Supplementary Information

Large Pore Donor–Acceptor Covalent Organic Frameworks

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A. Materials and Methods

Dehydrated *N,N*-dimethylformamide (DMF), dehydrated tetrahydrofuran (THF), dehydrated *N*, *N*-dimethylacetamide (DMAc), dehydrated dioxane, dehydrated toluene, *o*-dichlorobenzene (*o*-DCB), mesitylene and sodium periodate were purchased from Kanto Chemicals. Dehydrated acetone, imidazole, methanol and chloroform were purchased from Wako Chemicals. 4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)aniline and pyrromellitic 1,2,4,5-tetracarboxylic acid dianhydride were purchased from Tokyo Kasai Co. (TCI). COF-10 was synthesized according to the previous reported method.[1]

^{1}H-NMR spectra were recorded on JEOL models JNM-LA400 NMR spectrometers, where chemical shifts (δ in ppm) were determined with a residual proton of the solvent as standard. Fourier transform infrared (FT-IR) spectra were recorded on a JASCO model FT-IR-6100 infrared spectrometer. UV-Vis-IR diffuse reflectance spectrum (Kubelka-Munk spectrum) was recorded on a JASCO model V-670 spectrometer equipped with integration sphere model IJN-727. Matrix-assisted laser desorption ionization time-of-flight mass (MALDI-TOF MS) spectra were recorded on an Applied Biosystems BioSpectrometry model Voyager-DE-STR spectrometer in reflector or linear mode. Field-emission scanning electron microscopy (FE-SEM) was performed on a JEOL model JSM-6700 operating at an accelerating voltage of 5.0 kV. The sample was prepared by drop-casting an acetone suspension onto mica substrate and then coated with gold. High-resolution transmission electron microscopy (HR-TEM) images were obtained on a JEOL model JEM-3200 microscopy. The sample was prepared by drop-casting an acetone suspension of D_{TP}-A_{NDI}-COF or D_{TP}-A_{PyrDI}-COF onto a copper grid. TGA measurements were performed on a Mettler-Toledo model TGA/SDTA851^e under N_2, by heating to 800 °C at a rate of 10 °C min^{-1}. X-ray diffraction (XRD) data were recorded on a Rigaku model RINT Ultima III diffractometer by depositing powder on glass substrate, from 2θ = 1.5° up to 60° with 0.02° increment.

Nitrogen sorption isotherms were measured at 77 K with a Bel Japan Inc. model BELSORP-mini II analyzer. Before measurement, the samples were degassed in vacuum at 150 °C for more than 10 h. The Brunauer-Emmett-Teller (BET) method was utilized to calculate the specific surface areas. By using the non-local density functional theory (NLDFT) model, the pore volume was derived from the sorption curve.

Molecular modeling and Pawley refinement were carried out using Reflex, a software package for crystal determination from XRD pattern, implemented in MS modeling version

4.4 (Accelrys Inc.). Unit cell dimension was first manually determined from the observed XRD peak positions using the coordinates. We performed Pawley refinement to optimize the lattice parameters iteratively until the R_{WP} value converges. The pseudo-Voigt profile function was used for whole profile fitting and Berrar–Baldinozzi function was used for asymmetry correction during the refinement processes. The final R_{WP} and R_P values were 9.91% and 6.71% for D_{TP}-A_{NDI}-COF and 8.66% and 5.33% for D_{TP}-A_{PyrDI}-COF, respectively.

The molecular structure and electronic properties of monolayer and stacked D_{TP}-A_{NDI}-COF and D_{TP}-A_{PyrDI}-COF isomers were determined using the density-functional tight-binding (DFTB) method including Lennard–Jones (LJ) dispersion. The corresponding LJ and crystal stacking energies were computed. The calculations were carried out with the DFTB+ program package version 1.2.[2] DFTB is an approximate density functional theory method based on the tight binding approach and utilizes an optimized minimal LCAO Slater-type all-valence basis set in combination with a two-center approximation for Hamiltonian matrix elements. The Coulombic interaction between partial atomic charges was determined using the self-consistent charge (SCC) formalism. Lennard-Jones type dispersion was employed in all calculations to describe van der Waals (vdW) and π-stacking interactions. The lattice dimensions were optimized simultaneously with the geometry. Where possible, DFTB parameters from the dftb.org website[3] were employed as follows. Standard DFTB parameters for X–Y element pairs (X, Y = C, H, O and N) interactions were selected from the mio-0-1 set and X–B parameters (X = C, H, O, B and N) were selected from the rscc-materials set. The optimal single layer 2D model system consisted of 198 atoms with optimal lattice constant of $a = b = 52.9$ Å, then three different stacking configurations: perfect AA, AA slip-stacked by 0.8 Å in the a and b directions and AB were optimized. The third dimension of the lattice, c was initialized at 3.5 Å for all structures. The optimum structures and corresponding electronic properties of stacked isomers of D_{TP}-A_{NDI}-COF were calculated using density-functional tight-binding (DFTB) method including Lennard–Jones (LJ) dispersion. For the monolayer structure, the obtained optimal cell length is, $a = b = 52.9$ Å. The smallest H–H distance is 1.88 Å within the planar triphenylene unit, the smallest inter-group distance is 1.91 Å between the phenyl hydrogen and diimine oxygen atom, and the monolayer remains planar. Using the optimal monolayer structure, three stacked configurations; AA, slipped-AA and AB were generated and optimized.

Time-resolved fluorescence spectroscopy of powder samples under argon were measured by a Compact Fluorescence Lifetime Spectrometer C11367 (Quantaurus-Tau) that contains an light-emitting diode (LED) pulsed light source, nomochromator, PMT (photomultiplier tube),

iris (aperture) for adjusting light level, and filter for cutting excitation light. The samples were irradiated by light source from internal LED at 280 nm.

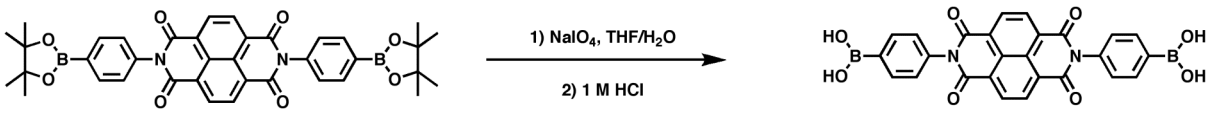
Time-resolved electron spin resonance (TR-ESR) spectra were measured by a Bruker model E680 spectrometer. The time dependence of the signal intensity at each magnetic field was recorded by Bruker SpecJet transient recorder. The laser pulse and detection systems were synchronized by a Stanford Research DG535 pulse generator. The laser for excitation at 355 nm were prepared by using the homemade BBO OPO system, pumped with the 3rd harmonics (355 nm) of a Nd:YAG laser (Continuum Surelite-I). The energy per pulse, pulse width, and repetition rate were 2 mJ, 5 ns, and 10 Hz, respectively. The temperature was controlled using an OXFORD CF931 cryostat and an OXFORD ITC503 temperature controller. In this measurements system, the field modulation was not used. Therefore, positive and negative signals stand for the absorption and emission of the microwave energy in the transient state, respectively.

B. Synthetic procedures

_N,N'_-Di-[4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-naphthalene-1,4,5,8-tetracarboxylic acid diimide.

