Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Comprehensive structure-function correlation of photoactive ionic π-conjugated supermolecular assemblies: an experimental and computational study

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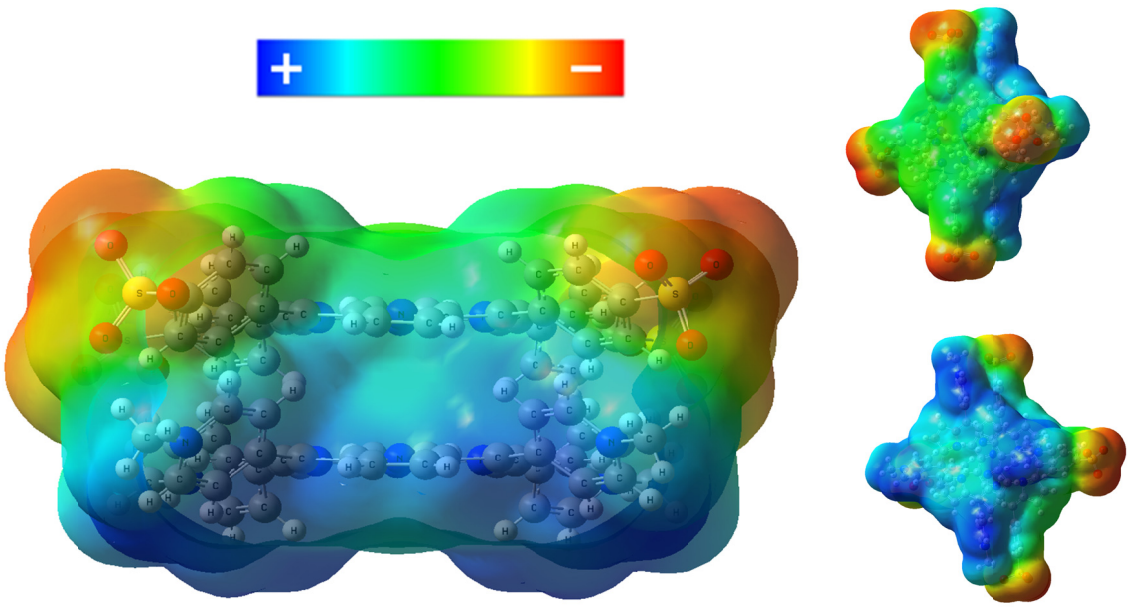
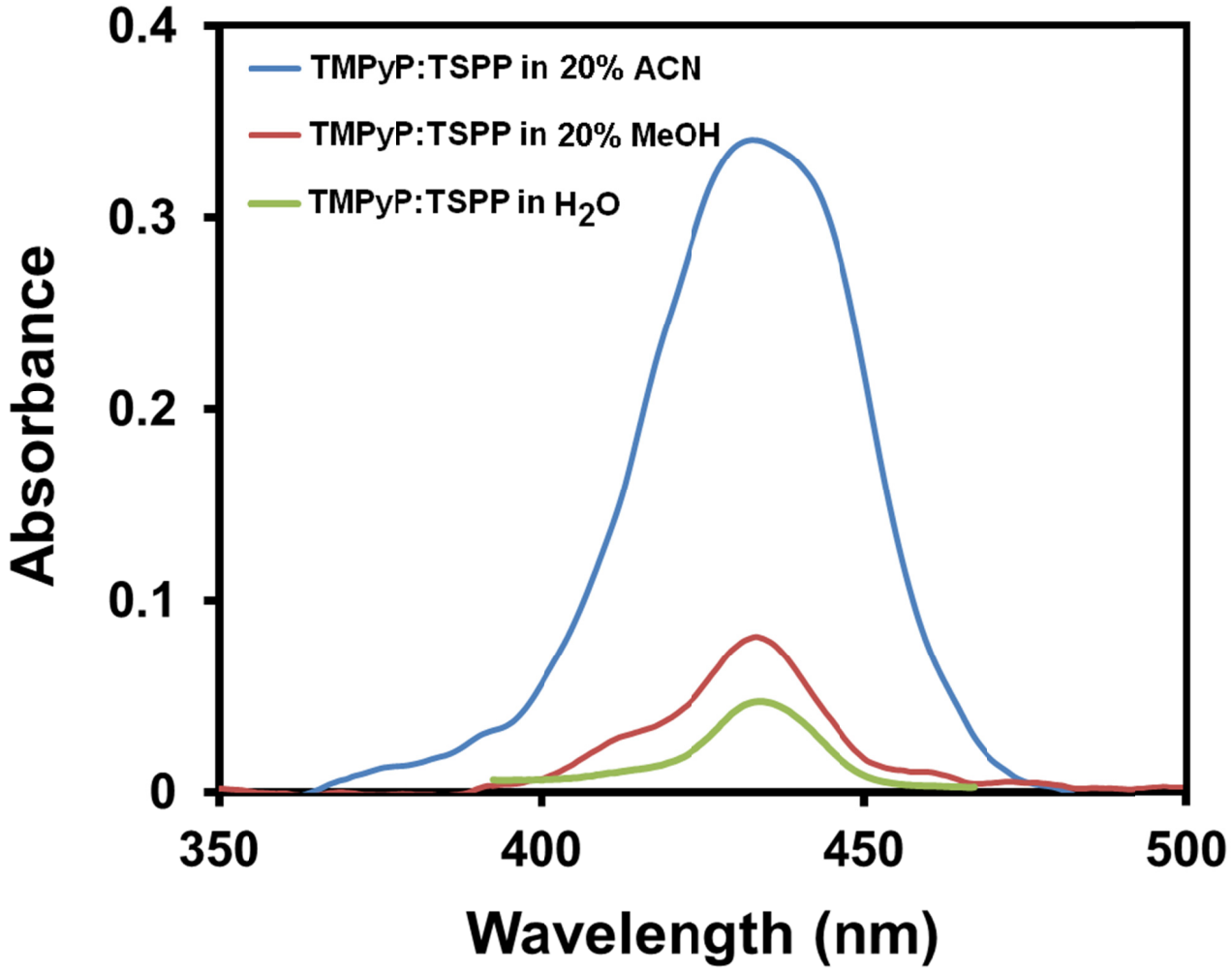
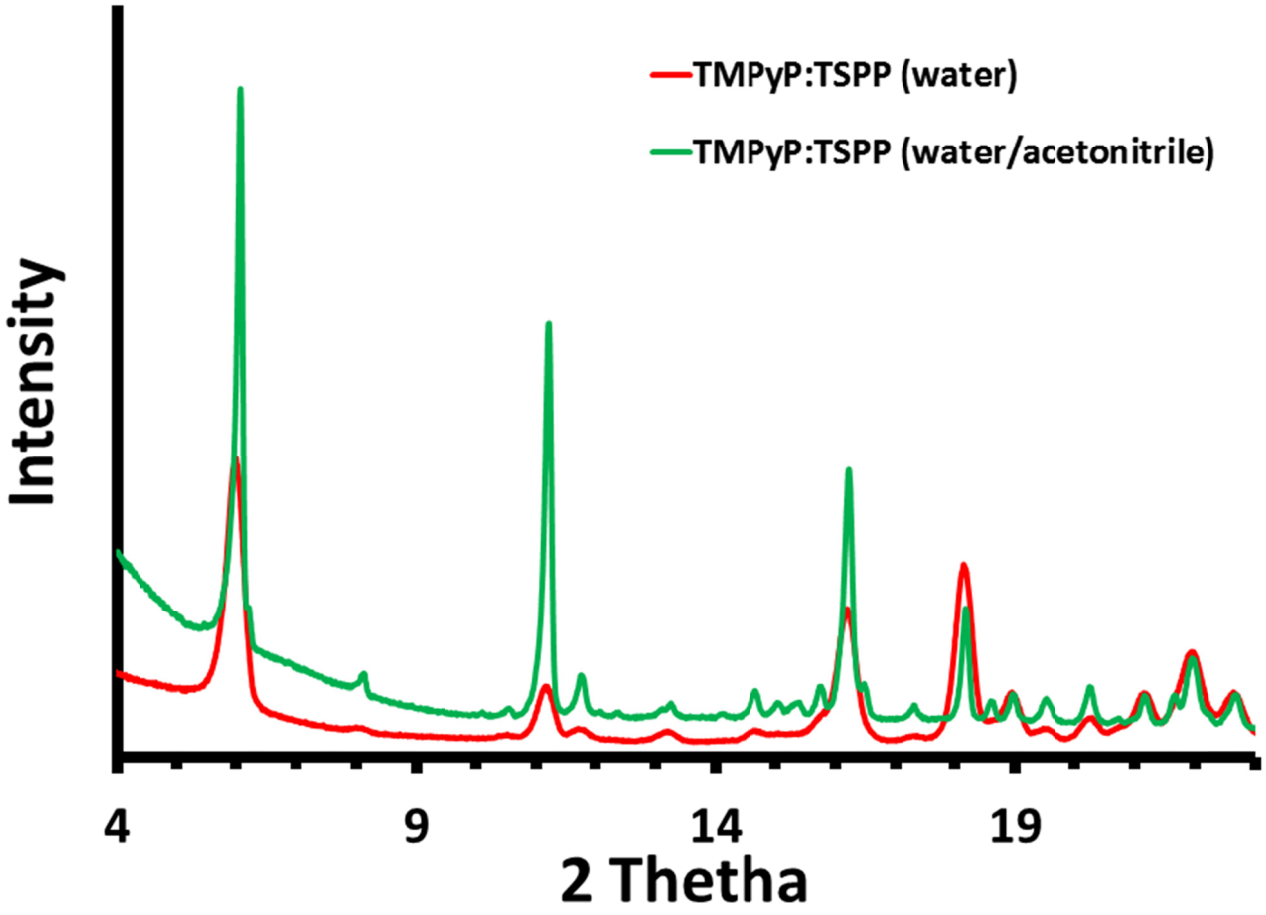


