Supporting Information for

Intralayer Anisotropy in Two-Dimensional Conjugated Covalent Organic Frameworks

This PDF file includes:

Computational details

Electronic structure calculations. The calculations conducted in this research, including lattice parameters and atomic coordinates optimization and electronic structure calculations, were performed within density functional theory (DFT) framework as implemented in the Vienna ab-initio simulation package (VASP 5.4.4)[1], using projector augmented wave (PAW)[2] method and the Perdew−Burke−Ernzerhof (PBE)[3] exchange-correlation functional. London dispersion was further corrected with Grimme's D3 approach[4] and Heyd−Scuseria−Ernzerhof (HSE06)[5] hybrid functional was used to calculate the band structures and density of states. For single-layer (SL) COFs, vacuum spacing in the out-of-plane direction was set to ~ 20 Å. The cut-off energy of 400 eV for plane-wave basis set was used in lattice and atom optimization, and 600 eV in other calculations. And the convergence criterion for forces in atomic coordinates optimization was set to 0.02 eVÅ^{-1}, while the energy convergence criterion in the self-consistent field iteration was set to 10^{-5} eV for lattice optimization and 10^{-6} eV for other calculations. And k-meshes of $2\times 2\times 10$ and $2\times 2\times 1$ were used in the optimization for bulk and SL structure while that of $4\times 4\times 10$ and $4\times 4\times 1$ were then used to obtain the converged charge density. The Brillouin zone and the corresponding high-symmetry k-points were shown in Figure S25.

Carrier mobility calculations. The carrier mobility was calculated by solving the Boltzmann transport equation (BTE) in the relaxation time approximation[6] using the BoltzTraP package[7]. It can be expressed as:

$$\mu^{e(h)} = \frac{e}{k_B T}\frac{\sum_{i\in CB(VB)}\int \tau(i,\mathbf{k})\mathbf{v}(i,\mathbf{k})^2 f^0(i,\mathbf{k})d\mathbf{k}}{\sum_{i\in CB(VB)}\int f^0(i,\mathbf{k})d\mathbf{k}}$$

where $\tau(\mathbf{k})$ is the relaxation time of charge carriers, $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}$ is the group velocity, f^0 is the Fermi-Dirac distribution function.

The total relaxation time, which measures how quickly the disturbed distribution of carriers in an electric field is back to equilibrium state via various scattering

mechanisms, can be described as follows according to Mathiessen's rule by assuming that different scattering mechanisms are independent of each other:

$$\frac{1}{\tau}=\frac{1}{\tau_{ac}}+\frac{1}{\tau_{op}}+\frac{1}{\tau_{imp}}+\ldots,$$

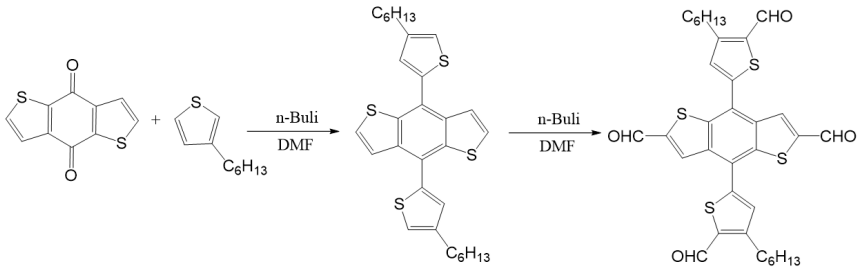
where τ_{ac}, τ_{op}, and τ_{imp} stand for the relaxation times due to acoustic phonon scattering, optical phonon scattering, and impurity scattering, respectively. The acoustic phonon scattering in the long wavelength limit was modeled based on deformation potential (DP) theory[6], and it was demonstrated as a dominating scattering mechanism in graphene and other carbon allotropes[8,9]. By applying Fermi's golden rule, the relaxation time due to acoustic phonon scattering can be derived as[10]

$$\frac{1}{\tau_{\mathbf{k}}}=\frac{2\pi}{\hbar}\sum_{\mathbf{k}'}k_B T E_1^2/C_{ii}\,\delta\left(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}\right)\left(1-\cos\theta\right),$$

where $\delta\left(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}\right)$ is the Dirac delta function to ensure energy conservation in elastic scattering events, θ is the scattering angle between $\mathbf{k}$ and $\mathbf{k}'$ states, the summation runs over all available final states, E_1 and C_{ii} are the DP constant and elastic constant. All these parameters can be obtained with first-principles calculations. $E_1=\Delta E_{\mathrm{CBM(VBM)}}/\left(\Delta l/l_0\right)$ was taken from a linear fitting of the CBM or VBM energy shift with the lattice deformation along the crystal directions *a, b* and *c* respectively, while the elastic constant C_{ii} was taken from a parabolic fitting of the total energy *E* with the dilation $\Delta l/l_0$ via $\frac{E-E_0}{\Omega_0}=C_{ii}(\Delta l/l_0)^2/2$, where E_0 and Ω_0 are the total energy and volume of the unit cell for the structure.

Experimental details.

Monomer 1 was synthesized according to literature and the procedure was as follows.[11] Monomer 2 was purchased from TCI Deutschland GmbH.



Nuclear magnetic resonance (NMR) spectroscopy. Solid-state nuclear magnetic resonance (NMR) spectroscopy measurements were carried out on BRUKER Ascend 300 MHz spectrometer using a commercial 2.5 mm MAS NMR probe and operating at a resonance frequency of 75.48 MHz for ^{13}C. The MAS frequency was 15 kHz. Cross polarization (CP) and SPINAL ^{1}H decoupling were used during signal acquisition. The ^{13}C chemical shift were referenced with adamantane. For prediction of ^{13}C NMR spectra, the program ACD/Labs was used (ACD/C+H NMR Predictors and DB 2020.1.0, Advanced Chemistry Development, Inc., Toronto, ON, Canada, www.acdlabs.com, 2020].

Fourier transform infrared (FT-IR) spectroscopy. FT-IR spectra was recorded with ca. 1 mg sample on a Bruker Optics ALPHA-E spectrometer in 400-4000 cm^{-1} at ambient condition.

Powder X-ray diffraction (PXRD) analysis. PXRD pattern was obtained on STOE STADI P diffractometer with Cu Kα line focused radiation at 40 kV and 40 mA from 2θ in the range of 2° to 50° with 0.02° increment.

Scanning electron microscopy (SEM). SEM (FESEM, Zeiss Gemini 500) was used to investigate the structure of the as-prepared TBDT-P-CN at an accelerating voltage of 5.0 kV. Sample was dispersed in ethanol then dropped onto silicon substrate, which was attached with conductive adhesive tapes to a flat aluminum sample holder and then coated with gold.

UV-visible-near IR absorption. UV-visible-near IR absorption spectra was collected on an Agilent Cary 5000 UV-Vis-NIR spectrophotometer.[11]

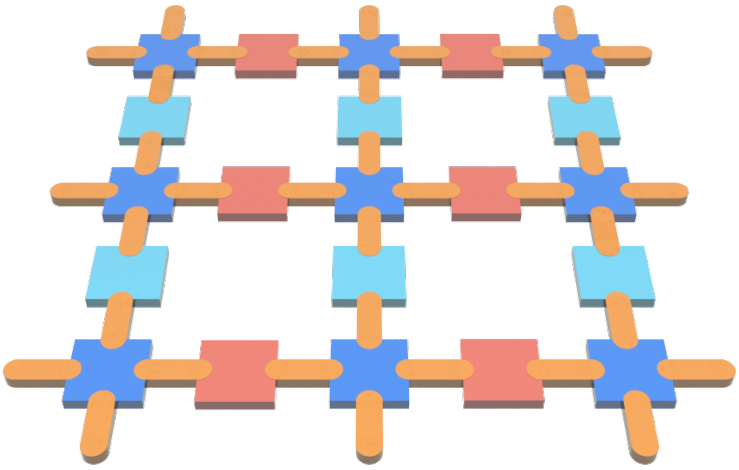


Figure S1. Illustration of the topological structure of multicomponent 2D COFs. The framework consists of node units (blue) and two distinct linker units (red and cyan), connected via conjugated linkages (orange), resulting in a periodic 2D architecture.

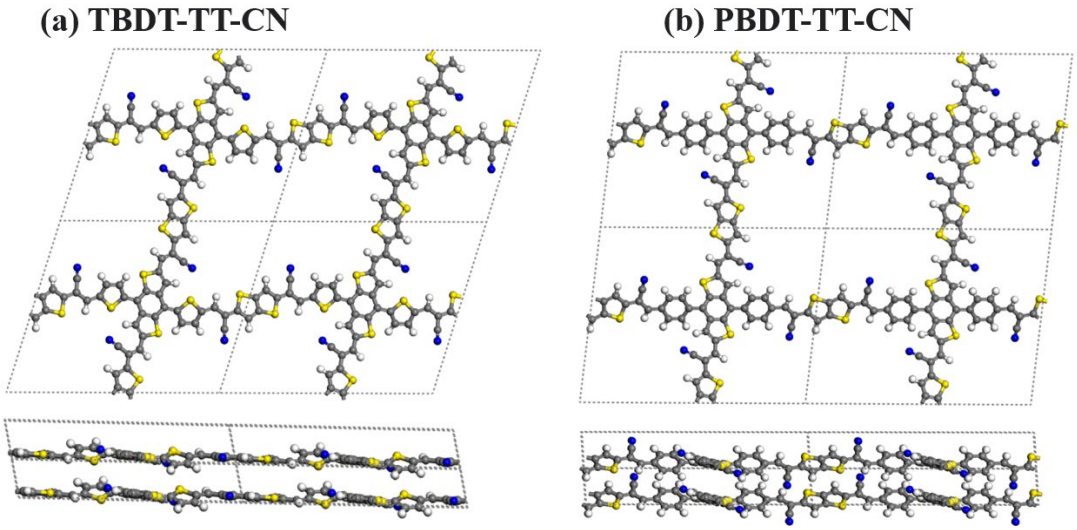


Figure S2. Crystal geometry of TBDT-TT-CN (a) and PBDT-TT-CN (b) for both top and side views.

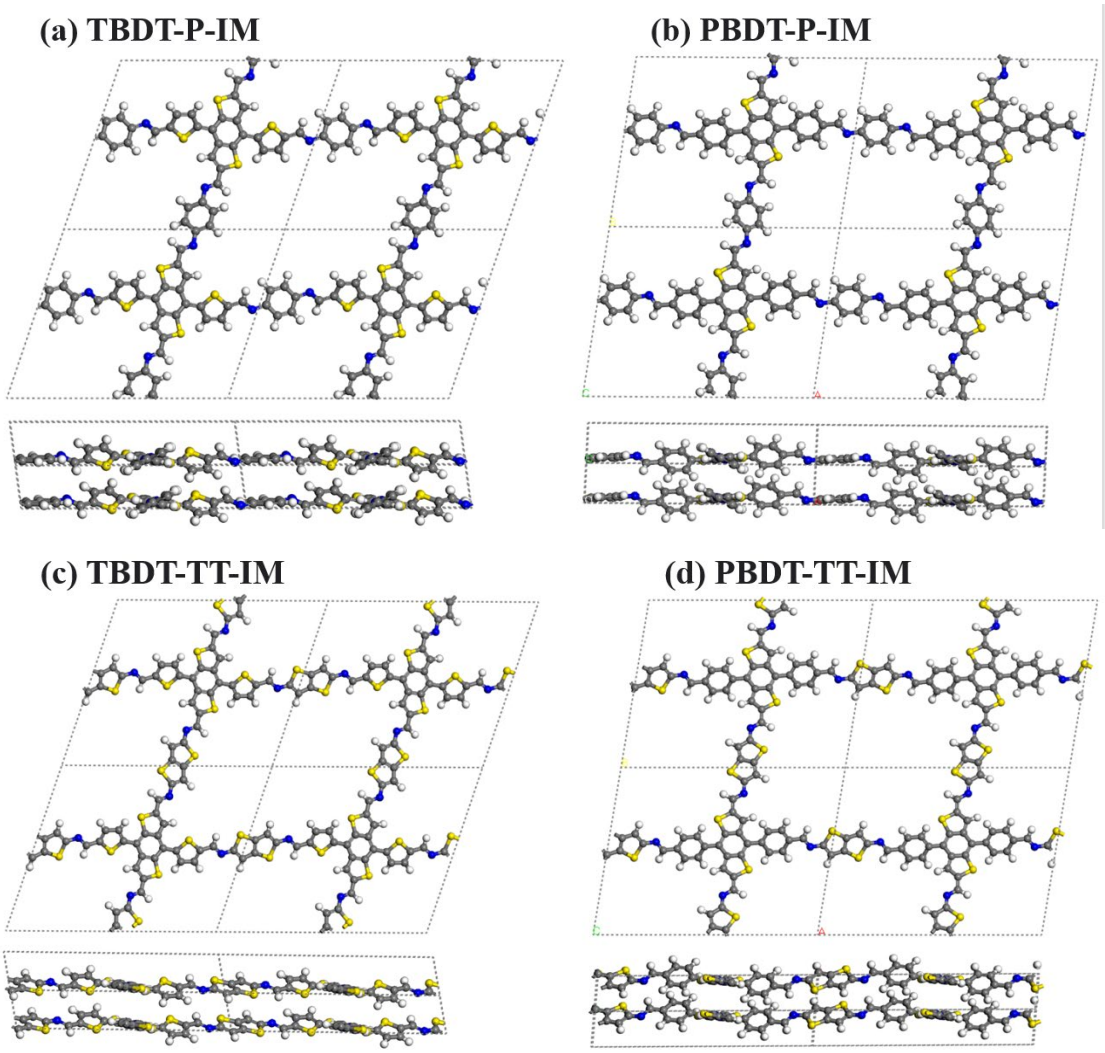


Figure S3. Crystal geometry of TBDT-P-IM (a), PBDT-P-IM (b), TBDT-TT-IM (c) and PBDT-TT-IM (d) for both top and side views.