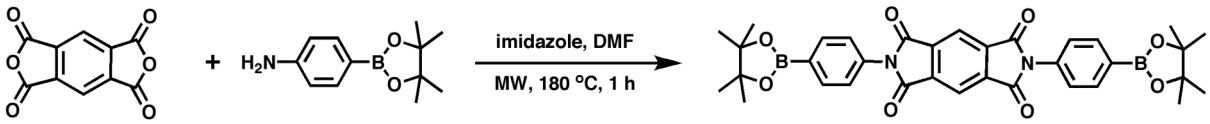
A DMF (2 mL) solution of naphthalene 1,4,5,8-tetracarboxylic dianhydride (26.6 mg, 0.1 mmol), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (48.2 mg, 0.22 mmol), and imidazole (0.50 g, 0.75 mmol) was purged with argon and reacted at 180 °C under microwave condition for 1 h. The mixture was cooled at room temperature, poured into water, and extracted with chloroform (3 × 25 mL). The chloroform layer was evaporated to yield a grey solid. The crude product was purified by column chromatography with chloroform as an eluent, to produce a white solid in 72% yield (48.5 mg). ^{1}H NMR ($CDCl_3$) δ (ppm): 8.84 (s, 4H), 8.04 (d, J = 8.04, 4H), 7.36 (d, J = 8.04, 4H), 1.37 (s, 24H). MALDI-TOF-MS for $C_{38}H_{36}B_2N_2O_8$ (calculated: 670.2658), found: 669.1053 ([M]$^+$).

_N,N'_-Di-(4-boronophenyl)-naphthalene-1,4,5,8-tetracarboxylic acid diimide (NDIDA).



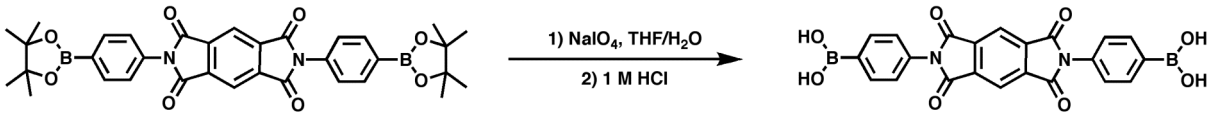
A THF/H_2O (10 mL, 4/1 by vol.) solution of _N,N'_-Di-[4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-naphthalene-1,4,5,8-tetracarboxylic acid diimide (67.6 mg, 0.1 mmol) and sodium periodate (128.3 mg, 0.6 mmol) was stirred at room temperature overnight, was added with an aqueous hydrochloride solution (1 M, 0.5 mL) and the mixture was stirred for 12 h. The yellowish precipitation was collected and washed with water, acetone and chloroform and dried under vacuum to produce NDIDA in 85% yield (42.9 mg). ^{1}H NMR (d^6-DMSO) δ (ppm) 8.72 (s, 4H), 8.21 (s, 4H), 7.93 (d, J = 8.04, 4H), 7.41 (d, J = 8.04, 4H). MALDI-TOF-MS for $C_{26}H_{16}B_2N_2O_8$ (calculated: 506.1093), found: 505.3103 ([M]$^+$).

_N,N'_-Di-[4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-pyrromellitic-1,2,4,5-tetracarboxylic acid diimide.



A DMF (2 mL) solution of pyrromellitic-1,2,4,5-tetracarboxylic dianhydride (21.7 mg, 0.1 mmol), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) aniline (48.2 mg, 0.22 mmol), and imidazole (0.50 g, 0.75 mmol) was purged with argon and reacted at 180 °C under microwave condition for 1 h. The mixture was cooled to room temperature, poured into methanol, and washed with water, methanol and acetone, respectively. The solid was dried at 100 °C under vacuum to produce the white powder in 83 % yield (52 mg). ^{1}H NMR ($CDCl_3$) δ (ppm): 8.47 (s, 2H), 7.97 (d, J = 8.4, 4H), 7.48 (d, J = 8.4, 4H), 1.35 (s, 24H). MALDI-TOF-MS for $C_{38}H_{36}B_2N_2O_8$ (calculated: 620.25), found: 619.52 ([M]$^+$).

***N,N'*-Di-(4-boronophenyl)-pyrromellitic-1,2,4,5-tetracarboxylic acid diimide (PyrDIDA).**



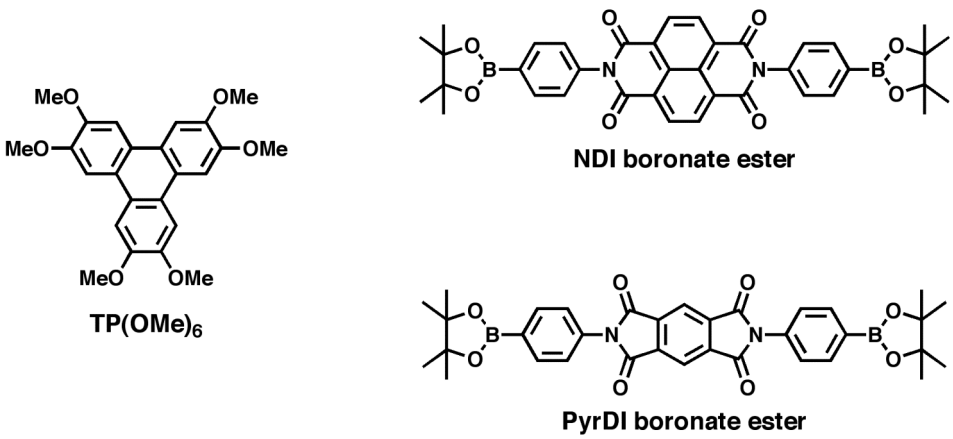
A THF/H_2O (10 mL, 4/1 by vol.) mixture of *N,N'*-di-[4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-pyrromellitic-1,2,4,5-tetracarboxylic acid diimide (62.0 mg, 0.1 mmol) and sodium periodate (128.3 mg, 0.6 mmol) was stirred at room temperature overnight, was added with an aqueous hydrochloride solution (1 M, 0.5 mL) and was stirred for 12 h. The yellowish precipitation was collected, washed with water, acetone and chloroform and dried under vacuum to give PyrDIDA in 81% yield (50 mg). ^{1}H NMR (d^6-DMSO) δ (ppm) 8.34 (s, 2H), 8.17 (s, 4H), 7.90 (d, J = 8.4, 4H), 7.44 (d, J = 8.4, 4H). MALDI-TOF-MS for $C_{26}H_{16}B_2N_2O_8$ (calculated: 456.09), found: 455.96 ([M]$^+$).

D_{TP}-A_{NDI}-COF. A 10-mL pyrex tube was charged with HHTP (13.0 mg, 0.04 mmol) and NDIDA (30.2 mg, 0.06 mmol) and 2 mL DMF/mesitylene (1/1 by vol) and the mixture was sonicated for 1 min, degassed through three freeze-pump-thaw cycles, sealed under vacuum, and then put in an oven at 120 °C for 7 days. The reaction mixture was cooled to room temperature and the precipitate was collected by centrifugation, washed with dehydrated DMAc for 3 times to remove any unreacted monomers, washed with dehydrated dioxane for 3 times and dried under vacuum at 100 °C overnight to obtain a light yellowish powder in 57% yield (23.4 mg). Theoretical elemental contents C = 70.20%, N = 4.31% and H = 2.48%. Observed: C = 67.55%, N = 3.91% and H = 3.39%.

D_{TP}-A_{PyrDI}-COF. A 10 mL pyrex tube was charged with HHTP (13.0 mg, 0.04 mmol) and PyrDIDA (27.3 mg, 0.06 mmol), 2 mL DMAc/o-dichlorobenzene (1/1 by vol) was added and sonicated for 1 min, degassed through three freeze-pump-thaw cycles, sealed under vacuum,

and then put in oven at 120 °C for 7 days. The reaction mixture was cooled to room temperature and the precipitate was collected by centrifugation, washed with dehydrated DMAc for 3 times to remove any unreacted monomers, washed with dehydrated dioxane for 3 times and dried under vacuum at 100 °C overnight to obtain a light yellowish powder in 68 % yield (26.2 mg). Theoretical elemental contents C = 68.05%, N = 4.67% and H = 2.35%. Observed: C = 61.35%, N = 4.82% and H = 2.88%.