Figure S1. Molecular electrostatic potential (MEP) surfaces of neutrally charged TMPyP:TSPP binary porphyrin complex. The electrostatic potential surface energies range from –67 (red) to +67 (blue) kcal mol^{-1}. The isodensity value for the MEP mapping is 0.03 a.u.


0.4
0.3
0.2
0.1
0
Absorbance
TMPyP:TSPP in 20% ACN
TMPyP:TSPP in 20% MeOH
TMPyP:TSPP in H_2O
350
400
450
500
Wavelength (nm)

),
K.


TMPyP:TSPP (water)
TMPyP:TSPP (water/acetonitrile)
Intensity
4
9
14
19
2 Thetha

(red)
re is

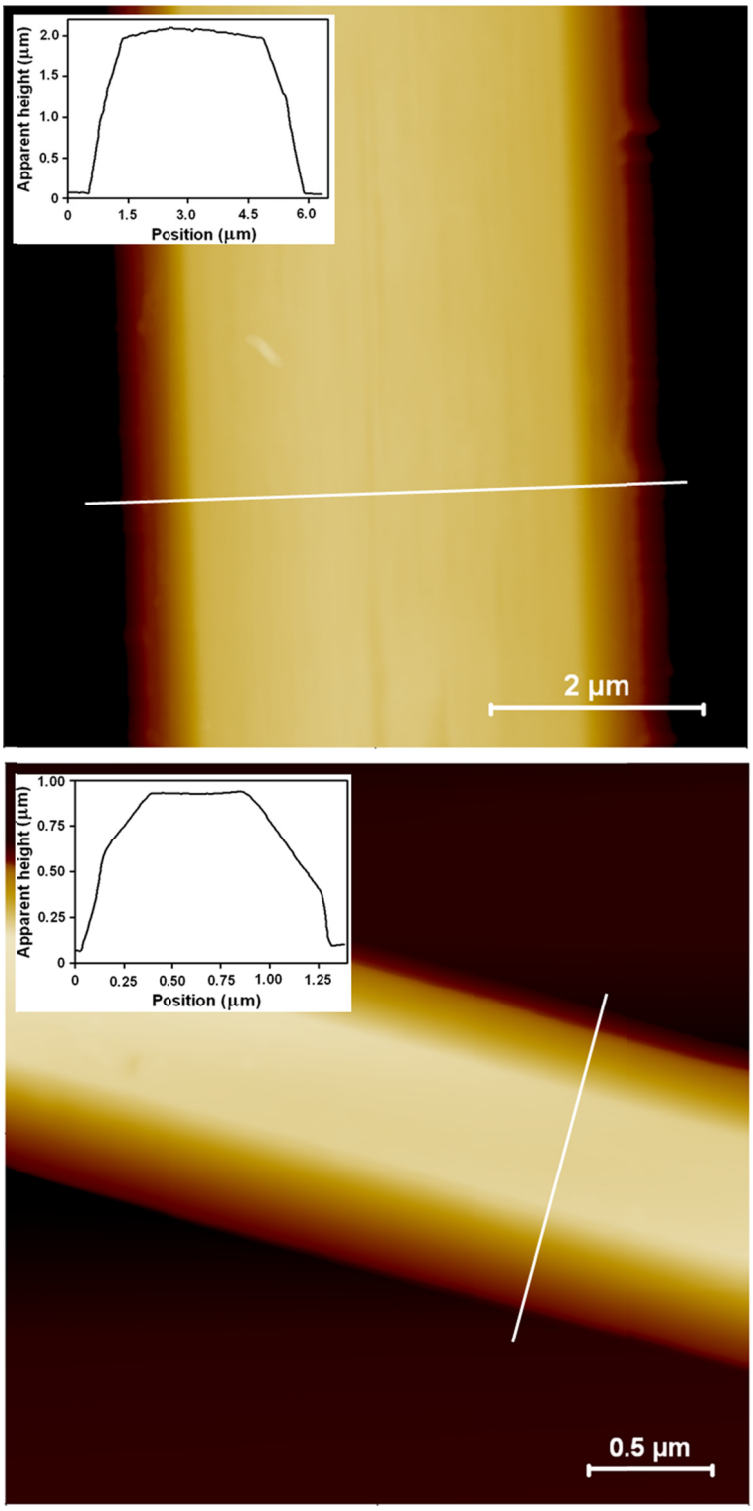


Figure S4. AFM images and corresponding cross sectional profiles of two different TMPyP:TSPP crystalline rods.

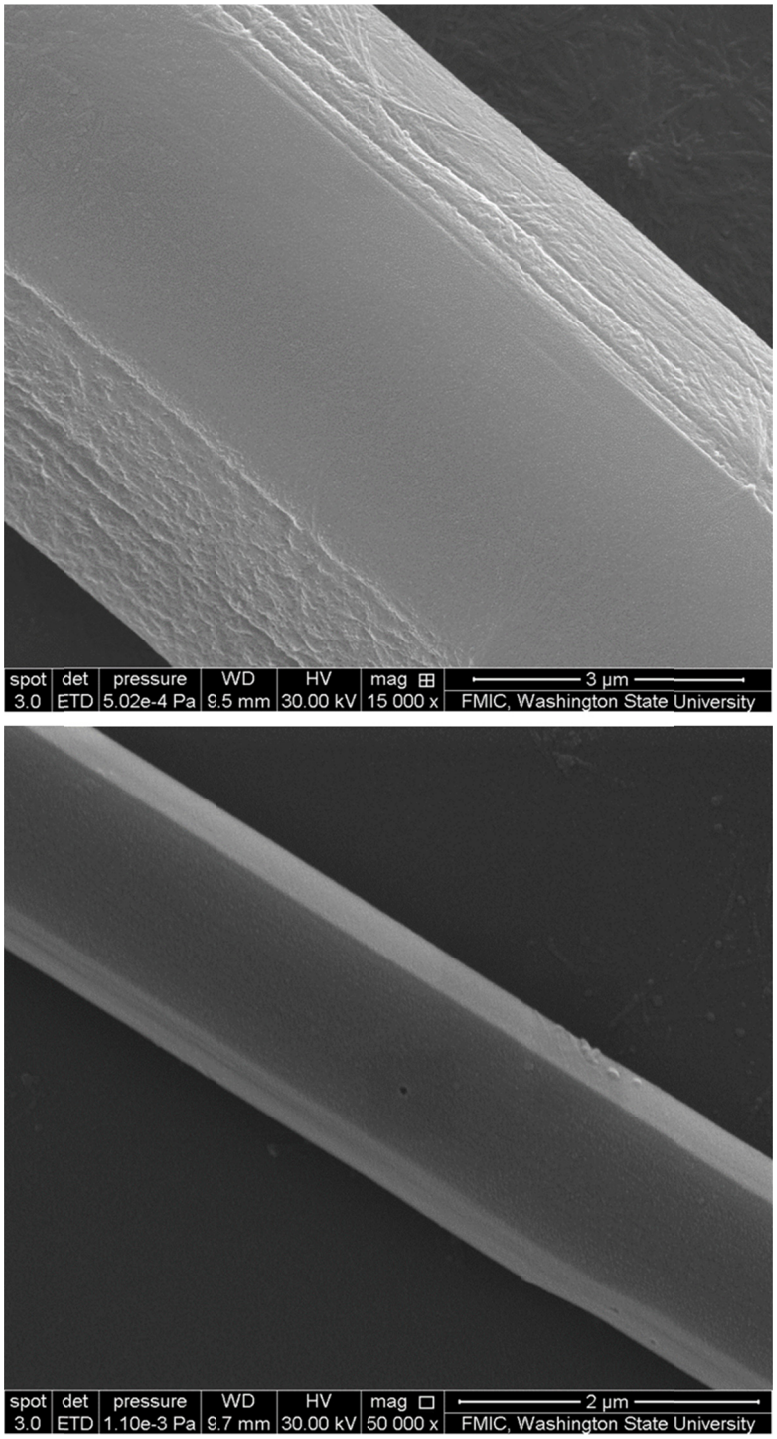


Figure S5. SEM micrographs illustrating morphology of a TMPyP:TSPP crystalline rod. The top surface and sloping sides of the crystals are flat with the top face being smoother than the sides.