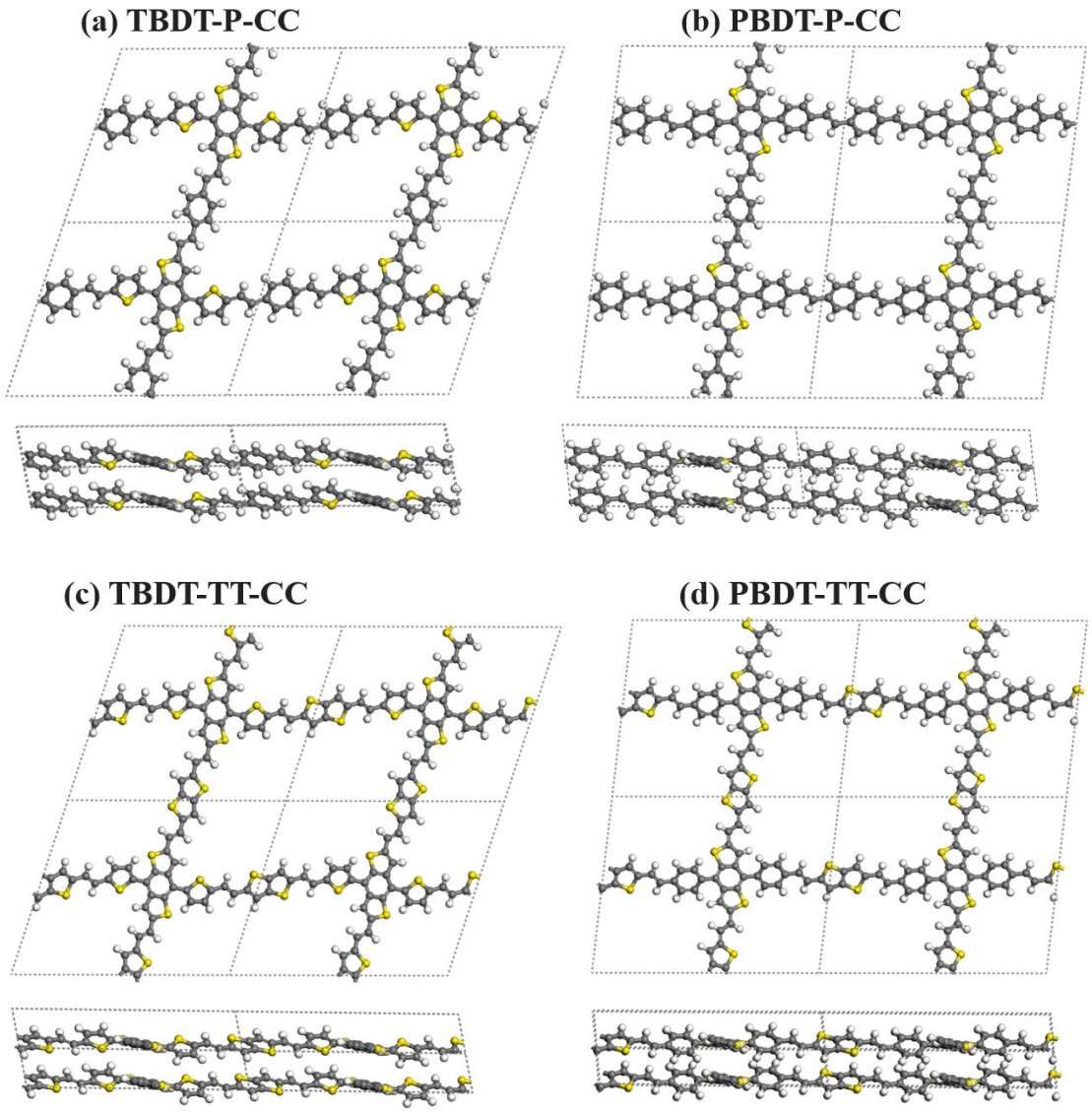


Figure S4. Crystal geometry of TBDT-P-CC (a), PBDT-P-CC (b), TBDT-TT-CC (c) and PBDT-TT-CC (d) for both top and side views.

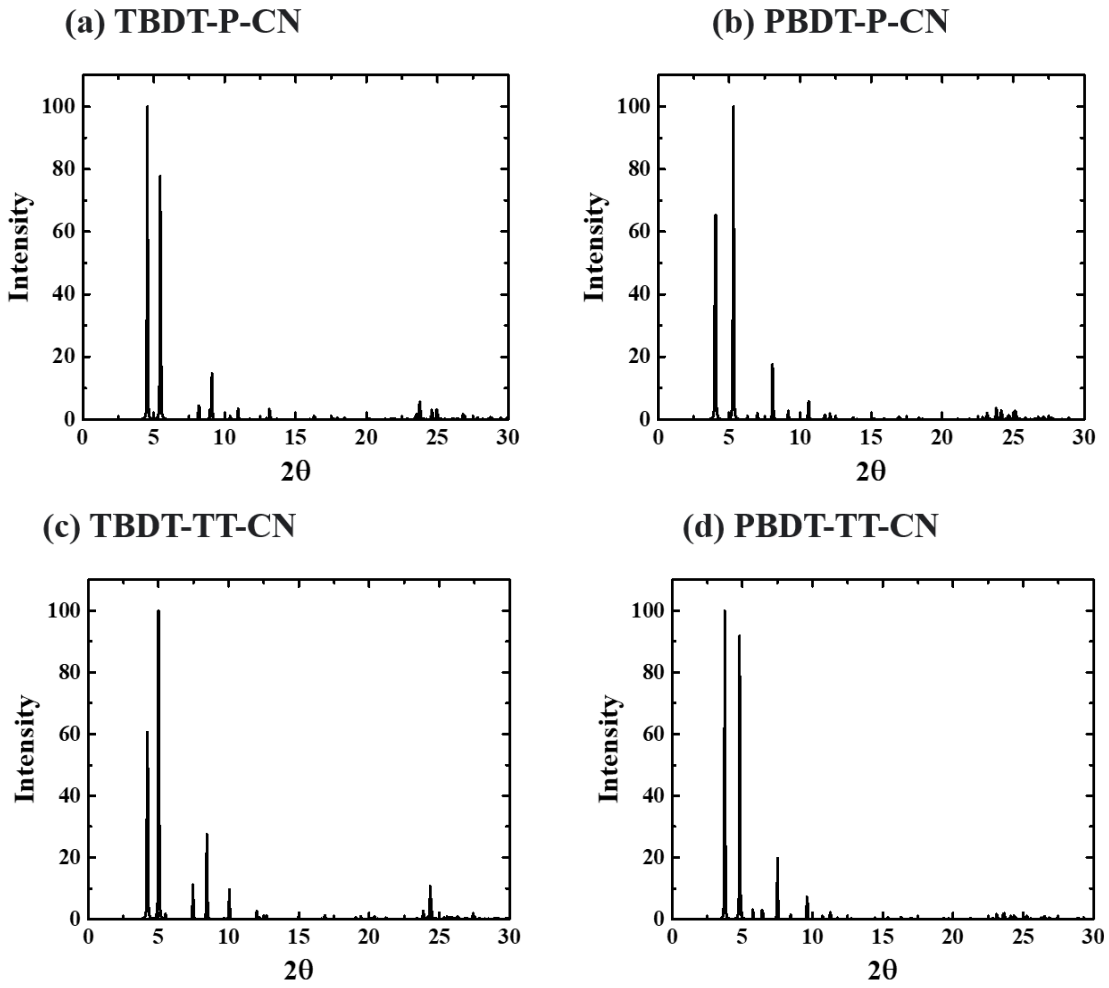


Figure S5. Simulated XRD of TBDT-P-CN (a), PBDT-P-CN (b), TBDT-TT-CN (c) and PBDT-TT-CN (d) for both top and side views.

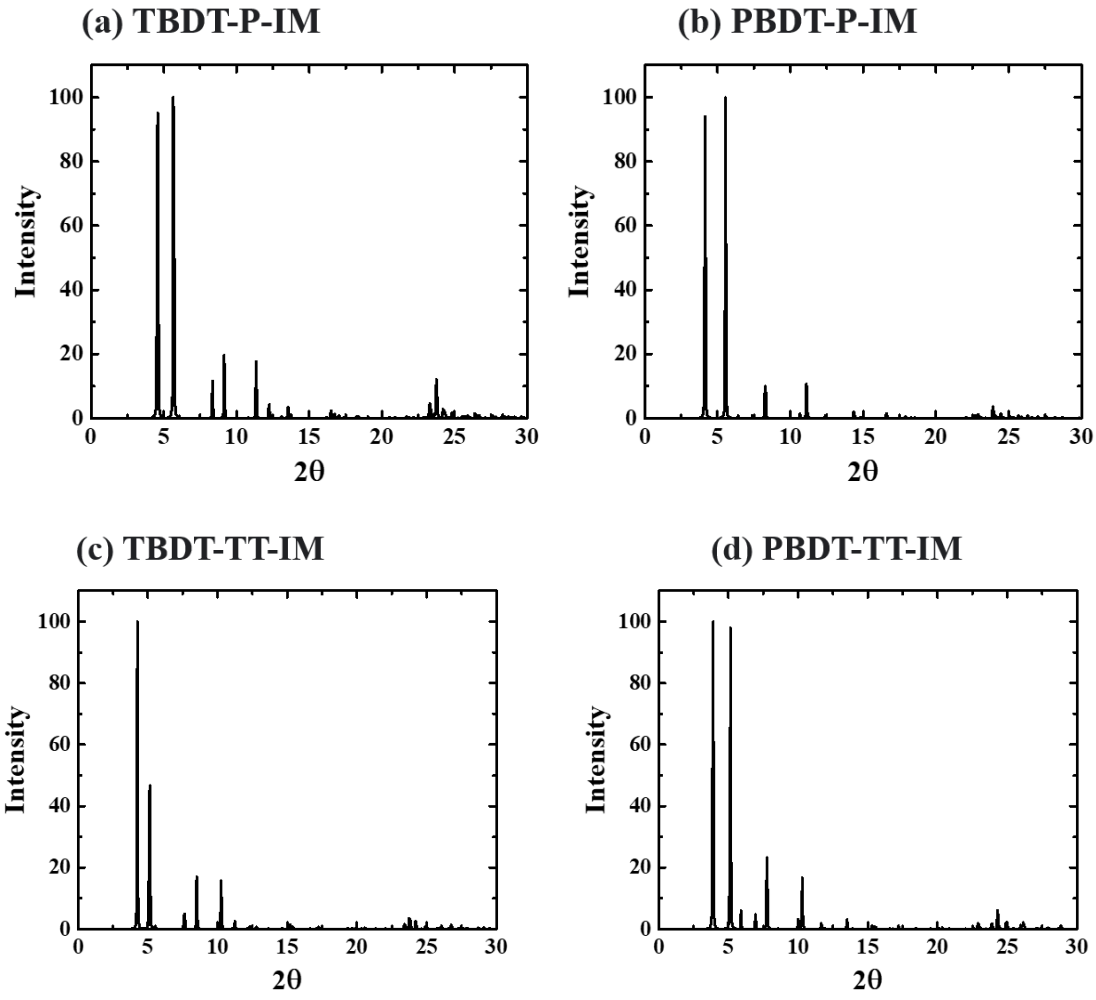


Figure S6. Simulated XRD of TBDT-P-IM (a), PBDT-P-IM (b), TBDT-TT-IM (c) and PBDT-TT- IM (d) for both top and side views.

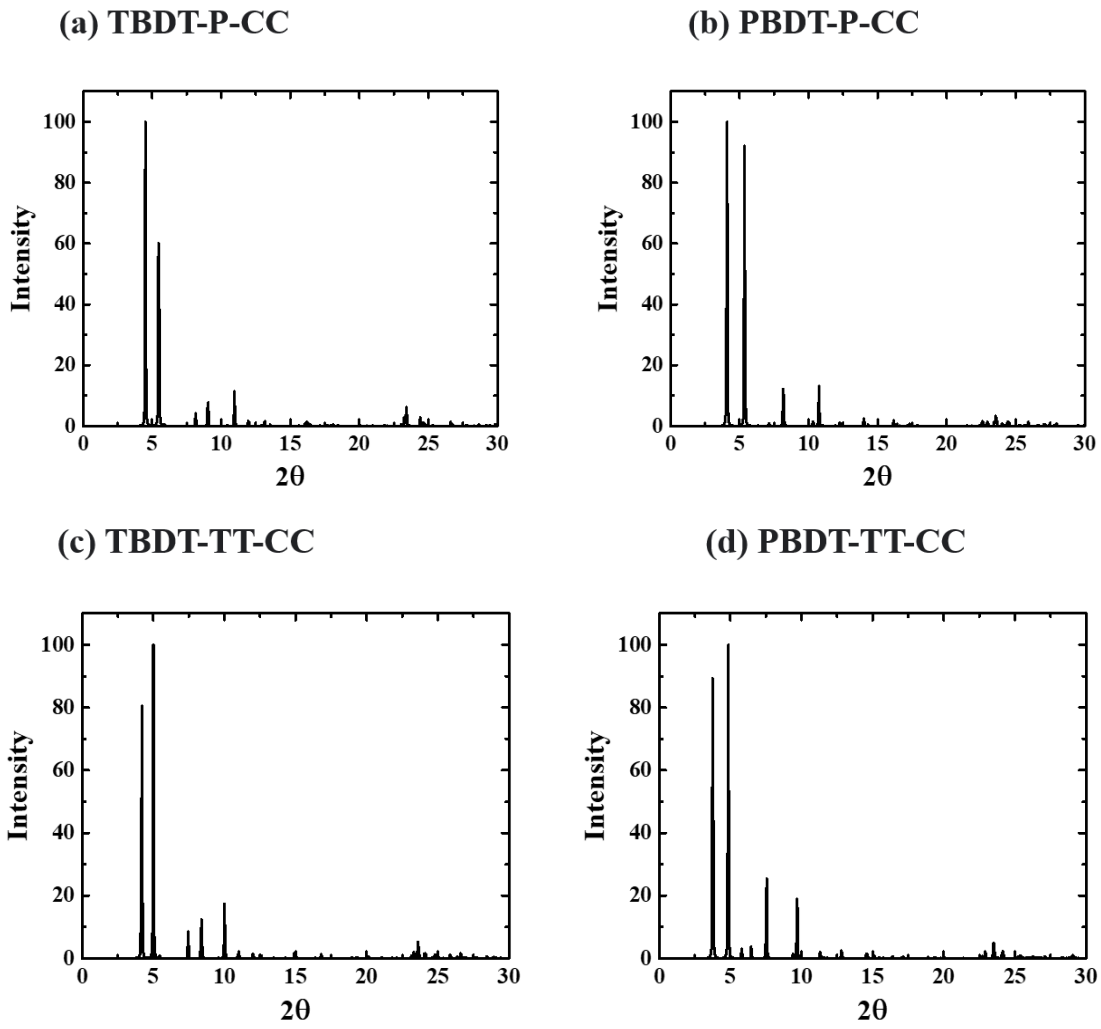


Figure S7. Simulated XRD of TBDT-P-CC (a), PBDT-P-CC (b), TBDT-TT-CC (c) and PBDT-TT-CC (d) for both top and side views.

