Supporting Information for

Rational Design of Charge-transfer Interactions in Halogen-bonded Co-crystals towards Versatile Solid-state Optoelectronics

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Contents

1. Molecular packing structures of Bpe, Bpe-IFB and Bpe-F_4DIB crystals

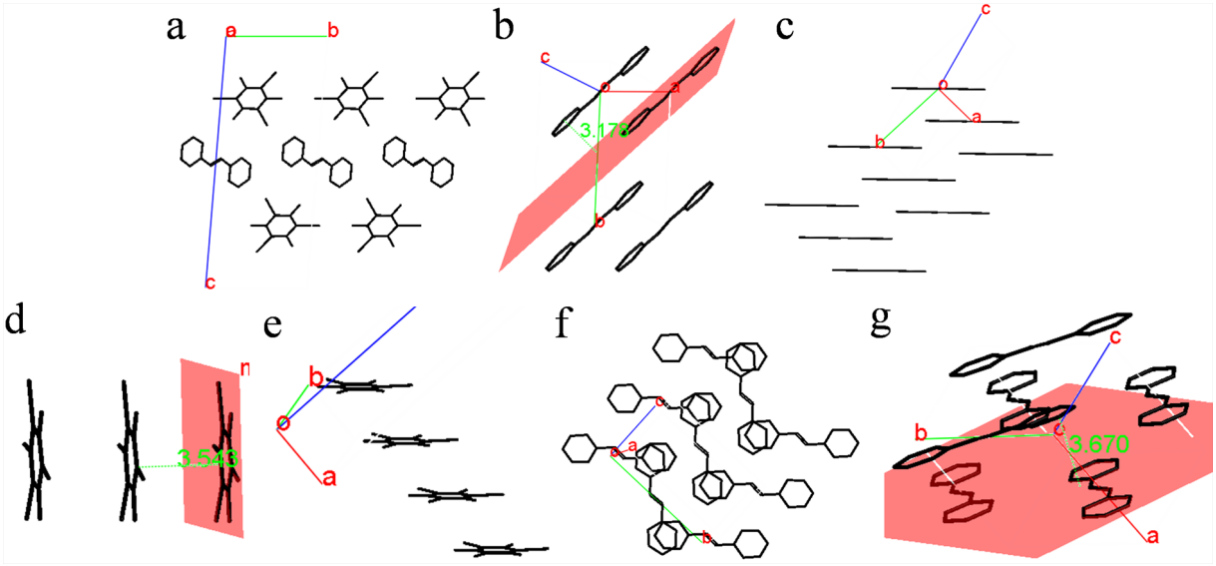


Figure S1. (a) Bpe and IFB molecules pack in a segregated form; (b) Bpe molecular columns in Bpe-IFB co-crystal. The distance is measured to be 3.178Å in Bpe column; (c) The "slipped stacking" of Bpe molecules in Bpe-IFB co-crystal; (d) and (e) Packing structure of IFB molecules in Bpe-IFB crystal. The distance is measured to be 3.543Å; (f) and (g) Molecular packing structures of Bpe single component crystal and the molecular distance is measured to be 3.67Å.

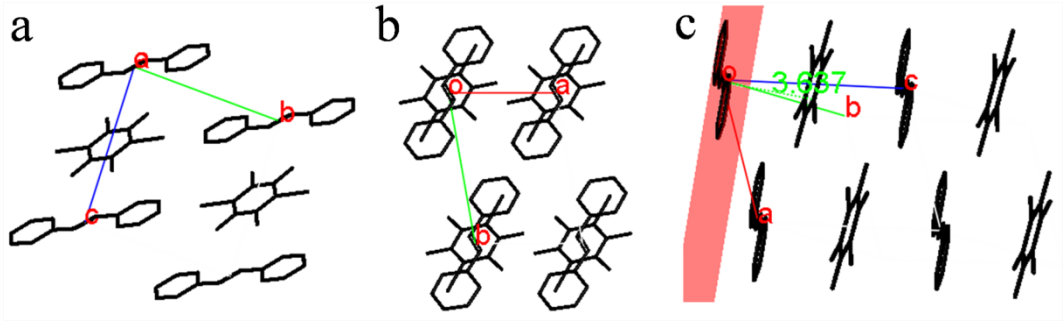
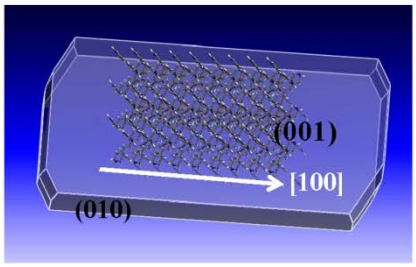


Figure S2. (a) and (b) The molecules pack in a mixed-stacking form in Bpe-F_4DIB co-crystal. (c) The donor-acceptor distance is measured to be 3.637 Å.

2. Morphology predictions of Bpe-IFB and Bpe-F_4DIB co-crystals

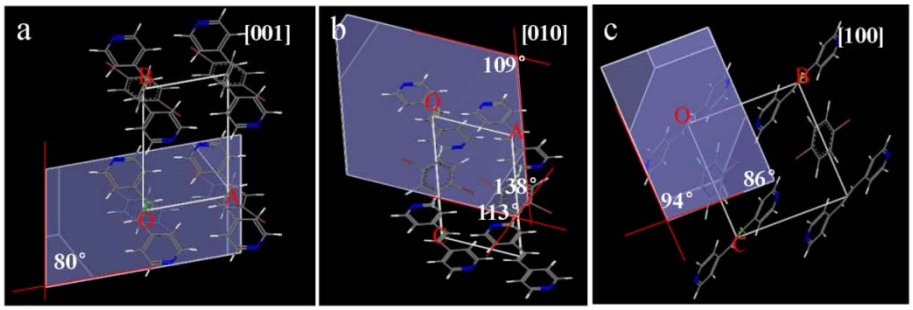
a



b

Miller Index	Eatt(total) (kcal/mol)	Total facet area
(001)	-8.30	69.69%
(010)	-28.34	18.54%
(10-2)	-53.47	3.5%
(10-1)	-56.31	2.66%

Figure S3. (a) The calculated growth morphology of Bpe-IFB crystal using Materials Studio software; (b) The calculated attachment energy of resulted crystal planes.



d

Miller Index	Eatt(total) (kcal/mol)	Total facet area
(010)	-9.06	43.76%
(001)	-13.29	28.27%
(100)	-15.24	22.56%
(111)	-20.72	3.54%

Figure S4. (a), (b) and (c) The calculated growth morphology of Bpe-F_4DIB crystal using Materials Studio software; (d) The calculated attachment energy of resulted crystal planes.