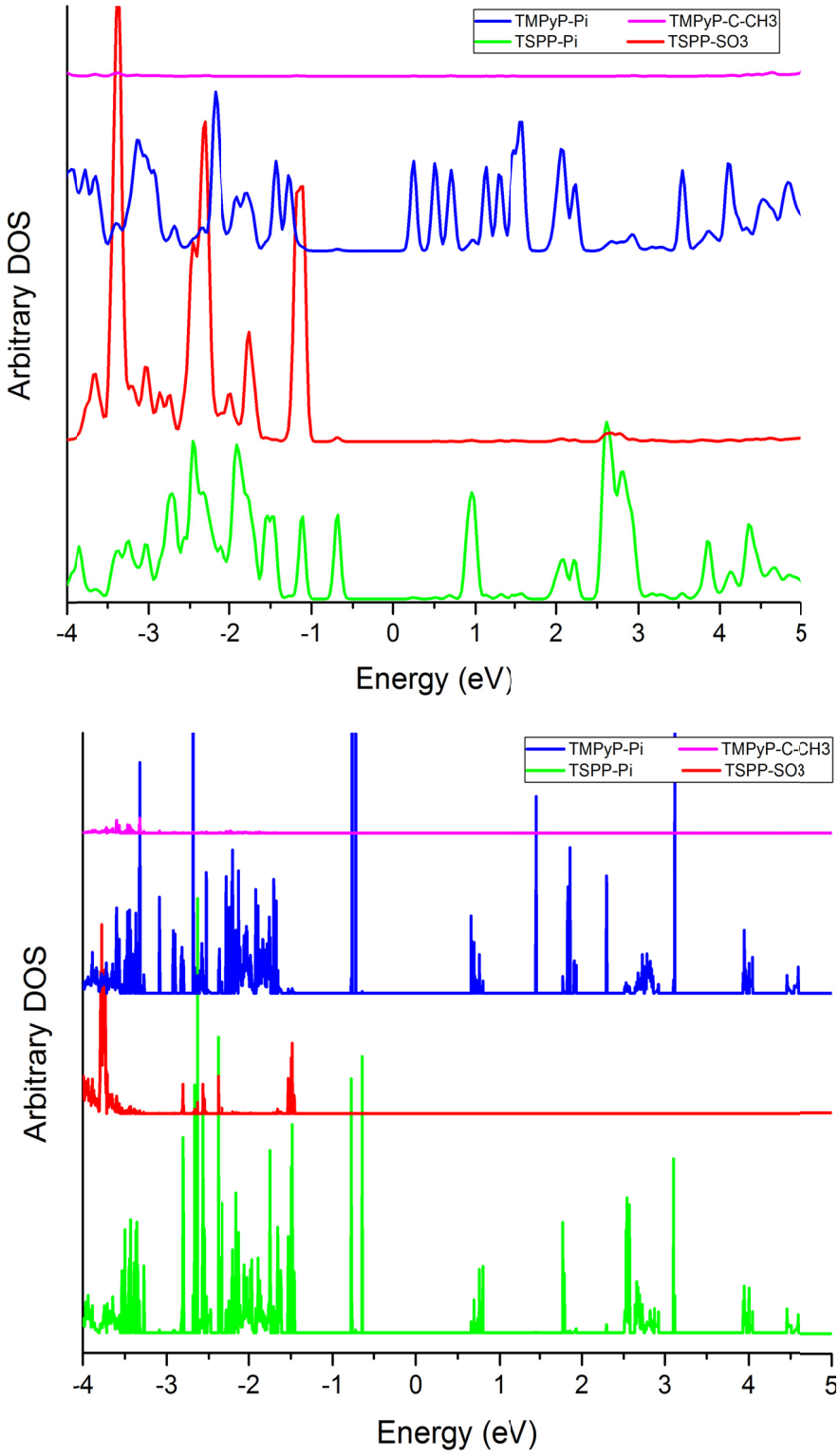


Figure S6. Projected density of states (pDOS) of TMPyP:TSPP crystal from DFT (top) and EHTB (bottom). In the images pDOS is plotted as a function of TMPyP, TSPP components and as a function of π-stacking components and non π-stacking components.

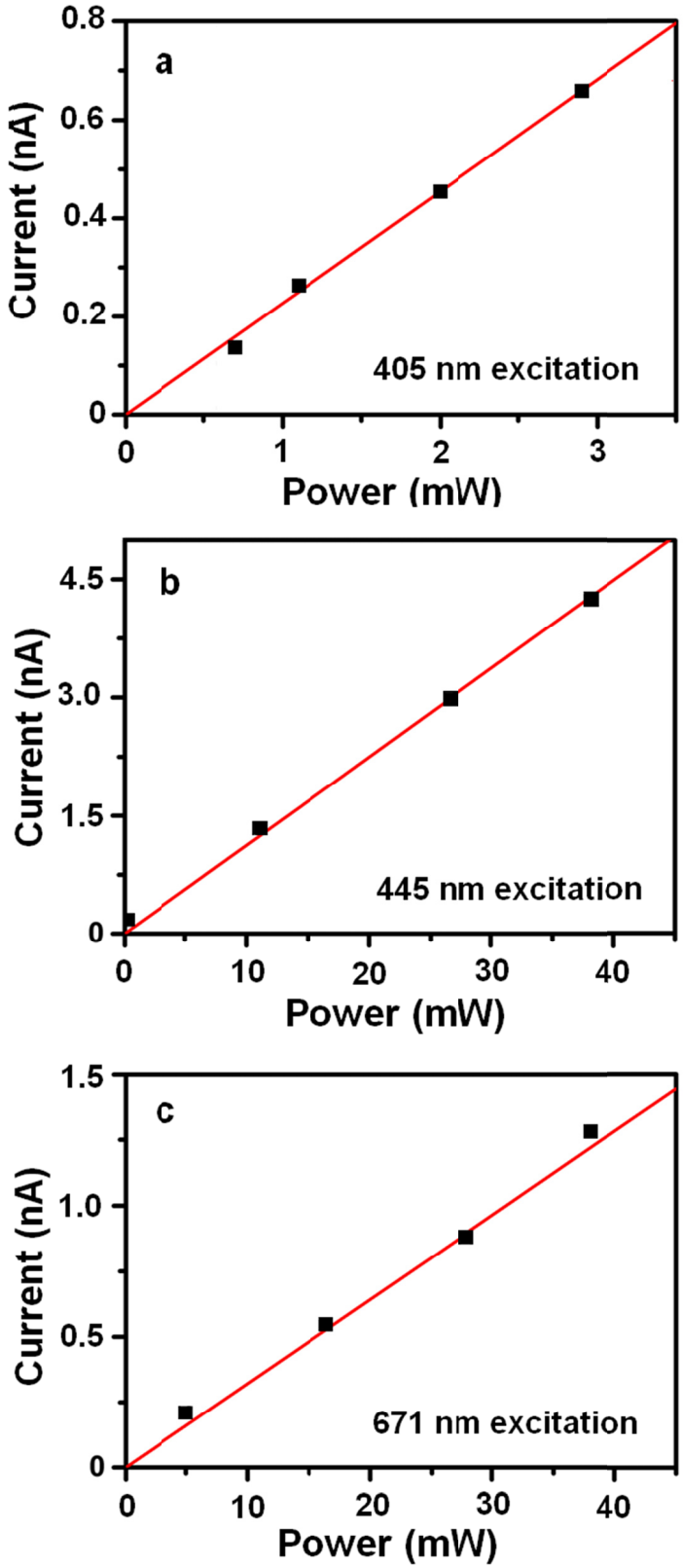


Figure S7. Power dependence of the photoconductivity of TMPyP:TSPP measured at different illumination wavelengths. Graph (a) was obtained with 405 nm excitation and has a slope of 0.223 nA/mW. Trace (b) was acquired with 445 nm excitation and has a slope of 0.133 nA/mW. Plot (c) was recorded with 671 nm excitation and has a slope of 0.032 nA/mW.