C. Schemes, Tables and Figures



Scheme S1. Structures of $TP(OMe)_6$, NDI boronate ester and PyrDI boronate ester.

Table S1. Summary of porous structures of D_{TP}-A_{NDI}-COF and D_{TP}-A_{PyrDI}-COF synthesized under different condition.

	Solvent (1/1 by vol)	BET surface area (m^2 g^{-1})	Langmuir surface area (m^2 g^{-1})	Pore volume (cm^3 g^{-1})
D_{TP}-A_{NDI}-COF	DMF/Mesitylene	1385	2175	1.57
	DMAc/Mesitylene	1504	2394	1.83
	DMAc/Mesitylene[a]	1910	2699	2.37
	DMAc/o–DCB	1193	2186	1.53
	DMAc/Toluene	1009	1812	1.23
	DMF/Toluene	822.8	1598	1.02
D_{TP}-A_{PyrDI}-COF	DMF/Mesitylene	1263	1833	1.61
	DMAc/Mesitylene	843.5	1351	1.12
	DMAc/o–DCB	1604	2063	1.98

[a] Under a condition of 50 mol% excess of HTTP.

Table S2. The total DFTB energies, Lennard-Jones contributions (LJ), and the crystal stacking energies per unit cell for D_{TP}-A_{NDI}-COF and D_{TP}-A_{PyrDI}-COF.

	Stacking mode	c (Å)	Total DFTB energy (a.u.)	LJ energy (a.u.)	Total crystal stacking energy (kcal mol^{-1})
D_{TP}-A_{NDI}-COF	Monolayer	-	-315.357259	1.2476	-
	Eclipsed AA	3.50	-631.225128	1.9250	160.21
	0.8 Å-Slipped AA	3.39	-631.264507	1.9213	172.56
	Staggered AB	3.18	-630.853510	2.3436	43.61
D_{TP}-A_{PyrDI}-COF	Monolayer	-	-292.585786	1.1052	-
	Eclipsed AA	3.51	-585.619133	1.7083	140.42
	0.8 Å-Slipped AA	3.41	-585.652753	1.7051	150.97
	Staggered AB	3.20	-585.305550	2.0670	42.04

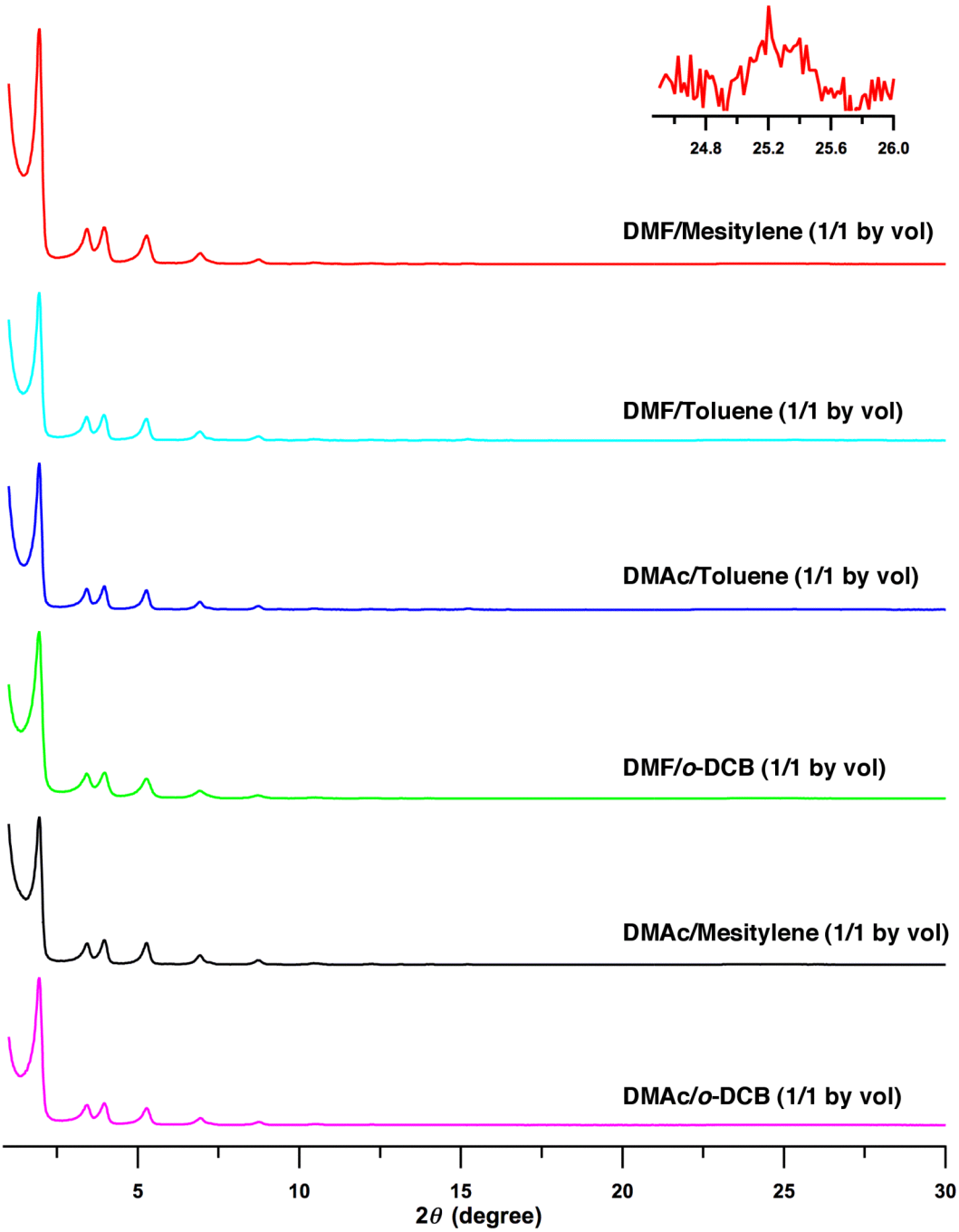


Fig. S1. XRD patterns of D_{TP}-A_{NDI}-COF synthesized in different solvents.