3. Morphology of Bpe, IFB, F_4DIB and co-crystals

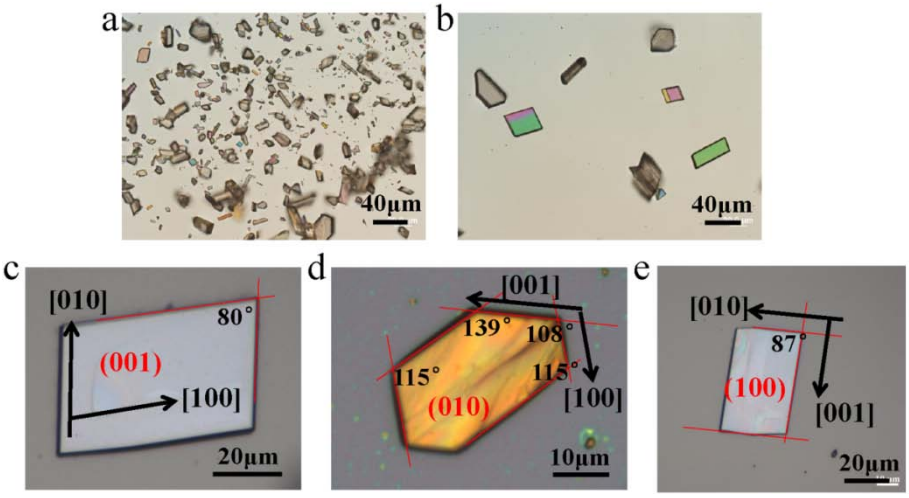


Figure S5. (a) and (b) Optical images of Bpe-F_4DIB crystals obtained from dichlormethane solution drop-casting. It shows mainly three polymorphs. And the co-crystals are indexed according to the calculation results obtained from Material Studio software, as displayed in (c), (d) and (e).

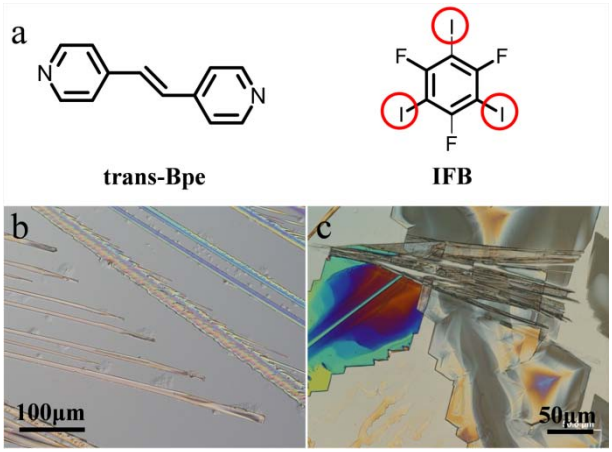


Figure S6. (a) Chemical structures of *tran*-Bpe and IFB; Optical images of (b) Bpe and (c) IFB crystals obtained from acetonitrile drop-casting.

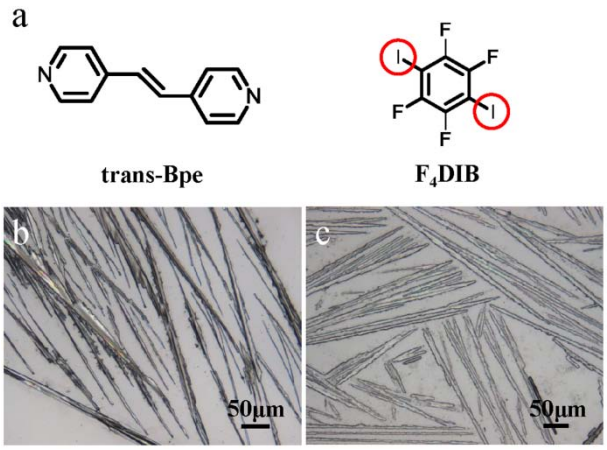


Figure S7. (a) Chemical structures of Bpe and F_4DIB; Optical images of (b) Bpe and (c) F_4DIB crystals obtained from dichlormethane solution drop-casting.

4. XRD analysis of Bpe-IFB and Bpe-F_4DIB co-crystals

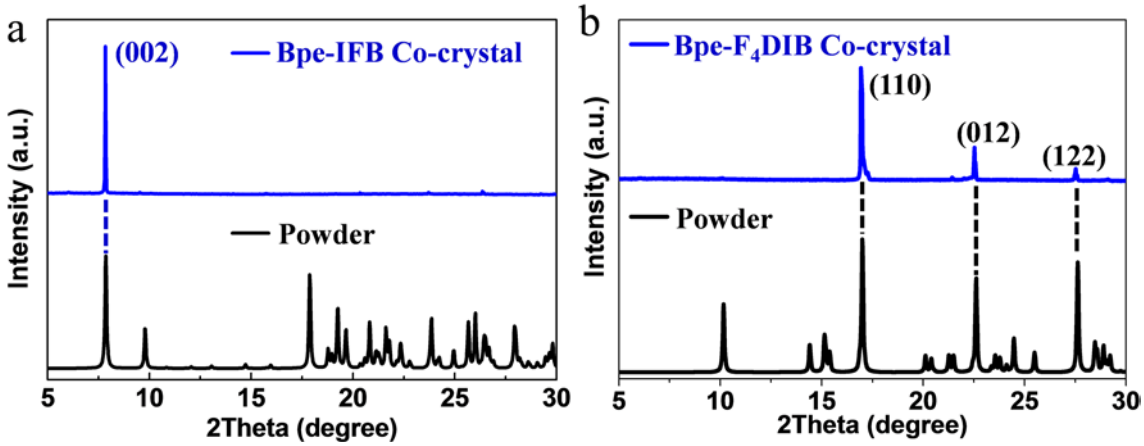


Figure S8. XRD results of (a) Bpe-IFB and (b) Bpe-F_4DIB crystals on the glass substrate. The b crystal planes are the most easily detected in Bpe-F_4DIB crystals. The calculated powder XRD patterns are exported from CIF files.