Field effect experiments were carried out by exciting the TMPyP:TSPP crystals at 445 nm (14 mW/mm^2) while applying V_{SD} = 120 mV and applying V_G of -300, -200, -100, 0, 100, 200, and 300 V to determine the sign of the primary charge carrier.

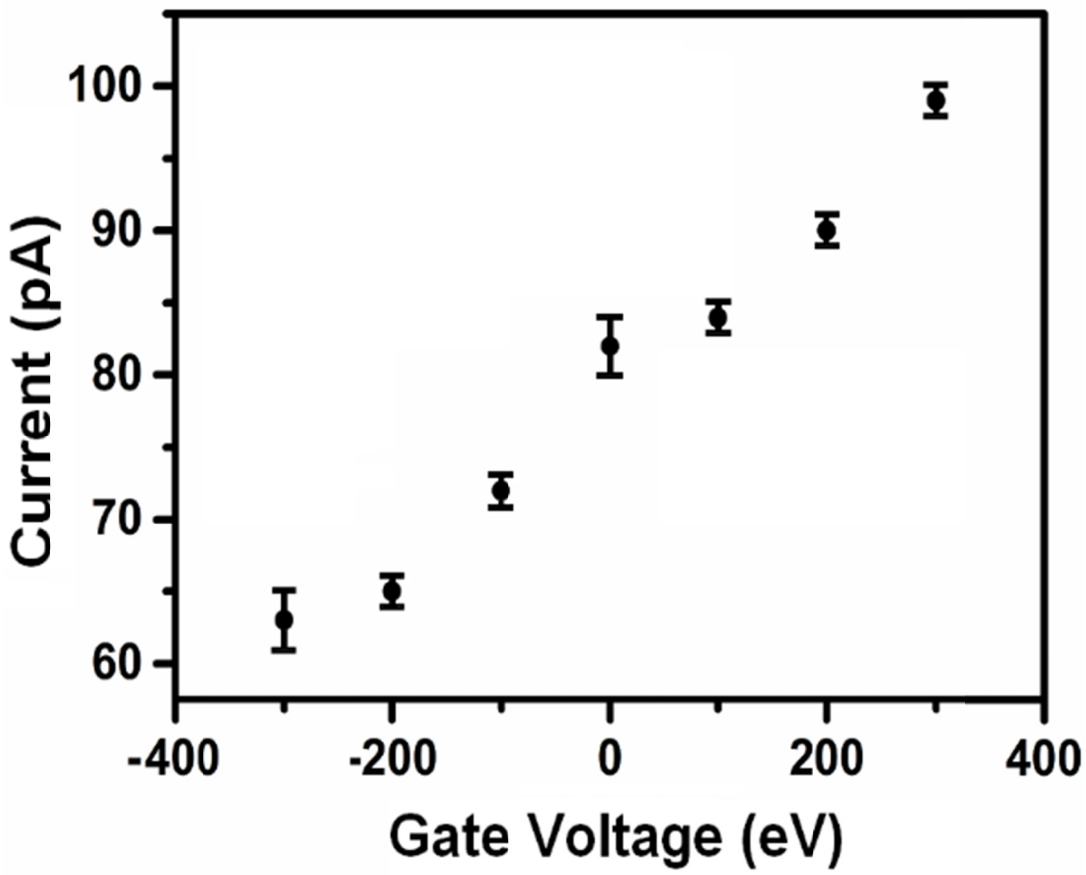


Figure S8. Gate Voltage (V_G) dependence of the TMPyP:TSPP photoconductivity. V_{SD} = 120 mV. The decrease in current with application of a negative voltage and increase in current with the application of a positive gate voltage is consistent with the behavior of an n-type photoconductor.

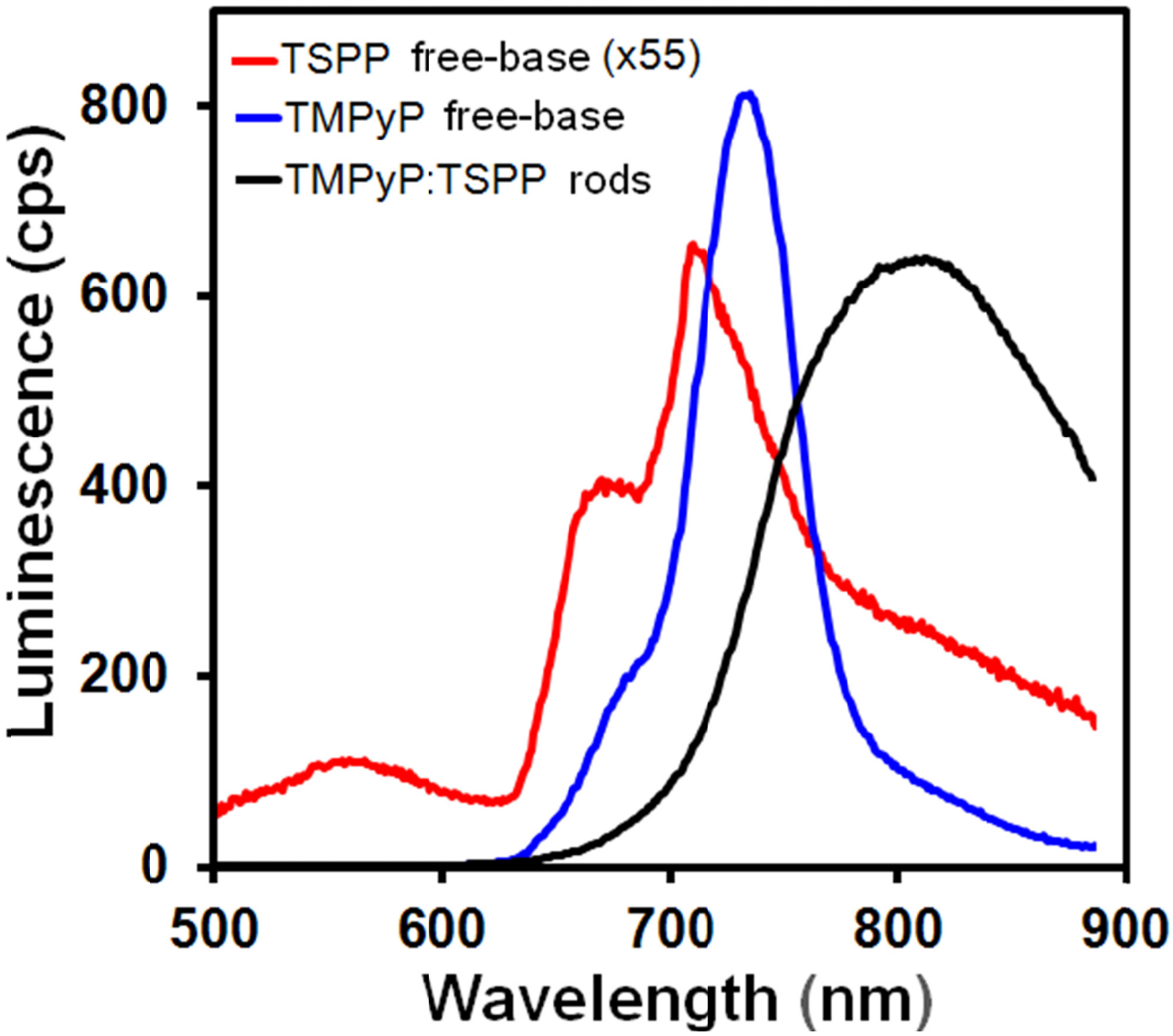


Figure S9. Solid state luminescence spectra of free-base forms of the TMPyP and TSPP tectons and the TMPyP:TSPP rods. Note the scale factor on the TSPP emission.

