Supplementary Information

Green-light wavelength-selective organic solar cells for agrivoltaics: dependence of wavelength on photosynthetic rate

Seihou Jinnai,[*, a,b] Naoto Shimohara,[a] Kazunori Ishikawa,[a] Kento Hama,[c] Yohei Iimuro,[c] Takashi Washio,[a] Yasuyuki Watanabe,[*, c] and Yutaka Ie[*,a,b]

[a] *The Institute of Scientific and Industrial Research (SANKEN), Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan*
[b] *Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (OTRI), Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan*
[c] *Department of Mechanical and Electrical Engineering, Faculty of Engineering, Suwa University of Science, 5000-1 Toyohira, Chino, Nagano 391-0292, Japan*

Table of Contents

Figures and tables

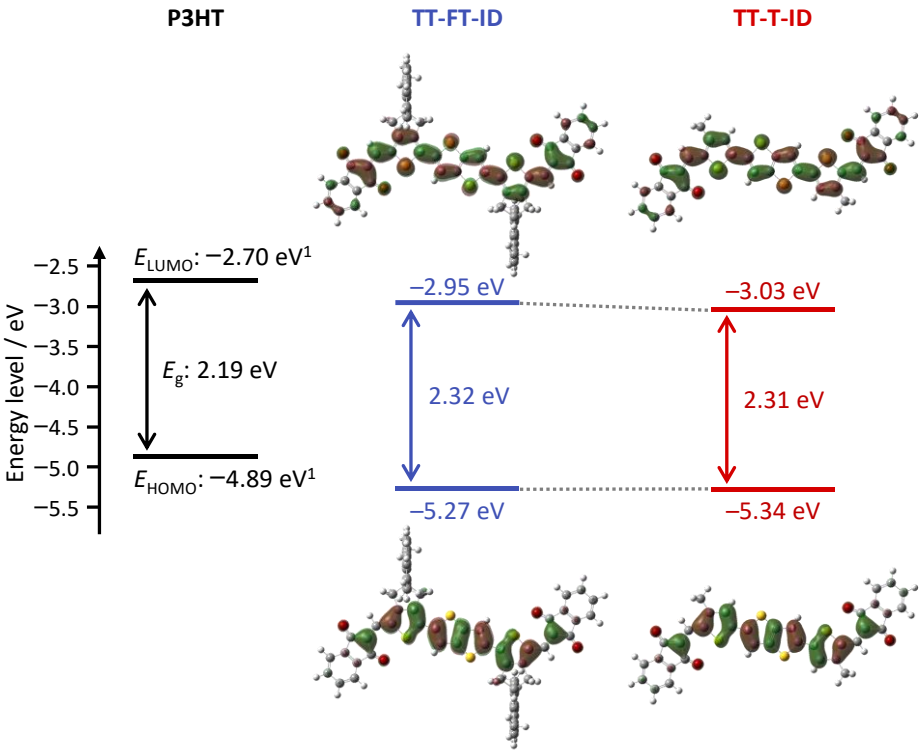


Fig. S1 Energy levels and distribution of the frontier orbitals for **TT-FT-ID** and **TT-T-ID** along with the experimental enegy levels of P3HT. All the alkyl groups for **TT-FT-ID** and **TT-T-ID** molecules were replaced with methyl groups to reduce the computational load.

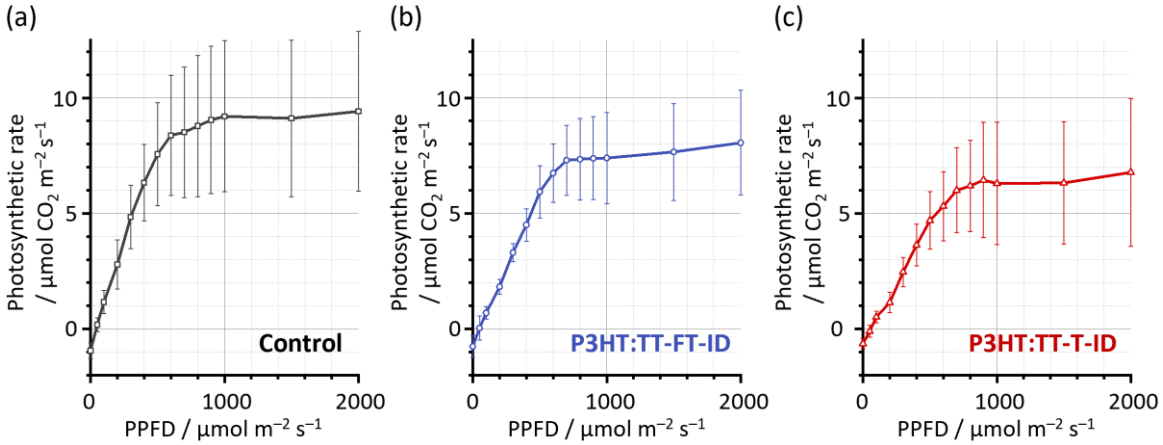


Fig. R1 Photosynthetic rates for green pepper under (a) control conditions, (b) P3HT:TT-FT-ID blend film, and (c) P3HT:TT-T-ID blend film. Each point is the average of 4 measurements, and error bars indicate standard deviation. Experimental data for the above are given in Tables S9-11.