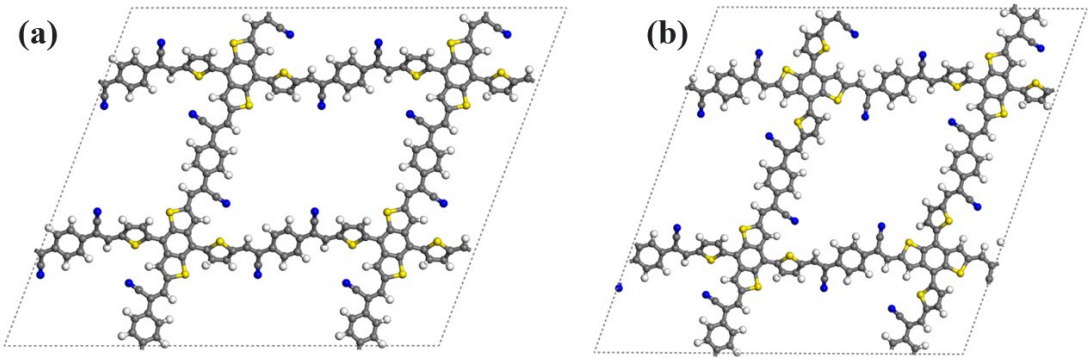


Figure S8. Two configurations of single-layer TBDT-P-CN: the unified configuration (a) and the chessboard configuration(b).

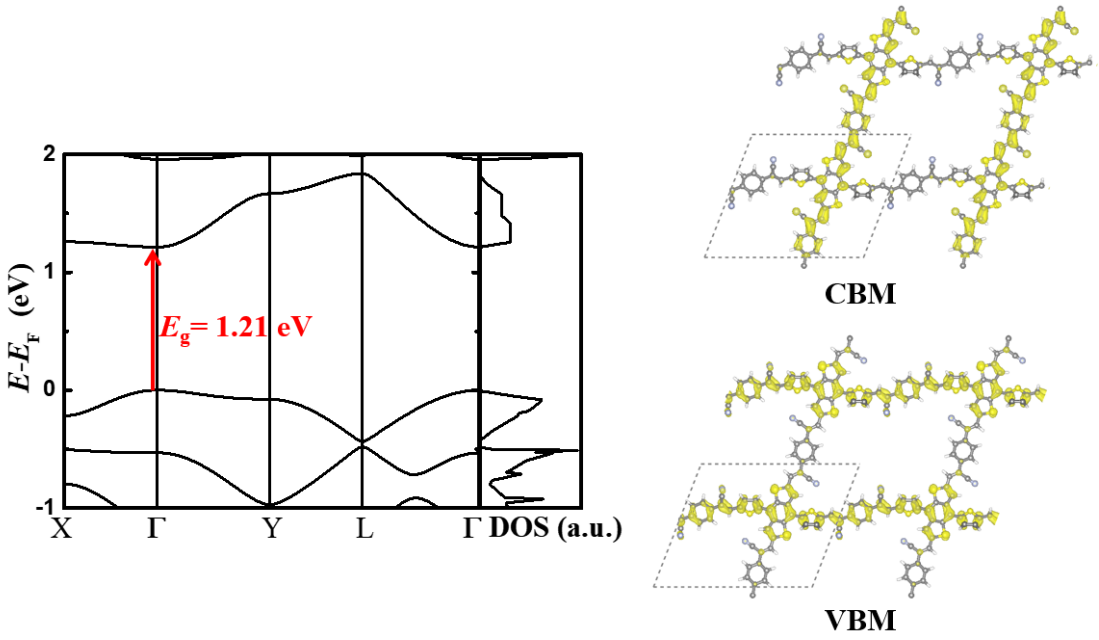


Figure S9. Band structure and density of states of single-layer (SL) TBDT-P-CN and charge density distribution at VBM and CBM calculated at the HSE06 level.

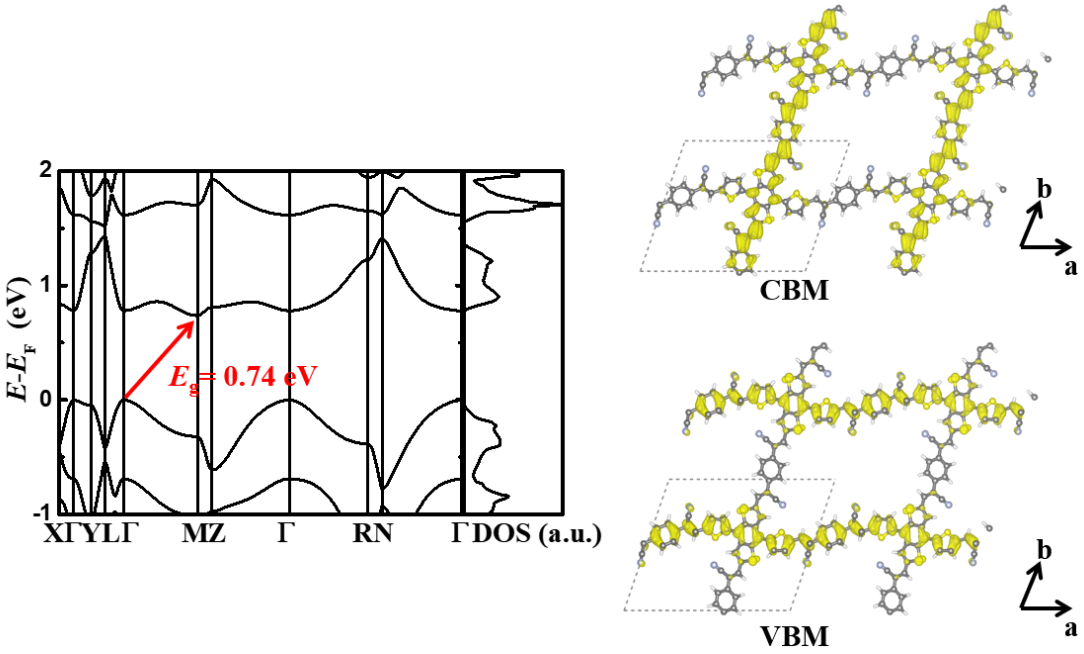


Figure S10. Band structure and density of states of TBDT-P-CN and charge density distribution at VBM and CBM calculated at the HSE06 level.

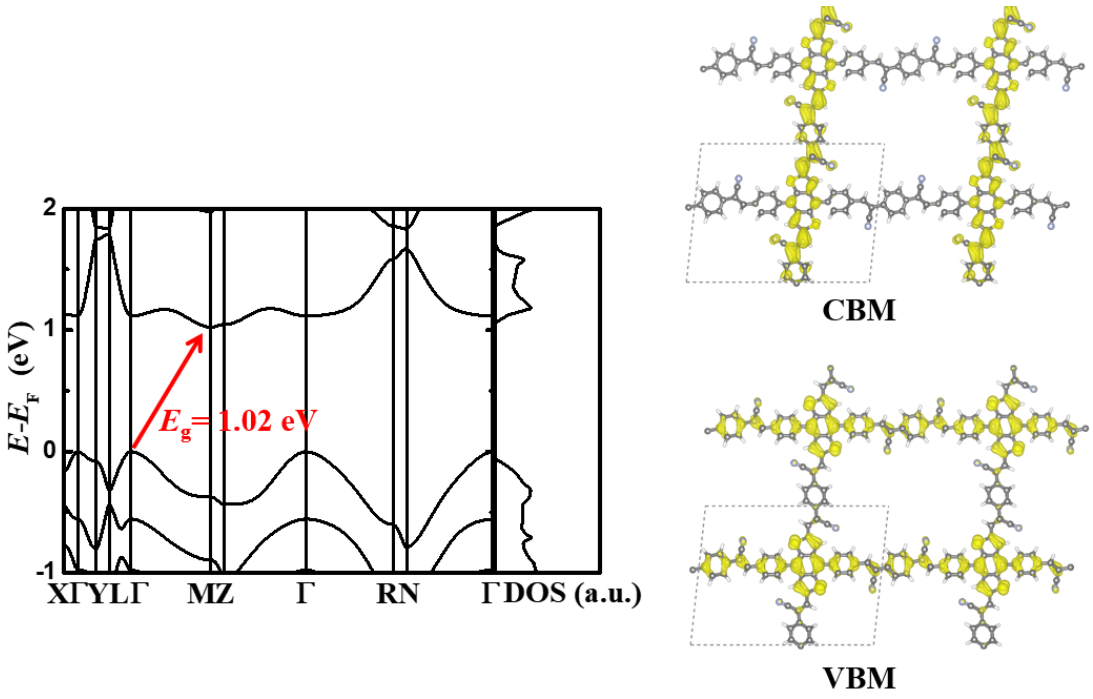


Figure S11. Band structure and density of states of PBDT-P-CN and charge density distribution at VBM and CBM calculated at the HSE06 level.

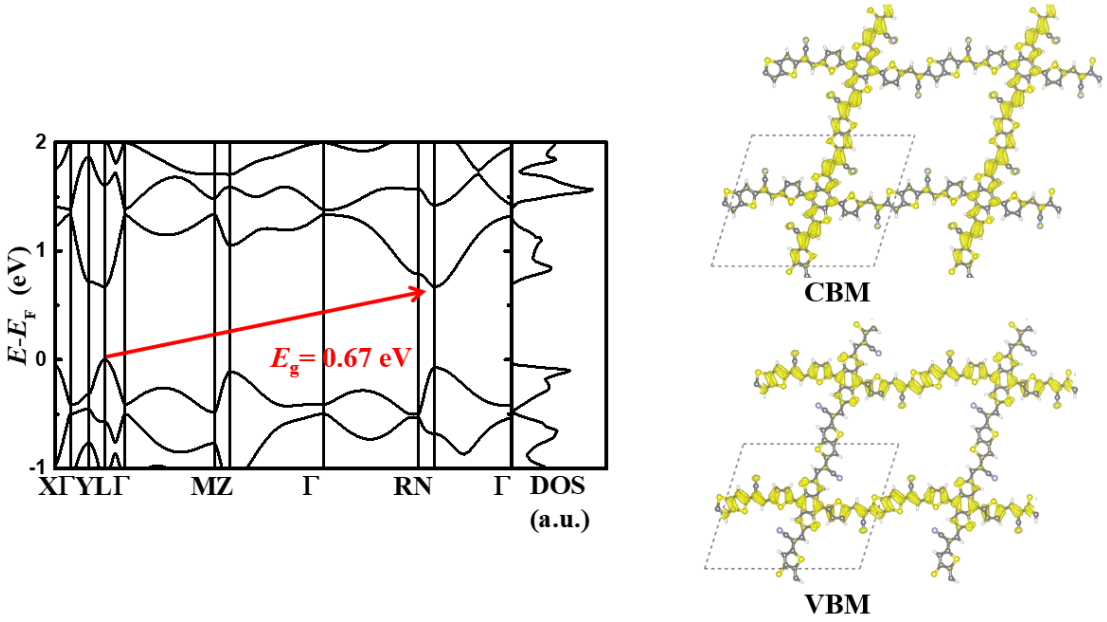


Figure S12. Band structure and density of states of TBDT-TT-CN and charge density distribution at VBM and CBM calculated at the HSE06 level.

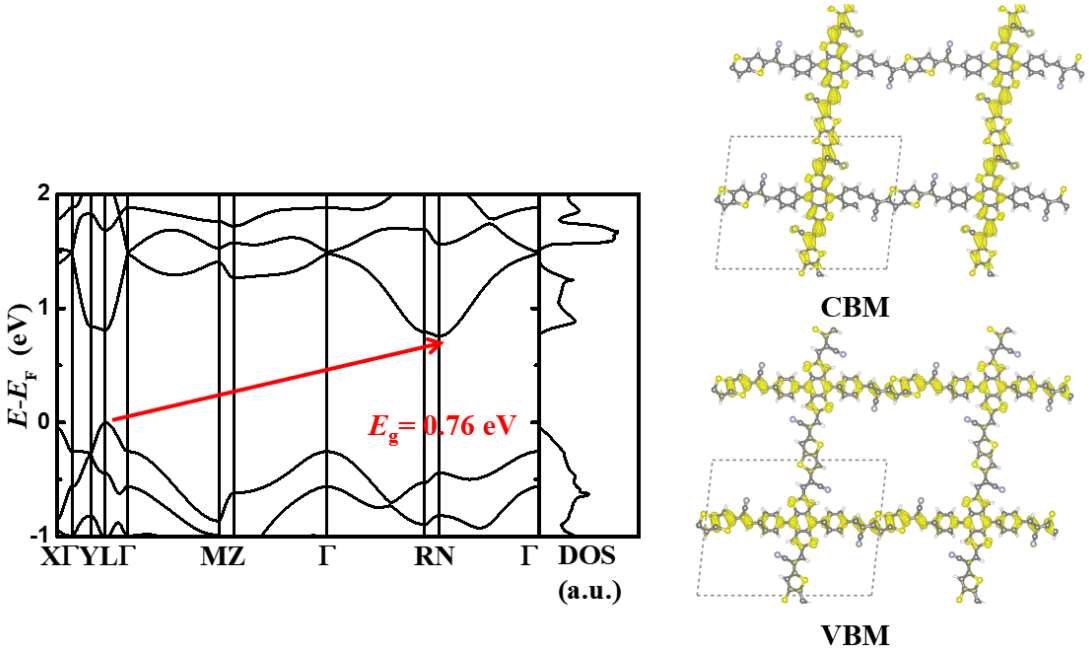


Figure S13. Band structure and density of states of PBDT-TT-CN and charge density distribution at VBM and CBM calculated at the HSE06 level.