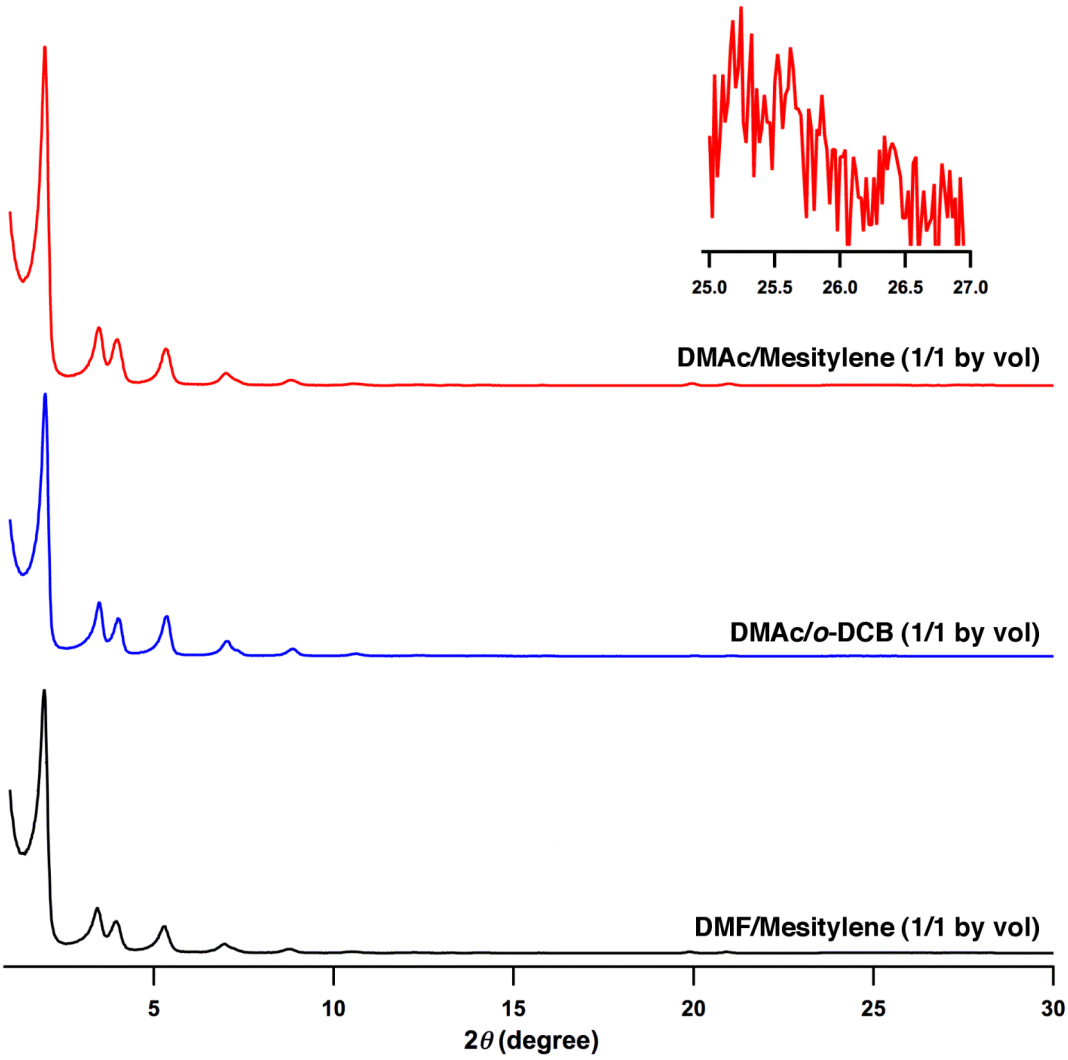


Fig. S2. XRD patterns of D_{TP}-A_{PyrDI}-COF synthesized in different solvents

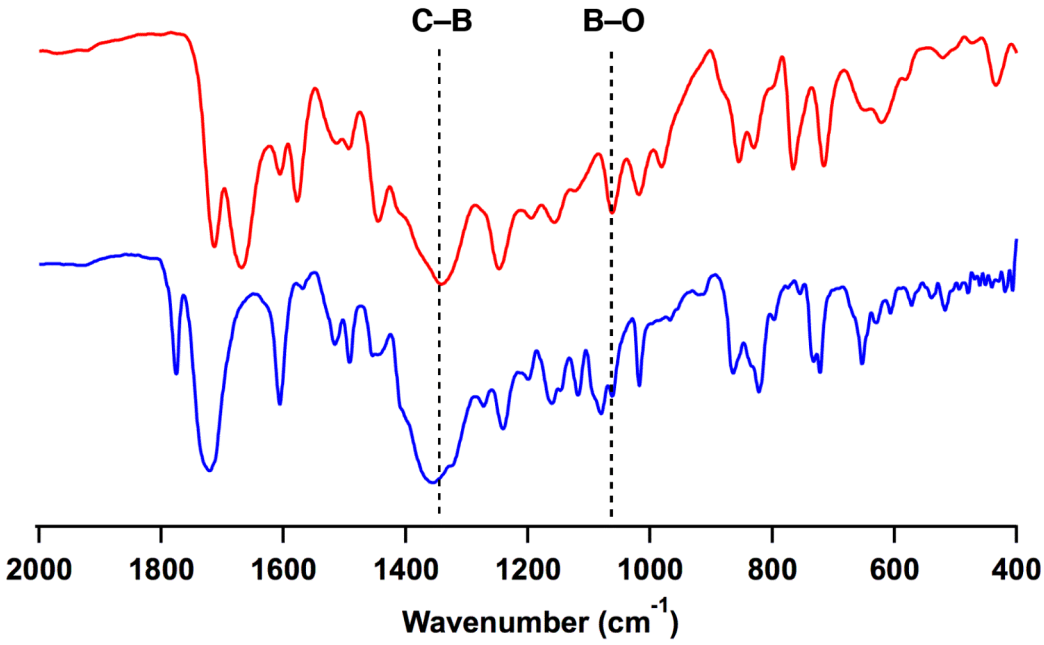


Fig. S3. FT-IR spectral profiles of D_{TP}-A_{NDI}-COF (red curve) and D_{TP}-A_{PyrDI}-COF (blue curve).

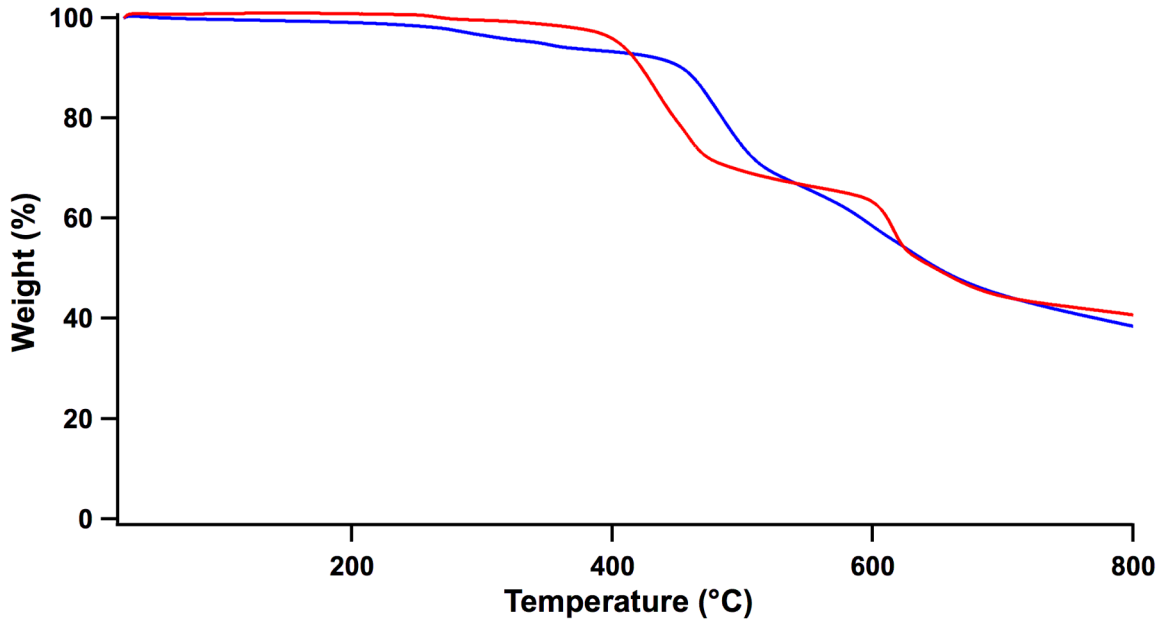


Fig. S4. TGA curves of D_{TP}-A_{NDI}-COF (blue) and D_{TP}-A_{PyrDI}-COF (red).