Table S1 OSC characteristics of the P3HT:TT-FT-ID based devices.

D:A [a]	solvent [b]	conc. [c] / mg mL^{-1}	rotation / rpm	T_a [d] / °C	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
1:1	CB	20	1000	-	0.95	3.29	0.86	34
1:1	CB	20	1000	130	1.43	4.27	0.84	40
1:1	DCB	20	1000	-	1.57	3.61	0.90	48
1:1	DCB	20	1000	130	1.26	3.39	0.86	43
1.5:1	CB	20	1000	130	0.48	3.01	0.41	39
1:1.5	CB	20	1000	130	0.40	2.36	0.53	32
2:1	DCB	20	1000	-	1.63	4.06	0.76	38
1.5:1	**DCB**	**20**	**1000**	**-**	**1.70**	**4.37**	**0.77**	**50**
1:1.5	DCB	20	1000	-	1.36	3.90	0.78	44

[a] Donor:acceptor weight ratio. [b] Process solvent (CB = chlorobenzene, DCB = 1,2-dichlorobenzene). [c] Concentration of total donor:acceptor weight. [d] Thermal annealing temperature in N_2 for 10 min.

Table S2 OSC characteristics of the P3HT:TT-T-ID based devices.

D:A [a]	solvent [b]	conc. [c] / mg mL^{-1}	rotation / rpm	T_a [d] / °C	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
1:1	CB	20	1000	-	0.14	0.50	0.78	36
1:1	CB	20	1000	130	0.51	2.25	0.58	39
1:1	DCB	20	1000	-	0.42	1.37	0.81	38
1:1	DCB	20	1000	130	0.52	2.25	0.51	45
2:1	DCB	20	1000	-	0.31	1.08	0.78	37
1.5:1	**DCB**	**20**	**1000**	**-**	**0.40**	**1.29**	**0.84**	**37**
1:1	DCB	20	1000	-	0.40	1.32	0.81	38
1:1.5	DCB	20	1000	-	0.31	1.10	0.77	37
1:2	DCB	20	1000	-	insoluble			

[a] Donor:acceptor weight ratio. [b] Process solvent (CB = chlorobenzene, DCB = 1,2-dichlorobenzene). [c] Concentration of total donor:acceptor weight. [d] Thermal annealing temperature in N_2 for 10 min.

Table S3 OSC characteristics of the P3HT:TT-FT-ID based devices.

D:A [a]	solvent [b]	conc. [c] / mg mL^{-1}	rotation / rpm	T_a [d] / °C	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
1.5:1	DCB	10	500	-	1.90	4.36	0.82	53
1.5:1	DCB	10	1000	-	1.25	3.11	0.74	54
1.5:1	DCB	20	1000	-	1.88	4.66	0.88	46
1.5:1	DCB	20	3000	-	1.49	3.75	0.80	50
1.5:1	DCB	30	1000	-	1.47	3.87	0.91	42
1.5:1	DCB	30	3000	-	1.93	4.49	0.90	48
1.5:1	DCB	40	2000	-	1.74	4.36	0.87	46
1.5:1	DCB	40	4000	-	1.16	3.33	0.84	41
1.5:1	DCB	10	5000	-	0.00	-	-	-
1.5:1	DCB	40	1000	-	0.00	-	-	-

[a] Donor:acceptor weight ratio. [b] Process solvent (CB = chlorobenzene, DCB = 1,2-dichlorobenzene). [c] Concentration of total donor:acceptor weight. [d] Thermal annealing temperature in N_2 for 10 min.

Table S4 OSC characteristics of the P3HT:TT-T-ID based devices.

D:A [a]	solvent [b]	conc. [c] / mg mL^{-1}	rotation / rpm	T_a [d] / °C	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
1.5:1	DCB	5	500	-	0.00	-	-	-
1.5:1	DCB	5	1000	-	0.00	-	-	-
1.5:1	DCB	5	3000	-	0.00	-	-	-
1.5:1	DCB	5	5000	-	0.00	-	-	-
1.5:1	DCB	10	1000	-	0.02	0.99	0.09	27
1.5:1	DCB	10	3000	-	0.00	-	-	-
1.5:1	DCB	20	1000	-	0.40	1.29	0.84	37
1.5:1	DCB	20	3000	-	0.09	0.87	0.27	37
1.5:1	DCB	20	5000	-	0.06	0.76	0.24	35
1.5:1	DCB	30	-	-	insoluble			

[a] Donor:acceptor weight ratio. [b] Process solvent (CB = chlorobenzene, DCB = 1,2-dichlorobenzene). [c] Concentration of total donor:acceptor weight. [d] Thermal annealing temperature in N_2 for 10 min.

