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Supporting Information

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1. Synthetic Procedure Synthesis of Boc-Glycine (Compound 1):

2g (26.3 mol) of glycine was dissolved in 60 mL of 1,4 dioxane: Water (2:1). To this solution was added 1.164g (26.6 mol) of Sodium hydroxide. The solution was cooled to 0^oC. To this solution 6.4g (29.2 mol) BOC-anhydride was added in portion wise. The solution was allowed to room temperature and stirred for 1hr. After completion of the reaction the solvent was removed by vacuum, the resultant residue was dissolved in 100 mL H₂O and washed with 2 portions of 50 ml EtOAc. The aq. solution was acidified using conc. HCl to PH 1-2. The aqueous fraction was extracted with three portions of 75 ml EtOAc. The organic fraction was dried over Na₂SO₄ and concentrated using rotary evaporator to get the compound 1. Yield:80% ¹H NMR (500 MHz, CDCl₃, δ): 9.00-8.80 (s,1H), 3.86- 4.00 (m, 2H), 1.50 (s, 9H), ¹³C (65 MHz, CDCl₃, δ): 174.29, 155.67, 80.47, 42.42, 28.31. Cal. Mass: 175.08 Found: 197 (M+Na)



Synthesis of L-Dibenzyl aspartate (Compound 2):

A mixture of L-aspartic acid (12.5g, 0.095 mol) and benzyl alcohol (30 mL), p-tolyl sulfonic acid monohydrate (19.0g, 0.1 mol) and (150 mL) of benzene was refluxed for 8 hrs using a dean stark apparatus. After getting in to the rt ether (150 mL) was added and stirred until to get the white ppt. The ppt was filtered off and washed with ether. The collected white solid was mixed with (200 mL) of water and treated with a saturated solution of NaHCO₃ (200 mL). The mixture was extracted with CHCl₃ (3x200 ml). The collected organic phase was dried over Na₂SO₄, filtered and concentrated under reduced pressure to afford the title compound as a color less oil. Yield: 90%

¹H NMR (400 MHz, CDCl₃, δ): 8.38 (s, 2H), 7.68 (s, 1H), 7.34-6.98 (m, 9H), 5.02-4.80 (m, 2H), 4.65 (s, 2H), 3.43 (s, 2H), 3.14-2.90 (m, 1H), ¹³C (100 MHz, CDCl₃, δ): 169.829, 167.741, 140.808, 129.713, 128.466, 127.537, 126.932, 125.893, 125.237, 65.171, 49.557, 33.583. Cal. Mass: 313.13 Found: 314 (M+1)



Synthesis of Dibenzyl 2-(2-((tert-butoxycarbonyl) amino) acetamido) succinate (Compound 3):

1g (5.71 mol) of Boc-glycine was dissolved in 40 mL of DCM. To this reaction mixture L-di benzyl aspartic ester 2.6g (8.5 mol) was added and the solution was stirred at rt for 20 min. To this solution DCC (0.30g) and N-hydroxy succinimide (0.900g, 8.5 mol) N-methyl morpholine (2 mL) was added then the mixture was stirred for 14 hrs at rt. White precipitate was removed by filtration, and the resulting crude material was purified by column chromatography (Hexane: EtOAc 5:1). We went to the next step without further purification. Yield: 70 %.

¹H NMR (400 MHz, CDCl₃, δ): 7.35-7.30 (m, 6H), 7.26-7.20 (m, 4H), 5.24-5.04 (m, 1H), 4.65-4.56 (s, 4H), 3.88-3.76 (m, 2H), 3.40-3.20 (m, 2H), 1.44-1.40 (s, 9H), ¹³C (100 CDCl₃, δ): 170.869, 170.269, 155.749, 140.822, 135.100, 128, 359, 127.388, 126.849, 71.949, 64.936, 52.131, 50.382, 42.121, 28. 172. Cal. Mass: 470.82, Found: 471.