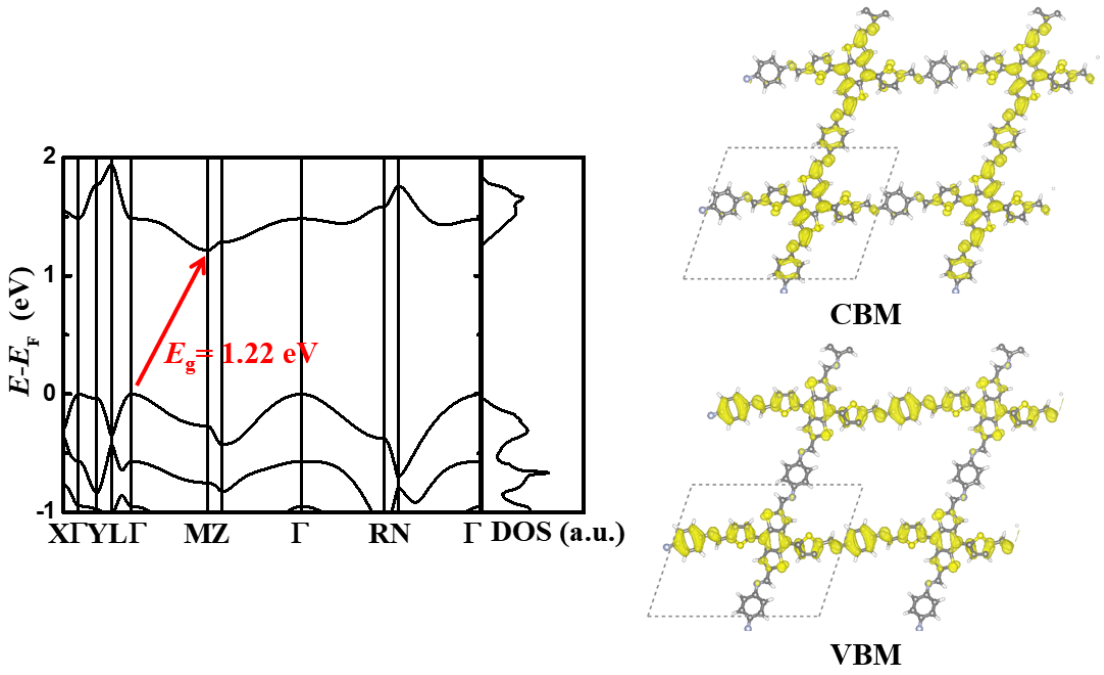


Figure S14. Band structure and density of states of TBDT-P-IM and charge density distribution at VBM and CBM calculated at the HSE06 level.

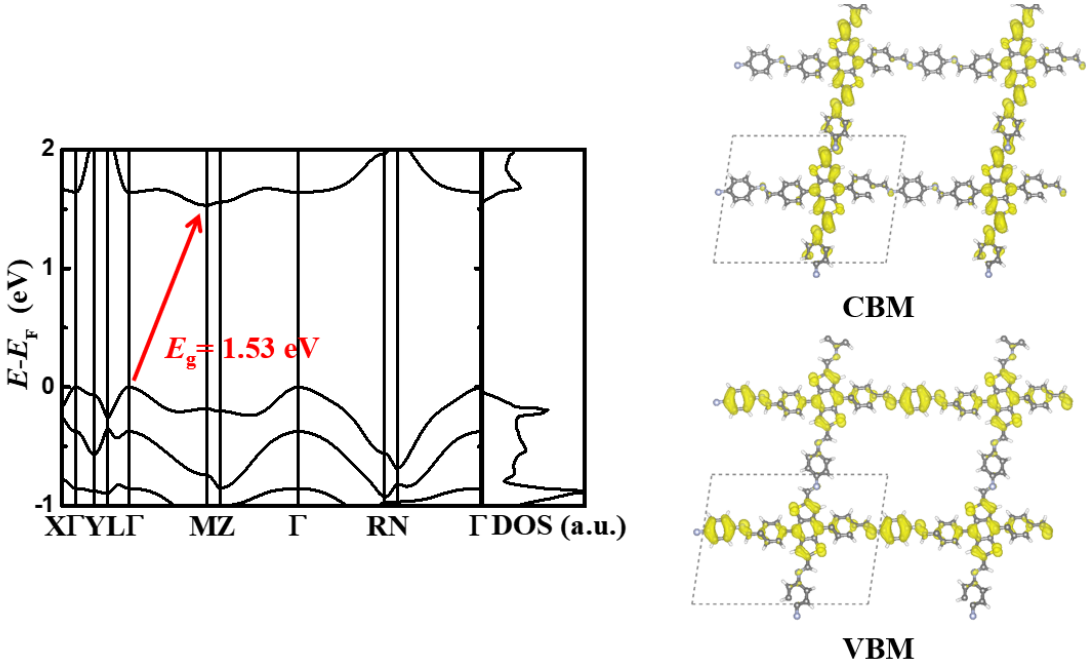


Figure S15. Band structure and density of states of PBDT-P-IM and charge density distribution at VBM and CBM calculated at the HSE06 level.

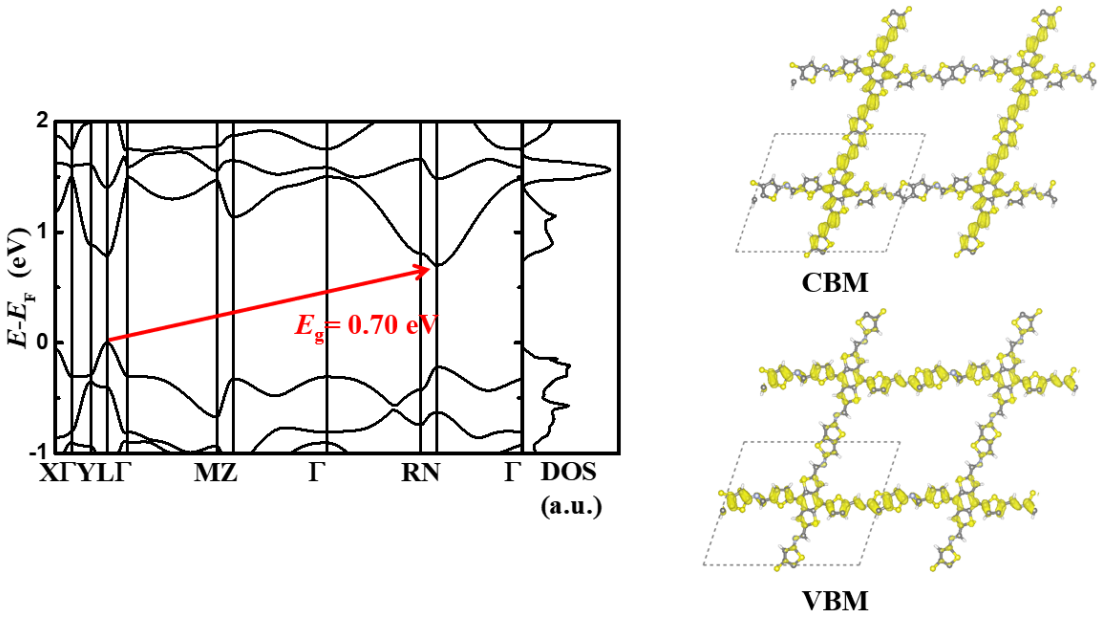


Figure S16. Band structure and density of states of TBDT-TT-IM and charge density distribution at VBM and CBM calculated at the HSE06 level.

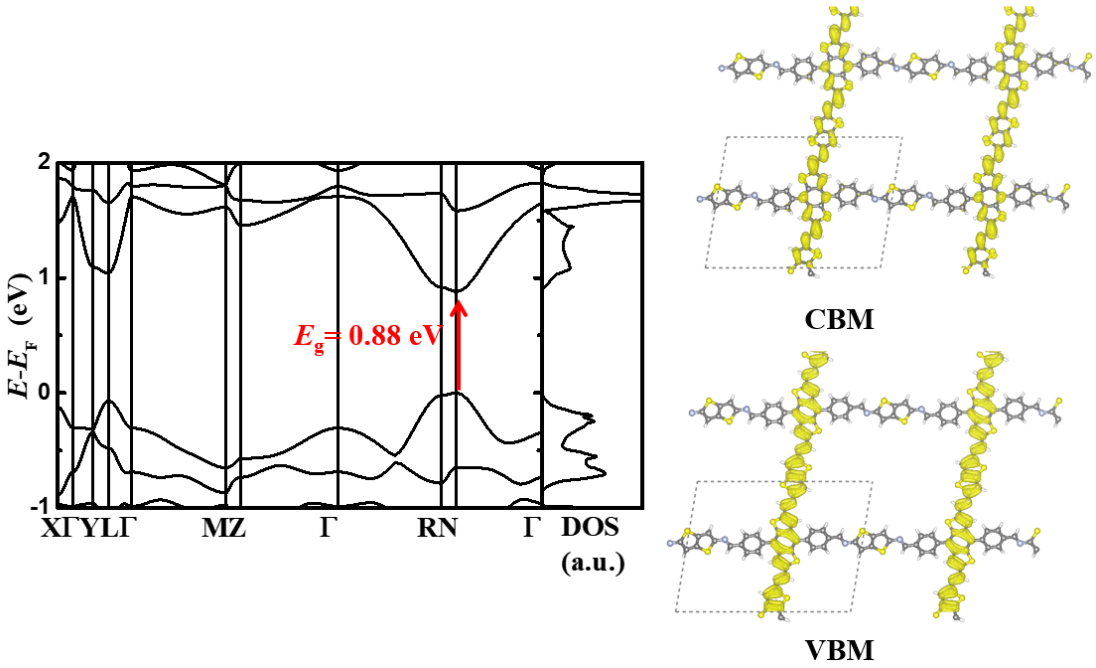


Figure S17. Band structure and density of states of PBDT-TT-IM and charge density distribution at VBM and CBM calculated at the HSE06 level.

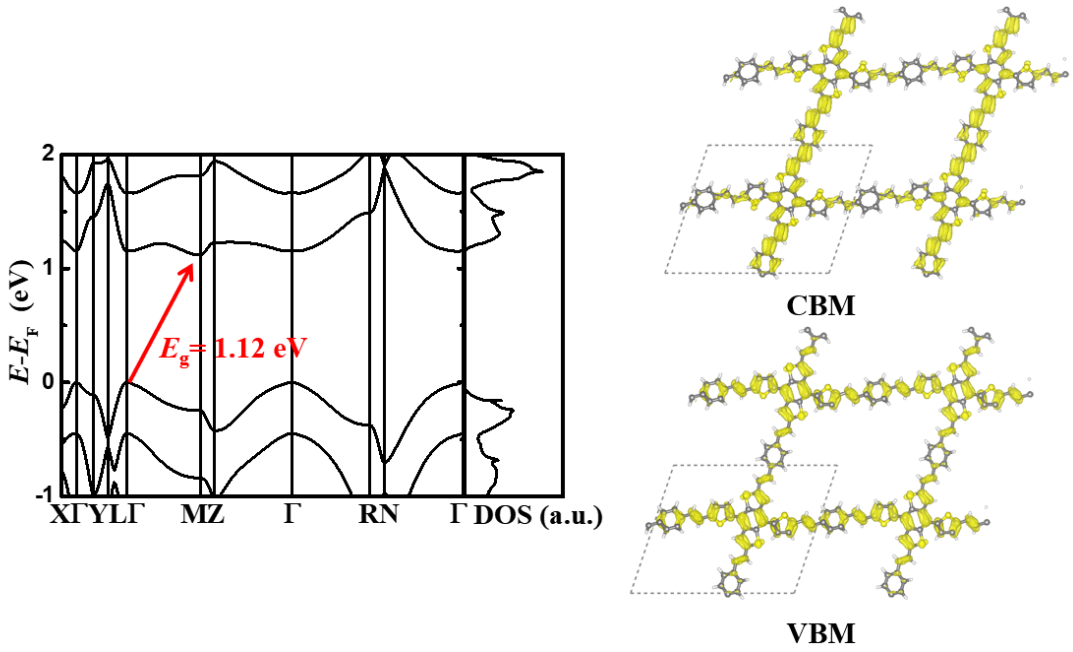


Figure S18. Band structure and density of states of TBDT-P-CC and charge density distribution at VBM and CBM calculated at the HSE06 level.

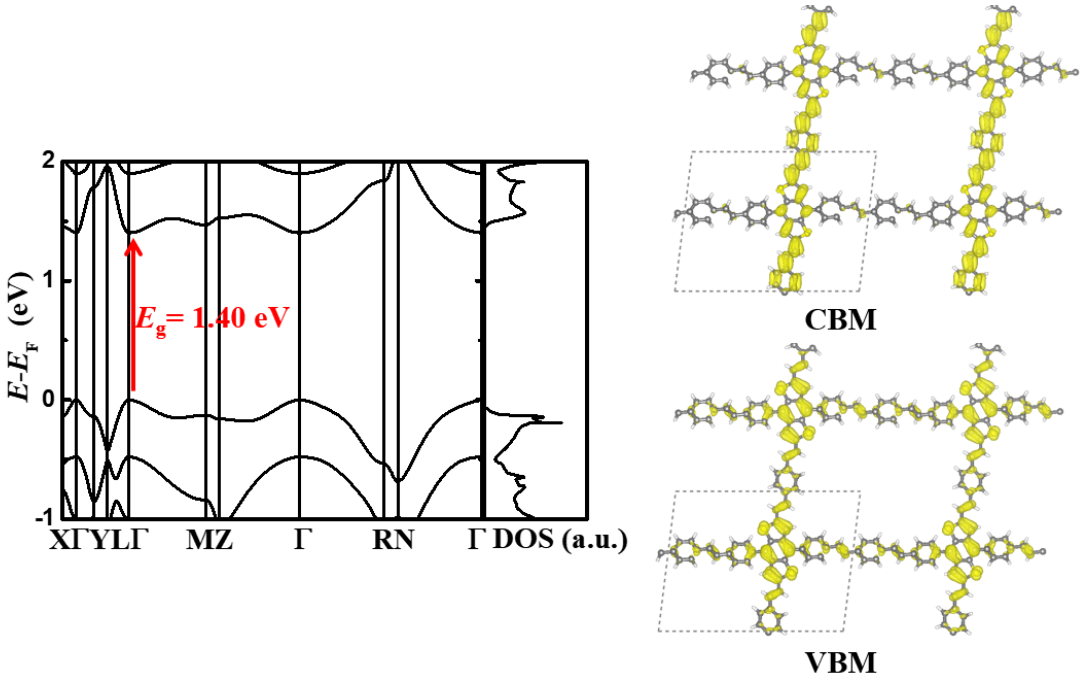


Figure S19. Band structure and density of states of PBDT-P-CC and charge density distribution at VBM and CBM calculated at the HSE06 level.