Table S5 OSC characteristics of the P3HT:TT-FT-ID based devices.

conc.[a] / mg mL^{-1}	rotation / rpm	predicted PCE[b] / %	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
28.3	**2216**	**1.96**	**2.04**	**5.93**	**0.80**	**43**
31.9	2457	1.98	2.00	5.94	0.79	43
17.6	500	2.11	1.98	4.42	0.86	52
40	2802	1.86	1.31	4.00	0.82	40

[a] Concentration of total donor:acceptor weight. [b] Predicted PCE by BO.

Table S6 OSC characteristics of the P3HT:TT-T-ID based devices.

conc.[a] / mg mL^{-1}	rotation / rpm	predicted PCE[b] / %	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
20.0	500	0.41	0.03	0.75	0.14	29
18.7	626	0.38	0.00	-	-	-
20.0	698	0.41	0.00	-	-	-
20.0	627	0.41	0.18	0.99	0.41	44

[a] Concentration of total donor:acceptor weight. [b] Predicted PCE by BO.

Table S7 OSC characteristics of the optimized P3HT:TT-FT-ID based devices.

Run	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
1	2.04	5.93	0.80	43
2	2.12	6.50	0.76	43
3	**2.43**	**5.83**	**0.78**	**53**
4	2.37	5.77	0.78	52
5	1.80	4.49	0.77	52
average	2.15 ± 0.26	5.70 ± 0.74	0.78 ± 0.01	49 ± 5

Table S8 OSC characteristics of the optimized P3HT:TT-T-ID based devices.

Run	PCE / %	J_{sc} / mAcm^{-2}	V_{oc} / V	FF / %
1	0.40	1.29	0.84	37
2	0.40	1.38	0.71	40
3	0.40	1.39	0.71	40
4	**0.55**	**1.78**	**0.79**	**39**
5	0.24	1.04	0.67	35
average	0.40 ± 0.11	1.38 ± 0.27	0.74 ± 0.07	38 ± 2

Table S9 The photosynthetic rate for green pepper under control conditions.

PPFD [a] / μmol m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}
	Batch 1	Batch 2	Batch 3	Batch 4	Average
0	-1.231704896	-1.042989088	-0.348542991	-1.139159675	-0.940599163
50	0.200240669	-0.006474152	0.64832943	-0.113694337	0.182100402
100	1.551144127	0.795560608	1.746363388	0.558814924	1.162970762
200	3.585932386	2.414174984	3.929976562	1.222454564	2.788134624
300	6.046457589	4.232693082	6.218539603	2.887496489	4.846296691
400	8.423985235	6.00390737	6.992365688	3.876391829	6.324162531
500	10.43899555	7.732516624	7.879711664	4.197258981	7.562120705
600	11.58580741	8.920801644	8.644713495	4.345319796	8.374160585
700	11.98170159	8.364336925	9.515883687	4.17518948	8.509277921
800	12.55597955	8.613533769	9.860548115	4.085974635	8.779009017
900	13.11503561	8.928202224	9.909685885	4.219497107	9.043105207
1000	13.23457186	9.27297488	10.15425693	4.139898395	9.200425515
1500	13.39292236	8.833746055	10.24816607	3.981990233	9.114206179
2000	13.73297193	9.498898918	10.33783577	4.096212009	9.416479657

[a] Photosynthetic photon flux density.

Table S10 Photosynthetic rate for green pepper using the P3HT:TT-FT-ID blend film.

PPFD [a] / μmol m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}
	Batch 1	Batch 2	Batch 3	Batch 4	Average
0	-1.441779833	-0.484825183	-0.948308864	-0.155683978	-0.757649465
50	-0.681074821	0.561408457	-0.232507033	0.500535347	0.037090488
100	0.274030794	1.013752031	0.708579314	0.769885196	0.691561834
200	1.754820634	2.277511971	1.880839327	1.387959967	1.825282975
300	3.330612199	3.929076491	3.019201869	2.936085169	3.303743932
400	4.67770562	5.561807291	4.047052587	3.715638547	4.500551011
500	6.87891455	7.183515527	5.174760831	4.500529224	5.934430033
600	7.684811606	8.229880197	5.922756165	5.142438632	6.74497165
700	8.856360744	8.650512459	6.443909534	5.249705052	7.300121947
800	9.090074924	9.088193863	5.92797715	5.274381027	7.345156741
900	9.020536583	9.302233847	5.912020063	5.309574786	7.38609132
1000	8.92505013	9.725731265	5.770586413	5.144683335	7.391512785
1500	9.525438576	9.93792437	6.019447874	5.148891028	7.657925462
2000	9.682972693	10.84754744	6.26107672	5.433171203	8.056192015

[a] Photosynthetic photon flux density.