Synthesis of Dibenzyl 2-(2-aminoacetamido) succinate (Compound 4):

To a stirred solution of dibenzyl 2-(2-((tert-butoxycarbonyl) amino) acetamido) succinate (2.35g, 0.005 mol) in dichloromethane (20 mL), added CF₃COOH (6 mL). After being stirred for 1 hr at rt, the reaction mixture was concentrated and precipitated with ethyl ether (200 mL). The white solid of N-de protected dibenzyl 2-(2-aminoacetamido) succinate was obtained by filtration in quantitative yield. Yield: 50%

¹H NMR (500 MHz, CDCl₃, δ): 7.40-7.26 (m, 6H), 7.28-7.20 (m, 4H), 5.28- 5.20 (m, 1H), 5.16-4.98 (m, 3H), 4.00-3.28 (m, 3H), 3.04-2.52 (m, 2H), ¹³C (100 MHz, CDCl₃, δ): 172. 832,

170.100, 161.202, 160.710, 155.773, 140.703, 135.054, 134.824, 129.568, 127.239, 126.795, 64.615, 53.290, 42.242, 35.952. Cal. Mass: 370.40 Found: 392 (M+Na).



Alkylated Perylene dibenzoic acid (Compound 5):

The commercialized di bromo perylene 0.5g (0.419 mol) was dissolved in 30 ml of toluene and benzene boronic ester (0.312g, 1.257 mol), K₂CO₃ (0.200g, 2.09 mol) was added to this reaction mixture. To the reaction mixture catalytic amount of Pd (PPh₃)₂Cl₂ was added and the mixture was refluxed for 24 hrs at 110 ^oC temperature. After time completion, toluene was evaporated by vacuum and the compound was isolated by column chromatography (hexane: EtOAc). A pink coloured solid was obtained with the yield of 60 %.

¹H NMR (500 MHz, CDCl₃, δ): 8.80-8.40 (m, 8H), 8.16-8.10 (m, 2H), 7.66-7.24 (m, 4H), 3.98-3.94 (m, 2H),1.64-1.48 (m, 8H), 1.40-1.04 (m, 72 H), 0.92-0.80 (m, 12 H) ¹³C (100 MHz, CDCl₃, δ): 142.756,142.674, 143.318, 133.391, 133.263, 133.622, 132.520, 132.411, 132.250, 133.144, 131.648, 13.460, 129.862, 129.049, 128.912. 128.518, 128.593, 127.534, 126.907, 125.900, 125.176, 125.350. Cal. Mass:1276.84 Found- 1295.97 (M+F).



Synthesis of Perylene di peptide (PDI-PEP):

0.130g (0.098 mol) of compound 5 was dissolved in dichloromethane (20 mL), 0.110 g (0.095 mol) of dibenzyl 2-(2-aminoacetamido) succinate, DCC (0.0063g, 0.030 mol), N-hydroxy succinimide (0.0045g, 0.038 mol) was added. The reaction was continued up to 24 hrs and removed the solvent by vacuum and the reaction mixture was isolated with the DCM and water and dried over Na_2SO_4 and required compound was purified by using separation techniques. Yield: 80 %.

¹H NMR (500 MHz, CDCl₃, δ): 8.96-8.86 (m, 4H), 7.78-7.76 (m, 2H), 7.74-7.72 (m, 2H), 7.68-7.60 (m, 2H), 7.46-7.34 (m, 20H), 7.14-7.06 (m, 8H), 4.72-4.70 (m, 4H) 4.12-3.96 (m, 10H), 3.58-3.53 (m, 2H), 2.40-2.20 (m, 4H), 1.40-1.20 (m, 80H), 0.90-0.82 (m, 12 H) ¹³C (100 MHz, CDCl₃, δ): 1167.122, 166.531, 157.987, 153.098, 151.903, 150.339, 148.254, 147.612, 143.915, 143.132, 138.547, 98.189, 87.625, 74.432, 53.968, 51.392, 49.654, 48.388, 46.395, 42.451, 42.199, 33.565, 20.448, 19. Cal. Mass: 1982.60 Found: 1983.080 (M+1).