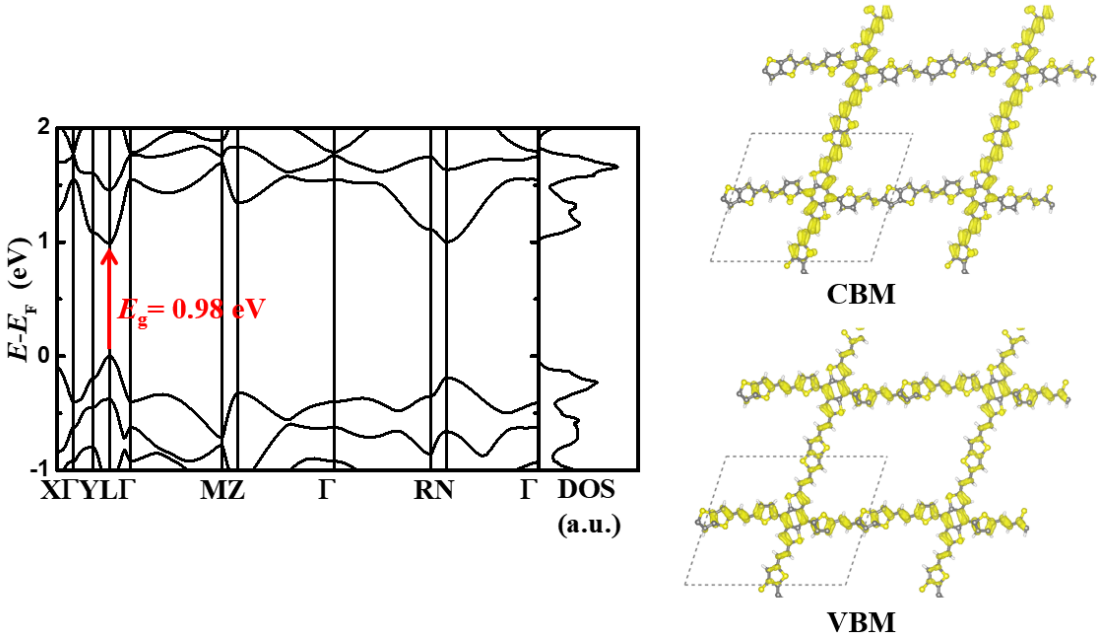


Figure S20. Band structure and density of states of TBDT-TT-CC and charge density distribution at VBM and CBM calculated at the HSE06 level.

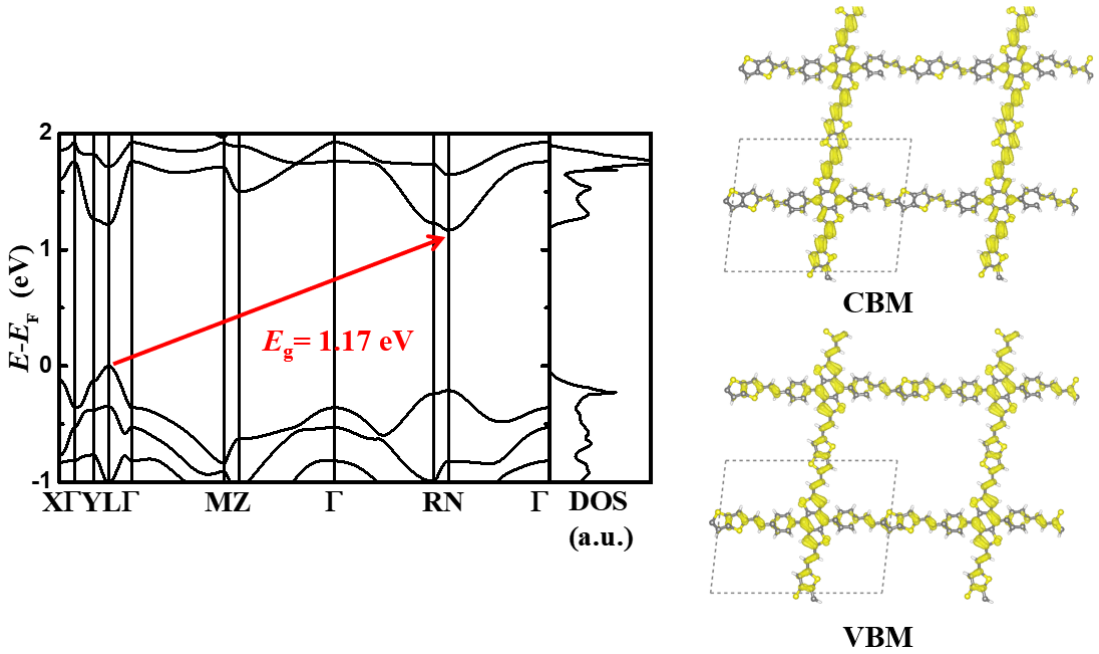


Figure S21. Band structure and density of states of PBDT-TT-CC and charge density distribution at VBM and CBM calculated at the HSE06 level.

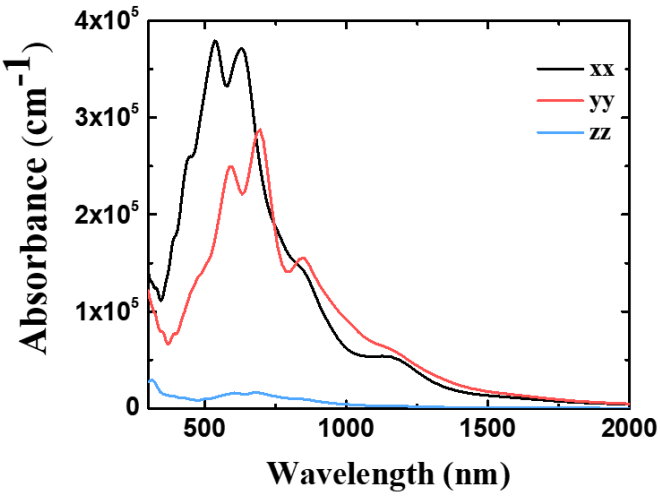


Figure S22. Optical absorption spectra of TBDT-P-CN calculated at HSE06 level.

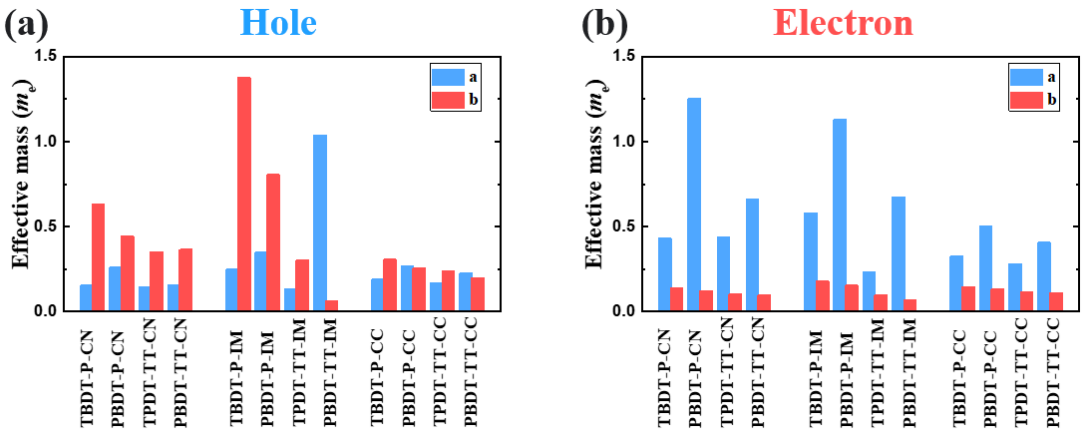


Figure S23.Effective masses of for hole (a) and electron (b) carriers along the a (blue) and b (red) directions.

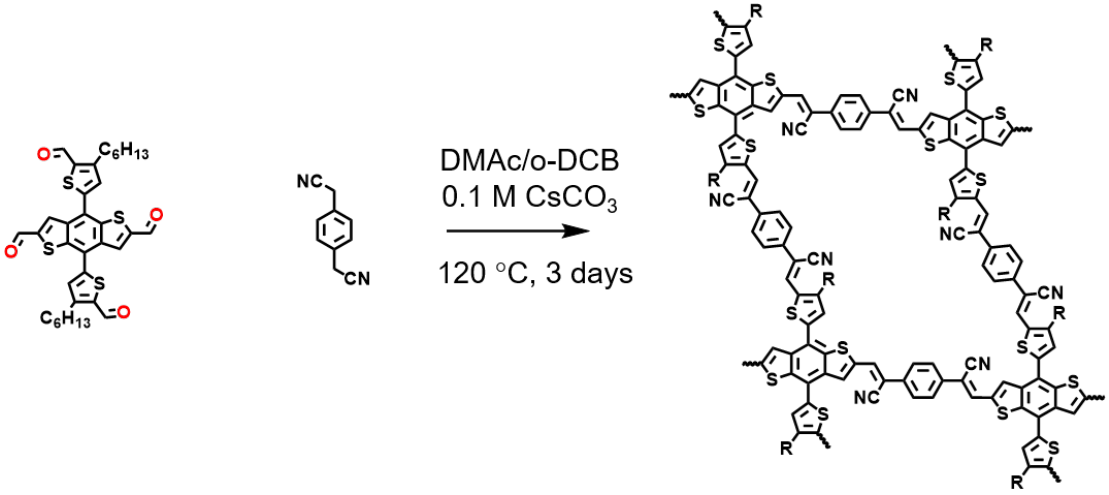


Figure S24. Synthetic route of TBDT-P-CN.

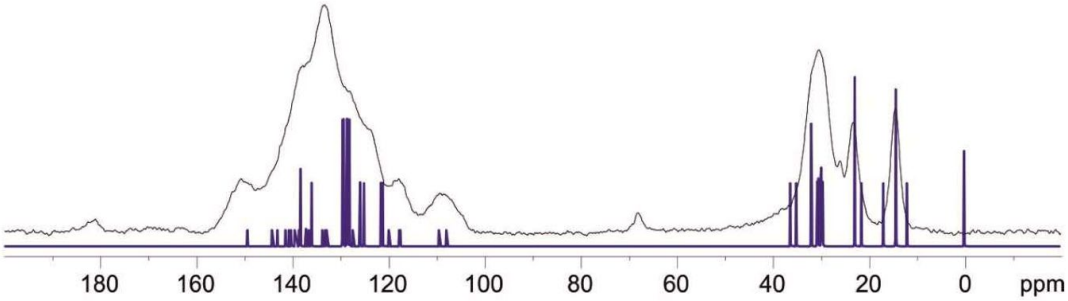


Figure S25. Comparison of the experimental (black) and predicted (purple) ^{13}C CP-MAS NMR spectrum of TBDT-P-CN. The prediction was performed using the program ACD/Labs (ACD/C+H NMR Predictors and DB 2020.1.0, Advanced Chemistry Development, Inc., Toronto, ON, Canada, www.acdlabs.com, 2020]).

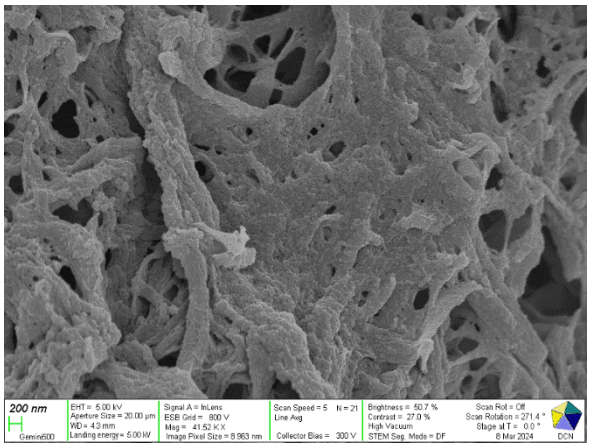
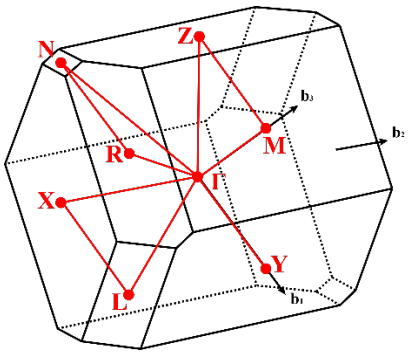


Figure S26. SEM image of TBDT-P-CN.



	$\times \mathbf{b_1}$	$\times \mathbf{b_2}$	$\times \mathbf{b_3}$		$\times \mathbf{b_1}$	$\times \mathbf{b_2}$	$\times \mathbf{b_3}$
Γ	0	0	0	R	0	0.5	0.5
L	0.5	0.5	0	X	0.5	0	0
M	0	0	0.5	Y	0	0.5	0
N	0.5	0.5	0.5	Z	0.5	0	0.5

Figure S27. Illustration of Brillouin zone of a generic triclinic lattice and the high-symmetry k-points.

Table S1. Electronic and charge carrier transport properties of 2D aniso-c-COFs, including bandgaps (E_g), effective masses (m^*), deformation potentials (E_1), elastic constants (C_{ii}), mean relaxation times (τ) and mobilities (μ) at 298 K.