Table S11 Photosynthetic rate for green pepper using the P3HT:TT-T-ID blend film.

PPFD [a] / μmol m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}	Photosynthetic rate /μmol CO_2 m^{-2} s^{-1}
	Batch 1	Batch 2	Batch 3	Batch 4	Average
0	-0.671871224	-0.735713658	-0.280411328	-0.863309956	-0.637826542
50	0.173048389	-0.508836828	0.036913232	-0.115170446	-0.103511413
100	0.828800456	0.620464945	0.473160557	0.128759401	0.51279634
200	1.691448507	1.458086846	0.752130743	0.690185871	1.147962992
300	3.402649227	2.649288874	1.935223702	1.852153682	2.459828871
400	4.902039106	4.005606882	3.049924085	2.555251271	3.628205336
500	6.389930447	5.159029797	4.258492209	2.970082161	4.694383654
600	7.297440488	5.994199582	4.66187171	3.290101891	5.310903418
700	8.617089643	6.649392732	5.004452571	3.719376106	5.997577763
800	8.882130175	6.897620445	5.509407984	3.485352416	6.193627755
900	10.21655004	6.736112897	5.476994822	3.344908589	6.443641588
1000	10.37061769	6.361857316	5.410536084	3.023832968	6.291711015
1500	10.2636043	6.652594886	5.457905169	2.905544377	6.319912182
2000	11.64075462	7.012521149	5.689293656	2.7479617	6.772632781

[a] Photosynthetic photon flux density.

Experimental information

Column chromatography was performed on silica gel, KANTO Chemical silica gel 60N (40–50 μm). Thin-layer chromatography plates were visualized by exposure to UV light. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constant (Hz). Mass spectra were obtained on a Shimadzu AXIMA-TOF system. UV-vis spectra were recorded on a Shimadzu UV-3600 spectrophotometer. Photoelectron yield spectroscopy (PYS) was performed using a Bunkoukeiki BIP-KV202GD instrument. Low-energy inverse photoemission spectroscopy (LEIPS) was performed by Ulvac-Phi, Inc. LEIPS system. The surface structures of the deposited organic films were observed by atomic force microscopy (AFM) (Shimadzu, SPM9600). Elemental analysis was performed on a Perkin Elmer LS-50B instrument by the Elemental Analysis Section of Comprehensive Analysis Center (CAC), SANKEN, Osaka University.

Preparation of materials.

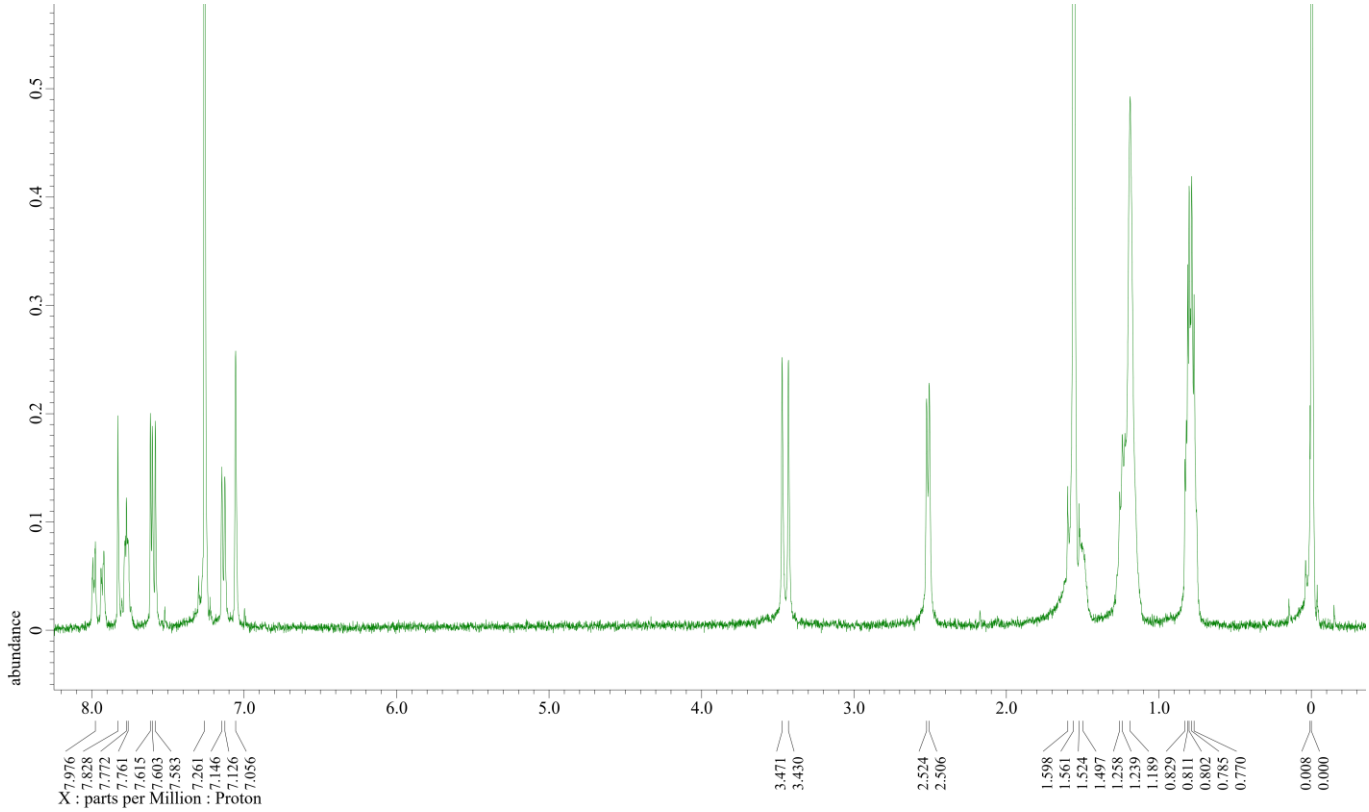
Commercially available reagents were used without further purification. All reactions were carried out under a nitrogen atmosphere. **1** and **2** was prepared by our previously reported procedure.[2]