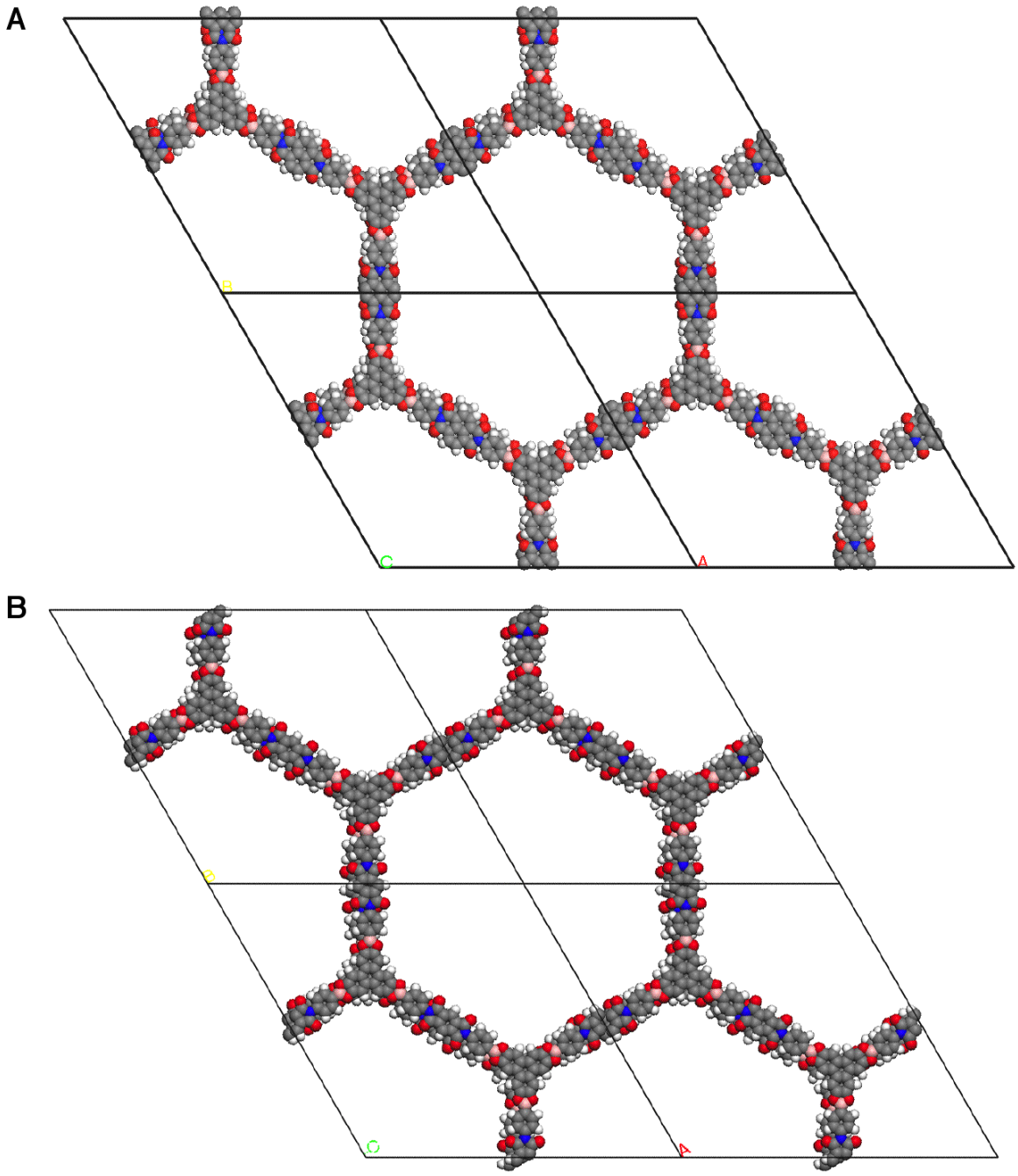


Fig. S5. Enlarged unit cells for the 0.8-Å slipped AA stacking modes of (A) D_{TP}-A_{NDI}-COF and (B) D_{TP}-A_{PyrDI}-COF.

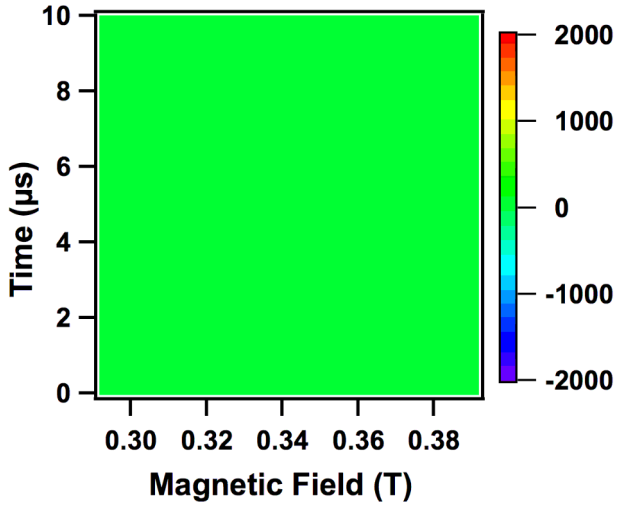


Fig. S6. Contour plot of the TR-ESR spectrum of the solid-state D_{TP}-A_{NDI}-COF at 80 K.

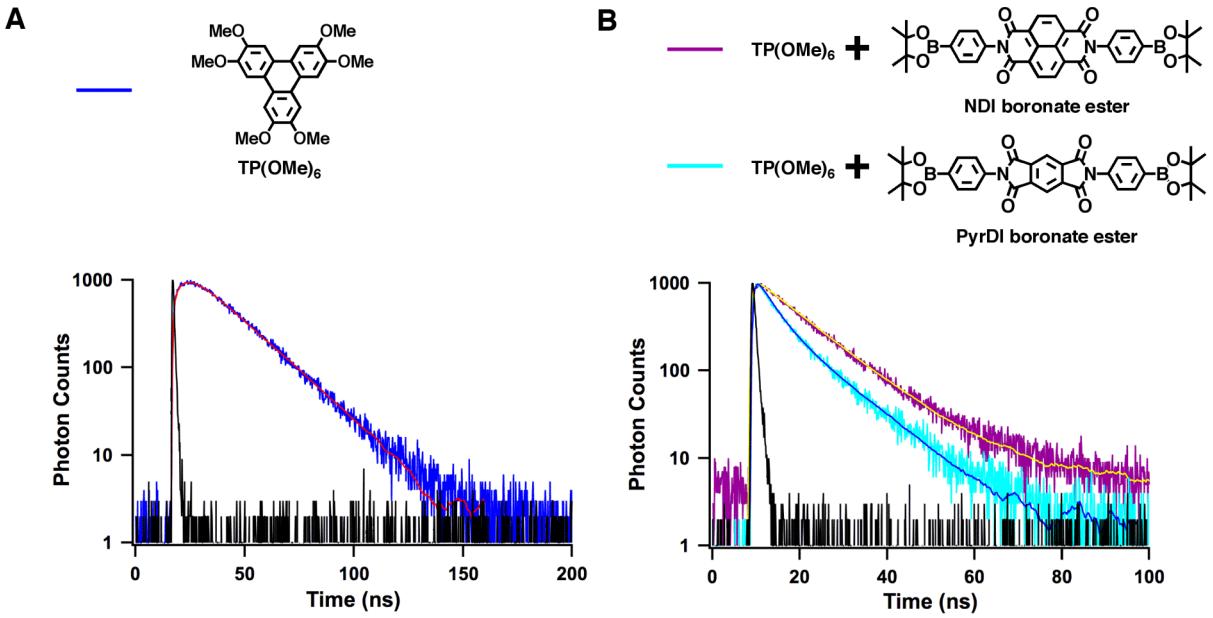


Fig. S7. Time resolved fluorescence decay profiles of (A) donor $TP(OMe)_6$ and (B) the mixtures of $TP(OMe)_6$ with NDI boronate ester and PyrDI boronate ester. IRF (instrument response function) is in black. The average lifetime for $TP(OMe)_6$ is 22.5 ns, whereas the average lifetimes of the mixtures of $TP(OMe)_6$ with NDI boronate ester and PyrDI boronate ester are 10.9 and 8.3 ns, respectively. The lifetime is shortened when the donor was mixed with the acceptors.