5. Raman and FTIR characterizations

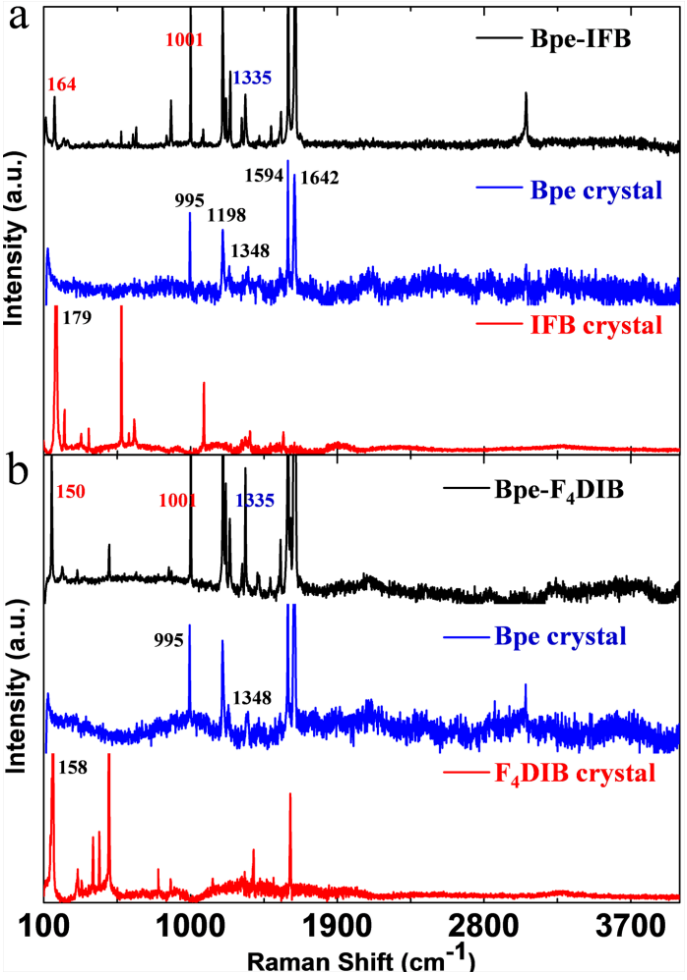


Figure S9. Raman spectra of (a) Bpe, IFB and Bpe-IFB crystals from acetonitrile solution drop-casting and (b) Bpe, F_4DIB and Bpe-F_4DIB crystals from dichlormethane solution drop-casting.

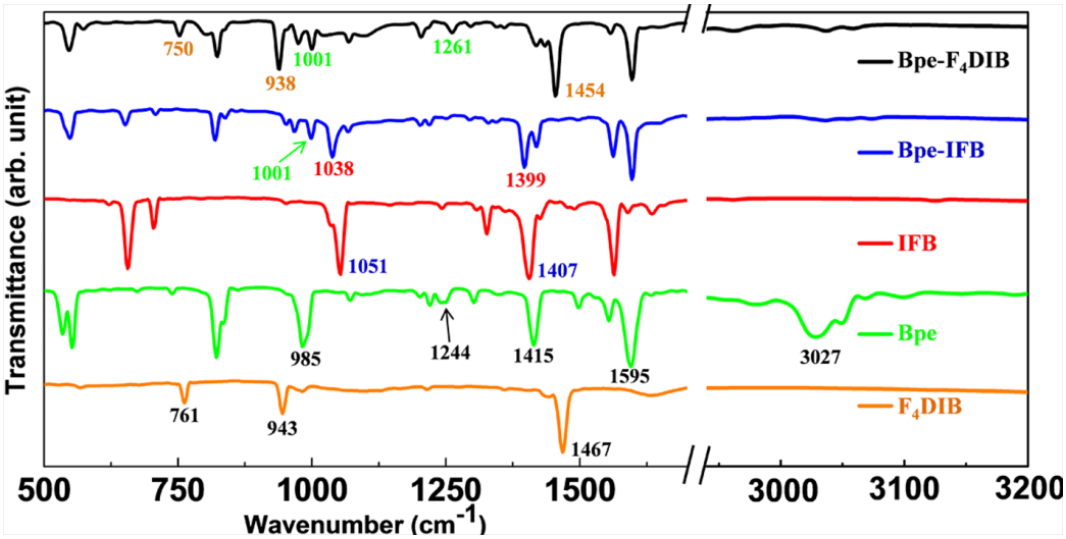


Figure S10. Infrared (IR) spectra of Bpe, IFB and F_4DIB powder, Bpe-IFB crystals and Bpe-F_4DIB crystals.

6. Optical and PL images of Bpe-F_4DIB co-crystals

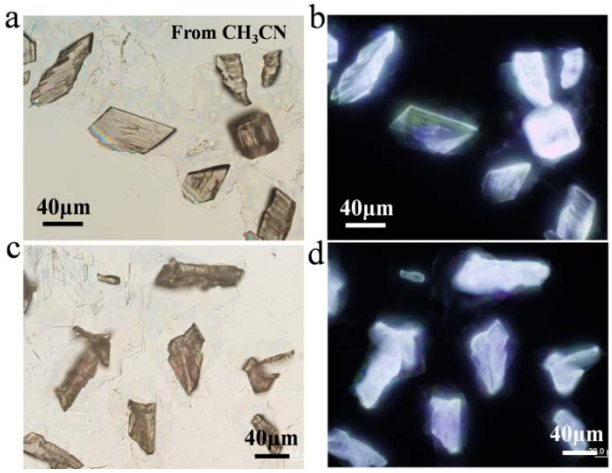


Figure S11. (a), (c) Optical images and (b), (d) corresponding confocal laser scan microscopy (CLSM) images of Bpe-F_4DIB crystals on the glass substrate under the excitation of an unfocused UV light (330-380 nm), indicating the white-light emission from these irregular co-crystals. The Bpe-F_4DIB crystals were obtained from acetonitrile solution drop-casting.

7. CIE coordinates of two types of co-crystals

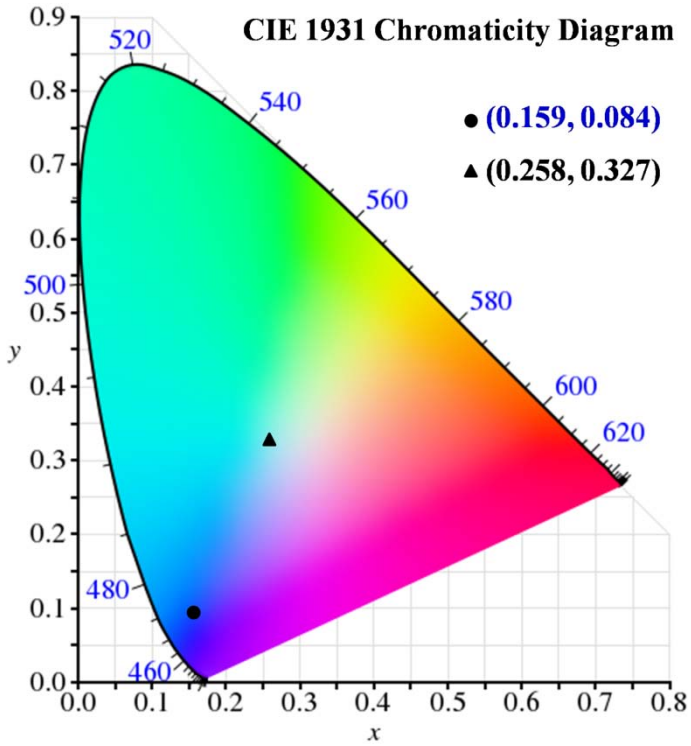


Figure S12. The calculated CIE coordinates according to the CIE 1931 chromaticity. The Bpe-F_4DIB crystals exhibit white light emission.