*Synthesis of **TT-FT-ID***: Piperidine (100 μL) was added to solution of **1** (65 mg, 0.055 mmol) and 1,3-indanone (64 mg, 0.44 mmol) in $CHCl_3$ (5 mL) and the resulting mixture was stirred at 65 °C for 12 h. Methanol (10mL) was added to the reaction mixture and the resulting precipitate was collected on a filtern. The crude product was purified by column chromatography on silica gel (hexane/$CHCl_3$=2/1, v/v, R_f = 0.3), followed by further purification with reprecipitation using $CHCl_3$ and acetone to give TT-FT-ID (61 mg, 77%). Deep purple solid. ^{1}H NMR (400 MHz, TMS) δ: 7.98 (m, 2H), 7.93 (m, 2H), 7.83 (s, 2H), 7.77 (m, 4H), 7.61 (s, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 4H), 7.14 (d, *J* = 8.0 Hz, 4H), 7.06 (s, 4H), 3.45 (d, *J* = 16.4 Hz, 8H), 2.52 (d, *J* = 7.2 Hz, 8H), 1.52 (m, 4H), 1.35-1.14 (br, 32H), 0.80 (m, 24H). ^{13}C NMR (100 MHz, TMS) δ: 190.13, 189.97, 164.01, 151.15, 144.13, 142.06, 141.83, 141.57, 140.55, 139.76, 139.64, 137.10, 134.94, 134.77, 133.32, 133.29, 128.90, 127.14, 123.06, 122.92, 122.77, 119.34, 118.61, 62.07, 41.86, 41.15, 40.75, 40.24, 32.26, 28.79, 25.46, 23.05, 14.14, 10.83. MS *m/z* calcd. for $C_{96}H_{100}O_4S_4$ (M^-): 1446; found: 1446. Anal. calcd for $C_{96}H_{100}O_4S_4$: C 79.74, H 6.97; found: C 79.57, H 6.99.