Table S3. Coordinates and atomic net charges for the 0.8-Å slipped AA model of D_{TP}-A_{NDI}-COF.

atom	*x*	*y*	*z*	charge
H	0.58046733	3.5656204	0.00622766	0.88702702
H	2.75758507	2.31702696	0.00602451	0.88960872
H	-2.78141345	-2.29229032	0.01138103	0.8852522
H	-0.60408192	-3.54186862	0.01161432	0.89043712
H	-9.76973676	8.50451715	0.00529589	0.90181659
H	-12.29139927	4.1189696	0.00759133	0.90046014
H	-10.70639373	10.12553582	0.00597116	0.90017657
H	-15.76301432	10.11883123	0.00591943	0.900015
H	-16.69533803	8.49306905	0.00553816	0.90203124
H	-14.16153862	4.11696534	0.00748089	0.90063462
H	-20.75215289	5.71197224	-0.00131102	0.92599106
H	-22.8728218	4.52484224	-0.00531918	0.87895538
H	-18.5995099	1.98588937	0.01417855	0.92502111
H	-20.68446752	0.74002156	0.01745378	0.87916472
H	-15.39868994	17.47969384	0.00904166	0.87428379
H	-15.38224656	15.05290501	0.00680486	0.92134336
H	-11.02518803	17.45114282	0.0087091	0.87408749
H	-11.07850402	15.02385805	0.00652715	0.92164975
H	-5.70343324	5.74101068	-0.00311342	0.92603249
H	-3.57745182	4.56438452	-0.00790255	0.87904005
H	-7.84161446	2.00450055	0.01568015	0.92478038
H	-5.75210378	0.76966142	0.0202523	0.8792218
H	5.72006486	-0.75888667	-0.00890155	0.8769329
H	7.81433073	-1.98900497	-0.00484683	0.9252884
H	3.55670379	-4.55992428	0.02348537	0.88089665
H	5.68208387	-5.72892603	0.01675907	0.92133274
H	9.75917813	-8.4839946	0.00736893	0.8992855
H	12.2745316	-4.09640879	0.0052378	0.90165562
H	14.1569893	-4.09394197	0.00534859	0.9017523
H	16.6864517	-8.47096686	0.00701969	0.89930851
H	10.69587009	-10.09856054	0.00588694	0.90191182
H	15.75469347	-10.09098286	0.00573956	0.90205987
H	11.06813974	-14.98362821	0.00864689	0.92525387
H	11.01453956	-17.41388436	0.00883346	0.87988876
H	15.37247694	-15.01435265	0.00863021	0.92519113
H	15.38708528	-17.44404721	0.0089883	0.87992266
H	22.87219753	-4.51909761	0.02118074	0.88051136
H	20.69528561	-0.72756889	-0.00553807	0.87664683
H	18.60563188	-1.96841636	-0.0027569	0.92524987
H	20.7516911	-5.69826637	0.01537135	0.92107111
H	0.54522508	2.07444633	3.39458484	0.89047199
H	2.72237327	0.82495166	3.39481233	0.88528752
H	-2.81666105	-3.78431818	3.40015548	0.88957737
H	-0.63938123	-5.033031	3.39995158	0.88699604
H	-9.82178957	7.01153822	3.39878188	0.89926891
H	-12.33600466	2.62330191	3.40091513	0.90167228
H	-10.75801842	8.62531456	3.4002789	0.9018942

H	-15.81684142	8.6181879	3.40042486	0.90206044
H	-16.74845992	6.99808541	3.39914765	0.89930848
H	-14.21938027	2.6208381	3.40080288	0.90176878
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H	-22.93502705	3.04824249	3.38508085	0.88054187
H	-18.6692782	0.49611416	3.40891606	0.92525211
H	-20.75929429	-0.74393955	3.41170441	0.87662558
H	-15.44688612	15.9716101	3.39704197	0.87989055
H	-15.43321808	13.54197215	3.39745469	0.92518852
H	-11.07433054	15.93992893	3.39745367	0.87991398
H	-11.12890654	13.50959375	3.39759691	0.92525363
H	-5.74394572	4.2595068	3.38954423	0.92133581
H	-3.61760378	3.09193601	3.38290056	0.8809508
H	-7.87360055	0.51811238	3.41103924	0.92528949
H	-5.77859261	-0.71045038	3.41513566	0.8768828
H	5.69356131	-2.23909499	3.38617697	0.87927539
H	7.78231488	-3.47550542	3.39063463	0.92478266
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C	15.54515153	-23.61358047	3.39794177	4.05297538
C	10.69952354	-23.58527088	3.39800101	4.05278981
C	19.45312118	-5.41266367	3.39972923	4.11536127
C	-13.28167624	13.34224019	3.39836884	4.11860364
C	20.68581415	-6.08302138	3.40474379	4.03683765
C	21.89611512	-5.39398498	3.40644577	4.14558025
C	21.93477608	-3.97785504	3.39990865	3.84998214
C	20.68904214	-3.30334687	3.39428622	4.13754294
C	19.48816778	-4.00950072	3.39549866	4.03040346
C	-12.07850765	14.06552586	3.39800275	4.03481079
C	-12.05737941	15.45856858	3.3981923	4.14144476
C	-13.25914103	16.20917677	3.39900647	3.84205689
C	-14.4715305	15.47561496	3.39798559	4.14206531
C	-14.47444893	14.08244354	3.39789946	4.03479293
C	-24.66812461	-3.27789173	3.40087144	4.05272337
C	-24.64271581	-1.88001699	3.40037067	4.0774593

C	-25.87189097	-1.17687233	3.40006032	3.98970323
C	-25.86563728	0.23881422	3.39811301	4.07727099
C	-27.08695941	0.92000727	3.39624605	4.05395039
C	-23.34229616	-1.14642471	3.39131076	3.52838031
C	-24.57620167	0.98972238	3.40323491	3.54991314
C	-14.4797399	18.40025467	3.40198215	3.52863108
C	-12.00764025	18.3849779	3.40144759	3.52938869
C	-14.45718675	19.89585147	3.40039898	4.07585314
C	-12.00924274	19.88122879	3.40032874	4.07677767
C	-15.65240872	20.62100716	3.39934892	4.04439784
C	-13.22899379	20.60196306	3.400304	4.01121419
C	-10.80564535	20.59251704	3.39924341	4.04491746
C	23.21498529	-1.82500423	3.40341638	3.54480365
C	24.44707295	-3.96379156	3.39152967	3.51961419
C	24.51495204	-1.08632675	3.39835707	4.08883544
C	25.73530027	-3.20670906	3.40005078	4.06540033
C	24.53790843	0.31217533	3.39638706	4.06027972
C	25.74361667	-1.79048087	3.39998971	3.99698431
C	26.95669733	-3.88559831	3.40065341	4.04793474
N	-3.17389099	1.82051024	0.00755532	5.1322452
N	3.14885766	-1.80086968	0.00882167	5.13909342
N	13.18915672	-19.14218	0.00588284	5.1349714
N	-23.26549641	1.78103814	0.00741968	5.13178185
N	-13.20030094	19.18691127	0.00941569	5.15045713
N	23.26961229	-1.76045262	0.00859067	5.1395298
N	-3.20813701	0.33296208	3.39731938	5.13908621
N	3.11458428	-3.2884748	3.39859405	5.13224428
N	13.14109663	-20.66013445	3.39675034	5.15046167
N	-23.33326736	0.28963469	3.39757149	5.13953041
N	-13.24845866	17.66895837	3.40028466	5.13496681
N	23.20185008	-3.25187061	3.39874389	5.13177708
B	-18.220776	4.68982406	0.00692145	2.72544934
B	-8.23246885	4.70706834	0.00667519	2.72513244
B	-13.2364831	13.35150281	0.00598367	2.7226522
B	8.21372664	-4.68970794	0.00583714	2.72513031
B	13.22711932	-13.319377	0.00745478	2.73040991
B	18.21820986	-4.67058654	0.00586794	2.72513009
B	-18.28081378	3.19809347	3.40029702	2.7251271
B	-8.2750101	3.21827184	3.40033062	2.72513222
B	-13.28860787	11.8462499	3.39871435	2.73041528
B	8.17114525	-6.17859317	3.39947955	2.72513148
B	13.17513751	-14.82463612	3.4001845	2.72264823
B	18.1581747	-6.16231425	3.39924203	2.72545428