Dipeptide thiophene diketopyrrolopyrrole (DPP-PEP):

In a sealed tube dibromo thiophene diketopyrrolopyrrole (dibromo DPP) 0.100 g (0.410 mol) was dissolved in toluene 20 mL, to this reaction mixture NaO^tBu (0.050 mg, 1.230 mol), dibenzyl 2-(2-aminoacetamido) succinate (0.163 g, 1.230 mol), triphenyl phosphine 20 mg was added. The reaction mixture was purged with nitrogen gas up to 30 min, added catalytic amount of $Pd_2(dba)_3$. The reaction mixture was refluxed at 110 °C up to 24 hr, after the completion of the reaction the toluene was removed by using rotary evaporator and extracted with the organic solvent and brine solution. The organic layer was collected the reduced the solvent by vacuum, purified by column chromatograph. Yield: 60%.

¹H NMR (500 MHz, CDCl₃, δ): 8.86-8.64 (m, 4H), 7.78-7.72 (m, 4H), 7.66-7.60 (m, 6H), 7.44-7.36 (m, 10H), 7.12-7.00 (m, 4H), 5.40-4.50 (m, 4H), 4.20-3.98 (m, 10 H), 1.40-1.20 (m, 18H),

1.06-1.08 (m, 12 H) ¹³C (100 MHz, CDCl₃, δ): 161.720, 143.502, 140.396, 135.228, 134.758, 132.104, 131.915,130.467, 130.030, 128.930, 128.526, 128.357, 126.095, 125.383, 125.497, 45.826, 39.639, 31.885, 31.165, 29.662, 28.324, 24.735, 23.504, 23.025, 22.658. 21.965, 14.093, 13,99. 10.45. MALDI-TOF: Experimental: 1260.52 Found: 1299.47 (M+K).



Computational Details

Time-Dependent DFT (TDDFT) and Density Functional Theory (DFT) calculations were performed using the *Gaussian09* program.¹ The **PDI-PEP** and **DPP-PEP** with neutral charge were optimized in the gas phase. B3LYP exchange-correlation functional with Hay and Wadt's double zeta quality Los Alamos electron effective core potential basis set 6-311 g (d,p) was adopted on all atoms.²⁻⁴ The optimized geometries were analyzed by vibrational frequencies, resulting in no imaginary frequencies. Thus, the optimized structures correspond to absolute minima on the potential energy surface. At the optimized geometry, TDDFT calculations were performed at B3LYP/6-311 g (d,p) level of theory in dichloromethane solvent utilizing the Polarizable Continuum Model^{5,6}. (PCM), as implemented in *Gaussian 09.50* singlet-singlet excitations at S₀ optimized geometry are calculated. The software *GaussSum 2.2.5*⁷ was used to simulate the major portion of the absorption spectrum and to interpret the nature of transitions. The *Gaussview*⁸ was used to make molecular orbital surfaces and *GaussSum* software was used to calculate the percentage contributions of the **PDI-PEP** and **DPP-PEP** molecular orbitals.



Figure S1. UV absorption images of the molecules of **PDI-PEP** (a,b) and **DPP-PEP** (c,d) under normal light and 365 nm.



Figure S2. Normalized plots of experimental and simulated absorption spectra of (A) DPP-PEP (B) PDI-PEP



re S3. (a) Cyclic voltammogram (b) Energy level diagram of PDI-PEP and DPP-PEP



Figure S4. Aggregated emission in THF in water (fw) for PDI-PEP a) absorption and b) emission



Figure S5. Aggregated emission in THF in water (fw) for DPP-PEP a) absorption and b) emission.



Figure S6. Chemical Structures of the Dopants



Figure S7. PXRD analysis of the molecules for comparison with different dopants, a) PDI-PEP and 2) DPP-PEP.



Figure S8. Halochromism effect of **DPP-PEP**, 1. Grinding, 2. TFA addition, 3. After 2 mins, 4. After 10 mins, 5. After few mins.