8. Absorption spectra of Bpe, Bpe-IFB and Bpe-F_4DIB crystals

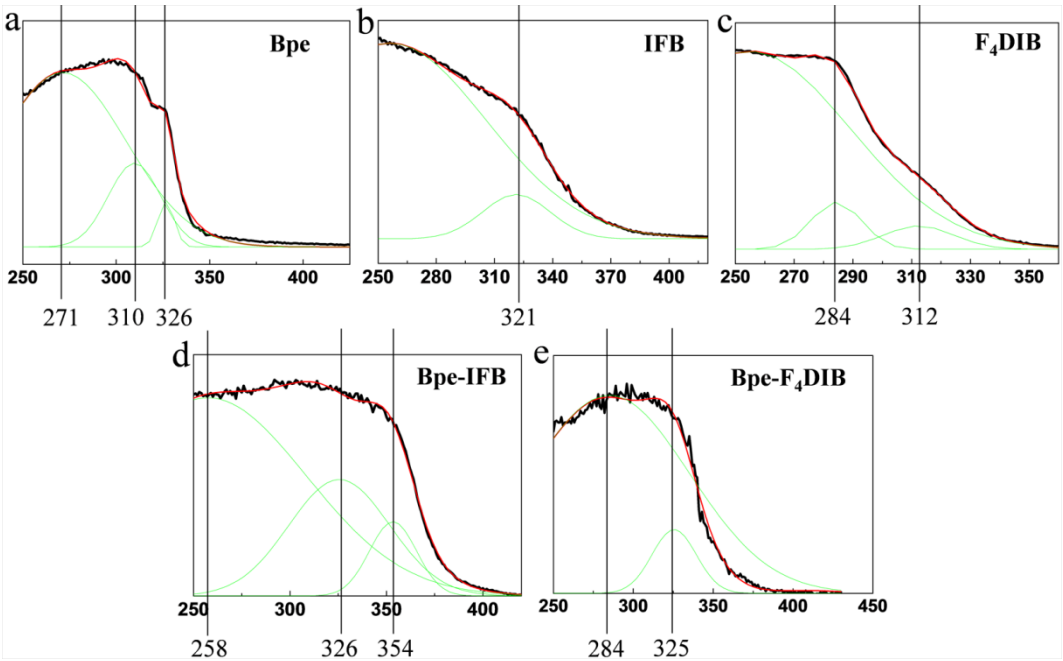


Figure S13. Absorption spectra of (a) Bpe, (b) IFB, (c) F_4DIB, (d) Bpe-IFB and (e) Bpe-F_4DIB crystals. The spectra are multi-peaks fitted.

9. The PL spectra of F_4DIB crystals

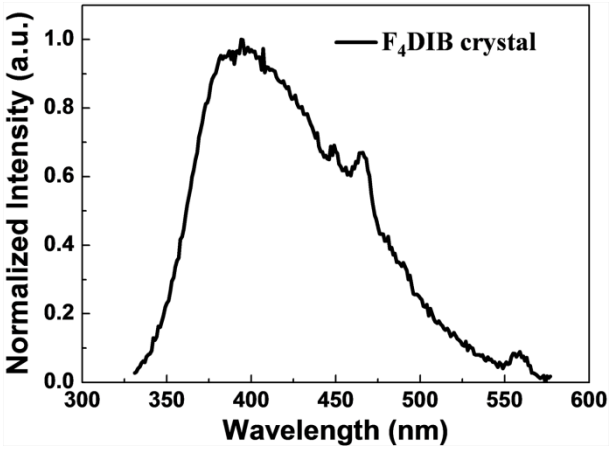
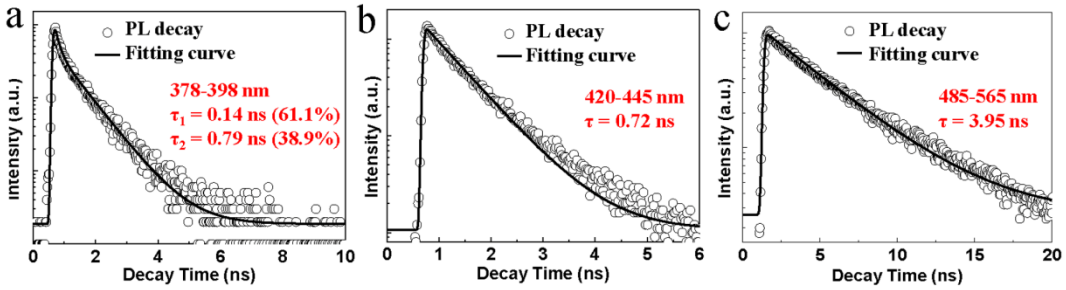


Figure S14. F_4DIB crystals show very weak photoluminescence and the spectrum was collected.

10. Results of PL decay measurements



d

	PL	τ	PLQY	k_f
Bpe crystal	350-390 nm	0.14ns(61.1%), 0.79ns(38.9%)	54.6%	/
	400-480 nm	0.72 ns		
	485-565 nm	3.95 ns		
Bpe-IFB co-crystal	425 nm	1.66 ns	26.14%	0.16 ns^{-1}
Bpe-F_4DIB co-crystal	360-425 nm	0.10 ns	/	/
	444-465 nm	0.1 ns(93%), 0.71 ns(7%)		
	470-495 nm	0.12 ns(71.2%), 1.55 ns(28.8%)		
	500-555 nm	1.59 ns		

Figure S15. (a), (b), (c) PL decay profiles of Bpe crystals; (d) The photophysical properties of Bpe crystals, Bpe-IFB crystals and Bpe-F_4DIB crystals.

11. ESR measurements of Bpe-IFB co-crystals

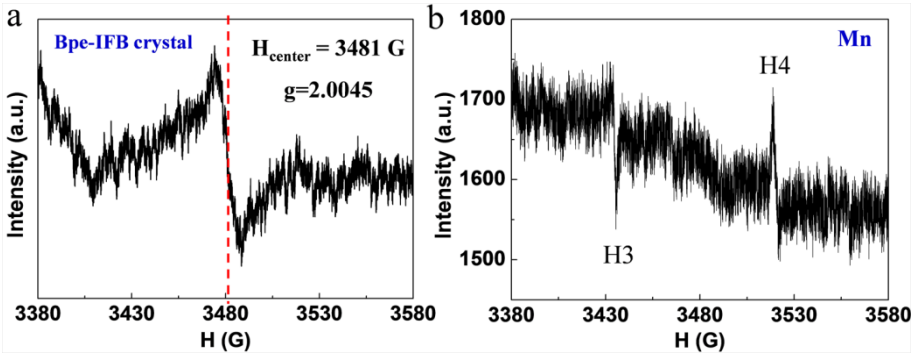


Figure S16. The ESR results of (a) Bpe-IFB crystals and (b) Mn sample measured at room temperature. A relative weak but sharp signal was observed, and the g factor was calculated to be 2.0045, referring to the Mn sample.

