.0088	2.9084
	2	0.7682	0.0579	-0.0107	1.9583
	3	-0.0815	-0.0611	-0.0012	0.2589
	All	1.5499	-0.7542	-0.0032	4.3810
4CNDPDBP-NDPA-1	1	-0.7351	-0.6917	0.0247	2.5663
	2	-0.7912	0.1141	0.0110	2.0320
	3	0.0545	-0.0385	-0.0056	0.1702

	All	-1.4718	-0.6161	0.0301	4.0561
4CNDPDBP-DBPPA	1	-0.5642	-0.8220	0.0420	2.5363
	2	-0.9076	0.0082	0.0169	2.3073
	3	0.0693	-0.0640	0.0115	0.2415
	All	-1.4025	-0.8778	0.0704	4.2092
4CNDPDBP-NDPA-2	1	0.5451	0.3852	-0.0267	1.6979
	2	0.5474	-0.0670	-0.0009	1.4017
	3	0.0030	-0.0294	0.0050	0.0762
	All	1.0956	0.2888	-0.0226	2.8804
4CNDPDBP-tBUTPA	1	-0.5632	-0.8042	0.0453	2.4981
	2	-0.8325	0.0179	-0.0055	2.1165
	3	0.0652	-0.0567	0.0049	0.2200
	All	-1.3305	-0.8430	0.0447	4.0050
4CNDPDBP-DPAC	1	0.0520	-0.0555	-0.0166	0.1979
	2	0.0604	0.0141	-0.0007	0.1577
	3	-0.0007	-0.0006	0.0000	0.0023
	All	0.1117	-0.0420	-0.0174	0.3065

Table S16. Intermolecular interaction energy analyses for selected dimers extracted from the solid phase of 4CNDPDBP-TPA. (Unit: kJ mol^{-1}).

		Electrostatic	Repulsion	Dispersion	Total
4CNDPDBP-TPA	Dimer-1	-16.65	60.79	-137.78	-93.64 kJ/mol
	Dimer-2	-7.28	32.47	-54.31	-29.12 kJ/mol
	Dimer-3	-17.49	27.41	-36.23	-26.31 kJ/mol
	Dimer-4	-31.67	141.13	-223.76	-114.3 kJ/mol
	Dimer-5	-0.42	8.70	-21.46	-13.18 kJ/mol

Table S17. Intermolecular interaction energy analyses for selected dimers extracted from the solid phase of 4CNDPDBP-NDPA-1. (Unit: kJ mol^{-1}).

		Electrostatic	Repulsion	Dispersion	Total
4CNDPDBP-NDPA-1	Dimer-1	-10.38	65.35	-140.75	-85.78 kJ/mol
	Dimer-2	-0.79	25.61	-41.80	-16.98 kJ/mol
	Dimer-3	-3.51	12.47	-17.24	-8.28 kJ/mol
	Dimer-4	-31.42	122.72	-195.69	-104.39 kJ/mol
	Dimer-5	-4.90	14.73	-18.49	-8.66 kJ/mol

Table S18. Intermolecular interaction energy analyses for selected dimers extracted from the solid phase of 4CNDPDBP-DBPPA. (Unit: kJ mol^{-1}).

		Electrostatic	Repulsion	Dispersion	Total
4CNDPDBP-DBPPA	Dimer-1	-10.37	35.96	-56.79	-31.20 kJ/mol
	Dimer-2	-7.61	28.37	-37.57	-16.81 kJ/mol
	Dimer-3	-38.66	133.13	-222.21	-127.74 kJ/mol
	Dimer-4	-3.18	10.21	-14.81	-7.78 kJ/mol
	Dimer-5	-6.28	19.62	-34.23	-20.89 kJ/mol

Table S19. Intermolecular interaction energy analyses for selected dimers extracted from the solid phase of 4CNDPDBP-NDPA-2. (Unit: kJ mol^{-1}).

		Electrostatic	Repulsion	Dispersion	Total
4CNDPDBP-NDPA-2	Dimer-1	-31.42	122.72	-195.69	-104.39 kJ/mol
	Dimer-2	-3.51	12.47	-17.24	-8.28 kJ/mol
	Dimer-3	-4.85	14.73	-18.49	-8.61 kJ/mol
	Dimer-4	-10.38	65.35	-140.75	-85.78 kJ/mol
	Dimer-5	-0.79	25.61	-41.80	-16.98 kJ/mol

Table S20. Intermolecular interaction energy analyses for selected dimers extracted from the solid phase of 4CNDPDBP-tBUTPA. (Unit: kJ mol^{-1}).

		Electrostatic	Repulsion	Dispersion	Total
4CNDPDBP-tBUTPA	Dimer-1	-46.32	150.12	-227.86	-124.06 kJ/mol
	Dimer-2	-4.06	0.17	-2.01	-5.90 kJ/mol
	Dimer-3	-57.45	170.71	-255.22	-141.96 kJ/mol
	Dimer-4	-16.90	57.95	-76.57	-35.52 kJ/mol
	Dimer-5	-11.88	43.64	-62.01	-30.25 kJ/mol

Table S21. Intermolecular interaction energy analyses for selected dimers extracted from the solid phase of 4CNDPDBP-DPAC. (Unit: kJ mol^{-1}).

		Electrostatic	Repulsion	Dispersion	Total
4CNDPDBP-DPAC	Dimer-1	-15.10	63.60	-111.04	-62.54 kJ/mol
	Dimer-2	-6.65	22.55	-35.94	-20.04 kJ/mol

	Dimer-3	-21.97	71.42	-117.53	-68.08 kJ/mol
	Dimer-4	-5.82	19.83	-32.68	-18.67 kJ/mol
	Dimer-5	-5.86	38.95	-64.06	-30.97 kJ/mol