Molecule Name	$\lambda_{max} [nm]^a$	НОМО	LUMO	E ₀₋₀ °
		[eV] ^b	(eV) ^b	
DPP-PEP	555	-5.87	-3.73	2.14
PDI-PEP	520	-5.80	-3.63	2.17

 Table S1. Optical Parameters of DPP-PEP and PDI-PEP

a. UV-Absorption spectra were recorded in DCM solution at 298K, b. Highest occupied molecular orbital values were calculated by adding 4.80 to E_{oxd} ; Lowest unoccupied molecular orbital was calculated by LUMO= E_{0-0} -HOMO d. The bandgap, E_{0-0} , was calculated from the intersection point of the absorption and emission spectra

Table S2. Solvatochromism UV absorption, emission and their molar extinction coefficient

 values of the **DPP-PEP** and **PDI-PEP**.

Solvent	DPP- PEP		PDI	-PEP	EMISSION (nm)		
	UV (nm)	Mol. Ext. Coeff (ε)	UV (nm)	Mol. Ext. Coeff (ε)	DPP-PEP	PDI-PEP	
TOL	556	7975	508	6310	565	541	

DCM	560	9560	515	16359	568	539
THF	551	10970	508	15358	570	543
ACN	557	20930	509	14355	570	536
DMF	560	17085	511	12301	574	539

Table S3. Experimental λ_{max} , calculated λ_{max} , (nm) and oscillator strengths (f) of **DPP-PEP** in DCM solvent, calculated at B3LYP/6-311g (d,p):

Table S4. Experimental λ_{max} , calculated λ_{max} , (nm) and oscillator strengths (f) of **PDI-PEP** in DCM solvent, calculated at B3LYP/6-311g (d,p):

	Wavelength		Osc.				
State	Wamelengt	h S	trenQtsc.		Major Contributions		Minor Contributions
State	(nm)		Strengt	th	Major Contributions	Mir	or Contributions
S1	520.391	1.	1163	Η	<u>OMŎ->LUMO (97%)</u>		
						HO	MO->L+1 (4%),
S1	859.324		0.0025	H	3HEIMIOLOL(2686%H-1->LU	M₽O	MO->L+4 (5%)
S2	336.445	0.	0053	(4	6%), HOMO->L+1 (24%)		
						HO	MO->L+5 (5%),
S2	714.766		0.0264	H	3HEIMIO4OL+6983%H-1->LU	M€O	MO->L+13 (6%)
S 3	324 393	0.	002	(1	6%). HOMO->L+1 (10%)		H-3->L+16 (2%)
S3	618.031		0.005	(-	H-1->LUMO (98%)		
				H	-1->LUMO (31%) HOMO->	.+1	
s\$4	305716167	0	00,0098	(6	1 b - 1 -> L + 1 (97%)	HO	$MO_{2} \rightarrow MO_{3} $
54	309.302	υ.	0000	(0			$11-2-2L+1(3\times0)$
\$5	307 102	0	7509	Н	HOMR(2L04%) (49%),	HO	$MQ_{t} \ge 1+21$ (6%(3%),
S5	528.600	0.	0.0038	11	HOMO -> L + 5 (33%)	НО	MO - >L + 6(7%)
S6	281.934	0.	0003	H	HOMOMO(8749) (36%),	HO	$MO^{1}S_{L}^{+1}(4\%),$
<u>- 56</u>	505,106		0.0023		HOMO->L+5 (49%)	но	MO->L+3 (4%)
~ ~	0000000		0.0020	H	1->L+17(18%), HOMO->L	+17	H-15->LUMO (3%),
S7	263.996	0.	0002	(7	1240MO -> L + 6 (54%).	HO	MtQMQ-3≥L+16(\$3%)
					$HOMO \rightarrow I + 9$ (11%)	НО	$MO \rightarrow I + 5 (4\%)$
S&7	262119870	0.	0801005	H	45004400-(77%)		$14_{1} + 1$
57	410.379		0.0005				MO - 2L + 0 (3.80)
				H	$1_{1} = 1_{1$	+18	157 LUMO ($3%$),
S9	260.343	0.	0001	(6	6400MO > 1 + 12 (18%)		HOMO - L + 14(9%)
C 0	406 500		0 000 4		HOMO- $>L+12$ (1070),		MO > L + 11 ((0/))
SN	251.451 ⁸²	0.	0221084	H	10->LUMO (84%)	но	MO->L+1 (0%) H-10->L+1 (9%)
S11	205.402		0 0 0 0 0	H	$13 - 210 MO^{+}(36\%), HOMO^{-},$	HO	H = 13 = 14 + 1 (4%), H = 13 = 14
S9	248.369	0.	1354	>]	L+161459%L+8 (22%)	HO	MO - 2L + 5 + (3%)
010	202 (11		0.0220	_			()/
S120	383.611		0.0322	Η	13-520MO (30%), HOMO-		H-13->L+1 (5%), H-
C11	247.877	0.	1716	\geq	+16 (28%)	TT	1 . 1-74-74-165%)11
511		•	0.01.0			H-	11->LUMU(3%),/H-
S13	361.351		0.0160	þ	H-2->LUMO (78%)		9->LUMO (7%)
							H-1->L+2(6%),
812	239.317	0.	0043	L	HUMHOMO-3 [42/(7,0%)		40MOL>10+3(6%)
	353.793		0.000	/	HOMO->L+9 (33%)	H	OMO->L+12 (9%)
S14					HOMO->L+11 (41%), HOMC)	H-2->L+11 (3%),
S13	230.362	0.	0053		H-18-≥ه 133240‰ H-8-	H-	17HOMO(329748%),
	351.386		0.031	7	>L+1 (17%)		>L+1 (9%)
S15							H-2->L+1 (8%), H-
S14					HOMD->L+14%)4%)7HOMC	_H-1	81-541(4°)/H-91-1-
	226.350,304	0.	010302	7	(14%) > L+19(44%)	>L-	1(8%) + 16(6%).
		5.					,
S15				•	HOMO->L+7 (30%),		H-15->L+1 (8%),
	347.837		0.0005	5	HOMO->L+9 (25%)	H	IOMO->L+11 (5%)
							· · · ·