12. The calculated static dipole moment of co-crystals

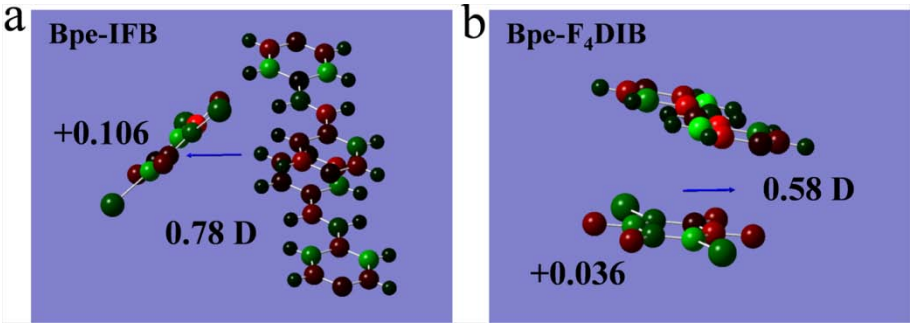


Figure S17. The calculated static dipole moment (SDM) of (a) Bpe-IFB and (b) Bpe-F_4DIB crystals in the ground state.

13. The calculated absorption spectra and vertical transition energies

a

Experimental ab	E_{vert}	Electronic transition	Calculated ab	Oscillator strength (f)
354 nm 3.50 eV	$CT_0 \rightarrow CT_1$	HOMO → LUMO	361.4 nm 3.43 eV	0.0021
326 nm 3.80 eV	$CT_0 \rightarrow CT_2$	HOMO → LUMO+2 (47.3%) HOMO-9 → LUMO (21.3%) HOMO-7 → LUMO (12.8%)	328.3 nm 3.78 eV	0.2027
258 nm 4.81 eV	$CT_0 \rightarrow CT_3$	HOMO-7 → LUMO+4 (18.9%) HOMO-9 → LUMO+3 (11.6%) HOMO-7 → LUMO+3 (11.0%)	257.5 nm 4.81 eV	0.0034

b

Experimental ab	E_{vert}	Electronic transition	Calculated ab	Oscillator strength (f)
325 nm 3.82 eV	$S_0 \rightarrow S_1$	HOMO-1 → LUMO+1 (81.8%) HOMO → LUMO+1 (6.2%)	312.1 nm 3.97 eV	0.0043

Figure S18. The vertical transition energies E_{vert} of (a) Bpe-IFB crystals and (b) Bpe-F_4DIB crystals as calculated by TD-DFT.

14. The calculated transition dipole moment of co-crystals

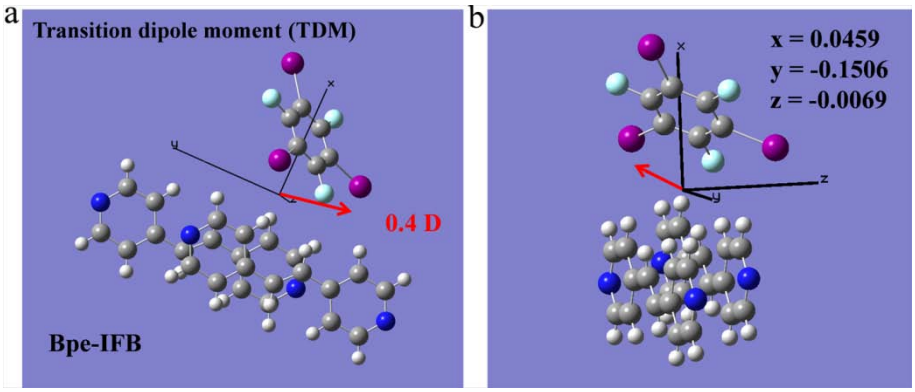


Figure S19. (a) and (b) The transition dipole moment (TDM) of Bpe-IFB crystal displayed along a different perspective.

15. The calculated energy levels of Bpe, Bpe-IFB and Bpe-F_4DIB crystals

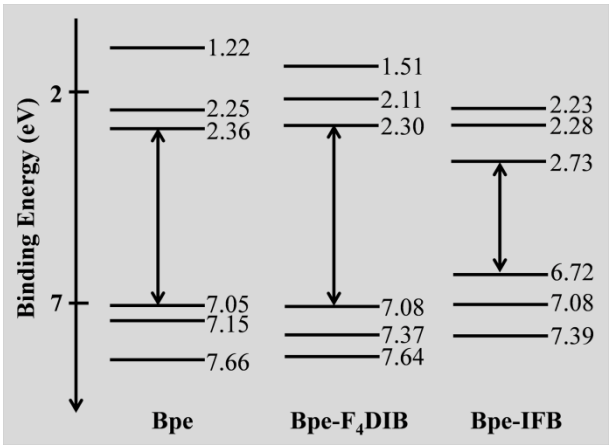
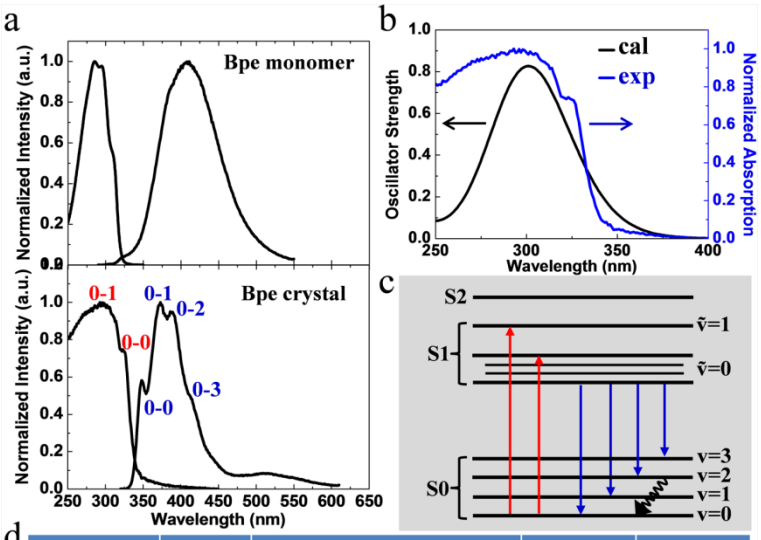


Figure S20. The calculated energy levels of Bpe, Bpe-F_4DIB and Bpe-IFB crystals by TD-DFT. The LUMO-HOMO gap narrows in the Bpe-IFB crystals and retains in Bpe-F_4DIB crystals as compared with Bpe crystals.

16. The spectroscopy and theoretical calculations of Bpe



d

Experimental ab	E_{vert}	Electronic transition	Calculated ab	Oscillator strength
326 nm 3.80 eV	$S_0 \rightarrow S_1$	HOMO → LUMO (76.1%) HOMO → LUMO+1 (8.6%) HOMO-1 → LUMO (6.2%)	305.2 nm 4.06 eV	0.2087
310 nm 4.0 eV				
271 nm 4.58 eV	$S_0 \rightarrow S_2$	HOMO-4 → LUMO+1 (51.3%) HOMO-2 → LUMO+1 (21.5%)	271.9 nm 4.56 eV	0.0173

Figure S21. (a) The absorption and PL spectra of Bpe monomer in acetonitrile and Bpe crystals; (b) The calculated absorption spectrum of Bpe crystals (black curve); (c) The Jablonski diagram for Bpe crystals; (d) The calculated vertical transition energies E_{vert} of Bpe crystals.