		E_g (eV)	m^* (m_e)		E_1 (eV)		C_{ii}	τ (fs)		μ ($cm^2V^{-1}s^{-1}$)	
			hole	electron	hole	electron	(GPa)	hole	electron	hole	electron
TBDT-P-CN	a	0.74	0.15	0.43	5.10	3.83	84	31.53	123.31	220.36	237.25
	b		0.63	0.14	4.64	5.36	114			37.68	814.96
	c		1.95	2.75	5.73	2.32	7			42.78	32.55
TBDT-P-CN	a	1.02	0.26	1.25	3.66	4.22	78	46.39	152.31	154.96	49.36
	b		0.44	0.12	3.86	3.24	94			64.12	1238.73
	c		2.05	2.50	5.56	1.83	7			30.62	57.53
TBDT-TT-	a	0.67	0.15	0.44	5.03	3.10	64	20.88	44.47	156.04	122.91
CN	b		0.35	0.10	4.47	4.26	99			27.81	399.23
	c		3.42	1.77	5.29	4.66	9			22.69	56.60
PBDT-TT-	a	0.76	0.16	0.66	6.81	2.72	92	55.39	44.57	277.19	32.00
CN	b		0.36	0.10	4.00	4.26	84			54.67	408.10
	c		1.83	2.81	5.37	4.19	6			37.32	17.22
TBDT-P-IM	a	1.22	0.25	0.58	5.04	4.57	94	19.72	189.62	103.55	325.21
	b		1.37	0.18	4.83	5.01	95			19.27	1111.63

	c		2.61	2.57	5.53	2.04	6			19.39	66.57
TBDT-P-IM	a	1.53	0.35	1.13	5.65	3.70	97	25.93	121.18	68.52	52.25
	b		0.80	0.15	4.53	4.76	78			19.44	819.07
	c		2.25	3.14	5.35	1.83	6			14.74	52.50
TBDT-TT-IM	a	0.70	0.13	0.23	6.67	3.17	95	36.00	85.72	254.10	295.58
	b		0.30	0.10	5.78	4.12	89			63.72	781.21
	c		2.49	2.75	5.54	4.45	7			46.06	27.33
PBDT-TT-IM	a	0.88	1.04	0.67	5.63	4.25	77	35.42	72.04	37.80	73.84
	b		0.06	0.07	6.13	6.38	76			437.70	968.02
	c		1.90	2.04	5.43	4.47	7			32.64	74.73
TBDT-P-CC	a	1.12	0.19	0.33	5.93	4.24	101	36.13	102.89	201.04	283.42
	b		0.31	0.14	5.55	5.11	91			92.25	673.87
	c		2.39	3.16	5.59	2.37	6			41.84	32.67
TBDT-P-CC	a	1.40	0.27	0.50	5.56	4.03	99	37.76	59.71	112.06	76.69
	b		0.25	0.13	5.78	3.80	77			139.79	462.44
	c		2.73	2.57	5.30	3.87	6			36.22	90.89
TBDT-TT-	a	0.98	0.17	0.28	5.96	3.40	82	35.84	36.68	221.9	130.83

CC	b		0.24	0.12	5.62	3.57	90			110.39	318.62
	c		2.59	2.20	5.49	4.35	6			47.15	38.2
PBDT-TT-	a	1.17	0.23	0.41	6.04	3.08	100	57.12	44.33	192.37	65.64
CC	b		0.20	0.11	6.03	4.62	78			244.89	354.11
	c		2.18	3.07	5.34	4.24	6			59.42	17.42

Appendix:

Geometry of conjugated 2D aniso-c-COFs.

TBDT-P-CC

a = 21.28 Å, b = 17.45 Å, c = 3.95 Å, alpha = 102.42º, beta = 103.70º, gamma = 69.22º

H	0.67112824	0.72233287	0.07273440
H	0.51300441	0.42986721	0.21109570
H	0.42844035	0.72609720	0.57919683
H	0.75517343	0.42603545	0.70253837
H	0.51219026	0.91772600	0.27249695
H	0.67195381	0.23451824	0.01193912
H	0.27444636	0.52213247	0.92609368
H	0.90974685	0.62935373	0.35353673
H	0.87879239	0.42616828	0.75898145
H	0.30491809	0.72546824	0.52205887
H	0.69367133	0.96279907	0.96994064
H	0.68674015	0.10671315	0.99063353
H	0.48982732	0.18959446	0.30842103
H	0.49677902	0.04566331	0.28781742
H	0.99448238	0.67357576	0.41581321
H	0.08543230	0.44150881	0.79098111
H	0.18994367	0.47682461	0.86775264
H	0.09896301	0.70890699	0.49237799
H	0.65097291	0.86123980	0.02971294
H	0.97328300	0.47093397	0.86415021
H	0.21091978	0.67966919	0.41973791
H	0.53255291	0.29113750	0.24838616
C	0.56905019	0.50947725	0.14183169
C	0.63653831	0.49638116	0.08507733
C	0.66213954	0.56096610	0.08951825
C	0.61496721	0.64274947	0.14110388
C	0.54744772	0.65583999	0.19753910
C	0.52183683	0.59125767	0.19323963
C	0.62476823	0.71870352	0.12907950
C	0.56925316	0.78812918	0.18384705
C	0.55929865	0.43351805	0.15404649
C	0.61482141	0.36411468	0.09904404
C	0.45150415	0.60769656	0.23176919
C	0.73245664	0.54436367	0.05065998
C	0.40969327	0.67746920	0.41373621
C	0.34289627	0.67687120	0.38564408
C	0.33076452	0.60629287	0.17970933
C	0.77409273	0.47450395	0.86823887
C	0.84093809	0.47483575	0.89593240
C	0.85324846	0.54531745	0.10189682

C	0.55968413	0.87442877	0.19310045
C	0.60401913	0.90520913	0.11330784
C	0.59614357	0.99180188	0.12695519
C	0.57967660	0.24714357	0.16671122
C	0.62431976	0.27785110	0.08957625
C	0.27131111	0.58021060	0.10483696
C	0.21332865	0.62142713	0.24265427
C	0.15317306	0.59637771	0.18640334
C	0.03119411	0.55411950	0.09647579
C	0.97091732	0.52932510	0.04000254
C	0.91283917	0.57107464	0.17638603
C	0.64885590	0.01276137	0.04675775
C	0.64492188	0.09425458	0.05950653
C	0.58744995	0.16057828	0.15242581
C	0.53469249	0.13963370	0.23216272
C	0.53864426	0.05813050	0.21948731
C	0.03683663	0.63003670	0.29220301
C	0.08845848	0.50033546	0.94738910
C	0.14755978	0.52039795	0.99107369
C	0.09591865	0.65010808	0.33577067
S	0.50198812	0.76126339	0.24914479
S	0.68202891	0.39095633	0.03307205
S	0.40412371	0.54211092	0.02133519
S	0.78002740	0.60969958	0.26109061

TBDT-P-CN

a = 21.13 Å, b = 17.54 Å, c = 3.89 Å, alpha = 102.93º, beta = 103.34º, gamma = 68.82º

H	0.68189538	0.70918913	0.06248149
H	0.50224766	0.44288880	0.22092100
H	0.42764155	0.74218974	0.56376087
H	0.75642632	0.40972464	0.72151870
H	0.52371142	0.91215147	0.23850548
H	0.66022515	0.23989127	0.04322689
H	0.27237439	0.53892239	0.98847952
H	0.91224915	0.61242057	0.29386690
H	0.88196719	0.40186598	0.75683738
H	0.30217167	0.74966397	0.52808224
H	0.70432552	0.97436169	0.01582718
H	0.68458634	0.12044538	0.04462432
H	0.47926811	0.17756939	0.26107876
H	0.49898162	0.03145703	0.23188598
H	0.98184008	0.66758355	0.33436056
H	0.10669125	0.43126950	0.84094874
H	0.20243490	0.48360958	0.94493579

H	0.07756492	0.71989132	0.43851093
C	0.56501970	0.51379225	0.14715313
C	0.63452090	0.49429515	0.09133600
C	0.66436833	0.55445820	0.09134818
C	0.61921860	0.63830484	0.13751221
C	0.54973032	0.65779772	0.19359745
C	0.51988134	0.59762766	0.19354112
C	0.63354039	0.71024422	0.11813578
C	0.57945670	0.78315887	0.16829018
C	0.55063430	0.44183869	0.16571412
C	0.60465806	0.36890579	0.11514815
C	0.44821730	0.61964835	0.23356844
C	0.73602633	0.53234537	0.05096259
C	0.40752021	0.69345753	0.41099808
C	0.33980947	0.69724726	0.39844487
C	0.32595235	0.62564796	0.20940028
C	0.77662089	0.45843260	0.87374757
C	0.84437091	0.45442749	0.88604089
C	0.85834075	0.52601313	0.07421888
C	0.57260571	0.86750602	0.17260950
C	0.61795025	0.90039133	0.10612407
C	0.68296263	0.84725609	0.01462396
C	0.60377198	0.98966495	0.12190080
C	0.56581539	0.25160302	0.17334824
C	0.61131749	0.28453715	0.10896531
C	0.50078923	0.30470552	0.26474768
C	0.26676746	0.60006483	0.14805043
C	0.20487829	0.64099657	0.26844135
C	0.19307928	0.72118970	0.47809462
C	0.14817262	0.60680702	0.20027331
C	0.03612117	0.54432091	0.07976126
C	0.97941448	0.51018100	0.01292472
C	0.91764206	0.55131009	0.13438548
C	0.99107135	0.42994684	0.80372243
C	0.65461189	0.01868081	0.07032663
C	0.64312040	0.10233340	0.08754092
C	0.57988463	0.16229102	0.15591942
C	0.52899323	0.13325313	0.20676638
C	0.54047460	0.04959728	0.18949377
C	0.02991068	0.62608245	0.24773825
C	0.09989677	0.49491159	0.97265258
C	0.15437076	0.52507641	0.03177436
C	0.08436984	0.65624316	0.30693901
S	0.50797073	0.76406628	0.23700760

S	0.67624694	0.38801363	0.04782565
S	0.39875809	0.55589208	0.04494809
S	0.78559390	0.59600680	0.23877524
N	0.73639276	0.80508085	0.93519997
N	0.44734224	0.34682417	0.34406436
N	0.18268490	0.78638492	0.65653569
N	0.00141904	0.36469298	0.62577832

TBDT-TT-CN

a = 22.82Å, b = 19.21Å, c = 3.88Å, alpha = 106.15º, beta = 106.13º, gamma = 69.40º

H	0.63305072	0.63705822	0.08231100
H	0.46133406	0.39574835	0.19231041
H	0.39188110	0.67323238	0.48825250
H	0.70259493	0.35997140	0.78652601
H	0.48574889	0.82236825	0.19213627
H	0.43890951	0.14051539	0.21285063
H	0.60870273	0.21052483	0.08001262
H	0.25068381	0.47455498	0.01641135
H	0.04377108	0.37401552	0.15851390
H	0.84370316	0.55870641	0.26503963
H	0.81927843	0.35584888	0.85145309
H	0.27530953	0.67750102	0.42678924
H	0.05068158	0.65910437	0.12459680
H	0.65565213	0.89192762	0.05687703
C	0.52118695	0.45973019	0.13668325
C	0.58657811	0.44210217	0.10692838
C	0.61516735	0.49696111	0.11396644
C	0.57316864	0.57321835	0.13881090
C	0.50777875	0.59085592	0.16856428
C	0.47919476	0.53600541	0.16200858
C	0.58736690	0.63827207	0.12115958
C	0.53701930	0.70462750	0.14926171
C	0.50699462	0.39461256	0.15349685
C	0.55733462	0.32825782	0.12457235
C	0.41214511	0.55591310	0.17890442
C	0.68224482	0.47709702	0.09811770
C	0.37352778	0.62595322	0.33503562
C	0.31047342	0.62834100	0.30628762
C	0.29818119	0.55938250	0.12717671
C	0.72093986	0.40716584	0.94154379
C	0.78404475	0.40485692	0.97229497
C	0.79624413	0.47378969	0.15336046
C	0.53179496	0.78088070	0.14984834
C	0.57597156	0.81015917	0.10582969

C	0.63772437	0.76275082	0.04444874
C	0.56375763	0.88998533	0.11523614
C	0.57930908	0.00275282	0.11353113
C	0.53077887	0.14254290	0.15476616
C	0.48764422	0.10851599	0.17934858
C	0.51525498	0.02970872	0.15541676
C	0.51850660	0.22244817	0.16567979
C	0.56263353	0.25191251	0.12260383
C	0.45676607	0.26976474	0.22769968
C	0.24300262	0.53591977	0.07648182
C	0.18174158	0.58179614	0.10630481
C	0.16476907	0.66174808	0.13094397
C	0.13039775	0.55465753	0.11188080
C	0.03019723	0.55505589	0.14009023
C	0.96405932	0.47844703	0.17070756
C	0.02710125	0.43452919	0.15797079
C	0.91270724	0.45141692	0.17688981
C	0.85141415	0.49734066	0.20546541
C	0.92967180	0.37153041	0.15416408
C	0.06422312	0.47799967	0.14175110
C	0.06734161	0.59855946	0.12451293
C	0.60690448	0.92394231	0.09003482
S	0.46935902	0.68740230	0.19236792
S	0.62501563	0.34555790	0.08239230
S	0.36650456	0.49353718	0.98991182
S	0.72784017	0.53943227	0.29009286
S	0.60533325	0.07640322	0.10489817
S	0.95126114	0.57323132	0.15832696
S	0.14316123	0.45983481	0.12351906
S	0.48920031	0.95611567	0.16425526
N	0.68864713	0.72560102	0.99049907
N	0.40589780	0.30690831	0.28261206
N	0.14901918	0.72710842	0.14028185
N	0.94545487	0.30625247	0.14704167

PBDT-P-CN

a = 22.08 Å, b = 17.53 Å, c = 3.90 Å, alpha = 106.50º, beta = 91.81º, gamma = 83.59º

H	0.67561453	0.73579180	0.07775056
H	0.50843810	0.41560148	0.19987269
H	0.44035834	0.68418462	0.58406608
H	0.74401556	0.46754549	0.69692743
H	0.52628962	0.88977877	0.19507670
H	0.65778409	0.26164883	0.08238108
H	0.25343245	0.50685777	0.94725124

H	0.93037956	0.64534147	0.33965719
H	0.69024894	0.00025383	0.89187054
H	0.67236964	0.14201348	0.94004627
H	0.49380226	0.15103921	0.38422046
H	0.51168214	0.00929031	0.33618926
H	0.01110218	0.68704071	0.15545298
H	0.06766592	0.43520484	0.97956340
H	0.17301980	0.46509347	0.13468176
H	0.11644585	0.71692763	0.31078502
H	0.85395701	0.46910013	0.70708366
H	0.83411837	0.69826025	0.51432867
H	0.72454185	0.69435383	0.51511404
H	0.33040996	0.68286116	0.57731252
H	0.34952269	0.45372633	0.76962083
H	0.45911789	0.45741564	0.76541388
C	0.56774597	0.50520993	0.14516833
C	0.63222357	0.50781092	0.11313404
C	0.65831851	0.57726766	0.11392444
C	0.61629861	0.64629428	0.13354639
C	0.55182708	0.64370310	0.16574853
C	0.52571982	0.57428371	0.16543661
C	0.62974448	0.72199123	0.10890532
C	0.57896443	0.77723627	0.13184215
C	0.55430942	0.42945221	0.16912740
C	0.60509545	0.37419490	0.14597826
C	0.45916204	0.57157859	0.17321420
C	0.72486853	0.58010274	0.10764451
C	0.42061544	0.63431605	0.39678663
C	0.76359498	0.51743789	0.88503839
C	0.57236217	0.85954053	0.13437901
C	0.61499139	0.90581844	0.07272036
C	0.67518077	0.87018019	0.96564076
C	0.60252807	0.99192289	0.10559834
C	0.56906190	0.24548888	0.20388273
C	0.61169367	0.29184041	0.14284465
C	0.50884829	0.28109701	0.31061616
C	0.26528443	0.56137832	0.14434157
C	0.21641523	0.61210048	0.30979497
C	0.22255159	0.68726353	0.56555369
C	0.15286485	0.59328934	0.23000442
C	0.03125240	0.55884431	0.06009927
C	0.96774136	0.53999555	0.97908096
C	0.91871637	0.59070614	0.14262931
C	0.96179574	0.46472216	0.72382936