Table S4. Coordinates and atomic net charges for the 0.8-Å slipped AA model of D_{TP}-A_{PyrDI}-COF.

atom	*x*	*y*	*z*	charge
C	-2.6006377	17.39820516	-0.00208112	3.80835064
C	-3.29865721	16.17878773	-0.00174213	3.80782754
C	-2.63971094	14.95942501	-0.00140346	4.16835755
C	-1.21489624	14.96618226	-0.00278623	3.99660157
C	-0.50067659	16.20966179	-0.00299097	3.99671226
C	-1.21451741	17.44408232	-0.00199842	4.16732335
C	-0.48074997	13.69827579	-0.00325641	3.98989405
C	0.952727	13.69761587	-0.00030117	3.98938833
C	1.68246483	14.96607665	-0.00025179	3.98910339
C	0.96509011	16.20821609	-0.00335284	3.99057435
C	3.10675049	14.95868567	0.00186048	4.1650062
C	3.76260524	16.17847823	-0.0012666	3.81395649
C	3.0618128	17.3961235	-0.00566025	3.81014317
C	1.67641908	17.4425454	-0.00611346	4.17183455
C	-1.19550834	12.4663477	-0.00613413	4.17206031
C	-0.46329445	11.2898382	-0.00592704	3.80964137
C	0.94145311	11.28932106	-0.00163535	3.81443449
C	1.67106396	12.46693694	0.00157587	4.1640905
O	5.12758966	16.44152239	-0.00049148	6.24818531
B	5.23151764	17.8331256	-0.00467769	2.72620811
O	3.97652707	18.44248897	-0.00776957	6.24446893
O	-3.52037547	18.44263759	-0.00128915	6.2428694
B	-4.7741689	17.82991907	-0.00082386	2.72420581
O	-4.66342042	16.43886438	-0.00072248	6.24286771
O	-0.91570654	9.97683402	-0.00818164	6.24493494
B	0.23700553	9.19088268	-0.00524614	2.72643419
O	1.39259847	9.97321971	-0.00105272	6.24835211
C	0.21818969	7.69448789	-0.0057951	4.11941211
C	6.52943392	18.57794908	-0.00503248	4.1193649
C	-6.08411128	18.55527768	-0.00026055	4.10858811
C	-1.00806955	7.00733105	-0.01004852	4.03277277
C	-1.06381583	5.61580637	-0.01053811	4.14436469
C	0.13365847	4.86622836	-0.00636899	3.84723253
C	1.37362799	5.54397961	-0.00170282	4.1387783
C	1.40363063	6.9373479	-0.0015162	4.02603475
C	7.75894513	17.89513127	-0.00063677	4.02563663
C	8.971269	18.58175077	-0.00058821	4.13906731
C	8.97842471	19.99497029	-0.00514421	3.84786547
C	7.74967985	20.69230685	-0.00944201	4.1440717
C	6.55050085	19.98348041	-0.00918944	4.03290928
C	-6.15360187	19.95998193	-0.00052102	4.02768184
C	-7.37733701	20.62908219	-0.00050564	4.14865563
C	-8.58396227	19.893016	-0.00012542	3.87645336
C	-8.52857256	18.48075832	0.00024667	4.15212751
C	-7.29237286	17.83625857	0.00025532	4.02726871
N	10.21515843	20.71543955	-0.00507311	5.14459434
C	11.50103781	20.11995581	-0.00213015	3.54252949

C	10.33709889	22.13829576	-0.00815858	3.51582828
O	11.75824543	18.92860396	0.00006808	6.42103236
O	9.43019985	22.9439139	-0.01100082	6.39761445
C	-0.12523903	-4.85604691	-0.00790071	3.85977158
C	-1.35749922	-5.54652414	-0.01207066	4.13678955
C	-1.37293337	-6.94018253	-0.01195813	4.03292469
C	-0.18177758	-7.68774131	-0.00788546	4.112308
C	1.03818259	-6.98866147	-0.00359187	4.02179227
C	1.079545	-5.59532099	-0.00364011	4.15402445
B	-0.20194271	-9.18456823	-0.00832354	2.72618473
O	-1.35923421	-9.9636806	-0.01315979	6.24319349
C	-0.9142897	-11.28117862	-0.01192889	3.80631599
C	0.49011516	-11.28630871	-0.00623382	3.81067808
O	0.94791268	-9.97487751	-0.00376778	6.24221946
C	-1.64843751	-12.45789788	-0.01415417	4.17078327
C	-0.93699333	-13.69283278	-0.01152624	3.99412072
C	0.49707895	-13.6954971	-0.00680341	3.99174464
C	1.21680185	-12.46645102	-0.00326862	4.17173202
C	-1.66940126	-14.96268122	-0.01171299	3.99396562
C	-0.95213273	-16.20528046	-0.00705283	3.99127295
C	0.51219415	-16.20618592	-0.0059661	3.98941472
C	1.22793096	-14.96414662	-0.00591656	3.98896543
C	1.22058733	-17.44186542	-0.005549	4.16335989
C	2.60540655	-17.39570711	-0.00658254	3.81192613
C	3.30531301	-16.178301	-0.00665225	3.81073371
C	2.65138915	-14.95727431	-0.00556516	4.16459605
C	-3.09393076	-14.9614522	-0.01463307	4.17133039
C	-3.74815669	-16.18401505	-0.01261084	3.80626826
C	-3.04498584	-17.39987469	-0.00691604	3.81132814
C	-1.65954242	-17.44167538	-0.0037898	4.17122965
O	3.5208071	-18.4428233	-0.00719618	6.24669506
B	4.77438013	-17.83102414	-0.00788515	2.73089842
O	4.66921673	-16.43995833	-0.00733825	6.24697746
O	-5.11163099	-16.4520061	-0.01404896	6.24329985
B	-5.21292922	-17.84339864	-0.00929983	2.72624244
O	-3.95622317	-18.44932942	-0.00464436	6.24223064
C	6.08164312	-18.5588013	-0.00868416	4.1220535
C	6.14514929	-19.96366562	-0.00859893	4.03050857
C	7.36786161	-20.63142455	-0.00931499	4.14071065
C	8.57305322	-19.89391649	-0.01009254	3.8405456
C	8.52119289	-18.4819416	-0.01019841	4.14172913
C	7.28777433	-17.83645766	-0.00941255	4.03071675
N	9.8339315	-20.56759574	-0.01040186	5.14473754
C	-6.51038856	-18.58977019	-0.00903246	4.11285203
C	-7.73415143	-17.89764932	-0.01320345	4.0331305
C	-8.95324297	-18.57218173	-0.01349045	4.13704865
C	-8.9744929	-19.98458124	-0.00937731	3.85892668
C	-7.75111764	-20.6929942	-0.00499892	4.15298225
C	-6.54399135	-19.99548425	-0.00480388	4.02147472
C	12.50505784	21.2298423	-0.00267176	4.09781527
C	11.80376778	22.45049489	-0.00673288	4.07272375