17. Relationship between molecular packing structures and CT interactions

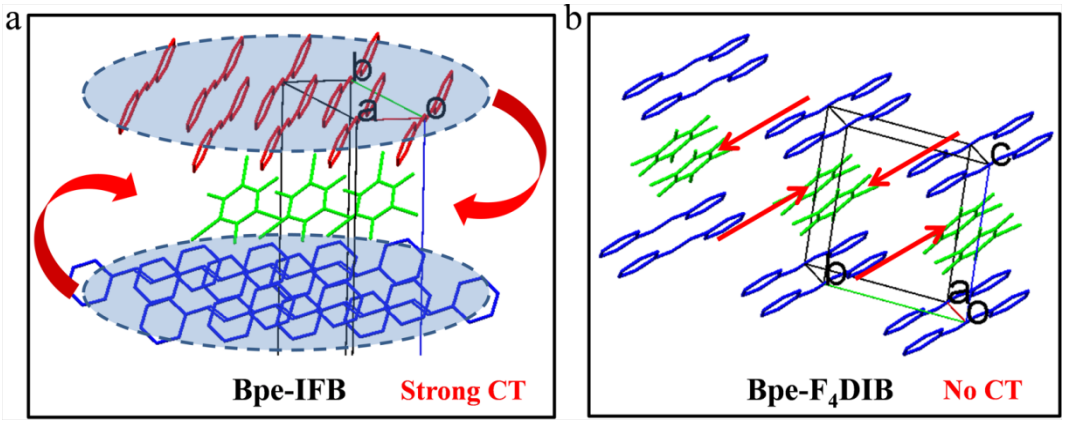


Figure S22. The molecular packing structures of (a) Bpe-IFB and (b) Bpe-F_4DIB co-crystals and the proposed mechanism for selective appearance of CT interactions.

18. The home-made platform for micro-area optical characterizations

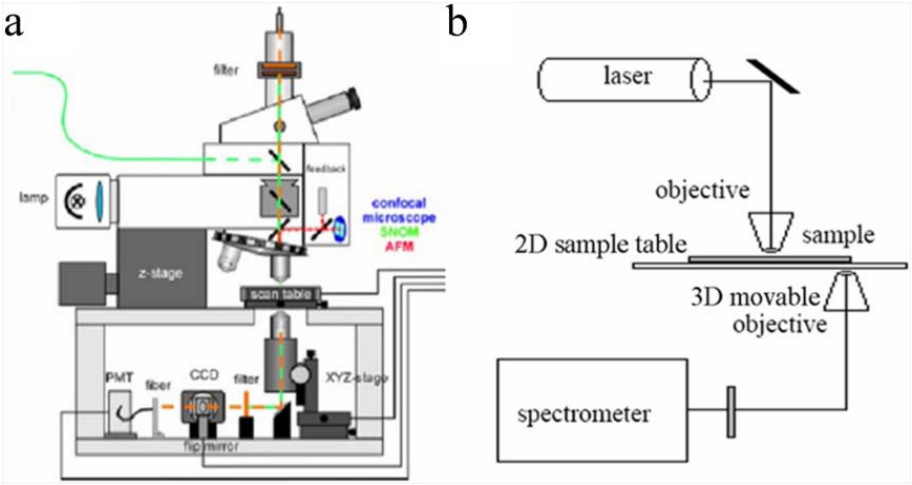


Figure S23. Schematic illustration of (a) the near-field scanning optical microscopy and (b) the transmittance optical path for the optical waveguide measurements.

19. The calculated excitation energies and oscillator strengths of crystals

Table S1. Excitation energies and oscillator strengths of Bpe-IFB crystals

Excited State	1:	Singlet-A	3.4311 eV	361.35 nm	f=0.0021 <S**2>=0.000
138 ->139		0.69829			
Excited State	2:	Singlet-A	3.6377 eV	340.83 nm	f=0.0099 <S**2>=0.000
138 ->140		0.67576			
138 ->141		-0.16819			
Excited State	3:	Singlet-A	3.7571 eV	330.00 nm	f=0.0078 <S**2>=0.000
128 ->139		-0.14118			
131 ->139		0.51153			
132 ->139		0.28395			
133 ->139		-0.14394			
134 ->139		-0.10266			
137 ->139		0.22009			
Excited State	4:	Singlet-A	3.7761 eV	328.34 nm	f=0.2027 <S**2>=0.000
129 ->139		-0.32671			
131 ->139		0.25270			
137 ->139		-0.18405			
137 ->140		0.15023			
138 ->140		0.11824			
138 ->141		0.48618			
Excited State	5:	Singlet-A	3.7806 eV	327.94 nm	f=0.1395 <S**2>=0.000
129 ->139		0.48641			
131 ->139		-0.15380			
132 ->139		0.18280			
137 ->140		0.12202			
138 ->141		0.39036			
Excited State	6:	Singlet-A	3.8184 eV	324.70 nm	f=0.0350 <S**2>=0.000
129 ->139		-0.16456			
132 ->139		-0.10728			
137 ->139		0.63512			
138 ->141		0.15302			
Excited State	7:	Singlet-A	3.9658 eV	312.63 nm	f=0.0019 <S**2>=0.000
136 ->139		0.20193			
136 ->140		-0.21288			
136 ->141		0.60458			
136 ->152		-0.11104			
Excited State	8:	Singlet-A	3.9691 eV	312.38 nm	f=0.0016 <S**2>=0.000
135 ->140		0.61083			
135 ->141		0.27504			
135 ->149		0.10131			
Excited State	9:	Singlet-A	4.0514 eV	306.03 nm	f=0.0622 <S**2>=0.000
129 ->140		0.13552			
131 ->140		0.15469			
132 ->140		-0.29325			
133 ->140		-0.17598			
133 ->141		-0.15570			