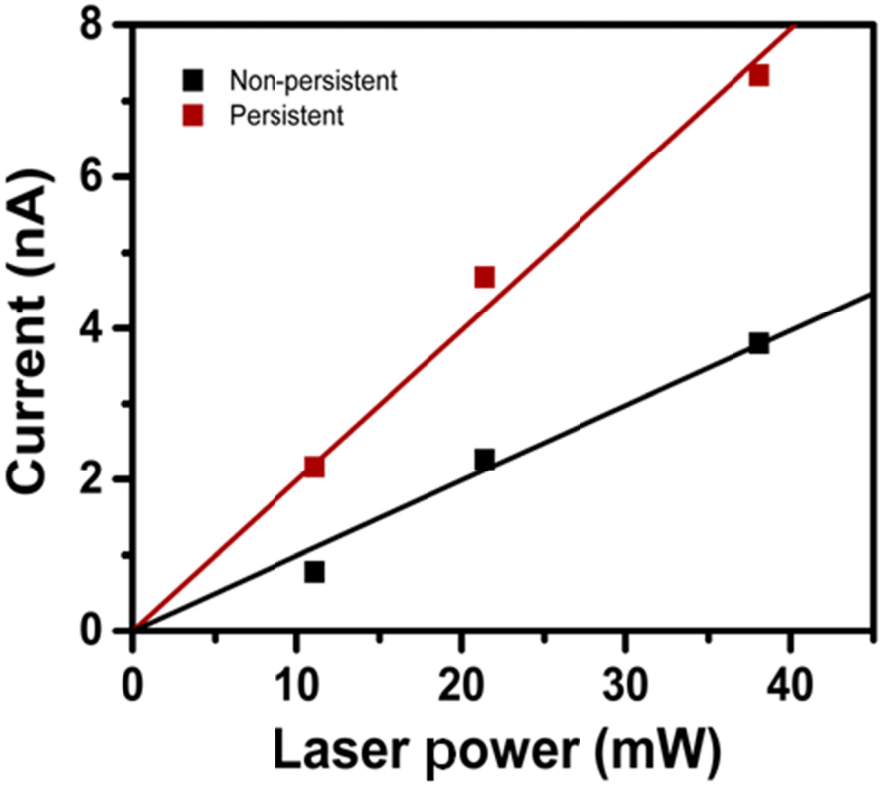


Figure S10. Photocurrent versus laser power of TMPyP:TSPP rods illuminated with 445 nm laser light.

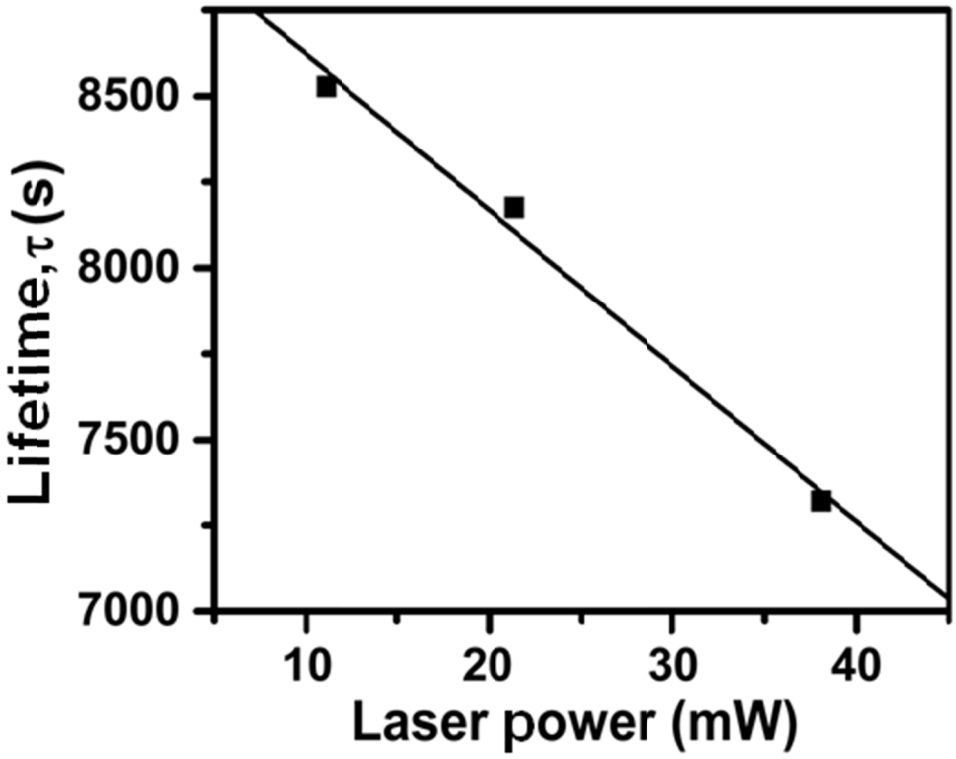


Figure S11. Lifetime of PPC versus laser power of TMPyP:TSPP rods illuminated with 445 nm laser light.

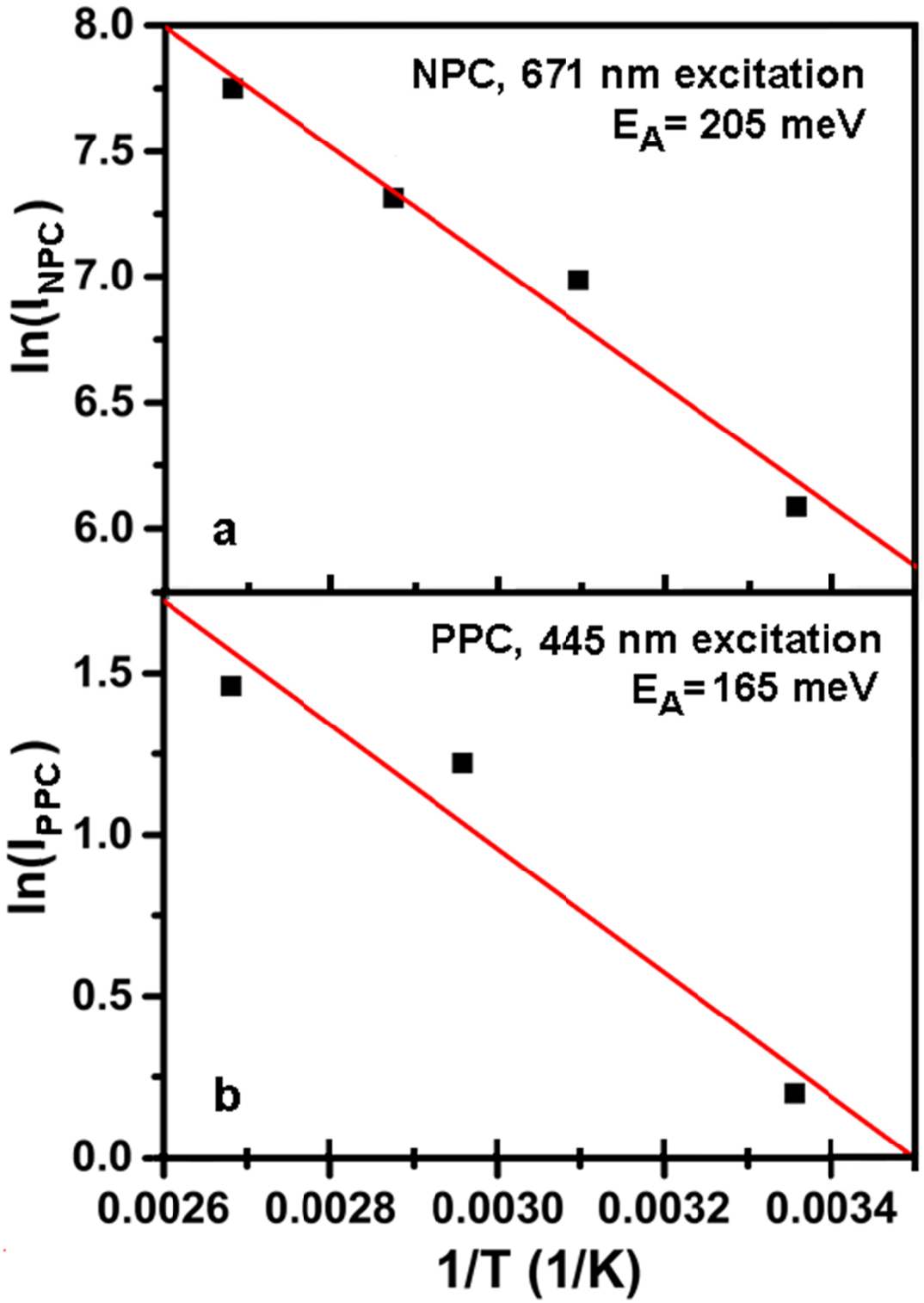


Figure S12. Arrhenius plots of the photoconductivity of TMPyP:TSPP assemblies as a function of temperature for: (a) nonpersistent photoconductivity with 671 nm excitation and (b) persistent photoconductivity with 445 nm excitation. Calculated activation energies associated with each plot are shown.

Table S1. Data collection and structure refinement parameters from XRD experiment of TMPyP:TSPP nanorods.