Table S5. Molecular orbital pictures of **DPP-PEP** calculated at B3LYP/6-311g (d,p) level of theory.

DPP-PEP



Table S6. Molecular orbital pictures of **PDI-PEP** calculated at B3LYP/6-311 g (d,p) level of theory.

PDI-PEP



Table S7. Aggregation emission and respective UV absorption of the DPP-PEP and PDI-PEP.

% <i>fw</i> of		DPP-PEP		PDI-PEP			
Water	UV (nm)	EMISSION (nm)	PLQY (%)	UV (nm)	EMISSION (nm)	PLQY (%)	
THF	554	570	0.0548	508	543	0.06536	

DPP-PEP % <i>fw</i> of Water	τ_1/ns	α ₁ (%)	τ ₂ /ns	8	α _z (%)	Avera lifetin τ (ns	age ne)
10	556	570	0.01503	521		547	7	0.00868
20	569	569	0.01943	521		548	3	0.00983
30	569	569	0.01805	521		550)	0.02829
40	556	570	0.02842	521		549)	0.01081
50	558	569	0.02116	521		543	3	0.06136
60	557	570	0.01043	527		543	3	0.0629
70	558	570	0.0196	539		612	2	0.06756
80	563	620	0.00995	539		612	2	0.07031
90	565	574	0.01111	523		612	2	0.07742

Table S8. TCPSC life-time data of d PDI-PEP.

PDI-PEP	τ_1/ns	α ₁ (%)	τ_2/ns	α _z (%)	Average lifetime τ
% <i>fw</i> of Water					
THF	0.002*10-9	99.95	4.33*10-9	0.05	0.82*10-9
90	1.57*10-9	60.15	6.82*10-9	39.85	5.46*10-9
80	0.81*10-9	72.15	8.30*10-9	27.49	6.72*10 ⁻⁹
70	0.63*10-9	65.47	4.65*10-9	34.53	3.82*10-9
60	0.83*10-9	63.14	5.52*10-9	36.86	4.55*10-9
50	1.00*10-9	24.91	4.22*10-9	75.00	3.98*10-9
40	0.76*10 ⁻⁹	16.40	4.03*10-9	83.60	3.91*10 ⁻⁹
30	0.0018*10-9	99.99	4.32* 10-9	0.01	0.83*10-9
20	0.004*10-9	100	4.34*10-9	0.00	3.97*10-9
10	0.0015*10-9	100	4.30*10-9	0.00	4.15*10-9