134 ->140 0.44180
137 ->140 -0.20993
Excited State 10: Singlet-A 4.0615 eV 305.27 nm f=0.0131 <S**2>=0.000
137 ->140 0.27633
137 ->141 0.61721
Excited State 11: Singlet-A 4.0746 eV 304.29 nm f=0.0347 <S**2>=0.000
130 ->140 -0.13946
130 ->141 0.23977
132 ->140 0.20563
133 ->140 0.33646
133 ->141 -0.27655
134 ->141 -0.30436
137 ->140 -0.13732
Excited State 12: Singlet-A 4.1380 eV 299.62 nm f=0.6946 <S**2>=0.000
134 ->140 0.10554
136 ->139 0.17321
137 ->140 0.52982
137 ->141 -0.29272
138 ->141 -0.16809
Excited State 13: Singlet-A 4.1584 eV 298.15 nm f=0.0604 <S**2>=0.000
136 ->139 0.63196
136 ->141 -0.17986
137 ->140 -0.14064
Excited State 14: Singlet-A 4.2314 eV 293.01 nm f=0.0022 <S**2>=0.000
133 ->139 -0.40793
134 ->139 0.52607
Excited State 15: Singlet-A 4.2899 eV 289.01 nm f=0.0004 <S**2>=0.000
125 ->139 0.11749
130 ->139 -0.11949
131 ->139 0.10635
133 ->139 0.41478
134 ->139 0.27015
135 ->139 0.41118
Excited State 16: Singlet-A 4.3053 eV 287.98 nm f=0.0012 <S**2>=0.000
125 ->139 -0.14299
132 ->139 -0.22246
133 ->139 -0.21687
134 ->139 -0.23852
135 ->139 0.51930
Excited State 17: Singlet-A 4.3176 eV 287.16 nm f=0.0029 <S**2>=0.000
122 ->139 -0.13595
126 ->139 0.33606
129 ->139 -0.22042
131 ->139 -0.22392
132 ->139 0.35279
134 ->139 -0.16950
135 ->139 0.22367
Excited State 18: Singlet-A 4.3576 eV 284.52 nm f=0.0014 <S**2>=0.000
125 ->139 -0.33034

126 ->139 0.37785
127 ->139 -0.17389
128 ->139 0.20589
129 ->139 0.12114
129 ->144 -0.10577
130 ->139 -0.16443
131 ->139 0.15989
131 ->145 0.11246
133 ->139 0.14633
Excited State 19: Singlet-A 4.3656 eV 284.00 nm f=0.0283 <S**2>=0.000
133 ->140 0.44715
133 ->141 0.24293
134 ->140 0.35353
134 ->141 0.25626
Excited State 20: Singlet-A 4.3881 eV 282.55 nm f=0.0011 <S**2>=0.000
124 ->139 0.11900
125 ->139 -0.25053
126 ->139 -0.37169
128 ->139 0.20725
129 ->139 -0.12054
130 ->139 -0.10360
132 ->139 0.38214
Excited State 21: Singlet-A 4.4006 eV 281.75 nm f=0.0219 <S**2>=0.000
133 ->139 0.10282
133 ->141 -0.43875
134 ->140 -0.15104
134 ->141 0.46028
Excited State 22: Singlet-A 4.4504 eV 278.59 nm f=0.0043 <S**2>=0.000
122 ->139 -0.23168
123 ->139 -0.12177
125 ->139 -0.32280
128 ->139 -0.29929
130 ->139 0.35692
133 ->139 0.14059
Excited State 23: Singlet-A 4.4810 eV 276.69 nm f=0.0072 <S**2>=0.000
124 ->139 -0.16469
128 ->140 -0.10856
130 ->140 0.54682
130 ->141 0.22196
132 ->140 -0.17394
Excited State 24: Singlet-A 4.4851 eV 276.43 nm f=0.0064 <S**2>=0.000
122 ->139 -0.28516
123 ->139 -0.11929
124 ->139 0.46942
125 ->139 0.13273
126 ->145 0.12493
127 ->139 -0.14069
130 ->139 -0.11565
130 ->140 0.17901

132 ->141 -0.10751
Excited State 25: Singlet-A 4.5067 eV 275.11 nm f=0.0035 <S**2>=0.000
124 ->139 0.13738
128 ->140 -0.14595
129 ->141 -0.12470
130 ->139 0.13586
131 ->141 -0.14038
132 ->139 -0.11060
132 ->140 -0.21831
132 ->141 0.50619
Excited State 26: Singlet-A 4.5172 eV 274.47 nm f=0.0030 <S**2>=0.000
122 ->139 0.19568
123 ->139 0.15301
124 ->139 0.21556
125 ->139 0.10795
128 ->139 0.22840
130 ->139 0.48553
132 ->141 -0.13916
133 ->139 0.10837
Excited State 27: Singlet-A 4.5327 eV 273.53 nm f=0.0002 <S**2>=0.000
122 ->139 0.15030
128 ->140 0.46404
129 ->141 -0.11121
130 ->140 0.10422
130 ->141 0.16308
131 ->140 0.14411
131 ->141 -0.19030
132 ->140 0.11702
132 ->141 0.17288
137 ->148 0.12513
138 ->149 -0.11028
Excited State 28: Singlet-A 4.5464 eV 272.71 nm f=0.0174 <S**2>=0.000
127 ->140 -0.14090
128 ->140 -0.12614
128 ->141 -0.20590
131 ->141 -0.12503
138 ->142 0.51033
138 ->148 0.22676
Excited State 29: Singlet-A 4.5672 eV 271.47 nm f=0.0269 <S**2>=0.000
127 ->140 0.13896
128 ->139 0.17822
128 ->140 0.13921
128 ->141 0.24320
130 ->139 0.10606
131 ->141 0.12678
138 ->142 0.43767
138 ->148 -0.22549
Excited State 30: Singlet-A 4.5848 eV 270.42 nm f=0.0055 <S**2>=0.000
122 ->139 -0.30626

123 ->139 -0.16376
124 ->139 -0.11826
127 ->139 0.21465
128 ->139 0.41549
131 ->141 -0.11381
138 ->142 -0.15269
138 ->148 0.10230
Excited State 31: Singlet-A 4.5992 eV 269.58 nm f=0.0003 <S**2>=0.000
136 ->140 0.65957
136 ->141 0.22334
Excited State 32: Singlet-A 4.6551 eV 266.34 nm f=0.0010 <S**2>=0.000
124 ->139 0.14599
127 ->139 0.29202
128 ->141 0.10363
138 ->143 0.52073
138 ->144 0.26207
Excited State 33: Singlet-A 4.6651 eV 265.77 nm f=0.0003 <S**2>=0.000
135 ->140 -0.29386
135 ->141 0.62872
Excited State 34: Singlet-A 4.6661 eV 265.71 nm f=0.0018 <S**2>=0.000
124 ->139 0.18430
126 ->139 0.11918
127 ->139 0.45684
138 ->143 -0.43715
Excited State 35: Singlet-A 4.6886 eV 264.44 nm f=0.0084 <S**2>=0.000
127 ->139 -0.10999
127 ->140 0.25979
128 ->141 -0.19447
131 ->140 -0.16208
131 ->141 -0.10452
132 ->140 -0.10686
138 ->143 -0.10039
138 ->144 0.49704
Excited State 36: Singlet-A 4.7027 eV 263.65 nm f=0.0100 <S**2>=0.000
127 ->139 -0.17704
127 ->140 -0.34953
127 ->141 -0.13137
128 ->141 0.11444
129 ->140 0.14612
131 ->140 0.25645
131 ->141 0.10919
138 ->143 -0.11097
138 ->144 0.36315
Excited State 37: Singlet-A 4.7450 eV 261.29 nm f=0.0043 <S**2>=0.000
127 ->140 -0.10341
127 ->141 0.21560
128 ->140 -0.22305
128 ->141 0.13755
129 ->141 -0.11759