C	0.64698111	0.03309074	0.00251670
C	0.63680183	0.11427919	0.03343510
C	0.58154642	0.15937752	0.17085630
C	0.53708502	0.11820284	0.27380544
C	0.54726835	0.03702209	0.24297800
C	0.04622934	0.63807651	0.15663692
C	0.07840195	0.49704791	0.04765215
C	0.13788132	0.51405474	0.13362934
C	0.10571090	0.65508240	0.24275636
C	0.82631836	0.51882472	0.88687961
C	0.85380054	0.58387129	0.11319565
C	0.81477746	0.64697871	0.33357993
C	0.75218306	0.64512572	0.33228474
C	0.35789247	0.63307033	0.39689051
C	0.33022263	0.56807084	0.17163484
C	0.36904454	0.50491370	0.94995014
C	0.43164372	0.50663412	0.94940545
S	0.51214236	0.73607199	0.18141786
S	0.67193603	0.41542698	0.09725760
N	0.72456713	0.84161273	0.87190144
N	0.45947836	0.30975470	0.40425378
N	0.22486416	0.74854554	0.78426216
N	0.95965960	0.40332592	0.50566298

PBDT-TT-CN

a = 23.81 Å, b = 19.17 Å, c = 3.91 Å, alpha = 105.19º, beta = 95.41º, gamma = 82.36º

H	0.63520099	0.68368841	0.07257506
H	0.47996005	0.39705744	0.21243777
H	0.41916818	0.64193091	0.55518635
H	0.69626900	0.43871365	0.72984741
H	0.49878552	0.82901251	0.18527906
H	0.61599967	0.25129488	0.09963747
H	0.24205606	0.48181870	0.94301912
H	0.87315879	0.59910116	0.34421455
H	0.65156551	0.93944044	0.94967800
H	0.00821082	0.41877374	0.74310008
H	0.79841503	0.43834909	0.74736445
H	0.78527182	0.64687008	0.52100225
H	0.68342264	0.64466064	0.51792154
H	0.31702848	0.64241433	0.53902153
H	0.32990964	0.43377279	0.76624565
H	0.43173698	0.43588945	0.76782792
H	0.10719571	0.66232759	0.54452467
H	0.46287208	0.14139514	0.33570744

C	0.53495628	0.47666037	0.15027759
C	0.59470332	0.47730313	0.12144732
C	0.61917202	0.53999630	0.12192760
C	0.58029371	0.60388178	0.13396247
C	0.52054740	0.60318511	0.16258347
C	0.49609892	0.54053783	0.16261585
C	0.59278739	0.67234519	0.10404665
C	0.54589174	0.72413064	0.12298017
C	0.52238230	0.40824856	0.18017421
C	0.56918082	0.35632711	0.16062166
C	0.43430080	0.53927038	0.16251623
C	0.68098599	0.54131377	0.12285369
C	0.39972447	0.59690972	0.37298830
C	0.71564539	0.48373698	0.91255742
C	0.54056497	0.79909530	0.12226451
C	0.58042211	0.83941575	0.05739595
C	0.63531543	0.80630859	0.94973710
C	0.57027471	0.91699257	0.08836880
C	0.53417965	0.24128022	0.22612701
C	0.57424596	0.28139506	0.16166352
C	0.47920336	0.27450527	0.33151449
C	0.25424921	0.53180036	0.12890239
C	0.21001294	0.57784319	0.29477199
C	0.21761080	0.64559732	0.54447749
C	0.15129701	0.56213491	0.23293046
C	0.96407351	0.51897955	0.05442536
C	0.90538163	0.50315637	0.99267387
C	0.86105877	0.54906264	0.15838490
C	0.89789750	0.43533144	0.74333577
C	0.60884117	0.96078202	0.03094637
C	0.01131770	0.47285383	0.91712660
C	0.77392202	0.48399327	0.91819088
C	0.80092901	0.54293344	0.13498659
C	0.76605257	0.60064108	0.34635864
C	0.70790889	0.59976791	0.34207222
C	0.34145871	0.59671568	0.36817475
C	0.31438777	0.53777808	0.15201712
C	0.34918645	0.47999652	0.94053916
C	0.40732317	0.48080782	0.94398224
C	0.58535279	0.03395264	0.09133995
C	0.52905570	0.04679807	0.19441811
C	0.05358771	0.57591656	0.25539788
C	0.06178303	0.50522167	0.03200600
C	0.10406958	0.60826999	0.37031197

C	0.50558772	0.11999939	0.25440752
C	0.54418268	0.16373521	0.19655143
S	0.48401988	0.68850029	0.17301052
S	0.63112331	0.39186339	0.11047310
S	0.50522387	0.96695524	0.21639004
S	0.98244998	0.60227043	0.32253625
S	0.13290328	0.47887624	0.96463948
S	0.60923564	0.11372744	0.06933326
N	0.68032650	0.78045835	0.85410972
N	0.43407570	0.30038327	0.42494565
N	0.22109318	0.70101372	0.75595746
N	0.89452677	0.37986190	0.53209057

TBDT-P-IM

a = 20.85 Å, b = 17.02 Å, c = 3.91Å, alpha = 104.93º, beta = 102.17º, gamma = 69.11º

H	0.67338579	0.72756011	0.08845916
H	0.51081302	0.42419327	0.19614817
H	0.42007570	0.73266003	0.57881201
H	0.76420284	0.41849078	0.70468842
H	0.50734098	0.92826015	0.23502783
H	0.67688659	0.22332877	0.05364322
H	0.26679329	0.51769230	0.87419997
H	0.91715562	0.63448262	0.39929936
H	0.89103898	0.42259732	0.77634711
H	0.29301335	0.72900397	0.50226374
H	0.70245291	0.98035157	0.40440180
H	0.69078845	0.13132765	0.41046964
H	0.48148442	0.17168908	0.88521905
H	0.49315650	0.02069838	0.87900086
H	0.97626727	0.68848397	0.13829673
H	0.10164479	0.42324629	0.07547574
H	0.20768851	0.46348393	0.13567894
H	0.08229805	0.72871456	0.19869879
C	0.56860729	0.50723784	0.13727520
C	0.63877319	0.49327037	0.09196557
C	0.66481643	0.55981018	0.10100931
C	0.61572889	0.64421991	0.14643078
C	0.54558907	0.65815516	0.19202341
C	0.51951312	0.59160132	0.18201178
C	0.62579342	0.72204864	0.13601270
C	0.56773276	0.79300395	0.18258470
C	0.55846880	0.42953388	0.14856611
C	0.61651956	0.35853936	0.10312185

C	0.44687727	0.60857851	0.21020532
C	0.73737908	0.54288388	0.07116219
C	0.40239704	0.68145917	0.40163151
C	0.33454777	0.67978692	0.36536136
C	0.32507098	0.60557851	0.14187232
C	0.78183082	0.46993637	0.87987672
C	0.84955806	0.47183912	0.91354344
C	0.85899807	0.54628210	0.13495348
C	0.55918332	0.88148982	0.19096443
C	0.59876636	0.99022097	0.14746193
C	0.62501983	0.27017263	0.09653295
C	0.26391862	0.57957875	0.06127616
C	0.15196378	0.59934225	0.16445495
C	0.03198051	0.55261270	0.10966626
C	0.92006063	0.57244053	0.21336910
C	0.65448275	0.02263347	0.28735677
C	0.64773796	0.10676233	0.28821243
C	0.58522760	0.16173924	0.14138201
C	0.52947045	0.12938264	0.00203657
C	0.53621983	0.04524731	0.00113298
C	0.02709149	0.63918255	0.14321654
C	0.09802815	0.49001530	0.10034021
C	0.15685727	0.51277039	0.13085320
C	0.08591400	0.66194090	0.17382275
N	0.60953955	0.90507974	0.15668521
N	0.57456076	0.24677468	0.13090389
N	0.20875010	0.62728755	0.20563054
N	0.97521813	0.52464922	0.06907453
S	0.49768602	0.76671581	0.23743501
S	0.68661566	0.38470791	0.04798162
S	0.40120834	0.53898710	0.97840920
S	0.78296079	0.61280667	0.29959257

TBDT-TT-IM

a = 22.64 Å, b = 18.76 Å, c = 3.93 Å, alpha = 104.39º, beta = 104.68º, gamma = 68.98º

H	0.62028629	0.65576065	0.09138672
H	0.47420788	0.37694043	0.18611994
H	0.39153013	0.65737093	0.56887168
H	0.70290804	0.37577170	0.70898235
H	0.46855020	0.83656877	0.25610471
H	0.44731477	0.15581392	0.20916851
H	0.62603587	0.19624050	0.01800340
H	0.24735203	0.46113512	0.90698111
H	0.01137337	0.38395235	0.83104920

H	0.84687298	0.57230395	0.37026325
H	0.81964296	0.37941167	0.77829987
H	0.27468866	0.65406823	0.49857175
H	0.08289111	0.64941227	0.44634345
H	0.64736330	0.87645322	0.06267307
C	0.52589649	0.45365739	0.12996802
C	0.58984852	0.44198516	0.08164941
C	0.61373311	0.50282019	0.09635758
C	0.56860280	0.57921159	0.14932008
C	0.50464708	0.59091526	0.19764125
C	0.48077047	0.53006476	0.18317184
C	0.57731968	0.65020031	0.14279415
C	0.52412116	0.71445787	0.19508506
C	0.51717144	0.38256180	0.13495316
C	0.57035089	0.31831926	0.08149739
C	0.41442800	0.54473871	0.21418221
C	0.68004698	0.48820961	0.06511214
C	0.37437087	0.61080265	0.39807499
C	0.31183347	0.60933429	0.36503228
C	0.30166209	0.54173809	0.15204161
C	0.72007644	0.42229894	0.88024855
C	0.78253943	0.42395964	0.91278619
C	0.79265165	0.49156347	0.12611479
C	0.51536340	0.79435366	0.20202817
C	0.55209416	0.89132839	0.14478020
C	0.57949239	0.99722278	0.11060314
C	0.54257828	0.14096239	0.12721530
C	0.49450961	0.11538486	0.17059512
C	0.51513183	0.03499667	0.15999417
C	0.57919574	0.23829228	0.07251465
C	0.24551562	0.51808298	0.07882047
C	0.14177793	0.54151094	0.17592712
C	0.03809031	0.55541325	0.23020187
C	0.95247656	0.49186945	0.10125843
C	0.00825609	0.44253424	0.97322202
C	0.84874380	0.51531249	0.19874549
C	0.05617675	0.47795597	0.04709694
C	0.08600937	0.59084112	0.30403817
C	0.60014325	0.91685748	0.10079705
N	0.56008232	0.81641609	0.14685485
N	0.53453517	0.21594940	0.12640859
N	0.19480856	0.56216419	0.21612851
N	0.89944649	0.47122845	0.06138350
S	0.46067619	0.68924969	0.25024331

S	0.63377577	0.34367692	0.02716658
S	0.37093854	0.48132509	0.99445152
S	0.72342467	0.55172896	0.28484189
S	0.61510402	0.06191370	0.07608432
S	0.96082103	0.58477145	0.31370935
S	0.13342759	0.44862276	0.96323305
S	0.47956699	0.97032201	0.19517639

PBDT-P-IM

a = 21.61Å, b = 17.01Å, c = 3.93Å, alpha = 108.67º, beta = 90.45º, gamma = 81.69º

H	0.66681203	0.75402601	0.15551162
H	0.51722772	0.39749013	0.12406343
H	0.42743260	0.67732399	0.50929759
H	0.75703051	0.47429403	0.77018690
H	0.51084997	0.89506956	0.07171374
H	0.67324982	0.25637882	0.20701885
H	0.25135213	0.47787978	0.81884258
H	0.93236814	0.67429108	0.46730334
H	0.68735294	0.97497057	0.86434660
H	0.67813908	0.12284306	0.87494630
H	0.49671513	0.17647278	0.41542710
H	0.50592798	0.02860222	0.40484468
H	0.01336082	0.69365122	0.09478199
H	0.05763313	0.44341494	0.15391459
H	0.17073488	0.45862218	0.19392235
H	0.12645605	0.70889365	0.13516454
H	0.87001727	0.48608253	0.82401624
H	0.82483554	0.72536913	0.65212672
H	0.71240771	0.71300320	0.60691322
H	0.31436165	0.66583976	0.45955856
H	0.35872858	0.42650432	0.63078603
H	0.47124801	0.43850556	0.67252188
C	0.57154855	0.49974887	0.12568625
C	0.63671187	0.50927558	0.14549052
C	0.65887711	0.58388911	0.16151256
C	0.61253188	0.65160568	0.15223096
C	0.54737610	0.64203835	0.13184231
C	0.52520664	0.56746392	0.11638301
C	0.62176202	0.73219744	0.14390822
C	0.56726657	0.78256219	0.11722241
C	0.56229931	0.41922689	0.13477118
C	0.61679436	0.36881915	0.16111508
C	0.45798068	0.55930090	0.09121273
C	0.72607548	0.59221942	0.18813653

C	0.41241722	0.62314415	0.30949050
C	0.77183660	0.52851600	0.97085345
C	0.55929638	0.86695206	0.09997898
C	0.59714085	0.99057328	0.12530105
C	0.62478697	0.28448197	0.17903477
C	0.26237134	0.53771260	0.00833554
C	0.15623305	0.58462273	0.16036133
C	0.02785911	0.56766349	0.12848591
C	0.92156512	0.61435485	0.27762276
C	0.64609348	0.02001396	0.98943354
C	0.64102000	0.10302715	0.00059975
C	0.58695442	0.16088902	0.15469873
C	0.53799707	0.13144341	0.29057061
C	0.54307120	0.04843000	0.27942463
C	0.04780987	0.64275487	0.12401380
C	0.07331690	0.50098990	0.14554932
C	0.13627632	0.50955209	0.16501785
C	0.11077236	0.65132733	0.14362272
C	0.83504037	0.53507999	0.99688326
C	0.85529435	0.60607510	0.24245191
C	0.80992503	0.67014814	0.45711672
C	0.74656082	0.66341688	0.43117058
C	0.34917419	0.61676049	0.28577154
C	0.32868790	0.54581440	0.04122292
C	0.37384739	0.48165879	0.82516772
C	0.43725445	0.48818565	0.84912219
N	0.60634596	0.90679733	0.11223233
N	0.57774966	0.24465014	0.16752492
N	0.21882133	0.59681840	0.18173126
N	0.96529839	0.55532282	0.10582036
S	0.50171314	0.73311082	0.10674796
S	0.68236640	0.41816622	0.17023037