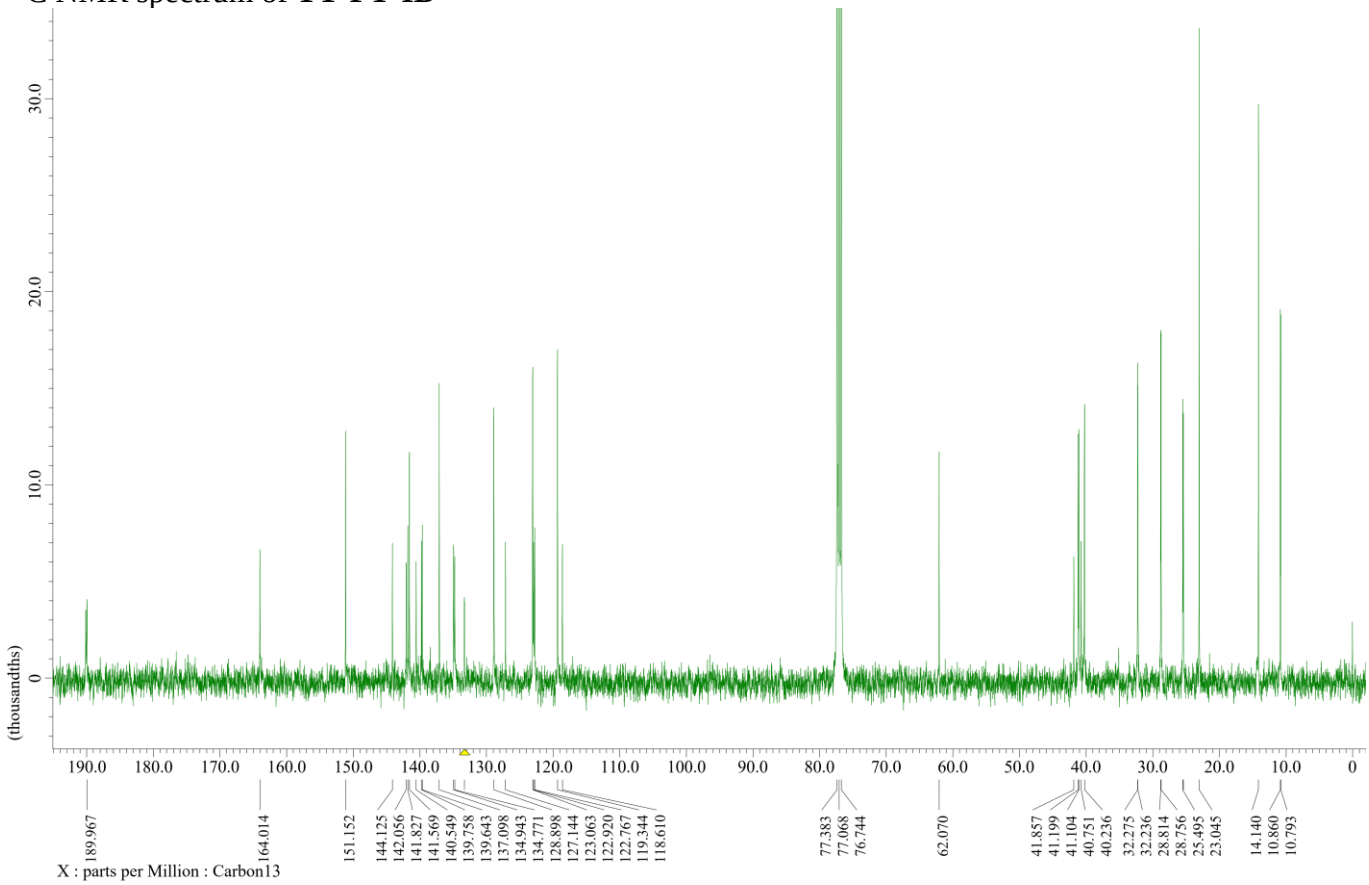
*Synthesis of **TT-T-ID***: Compound **TT-T-ID** was synthesized from **2** (60 mg, 0.103 mmol) by following the procedure used for the preparation of **TT-FT-ID**. Yield: 51 mg (60%). Deep purple solid. ^{1}H NMR (400 MHz, TMS) δ: 8.00-7.97 (m, 4H), 7.91 (s, 2H), 7.80-7.78 (m, 4H), 7.59 (s, 2H), 2.84 (d, *J* = 7.2 Hz, 4H), 1.76 (m, 2H), 1.41-1.26 (br, 16H), 0.90 (m, 12H). ^{13}C NMR (100 MHz, TMS) showed no distinct peaks due to its limited solubility in $CDCl_3$. MS *m/z* calcd. for $C_{50}H_{48}O_4S_4$ (M^-): 841; found: 841. Anal. calcd for $C_{50}H_{48}O_4S_4$: C 71.39, H 5.75; found: C 71.19, H 5.78.