Parameter type	**Parameter value**	
Theta range for data collection	3.09 to 66.76°	
Index ranges	$9 \leq h \leq 9$, $-19 \leq k \leq 19$, $-32 \leq l \leq 34$	
Reflections collected	33146	
Independent reflections	6977 [R(int) = 0.0818]	
Coverage of independent reflections	99.1%	
Absorption correction	Multi-Scan	
Refinement method	Full-matrix least-squares on F2	
Refinement program	SHELXL-2014/7[a]	
Function minimized	$\Sigma\, w(Fo^2 - Fc^2)2$	
Data / restraints / parameters	6977 / 852 / 591	
Goodness-of-fit on F2	1.023	
Final R indices	4493 data; I>2σ(I)	R1 = 0.0625, wR2 = 0.1591
	all data	R1 = 0.1056, wR2 = 0.1808
Weighting scheme	w=1/[σ2(Fo2)+(0.0917P)2+1.2876P] where $P=(Fo^2+2Fc^2)/3$	
Extinction coefficient	0.0007(1)	
Largest diff. peak and hole	1.183 and -0.460 eÅ-3	
R.M.S. deviation from mean	0.087 eÅ-3	
Density	1.47 g/cm^3	

[a]Reference 1.

Table S2. Atomic coordinates and equivalent isotropic atomic displacement parameters of TMPyP:TSPP crystals.				
	x/a	**y/b**	**z/c**	**U(eq)***
S1	0.21791(12)	0.03741(5)	0.09218(4)	0.0325(3)
S2	0.28441(12)	0.31794(6)	0.30155(4)	0.0376(3)
O1	0.0895(3)	0.06436(14)	0.06061(10)	0.0363(7)
O2	0.3631(3)	0.08680(14)	0.09083(11)	0.0397(7)
O3	0.1632(4)	0.02518(15)	0.13852(10)	0.0408(8)
O4	0.4038(4)	0.25514(19)	0.31112(11)	0.0512(8)
O5	0.1200(3)	0.28807(18)	0.30180(10)	0.0448(8)
O6	0.3146(4)	0.38902(19)	0.33054(11)	0.0519(9)
O7	0.5783(5)	0.1492(2)	0.25796(13)	0.0646(10)
O8	0.9245(5)	0.14459(19)	0.27490(13)	0.0611(10)
O9	0.9427(5)	0.1389(2)	0.17849(12)	0.0579(9)
O10	0.5992(4)	0.14264(19)	0.16284(14)	0.0535(9)
N1	0.9105(4)	0.55249(16)	0.05771(11)	0.0265(7)
N2	0.0075(4)	0.39021(16)	0.03590(11)	0.0256(7)
N3	0.8119(4)	0.37150(18)	0.24805(11)	0.0295(7)
N4	0.2240(4)	0.06609(16)	0.93015(12)	0.0281(7)
N5	0.4896(3)	0.61127(16)	0.96641(10)	0.0236(7)
N6	0.4118(4)	0.55367(16)	0.05769(11)	0.0259(7)
C5	0.8635(4)	0.63281(19)	0.06012(13)	0.0249(8)
C6	0.7881(4)	0.6455(2)	0.10317(14)	0.0286(9)
C7	0.7928(4)	0.5744(2)	0.12637(14)	0.0296(9)
C8	0.8728(4)	0.5158(2)	0.09813(13)	0.0259(8)
C9	0.9031(4)	0.4344(2)	0.10984(13)	0.0261(8)
C10	0.9605(4)	0.3750(2)	0.07925(13)	0.0250(8)
C11	0.9862(4)	0.2898(2)	0.08923(14)	0.0263(8)
O11	0.6887(16)	0.5557(10)	0.2699(5)	0.068(4)
C12	0.0445(4)	0.2556(2)	0.05168(13)	0.0268(8)
C13	0.0595(4)	0.3186(2)	0.01771(13)	0.0256(8)
C14	0.1155(4)	0.30715(19)	0.97324(13)	0.0252(8)
C15	0.8737(4)	0.4096(2)	0.15780(13)	0.0249(8)
C16	0.9381(5)	0.4554(2)	0.19467(14)	0.0297(9)
C17	0.9056(5)	0.4356(2)	0.23909(14)	0.0315(9)
C18	0.7514(4)	0.3239(2)	0.21344(14)	0.0288(8)
C19	0.7808(4)	0.3416(2)	0.16892(14)	0.0278(8)
C20	0.7721(5)	0.3534(3)	0.29615(14)	0.0367(10)
C21	0.1530(4)	0.2220(2)	0.95933(13)	0.0248(8)
C22	0.2592(4)	0.1712(2)	0.98507(14)	0.0277(8)
C23	0.2916(4)	0.0948(2)	0.96964(14)	0.0279(8)
C24	0.2668(5)	0.9845(2)	0.91282(16)	0.0359(10)
C25	0.1178(5)	0.1120(2)	0.90541(14)	0.0291(9)
C26	0.0816(4)	0.1897(2)	0.91914(13)	0.0262(8)
C27	0.5325(4)	0.62550(19)	0.92269(13)	0.0246(8)
C28	0.5036(4)	0.7104(2)	0.91185(14)	0.0264(8)
C29	0.4481(4)	0.7455(2)	0.94973(13)	0.0268(8)

C30	0.4369(4)	0.6836(2)	0.98445(13)	0.0245(8)
C31	0.3831(4)	0.69569(19)	0.02895(13)	0.0249(8)
C32	0.3634(4)	0.6338(2)	0.06163(13)	0.0255(8)
C33	0.2867(4)	0.6436(2)	0.10458(13)	0.0261(8)
C34	0.2891(4)	0.5705(2)	0.12592(14)	0.0284(9)
C35	0.3712(4)	0.5140(2)	0.09702(13)	0.0249(8)
C36	0.4039(4)	0.4318(2)	0.10788(13)	0.0241(8)
C37	0.3448(4)	0.7804(2)	0.04356(13)	0.0243(8)
C38	0.4146(4)	0.8122(2)	0.08427(13)	0.0254(8)
C39	0.3796(4)	0.8911(2)	0.09871(14)	0.0272(8)
C40	0.2725(5)	0.9389(2)	0.07239(14)	0.0281(8)
C41	0.2046(4)	0.9092(2)	0.03168(14)	0.0287(9)
C42	0.2395(4)	0.8307(2)	0.01754(14)	0.0259(8)
C43	0.3705(4)	0.4044(2)	0.15556(13)	0.0259(8)
C44	0.2805(4)	0.3337(2)	0.16301(14)	0.0284(9)
C45	0.2535(4)	0.3074(2)	0.20748(14)	0.0311(9)
C46	0.3133(4)	0.3523(2)	0.24450(14)	0.0308(9)
C47	0.3995(5)	0.4227(2)	0.23786(14)	0.0318(9)
C48	0.4290(4)	0.4483(2)	0.19350(14)	0.0293(9)
*U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.				

Table S3. Interatomic distances (Å) in TMPyP:TSPP crystal structure.

S1-O1	1.448(3)	**S1-O2**	1.455(3)
S1-O3	1.459(3)	**S1-C40**	1.782(3)
S2-O4	1.449(3)	**S2-O5**	1.451(3)
S2-O6	1.456(3)	**S2-C46**	1.784(4)
O7-H7	1.12(5)	**O8-H8**	1.02(4)
O9-H9	0.98(8)	**O10-H10**	0.85(5)
N1-C8	1.373(5)	**N1-C5**	1.377(4)
N2-C10	1.363(5)	**N2-C13**	1.366(4)
N2-H2	0.88	**N3-C17**	1.341(5)
N3-C18	1.356(5)	**N3-C20**	1.486(5)
N4-C23	1.345(5)	**N4-C25**	1.345(5)
N4-C24	1.480(4)	**N5-C27**	1.360(5)
N5-C30	1.377(4)	**N5-H5**	0.88
N6-C35	1.374(5)	**N6-C32**	1.382(4)
C5-C14	1.401(5)	**C5-C6**	1.443(5)
C6-C7	1.349(5)	**C6-H6**	0.95
C7-C8	1.447(5)	**C7-H7**	0.95
C8-C9	1.399(5)	**C9-C10**	1.418(5)
C9-C15	1.488(5)	**C10-C11**	1.443(5)
C11-C12	1.341(5)	**C11-H11**	0.95
O11-H11	1.17(6)	**C12-C13**	1.443(5)
C12-H12	0.95	**C13-C14**	1.411(5)
C14-C5	1.401(5)	**C14-C21**	1.492(5)
C15-C16	1.400(5)	**C15-C19**	1.404(5)