131 ->140 -0.17590
131 ->141 -0.14839
132 ->140 0.33709
132 ->141 0.10252
133 ->140 -0.23564
134 ->140 0.24270
134 ->141 0.11425
138 ->146 0.10892

Excited State 38: Singlet-A 4.7715 eV 259.84 nm f=0.0036 <S**2>=0.000
127 ->141 0.13989
128 ->141 0.13552
132 ->140 -0.12175
133 ->140 0.10137
137 ->146 -0.11319
138 ->146 0.61178

Excited State 39: Singlet-A 4.7790 eV 259.43 nm f=0.0050 <S**2>=0.000
127 ->141 0.37770
128 ->141 0.36642
129 ->141 -0.12810
131 ->140 0.11570
132 ->140 -0.13102
132 ->141 -0.14490
133 ->140 0.10069
134 ->140 -0.13458
138 ->146 -0.25882

Excited State 40: Singlet-A 4.8142 eV 257.54 nm f=0.0034 <S**2>=0.000
129 ->142 -0.24039
129 ->143 -0.23169
129 ->144 0.14403
131 ->140 0.11078
131 ->141 -0.14712
131 ->142 -0.23490
131 ->143 0.30722
132 ->142 -0.22602
138 ->148 -0.10731

Table S2. Excitation energies and oscillator strengths of Bpe-F_4DIB co-crystals

Excited State 1:	Singlet-A	3.9725 eV	312.11 nm	f=0.0043	<S**2>=0.000
82 -> 95	0.11260				
90 -> 92	0.12823				
90 -> 93	0.63943				
91 -> 92	0.10167				
91 -> 93	0.17544				
Excited State 2:	Singlet-A	4.0922 eV	302.98 nm	f=0.3899	<S**2>=0.000
89 -> 92	-0.26560				
90 -> 92	0.12058				
90 -> 93	-0.11751				
91 -> 92	0.61135				
Excited State 3:	Singlet-A	4.1216 eV	300.81 nm	f=0.1043	<S**2>=0.000
88 -> 92	0.44714				
89 -> 92	-0.38878				
90 -> 92	0.17385				
91 -> 92	-0.27799				
Excited State 4:	Singlet-A	4.1362 eV	299.75 nm	f=0.0222	<S**2>=0.000
88 -> 92	0.45066				
89 -> 92	0.47178				
91 -> 92	0.12809				
Excited State 5:	Singlet-A	4.1975 eV	295.37 nm	f=0.0182	<S**2>=0.000
90 -> 93	-0.15316				
91 -> 93	0.66402				
Excited State 6:	Singlet-A	4.3302 eV	286.33 nm	f=0.0585	<S**2>=0.000
88 -> 92	-0.19655				
90 -> 92	0.62746				
90 -> 93	-0.12664				
Excited State 7:	Singlet-A	4.4759 eV	277.01 nm	f=0.0006	<S**2>=0.000
85 -> 93	0.61490				
86 -> 93	0.29677				
Excited State 8:	Singlet-A	4.4899 eV	276.14 nm	f=0.0005	<S**2>=0.000
82 -> 93	0.29659				
87 -> 93	-0.14544				
90 -> 92	-0.10004				
90 -> 94	0.11066				
90 -> 95	0.54853				
91 -> 95	0.15635				
Excited State 9:	Singlet-A	4.5910 eV	270.06 nm	f=0.0342	<S**2>=0.000
85 -> 92	-0.10260				
86 -> 92	0.46082				
87 -> 92	-0.43257				
91 -> 98	-0.17685				
91 -> 99	0.11246				
Excited State 10:	Singlet-A	4.6109 eV	268.89 nm	f=0.0011	<S**2>=0.000
86 -> 92	0.43066				
87 -> 92	0.47198				
91 ->100	0.15232				
91 ->101	0.13112				

Table S3. Excitation energies and oscillator strengths of Bpe crystals

Excited State 1:	Singlet-A	4.0625 eV	305.19 nm	f=0.2087	<S**2>=0.000
90 -> 97	-0.11751				
91 -> 97	-0.12466				
95 -> 97	-0.17665				
96 -> 97	0.61685				
96 -> 98	0.20715				
Excited State 2:	Singlet-A	4.0725 eV	304.44 nm	f=0.8318	<S**2>=0.000
95 -> 97	0.47780				
96 -> 97	0.26332				
96 -> 98	-0.42814				
Excited State 3:	Singlet-A	4.1617 eV	297.92 nm	f=0.0719	<S**2>=0.000
90 -> 97	-0.16166				
91 -> 97	0.57513				
92 -> 97	-0.16846				
95 -> 97	0.14082				
96 -> 98	0.20507				
Excited State 4:	Singlet-A	4.1714 eV	297.22 nm	f=0.3203	<S**2>=0.000
90 -> 97	-0.23829				
91 -> 97	-0.20715				
92 -> 97	0.18240				
95 -> 97	0.39273				
96 -> 97	-0.14665				
96 -> 98	0.39663				
Excited State 5:	Singlet-A	4.1811 eV	296.53 nm	f=0.1155	<S**2>=0.000
90 -> 97	0.53713				
92 -> 97	-0.18568				
95 -> 97	0.22749				
96 -> 97	0.11403				
96 -> 98	0.23594				
Excited State 6:	Singlet-A	4.1995 eV	295.23 nm	f=0.0052	<S**2>=0.000
92 -> 98	-0.14375				
93 -> 98	0.46804				
94 -> 98	0.45208				
Excited State 7:	Singlet-A	4.2171 eV	294.00 nm	f=0.0124	<S**2>=0.000
92 -> 98	0.32571				
93 -> 98	0.44383				
94 -> 98	-0.36752				
Excited State 8:	Singlet-A	4.2742 eV	290.08 nm	f=0.0060	<S**2>=0.000
92 -> 98	-0.11608				
95 -> 98	0.68692				
Excited State 9:	Singlet-A	4.5134 eV	274.70 nm	f=0.0652	<S**2>=0.000
87 -> 97	-0.26359				
90 -> 97	0.22215				
91 -> 97	0.20491				
92 -> 97	0.32229				
93 -> 97	-0.13021				
94 -> 97	0.40397				

95 ->101 0.11653

Excited State 10: Singlet-A 4.5594 eV 271.93 nm f=0.0173 <S**2>=0.000

87 -> 98 0.12065

90 -> 98 0.10850

91 -> 98 0.13949

92 -> 98 0.50650

93 -> 98 -0.14236

94 -> 98 0.32823

95 -> 98 0.13234

96 ->107 -0.11732

Excited State 11: Singlet-A 4.5920 eV 270.00 nm f=0.0258 <S**2>=0.000

88 -> 97 0.65230

95 ->104 0.13971

95 ->106 -0.10178

Excited State 12: Singlet-A 4.6268 eV 267.97 nm f=0.0192 <S**2>=0.000

89 -> 98 0.63859

96 ->105 0.17022

96 ->107 -0.12745