NMR Spectra

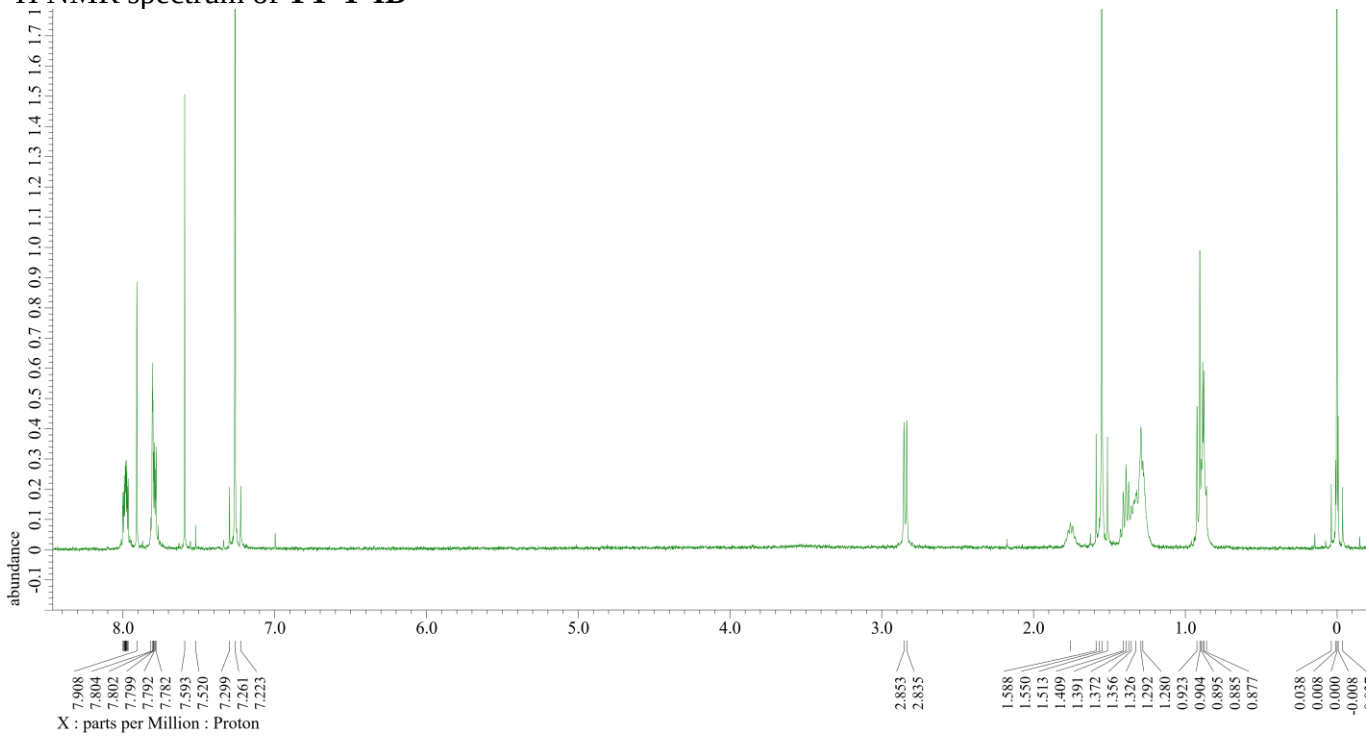
^{1}H NMR spectrum of **TT-FT-ID**



^{13}C NMR spectrum of **TT-FT-ID**



^{1}H NMR spectrum of **TT-T-ID**



Script for Bayesian optimization

Bayesian optimizations were performed for the experimental data (Table S3 and S4) based on the following Python script.

```
import numpy as np
import pandas as pd
import GPy
import GPyOpt
import datetime

# Prediction number
batch_size = 4

# Display GPR results (only for num_x=2): True/False
gpr_output = False

# Data file loading. File name: data.csv
data = pd.read_csv("data.csv")

# Experimental data storing
x_results = data.iloc[:,1:] # Conditions
y_results = data.iloc[:,0] # Power conversion efficiency

# Number of experimental variables
num_x = len(data.columns)-1

# Variables for GPR
norm_x_suggest = []
y_predict = []
y_mean = []
y_variance = []

# List XY data
x_data = np.asarray(x_results).astype(float)
y_data = np.asarray(y_results)
y_data = y_data.reshape(len(y_data),1)
y_data = -y_data

# Standardization of Conditions (x_results) : Min-Max standardization
# x0:Concentration, x1:Rotational speed.
norm_x_data = x_data
norm_x_data[:,0] = norm_x_data[:,0] / 40 # Scale 0-40 mg/mL to 0-1
norm_x_data[:,1] = norm_x_data[:,1] / 5000 # Scale 0-5000 rpm to 0-1

# Range of experimental conditions
bounds = [{'name': 'x1', 'type': 'continuous', 'domain': (0.1, 1)},
        {'name': 'x2', 'type': 'continuous', 'domain': (0.1, 1)},
       ]

print("GPR started for {} batches".format(batch_size))

for i in range(batch_size):

   # Parameter for GPR
   params = {'acquisition_type':'LCB',
           'kernel':GPy.kern.Matern52(input_dim=len(bounds)), # Define the dimension of input by bounds
           'f':None,
           'domain':bounds,
           'X':norm_x_data,
           'Y':y_data,
           'normalize_Y': False,
           'acquisition_weight': 2,
```

	A	B	C
1	y	x0	x1
2	1.9	10	500
3	1.25	10	1000
4	1.88	20	1000
5	1.49	20	3000
6	1.47	30	1000
7	1.93	30	3000
	⋮	⋮	⋮