C16-C17	1.375(6)	**C16-H16**	0.95
C17-H17	0.95	**C18-C19**	1.364(5)
C18-H18	0.95	**C19-H19**	0.95
C20-H20A	0.98	**C20-H20B**	0.98
C20-H20C	0.98	**C21-C26**	1.396(5)
C21-C22	1.407(5)	**C22-C23**	1.364(5)
C22-H22	0.95	**C23-H23**	0.95
C24-H24A	0.98	**C24-H24B**	0.98
C24-H24C	0.98	**C25-C26**	1.375(5)
C25-H25	0.95	**C26-H26**	0.95
C27-C36	1.414(5)	**C27-C28**	1.447(5)
C28-C29	1.345(5)	**C28-H28**	0.95
C29-C30	1.441(5)	**C29-H29**	0.95
C30-C31	1.406(5)	**C31-C32**	1.407(5)
C31-C37	1.492(5)	**C32-C33**	1.439(5)
C33-C34	1.352(5)	**C33-H33**	0.95
C34-C35	1.444(5)	**C34-H34**	0.95
C35-C36	1.410(5)	**C36-C27**	1.414(5)
C36-C43	1.500(5)	**C37-C38**	1.401(5)
C37-C42	1.402(5)	**C38-C39**	1.396(5)
C38-H38	0.95	**C39-C40**	1.393(5)
C39-H39	0.95	**C40-C41**	1.382(6)
C41-C42	1.389(5)	**C41-H41**	0.95
C42-H42	0.95	**C43-C48**	1.391(5)
C43-C44	1.402(5)	**C44-C45**	1.395(5)
C44-H44	0.95	**C45-C46**	1.382(6)
C45-H45	0.95	**C46-C47**	1.377(5)
C47-C48	1.393(6)	**C47-H47**	0.95
C48-H48	0.95		

Table S4. Bond angles (°) in TMPyP:TSPP crystal structure.			
O1-S1-O2	113.63(16)	**O1-S1-O3**	112.43(17)
O2-S1-O3	113.16(18)	**O1-S1-C40**	105.16(18)
O2-S1-C40	105.90(16)	**O3-S1-C40**	105.64(16)
O4-S2-O5	113.26(19)	**O4-S2-O6**	111.0(2)
O5-S2-O6	113.95(19)	**O4-S2-C46**	106.66(17)
O5-S2-C46	106.01(18)	**O6-S2-C46**	105.19(18)
C8-N1-C5	107.5(3)	**C10-N2-C13**	108.1(3)
C10-N2-H2	125.9	**C13-N2-H2**	125.9
C17-N3-C18	120.4(3)	**C17-N3-C20**	119.7(3)
C18-N3-C20	119.9(3)	**C23-N4-C25**	120.2(3)
C23-N4-C24	120.8(3)	**C25-N4-C24**	119.0(3)
C27-N5-C30	108.1(3)	**C27-N5-H5**	125.9
C30-N5-H5	125.9	**C35-N6-C32**	107.4(3)
N1-C5-C14	126.4(3)	**N1-C5-C6**	108.5(3)
C14-C5-C6	125.1(3)	**C7-C6-C5**	107.9(3)
C7-C6-H6	126.0	**C5-C6-H6**	126.0
C6-C7-C8	107.1(3)	**C6-C7-H7**	126.5
C8-C7-H7	126.5	**N1-C8-C9**	125.7(3)
N1-C8-C7	108.9(3)	**C9-C8-C7**	125.3(3)
C8-C9-C10	124.3(3)	**C8-C9-C15**	117.1(3)
C10-C9-C15	118.5(3)	**N2-C10-C9**	125.2(3)
N2-C10-C11	108.6(3)	**C9-C10-C11**	126.2(3)
C12-C11-C10	107.3(3)	**C12-C11-H11**	126.4
C10-C11-H11	126.4	**C11-C12-C13**	107.8(3)
C11-C12-H12	126.1	**C13-C12-H12**	126.1
N2-C13-C14	126.5(3)	**N2-C13-C12**	108.2(3)
C14-C13-C12	125.3(3)	**C5-C14-C13**	126.9(3)
C5-C14-C21	115.8(3)	**C13-C14-C21**	117.2(3)
C16-C15-C19	116.5(3)	**C16-C15-C9**	120.2(3)
C19-C15-C9	123.3(4)	**C17-C16-C15**	120.9(3)
C17-C16-H16	119.6	**C15-C16-H16**	119.6
N3-C17-C16	120.6(4)	**N3-C17-H17**	119.7
C16-C17-H17	119.7	**N3-C18-C19**	120.8(3)
N3-C18-H18	119.6	**C19-C18-H18**	119.6
C18-C19-C15	120.8(4)	**C18-C19-H19**	119.6
C15-C19-H19	119.6	**N3-C20-H20A**	109.5
N3-C20-H20B	109.5	**H20A-C20-H20B**	109.5
N3-C20-H20C	109.5	**H20A-C20-H20C**	109.5
H20B-C20-H20C	109.5	**C26-C21-C22**	117.2(3)
C26-C21-C14	119.9(3)	**C22-C21-C14**	122.9(3)
C23-C22-C21	119.8(4)	**C23-C22-H22**	120.1
C21-C22-H22	120.1	**N4-C23-C22**	121.6(4)
N4-C23-H23	119.2	**C22-C23-H23**	119.2
N4-C24-H24A	109.5	**N4-C24-H24B**	109.5
H24A-C24-H24B	109.5	**N4-C24-H24C**	109.5
H24A-C24-H24C	109.5	**H24B-C24-H24C**	109.5
N4-C25-C26	120.6(4)	**N4-C25-H25**	119.7

C26-C25-H25	119.7	**C25-C26-C21**	120.5(4)
C25-C26-H26	119.8	**C21-C26-H26**	119.8
N5-C27-C36	126.7(3)	**N5-C27-C28**	108.8(3)
C36-C27-C28	124.4(3)	**C29-C28-C27**	107.0(3)
C29-C28-H28	126.5	**C27-C28-H28**	126.5
C28-C29-C30	108.1(3)	**C28-C29-H29**	126.0
C30-C29-H29	126.0	**N5-C30-C31**	126.5(3)
N5-C30-C29	107.9(3)	**C31-C30-C29**	125.6(3)
C30-C31-C32	125.1(3)	**C30-C31-C37**	118.4(3)
C32-C31-C37	116.5(3)	**N6-C32-C31**	126.0(3)
N6-C32-C33	108.6(3)	**C31-C32-C33**	125.4(3)
C34-C33-C32	107.7(3)	**C34-C33-H33**	126.1
C32-C33-H33	126.1	**C33-C34-C35**	107.4(3)
C33-C34-H34	126.3	**C35-C34-H34**	126.3
N6-C35-C36	126.1(3)	**N6-C35-C34**	108.9(3)
C36-C35-C34	125.0(3)	**C35-C36-C27**	124.6(3)
C35-C36-C43	117.0(3)	**C27-C36-C43**	118.4(3)
C38-C37-C42	117.7(3)	**C38-C37-C31**	120.3(3)
C42-C37-C31	122.0(3)	**C39-C38-C37**	121.2(4)
C39-C38-H38	119.4	**C37-C38-H38**	119.4
C40-C39-C38	119.5(4)	**C40-C39-H39**	120.2
C38-C39-H39	120.2	**C41-C40-C39**	120.2(3)
C41-C40-S1	119.9(3)	**C39-C40-S1**	119.9(3)
C40-C41-C42	120.0(4)	**C40-C41-H41**	120.0
C42-C41-H41	120.0	**C41-C42-C37**	121.3(4)
C41-C42-H42	119.4	**C37-C42-H42**	119.4
C48-C43-C44	118.4(4)	**C48-C43-C36**	120.8(3)
C44-C43-C36	120.9(3)	**C45-C44-C43**	120.6(4)
C45-C44-H44	119.7	**C43-C44-H44**	119.7
C46-C45-C44	119.7(3)	**C46-C45-H45**	120.2
C44-C45-H45	120.2	**C47-C46-C45**	120.6(4)
C47-C46-S2	119.2(3)	**C45-C46-S2**	120.2(3)
C46-C47-C48	119.8(4)	**C46-C47-H47**	120.1
C48-C47-H47	120.1	**C43-C48-C47**	121.0(4)
C43-C48-H48	119.5	**C47-C48-H48**	119.5