THF	3.13*10-9	56.98	5.70*10-9	43.02	4.61*10-9
90	0.0697*10 ⁻⁹	84.42	2.83*10-9	15.58	2.49*10-9
80	0.70*10-9	38.50	2.85*10-9	61.50	2.56*10-9
70	0.85*10-9	22.92	4.29*10-9	77.08	4.09*10-9
60	0.46*10-9	24.46	4.70*10-9	75.54	4.57*10-9
50	1.74*10-9	36.55	6.72*10-9	63.45	6.07*10-9
40	2.18*10-9	33.68	6.57*10 ⁻⁹	66.32	5.93*10 ⁻⁹
30	0.012*10-9	100	5.34*10-9	0.00	4.36*10 ⁻⁹
20	3.20*10-9	35.35	1.92* 10-9	55.15	2.58*10-9
10	2.40*10-9	39.09	6.08*10-9	60.91	5.33*10-9

 Table S9. TCPSC life-time data of d DPP-PEP.

Table S10. TCPSC life-tim	ne data of d DPP-PEP	and PDI-PEP in	various solvents.
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Solvents	DPP-PEP						Р	DI-PEP		
	τ_1/ns	α ₁ (%)	τ_2/ns	α ₂ (%)	Avera ge lifetim e τ (ns)	τ_1/ns	α ₁ (%)	τ_2/ns	α ₂ (%)	Averag e lifetim e τ (ns)
DCM	1.00*10 ⁻⁹	3.79	5.91*10 ⁻⁹	96.2 1	5.87*1 0 ⁻⁹	0.922 *10 ⁻⁹	28.36	3.22*10 -9	71. 64	2.99*1 0 ⁻⁹
THF	3.13*10 ⁻⁹	56.98	5.70*10 ⁻⁹	43.0 2	4.61*1 0 ⁻⁹	0.002 *10 ⁻⁹	99.95	4.33*10 -9	0.0 5	0.82*1 0 ⁻⁹
TOL	0.39*10 ⁻⁹	2.14	5.64*10 ⁻⁹	97.8 8	5.63*1 0 ⁻⁹	0.811 *10 ⁻⁹	23.64	3.13*10 -9	76. 36	3.13*1 0 ⁻⁹
DMF	0.44*10 ⁻⁹	1.89	5.98*10 ⁻⁹	98.1 1	5.97*1 0 ⁻⁹	1.13* 10 ⁻⁹	72.74	2.81*10 -9	27. 26	1.94*1 0 ⁻⁹
ACN	0.42*10 ⁻⁹	1.08	5.85*10 ⁻⁹	98.9 2	5.84*1 0 ⁻⁹	0.13* 10 ⁻⁹	80.75	3.85*10 -9	19. 25	3.81*1 0 ⁻⁹

NMR, Mass Spectra:



Figure S8. ¹H NMR spectrum of compound 1



Figure S9 ¹³C NMR spectrum of compound **1**



Figure S10. ESI-Mass spectrum of compound 1



Figure S11. ¹H NMR spectrum of compound 2



Figure S12. ¹³C NMR spectrum of compound 2



Figure S13. ESI-Mass spectrum of compound 2



Figure S14. ¹H NMR spectrum of compound



Figure S15. ¹³CNMR spectrum of compound 3



Figure S16. ESI-Mass spectrum of compound 3



Figure S17. ¹NMR spectrum of compound 4



Figure S18. ¹³C NMR spectrum of compound 4



Figure S19. EIS spectrum of compound 4



Figure S20. ¹H NMR spectrum of compound 5



Figure S21. ¹³C NMR spectrum of compound 5



Figure S22. Mass spectrum of compound 5



Figure S24. ¹³CNMR spectrum of PER-PEP



Figure S25. MALDI-TOF spectrum of PER-PEP



Figure S26. ¹H NMR spectrum of DPP-PEP





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