PBDT-TT-IM

a = 23.34 Å, b = 18.72Å, c = 3.94 Å, alpha = 111.27º, beta = 98.61º, gamma = 78.11º

H	0.62529032	0.70128125	0.19585837
H	0.48991267	0.37934177	0.09457573
H	0.40583179	0.63715882	0.48851726
H	0.70910534	0.44327722	0.79997488
H	0.47670723	0.84024457	0.13194170
H	0.63851288	0.24033760	0.15886753
H	0.23808937	0.45167424	0.71949264
H	0.87699040	0.62930362	0.55803715
H	0.65215277	0.93125243	0.26298890

H	0.99143202	0.42323419	0.75182304
H	0.81416095	0.45544623	0.87077320
H	0.77866422	0.67528512	0.73901281
H	0.67398885	0.66297661	0.67189852
H	0.30067931	0.62515693	0.41195306
H	0.33672104	0.40553044	0.54328036
H	0.44151546	0.41761510	0.61627923
H	0.12329021	0.65793535	0.52302274
H	0.46309907	0.14932052	0.02907004
C	0.53948936	0.47054754	0.11131343
C	0.60064875	0.47684506	0.14258263
C	0.62042386	0.54556209	0.18269227
C	0.57575810	0.61002836	0.17928006
C	0.51460244	0.60370478	0.14781378
C	0.49482555	0.53498564	0.10754310
C	0.58320515	0.68378985	0.18318102
C	0.53105082	0.73332554	0.16348272
C	0.53202063	0.39678278	0.10727729
C	0.58415957	0.34721343	0.12697697
C	0.43192872	0.52822660	0.05903735
C	0.68329524	0.55231375	0.22932637
C	0.39066050	0.58698317	0.27517772
C	0.72439715	0.49354856	0.01188455
C	0.52257320	0.81085283	0.15617052
C	0.56042602	0.91728604	0.16212508
C	0.59263725	0.26970367	0.13473861
C	0.25019504	0.50479228	0.93636386
C	0.15514949	0.54586650	0.12897780
C	0.95959115	0.53526038	0.14625558
C	0.86478936	0.57613156	0.34206131
C	0.60708540	0.95719045	0.20988939
C	0.00209746	0.47863270	0.94113351
C	0.78320841	0.50023928	0.04820028
C	0.80391798	0.56627289	0.30740385
C	0.76332003	0.62439169	0.53069874
C	0.70430669	0.61770528	0.49197610
C	0.33178474	0.58038769	0.23559405
C	0.31116407	0.51449907	0.97438037
C	0.35195937	0.45634707	0.75285941
C	0.41103851	0.46290694	0.79489757
C	0.58831131	0.03118111	0.18259692
C	0.52692775	0.04948635	0.11052117
C	0.05758560	0.57852421	0.26493052
C	0.05709828	0.50273932	0.00947974

C	0.11260746	0.60256562	0.33350063
C	0.50816220	0.12342818	0.08265641
C	0.55481435	0.16334495	0.13033625
N	0.56700296	0.84506715	0.17737202
N	0.54822755	0.23551242	0.11434388
N	0.21173853	0.55506431	0.14682604
N	0.90308136	0.52591281	0.13014316
S	0.47023523	0.69050793	0.14108951
S	0.64499387	0.38998073	0.14869161
S	0.49181202	0.97433626	0.07803505
S	0.98936695	0.62050904	0.42528584
S	0.12533225	0.46068456	0.84957612
S	0.62341847	0.10634958	0.21523290

TBDT-TT-CC

a = 22.97 Å, b = 19.15 Å, c = 3.96 Å, alpha = 104.00º, beta = 105.08º, gamma = 69.43º

H	0.62319536	0.64796374	0.07989074
H	0.47129374	0.38559490	0.19770483
H	0.39730484	0.65741213	0.57108349
H	0.69664437	0.37648680	0.70218987
H	0.47601462	0.82783713	0.25457328
H	0.44684612	0.14884642	0.24271193
H	0.61773914	0.20554888	0.01712503
H	0.25024008	0.46966279	0.93231535
H	0.01525660	0.38509141	0.81487978
H	0.84489231	0.56252228	0.35009873
H	0.81149679	0.37552803	0.75781397
H	0.28273606	0.65766714	0.51793072
H	0.08005730	0.64658924	0.47027948
H	0.64652579	0.88490845	0.02600196
H	0.60835195	0.77556128	0.06092987
H	0.90130487	0.41156086	0.87788697
H	0.19374786	0.62039528	0.40567588
H	0.48524561	0.25833382	0.20949526
C	0.52459908	0.45663588	0.13255899
C	0.58741384	0.44362355	0.08046542
C	0.61252375	0.50180488	0.09150525
C	0.56982499	0.57693349	0.14440677
C	0.50696234	0.58992219	0.19582810
C	0.48188378	0.53174648	0.18552020
C	0.58006778	0.64556458	0.13543803
C	0.52910696	0.70950640	0.18707112
C	0.51431109	0.38801296	0.14094251
C	0.56511070	0.32402141	0.08716905

C	0.41661563	0.54782292	0.22113232
C	0.67781576	0.48559142	0.05597929
C	0.37894382	0.61262612	0.40429839
C	0.31691376	0.61262230	0.37795716
C	0.30430285	0.54749563	0.17168116
C	0.71526046	0.42089627	0.87107715
C	0.77744896	0.42051664	0.89887973
C	0.79040574	0.48523118	0.10803698
C	0.52087048	0.78755876	0.19171866
C	0.56333784	0.81507106	0.12468468
C	0.55529423	0.89270715	0.12767179
C	0.57772765	0.00031423	0.10033954
C	0.53803722	0.14106791	0.14052145
C	0.49321333	0.11254757	0.19010906
C	0.51555600	0.03343220	0.16640198
C	0.53020909	0.21871739	0.14554027
C	0.57296668	0.24600973	0.08026246
C	0.24868928	0.52443637	0.10252305
C	0.19540071	0.56530971	0.23865579
C	0.13971593	0.54428728	0.19444820
C	0.03823871	0.55292445	0.23731791
C	0.95554648	0.48743993	0.09024771
C	0.01057807	0.44200128	0.96364183
C	0.89972423	0.46663020	0.04494149
C	0.84631877	0.50781195	0.17953116
C	0.05703383	0.47878132	0.04750525
C	0.08470345	0.58969660	0.32132577
C	0.60009558	0.92121365	0.07757670
S	0.46605304	0.68629911	0.24788125
S	0.62819244	0.34718010	0.02626312
S	0.37122219	0.48767311	0.00973067
S	0.72354474	0.54516122	0.27060692
S	0.60817847	0.06852233	0.06768805
S	0.96217730	0.57642162	0.31041838
S	0.13307856	0.45532711	0.97405217
S	0.48510093	0.96526171	0.19926002

PBDT-P-CC

a = 22.10 Å, b = 17.43 Å, c = 3.99 Å, alpha = 107.81º, beta = 99.36º, gamma = 80.49º

H	0.66681785	0.74456418	0.14547270
H	0.51717004	0.40731288	0.13972128
H	0.43870409	0.67508028	0.52589573
H	0.74490689	0.47635649	0.75606505
H	0.51414624	0.89906768	0.22710109

H	0.67002847	0.25304690	0.06006126
H	0.25124680	0.49044142	0.78320544
H	0.93277433	0.66076934	0.49235524
H	0.68614270	0.98246971	0.96447257
H	0.68013660	0.12562616	0.98992268
H	0.49843962	0.16981383	0.32786533
H	0.50445155	0.02665365	0.30239966
H	0.02566756	0.68527779	0.52375220
H	0.04726115	0.45724818	0.70539792
H	0.15791992	0.46620630	0.74874495
H	0.13632198	0.69418882	0.56733867
H	0.85517034	0.48528052	0.81120243
H	0.83363283	0.70854047	0.65611265
H	0.72260413	0.69787232	0.60596769
H	0.32842150	0.66594030	0.46754543
H	0.35063597	0.44292150	0.62182929
H	0.46170065	0.45378968	0.67556812
H	0.64723154	0.87271530	0.03918578
H	0.94823483	0.50767520	0.85870519
H	0.23529337	0.64376681	0.41522957
H	0.53722058	0.27950504	0.25216635
C	0.57122369	0.50237802	0.12444513
C	0.63527871	0.50813956	0.12306148
C	0.65790307	0.58058100	0.14805937
C	0.61270183	0.64943506	0.15921302
C	0.54863363	0.64367163	0.16045382
C	0.52601327	0.57118977	0.13499147
C	0.62183826	0.72813620	0.15435651
C	0.56859681	0.78224570	0.16246725
C	0.56213484	0.42373493	0.13047086
C	0.61542471	0.36971746	0.12329601
C	0.45939897	0.56488697	0.10708170
C	0.72452194	0.58672603	0.17459889
C	0.41956750	0.62461449	0.32125738
C	0.76417833	0.52685196	0.95978170
C	0.55969552	0.86637879	0.16883162
C	0.60260990	0.90690649	0.10986351
C	0.59592439	0.99222267	0.12872150
C	0.58179538	0.24529995	0.18066636
C	0.62450587	0.28572758	0.11906735
C	0.26500544	0.54290429	0.99996852
C	0.22141640	0.59115536	0.19973979
C	0.15636125	0.58139465	0.16209472
C	0.02723935	0.57002719	0.11069713

C	0.96222382	0.56021254	0.07424557
C	0.91883683	0.60840102	0.27564196
C	0.64485117	0.02382281	0.04684059
C	0.64151178	0.10491710	0.06301998
C	0.58860698	0.16003760	0.16297180
C	0.53971863	0.12845398	0.24532974
C	0.54305048	0.04735806	0.22904033
C	0.05410716	0.63698951	0.35070180
C	0.06690401	0.50933114	0.89706968
C	0.12947531	0.51447260	0.92185803
C	0.11667933	0.64210880	0.37563387
C	0.82686289	0.53241924	0.98972329
C	0.85372766	0.59845901	0.23664488
C	0.81406456	0.65778570	0.45442795
C	0.75132452	0.65222072	0.42458981
C	0.35686484	0.61891989	0.28937815
C	0.33015835	0.55291393	0.04109382
C	0.37003679	0.49368441	0.82433820
C	0.43279290	0.49936597	0.85611569
S	0.50444284	0.73699043	0.17523732
S	0.67950857	0.41487923	0.10900811

PBDT-TT-CC

a = 23.80Å, b = 19.15 Å, c = 3.95 Å, alpha = 106.39º, beta = 97.26º, gamma = 81.71º

H	0.62812037	0.69224964	0.11458993
H	0.48696832	0.38843412	0.17261635
H	0.41590786	0.63028057	0.54126207
H	0.69928163	0.45007184	0.74518209
H	0.48727815	0.83130312	0.20534608
H	0.62756752	0.24910925	0.08380888
H	0.24249250	0.46323928	0.84032761
H	0.87267336	0.61749820	0.44228624
H	0.64677935	0.92968688	0.97726619
H	0.99476170	0.42861260	0.74013571
H	0.80127142	0.45779547	0.78863915
H	0.78101609	0.66019810	0.61370902
H	0.67820504	0.65093056	0.57443512
H	0.31384484	0.62273347	0.49561726
H	0.33420293	0.42048263	0.66966301
H	0.43709412	0.42958598	0.71120072
H	0.12035040	0.65255180	0.54029865
H	0.46774111	0.15139710	0.31409732
H	0.61187199	0.81203672	0.02353205
H	0.22464181	0.60899181	0.41971747

H	0.50296756	0.26911623	0.26671631
H	0.89051103	0.47208624	0.86068227
C	0.53782744	0.47390809	0.13751282
C	0.59711270	0.47908632	0.12473500
C	0.61860036	0.54441591	0.13817595
C	0.57734900	0.60659074	0.14892996
C	0.51807508	0.60138638	0.16178184
C	0.49659184	0.53605797	0.14809420
C	0.58639345	0.67754068	0.13369034
C	0.53751822	0.72643943	0.14591789
C	0.52872191	0.40304510	0.15339027
C	0.57755638	0.35410996	0.14194866
C	0.43498405	0.53050868	0.13016191
C	0.68021372	0.54996164	0.15564389
C	0.39815941	0.58480082	0.34286188
C	0.71702590	0.49565496	0.94286473
C	0.52964017	0.80234660	0.14854468
C	0.56986400	0.84072618	0.09120440
C	0.56333539	0.91714964	0.11106011
C	0.54490999	0.24019661	0.19915135
C	0.58526817	0.27827134	0.14066394
C	0.25492396	0.51247239	0.04004478
C	0.21341685	0.55900501	0.22191355
C	0.15399168	0.55004431	0.18436938
C	0.96109426	0.53110772	0.09619712
C	0.90170028	0.52201770	0.05902079
C	0.86022428	0.56832520	0.24219546
C	0.60479127	0.95599013	0.05230883
C	0.00376104	0.48060631	0.92569181
C	0.77506825	0.50042708	0.96661683
C	0.79993053	0.56002847	0.20571772
C	0.76301198	0.61420900	0.41933519
C	0.70494033	0.60936363	0.39557870
C	0.34008899	0.58013082	0.31778058
C	0.31524195	0.52063383	0.07770715
C	0.35219438	0.46639975	0.86463059
C	0.41029056	0.47116013	0.88959660
C	0.58543909	0.03073489	0.09849096
C	0.52900835	0.05024776	0.19284526
C	0.05721494	0.57557765	0.26093569
C	0.05787489	0.50557299	0.01970415
C	0.11132723	0.60056108	0.35478181
C	0.50972572	0.12504490	0.23923121
C	0.55123707	0.16381780	0.18030246

S	0.47787536	0.68546820	0.17351724
S	0.63725985	0.39497149	0.11377981
S	0.50020677	0.97468532	0.22378240
S	0.98880088	0.61002775	0.37067145
S	0.12628950	0.47113446	0.90980845
S	0.61430353	0.10619525	0.06761075

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