Table S5. Anisotropic atomic displacement parameters (Å2) in TMPyP:TSPP crystal structure. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	0.0438(6)	0.0156(4)	0.0388(7)	-0.0001(4)	0.0099(5)	0.0027(4)
S2	0.0409(6)	0.0451(6)	0.0272(6)	0.0063(5)	0.0063(4)	0.0049(5)
O1	0.0378(15)	0.0221(12)	0.0493(19)	0.0011(12)	0.0056(13)	0.0047(11)
O2	0.0437(16)	0.0200(12)	0.056(2)	-0.0006(13)	0.0060(14)	-0.0002(11)
O3	0.0633(19)	0.0240(13)	0.0361(18)	-0.0039(12)	0.0147(15)	0.0102(12)
O4	0.0530(18)	0.0634(19)	0.0376(19)	0.0167(16)	0.0084(15)	0.0183(15)
O5	0.0399(16)	0.0599(18)	0.0344(18)	0.0127(15)	0.0023(13)	-0.0037(14)
O6	0.071(2)	0.0539(18)	0.0317(19)	-0.0063(15)	0.0088(16)	-0.0065(16)
O7	0.078(3)	0.064(2)	0.052(2)	0.0024(19)	0.005(2)	0.0074(19)
O8	0.075(3)	0.0474(19)	0.061(3)	0.0069(18)	0.009(2)	0.0066(17)
O9	0.070(2)	0.0526(19)	0.052(2)	-0.0114(17)	0.0121(19)	0.0027(18)
O10	0.069(2)	0.0429(18)	0.049(2)	0.0015(17)	0.006(2)	0.0103(16)
N1	0.0381(18)	0.0162(13)	0.0254(18)	0.0005(12)	0.0034(14)	0.0011(12)
N2	0.0373(18)	0.0148(13)	0.0248(18)	-0.0008(12)	0.0022(14)	0.0015(12)
N3	0.0336(17)	0.0319(16)	0.0230(18)	0.0012(14)	0.0022(14)	0.0052(13)
N4	0.0359(17)	0.0172(13)	0.032(2)	-0.0015(13)	0.0082(14)	-0.0009(12)
N5	0.0351(17)	0.0127(12)	0.0232(18)	-0.0006(12)	0.0031(14)	0.0002(11)
N6	0.0351(17)	0.0186(13)	0.0239(18)	0.0028(12)	0.0009(14)	0.0004(12)
C5	0.032(2)	0.0169(15)	0.026(2)	0.0000(15)	0.0030(16)	-0.0006(14)
C6	0.036(2)	0.0184(16)	0.032(2)	-0.0020(15)	0.0054(17)	0.0047(14)
C7	0.038(2)	0.0220(16)	0.029(2)	-0.0011(16)	0.0074(18)	0.0036(15)
C8	0.034(2)	0.0199(15)	0.024(2)	0.0000(14)	0.0048(16)	-0.0003(14)
C9	0.033(2)	0.0215(16)	0.025(2)	0.0018(14)	0.0038(16)	-0.0002(14)
C10	0.031(2)	0.0184(15)	0.026(2)	0.0010(14)	0.0024(16)	-0.0004(14)
C11	0.037(2)	0.0172(16)	0.025(2)	0.0009(14)	0.0020(17)	-0.0004(14)
O11	0.059(9)	0.081(10)	0.060(10)	-0.023(9)	-0.035(7)	0.022(7)
C12	0.036(2)	0.0148(15)	0.029(2)	0.0002(15)	-0.0003(17)	0.0016(14)
C13	0.034(2)	0.0172(15)	0.025(2)	0.0024(14)	0.0003(16)	0.0024(14)
C14	0.032(2)	0.0182(16)	0.025(2)	0.0003(15)	0.0013(16)	0.0019(14)
C15	0.0301(19)	0.0199(16)	0.025(2)	0.0016(14)	0.0034(15)	0.0062(14)
C16	0.035(2)	0.0251(17)	0.029(2)	-0.0018(16)	0.0022(17)	-0.0036(15)
C17	0.036(2)	0.0321(19)	0.026(2)	-0.0010(17)	-0.0006(17)	0.0001(16)
C18	0.033(2)	0.0248(17)	0.029(2)	0.0031(16)	0.0045(16)	0.0045(15)
C19	0.035(2)	0.0215(16)	0.027(2)	-0.0026(15)	0.0030(17)	0.0030(14)
C20	0.043(2)	0.044(2)	0.023(2)	0.0025(18)	0.0039(18)	0.0058(18)
C21	0.0304(19)	0.0200(16)	0.025(2)	0.0003(14)	0.0074(16)	-0.0002(14)
C22	0.033(2)	0.0211(16)	0.029(2)	0.0011(15)	0.0011(16)	-0.0036(14)
C23	0.031(2)	0.0235(17)	0.030(2)	0.0031(16)	0.0048(16)	0.0012(14)
C24	0.044(2)	0.0172(16)	0.047(3)	-0.0088(17)	0.010(2)	0.0030(15)
C25	0.035(2)	0.0258(17)	0.027(2)	0.0002(16)	0.0054(17)	-0.0002(15)
C26	0.0313(19)	0.0215(16)	0.026(2)	0.0005(15)	0.0029(16)	0.0022(14)
C27	0.034(2)	0.0172(16)	0.022(2)	0.0017(15)	0.0007(16)	-0.0020(14)
C28	0.033(2)	0.0202(16)	0.026(2)	0.0038(15)	0.0028(16)	-0.0014(14)

C29	0.036(2)	0.0173(15)	0.027(2)	0.0008(15)	-0.0001(16)	-0.0007(14)
C30	0.0315(19)	0.0174(15)	0.025(2)	0.0025(14)	-0.0001(15)	-0.0022(14)
C31	0.0308(19)	0.0174(15)	0.026(2)	-0.0008(14)	-0.0011(15)	0.0001(14)
C32	0.032(2)	0.0184(15)	0.026(2)	-0.0016(14)	0.0012(16)	0.0011(13)
C33	0.034(2)	0.0176(16)	0.027(2)	-0.0017(15)	0.0020(17)	0.0029(14)
C34	0.033(2)	0.0246(16)	0.028(2)	0.0030(16)	0.0056(17)	0.0020(15)
C35	0.0283(19)	0.0211(15)	0.025(2)	-0.0001(14)	0.0018(16)	-0.0001(13)
C36	0.0292(19)	0.0212(16)	0.022(2)	0.0014(15)	0.0008(16)	0.0000(14)
C37	0.0281(19)	0.0182(15)	0.027(2)	0.0001(14)	0.0045(15)	-0.0004(13)
C38	0.032(2)	0.0212(16)	0.023(2)	0.0032(15)	0.0031(15)	-0.0002(14)
C39	0.034(2)	0.0205(16)	0.027(2)	-0.0007(15)	0.0079(17)	-0.0016(14)
C40	0.036(2)	0.0186(16)	0.031(2)	-0.0011(15)	0.0082(16)	0.0003(14)
C41	0.033(2)	0.0223(16)	0.031(2)	0.0046(16)	0.0061(17)	0.0013(14)
C42	0.0302(19)	0.0204(16)	0.027(2)	0.0002(15)	0.0021(16)	-0.0002(14)
C43	0.0296(19)	0.0223(16)	0.026(2)	0.0019(15)	0.0031(15)	0.0054(14)
C44	0.033(2)	0.0273(17)	0.024(2)	0.0018(15)	0.0023(16)	0.0044(15)
C45	0.035(2)	0.0275(18)	0.032(2)	0.0063(16)	0.0066(17)	0.0029(15)
C46	0.032(2)	0.0350(19)	0.026(2)	0.0019(16)	0.0046(16)	0.0084(15)
C47	0.035(2)	0.0366(19)	0.024(2)	-0.0025(17)	0.0006(17)	0.0076(16)
C48	0.032(2)	0.0285(18)	0.027(2)	-0.0033(16)	-0.0002(16)	0.0049(15)

Table S6. Miller index, multiplicity, attachment energy and percent of coverage for the predicted TMPyP:TSPP crystal morphology using the AE method.

hkl	**Multiplicity**	**d_{hkl} (Å)**	**E_{att}(kcal/mol)**	**%Total facet area**
{0 0 2}	2	14.579	-51.0195	35.4174
{0 1 1}	4	14.3027	-65.8419	44.2718
{0 1 2}	4	10.8998	-79.2946	0
{0 1 3}	4	8.3630	-92.7473	0
{1 0 0}	2	8.2971	-116.2424	20.3106
{0 2 0}	2	8.2065	-91.8112	0
{0 2 1}	4	7.8995	-80.3633	0
{1 1 0}	4	7.4047	-142.8662	0
{1 0 -2}	2	7.3489	-161.3968	0
{1 1 -1}	4	7.2439	-146.8707	0

Table S7. Effective masses at Gamma point (Γ) from EHTB calculations of TMPyP:TSPP crystals as a function of π-stacking distances.

Interaction Distance	**Bands and Effective Masses (m*) at Γ (units: m_e)**‡	
π-π stacking distances	**HOMO (top of valence band)**	**LUMO (bottom of conduction band)**
3.67 Å	-18.642	7.337
3.84 Å	-63.848	13.032
4.01 Å	-129.711	18.115

‡ m_e is the mass of an electron, 9.11 x 10^{-31} kilograms.

Table S8. Photoconductivity parameters at different laser power levels for TMPyP:TSPP illuminated with 445 nm laser light at 25 °C.

Power (mW)	**I_{npc} (nA)**	**I_{ppc} (nA)**	**I_{ppc}/I_{npc}**	**τ (s)**	**β**
11	0.8	2.2	2.8	8528	0.43
21	2.3	4.7	2.1	8176	0.44
38	3.8	7.3	1.9	7320	0.40