C	13.90746117	21.1732638	0.00000601	4.03744502
N	0.08615644	3.43598865	-0.00652472	5.14474066
C	-1.10899824	2.65462175	-0.00981922	3.5161941
C	1.22039377	2.58612619	-0.00361685	3.54193357
O	-2.24845276	3.07078952	-0.01272588	6.39787431
O	2.3909203	2.9245255	-0.00121555	6.41976462
C	-1.25197352	-2.57787945	-0.01060816	3.52198093
N	-0.09882625	-3.42321865	-0.00758724	5.15172435
C	1.07741101	-2.63204352	-0.00435136	3.54434366
O	2.22831261	-3.03642532	-0.00209409	6.42832405
O	-2.4112494	-2.93351377	-0.01350785	6.39451243
C	-0.68921373	1.21551978	-0.00855201	4.07262272
C	0.71790805	1.17610615	-0.00442943	4.09834328
C	-1.46631466	0.04648754	-0.01052762	4.02389832
C	-0.75532199	-1.16369007	-0.00907295	4.08346537
C	0.65248871	-1.19972194	-0.0048174	4.08490872
C	1.43097135	-0.03282767	-0.00187566	4.03779085
C	11.10203669	-19.92165261	-0.01106703	3.52662399
C	10.00405686	-21.97983715	-0.01036641	3.52840705
O	9.12662203	-22.82017223	-0.01017198	6.40329692
O	11.31182352	-18.72514165	-0.01165815	6.4024091
C	13.54236512	-20.89957584	-0.01062043	4.03030596
C	12.14266128	-21.00002214	-0.01080201	4.08923109
C	11.4802332	-22.24271217	-0.01043605	4.09265589
H	-3.22796021	14.03414945	0.0010775	0.89953347
H	-0.71132682	18.41865382	-0.00009007	0.8999374
H	3.69602787	14.0340125	0.00633031	0.90021473
H	1.17223125	18.41651948	-0.00821005	0.90164576
H	-2.29082474	12.41534193	-0.00816459	0.90147437
H	2.76655003	12.41735383	0.00590597	0.90028696
H	-1.93775609	7.59503553	-0.0127771	0.92259251
H	-2.04128413	5.11689067	-0.01392273	0.88736216
H	2.32000866	4.98846425	0.00166366	0.88897095
H	2.36979265	7.46332546	0.00234433	0.92222186
H	7.75086176	16.79512965	0.00309174	0.92210888
H	9.90928309	18.01225185	0.0028553	0.88883968
H	7.72606155	21.78949153	-0.01277032	0.88745753
H	5.59214082	20.5233129	-0.01206009	0.92256012
H	-5.2174663	20.53732456	-0.00030472	0.91904529
H	-7.38850399	21.72658076	-0.0006578	0.88227785
H	-9.44673601	17.87938805	0.00071669	0.88240142
H	-7.24874213	16.73741908	0.00107223	0.91858981
H	-2.30786244	-4.99799836	-0.01539601	0.88459651
H	-2.33360574	-7.47606103	-0.01478492	0.92183231
H	1.97520626	-7.5641013	-0.00005335	0.91896926
H	2.0542814	-5.09043113	-0.0002255	0.88933106
H	-2.74406278	-12.40524292	-0.01718009	0.9010592
H	2.31221693	-12.41940535	0.00273972	0.89889599
H	0.71728587	-18.41622187	-0.00430896	0.90165567
H	3.24221868	-14.0336951	-0.00432757	0.90158311
H	-3.68485876	-14.0374803	-0.01773243	0.90109356

H	-1.15340609	-18.41447132	0.00210828	0.8991636
H	5.20645268	-20.53689226	-0.00753316	0.92202232
H	7.38032554	-21.72879174	-0.00909829	0.88889869
H	9.44084634	-17.88323231	-0.01066106	0.88827176
H	7.23996586	-16.73773293	-0.00899066	0.92209521
H	-7.71472656	-16.79781977	-0.01599128	0.92187594
H	-9.88729469	-17.99640015	-0.01688737	0.88456078
H	-7.73363043	-21.79058817	-0.0016213	0.88975587
H	-5.59242114	-20.54669286	-0.00121513	0.91911532
H	14.45366918	20.21893969	0.00442899	0.88270622
H	-2.56507452	0.07799028	-0.01285947	0.87653346
H	2.53014146	-0.06336437	0.00259165	0.88229631
H	14.05626716	-19.92780846	-0.00966877	0.87406702
N	-9.84885605	20.56921648	0.00010096	5.16122317
C	-11.12062099	19.92704082	0.00043556	3.53531424
C	-10.02332998	21.98417826	-0.0001715	3.53379014
O	-11.32779003	18.72898002	0.00014904	6.40886631
O	-9.14337422	22.82208544	-0.00108482	6.40550745
C	-12.15918372	21.00351565	0.00091245	4.08521784
C	-11.4970395	22.24588251	0.00054493	4.08547396
C	-13.55948764	20.90309328	0.00179277	4.03295282
H	-14.07646957	19.93287516	0.00329873	0.87458925
N	-10.22325835	-20.68765123	-0.00922706	5.15079848
C	-10.36279857	-22.09802084	-0.00625396	3.54463011
C	-11.51409961	-20.07283837	-0.01225348	3.52132515
O	-9.46093552	-22.9196564	-0.00418346	6.42883721
O	-11.75070324	-18.88341148	-0.01494142	6.39464423
C	-11.82597303	-22.40260361	-0.00681543	4.08536423
C	-12.5245616	-21.17972193	-0.01098213	4.08303752
C	-13.92706318	-21.12562605	-0.01256121	4.02402264
H	-14.47374163	-20.17201102	-0.01484131	0.87673754
C	-1.44597818	16.66959947	3.40088809	3.81195925
C	-2.14443583	15.45136237	3.40096265	3.81068019
C	-1.48927041	14.23114188	3.39987559	4.16468769
C	-0.06588331	14.23977123	3.40021917	3.98894406
C	0.64851372	15.48238094	3.40026906	3.98942246
C	-0.06119546	16.71735277	3.39985452	4.16335602
C	0.66613579	12.97199683	3.4010991	3.99169392
C	2.1002407	12.96973125	3.40581705	3.99418409
C	2.8315944	14.24044581	3.40600477	3.99400076
C	2.11280128	15.4823302	3.40135266	3.9912439
C	4.25623366	14.24135593	3.40892312	4.17121408
C	4.90893041	15.46493599	3.40691153	3.80635805
C	4.20391414	16.67972502	3.40122317	3.81125799
C	2.81850504	16.71959581	3.39809394	4.17127786
C	-0.05357423	11.74312979	3.3975637	4.17187261
C	0.67303523	10.56317572	3.40053761	3.81053374
C	2.07743539	10.55763777	3.4062301	3.80645321
C	2.81164653	11.73457764	3.40844409	4.17063
O	6.27209064	15.73560402	3.40835662	6.24333206
B	6.37090151	17.12725365	3.4036183	2.72623425

O	5.11309248	17.73079492	3.39896151	6.24221685
O	-2.36282986	17.71549077	3.40150019	6.2467091
B	-3.61554556	17.10191056	3.40219315	2.7309158
O	-3.50858038	15.71103791	3.40165119	6.24694587
O	0.21416752	9.25242927	3.39808305	6.24219442
B	1.36329447	8.46120676	3.40264546	2.72619314
O	2.52129094	9.23944158	3.40747126	6.24321871
C	1.33907873	6.96443538	3.40221108	4.11233261
C	7.66639055	17.87707682	3.40335381	4.11285985
C	-4.92401388	17.82746888	3.40299043	4.12206776
C	0.11678791	6.26924278	3.39790441	4.02180728
C	0.07055636	4.87598455	3.39794338	4.15379155
C	1.27296653	4.13291257	3.40221173	3.8597395
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D. Supporting References

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