Example for “data.csv”

```
        }

    # Execution of GPR
    b_opt = GPyOpt.methods.BayesianOptimization(**params)

    norm_x_suggest.append(b_opt.suggest_next_locations(ignored_X = norm_x_data))
    y_predict.append(b_opt.model.model.predict(norm_x_suggest[i]))

    norm_x_data = np.append(norm_x_data, norm_x_suggest[i], axis=0)
    y_data = np.append(y_data, y_predict[i][0], axis=0)

    # Separation of mean values and variance values
    y_mean.append(y_predict[i][0])
    y_variance.append(y_predict[i][1])

    # Show/Save GPR results
    if gpr_output == True:
        b_opt.plot_acquisition()
    else:
        date = str(datetime.date.today())
        batch = str(i + 1)
        filename = date + '_' + batch
        b_opt.plot_acquisition(filename)

    print('GPR for batch: {} completed'.format(i+1))

# Output of prediction
print("\nNext {} experiment conditions are as follow:".format(batch_size))
for i in range(batch_size):
    print("\nCondition for batch {} :".format(i+1))
    print("Concentration [variable 1]: {:.1f} mg/mL".format(norm_x_suggest[i][0][0] * 40))
    print("Rotational speed [variable 2]: {:.0f} rpm".format(norm_x_suggest[i][0][1] * 5000))
    print("Predicted PCE (mean): {:.2f}%".format(-y_mean[i][0][0]))
    print("Variance: {:.3f}%".format(y_variance[i][0][0]))
```

References

1 S. Jinnai, Y. Ie, M. Karakawa, T. Aernouts, Y. Nakajima, S. Mori, and Y. Aso, *Chem. Mater.* **2016**, *28*, 1705–1713.

2 S. Jinnai, K. Murayama, K. Nagai, M. Mineshita, K. Kato, A. Muraoka, A. Yamakata, S. Saeki, Y. Kobori, and Y. Ie, *J. Mater. Chem. A* **2022**, *10*, 20035–20047.

Density functional theory (DFT) calculations

All calculations were conducted using the Gaussian 16 program. The geometry was optimized with the Becke Hybrid (B3LYP) at 6-31G(d,p) level. All of the alkyl groups were replaced with methyl groups to reduce the computational load.

Optimized structure of **TT-FT-ID**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.089349	0.102024	0.148954
2	6	0	3.434214	0.185604	0.227746
3	6	0	4.335984	-0.788011	0.403500
4	16	0	4.175467	1.457824	0.132198
5	6	0	5.574942	1.040406	0.272535
6	6	0	5.567575	-0.288415	0.435428
7	6	0	6.707321	1.767596	0.255220
8	6	0	7.021719	3.072898	0.101791
9	6	0	8.332846	3.469140	0.140848
10	6	0	8.314612	4.809057	-0.043704
11	6	0	7.054434	5.216159	-0.188964
12	6	0	6.211468	4.156976	-0.104275
13	6	0	9.344547	5.663624	-0.087870
14	6	0	9.058022	6.962492	-0.286324
15	6	0	7.786028	7.377655	-0.434000
16	6	0	6.760715	6.508374	-0.387092
17	8	0	9.331144	2.799312	0.303033
18	6	0	-6.192364	-4.130043	-0.366857
19	6	0	6.631616	-1.324755	0.629918
20	6	0	5.801575	-2.601951	0.364206
21	6	0	4.302725	-2.277289	0.571410
22	6	0	6.059312	-3.144039	-1.030121
23	6	0	6.570241	-4.385116	-1.024770
24	6	0	6.711136	-4.802511	0.241928
25	6	0	6.292728	-3.839187	1.077140
26	6	0	7.178024	-5.962703	0.722643
27	6	0	7.218019	-6.139484	2.053716
28	6	0	6.801388	-5.183006	2.905372
29	6	0	6.335629	-4.024216	2.404228
30	6	0	5.826996	-2.513531	-2.190319
31	6	0	6.105809	-3.124447	-3.356296
32	6	0	6.619081	-4.369285	-3.333307
33	6	0	6.855174	-5.008956	-2.175620
34	6	0	6.862853	-5.421131	4.395788
35	6	0	5.841866	-2.407097	-4.659336
36	16	0	1.350145	-1.179982	0.228777
37	6	0	0.007273	-0.632703	0.074846
38	6	0	-0.009637	0.690501	-0.043670
39	6	0	1.243330	1.144911	-0.004618
40	6	0	-1.243905	-1.089236	0.010850
41	6	0	-2.089549	-0.046227	-0.142134
42	16	0	-1.353281	1.239403	-0.184379
43	6	0	-3.432534	-0.131003	-0.247946
44	6	0	-4.336352	0.849831	-0.361115
45	16	0	-4.170212	-1.409016	-0.250414
46	6	0	-5.566884	-0.988055	-0.409381
47	6	0	-5.564751	0.349914	-0.454867
48	6	0	-6.693453	-1.718490	-0.500577
49	6	0	-7.002997	-3.033669	-0.488967
50	6	0	-8.308972	-3.428766	-0.614951
51	6	0	-8.286936	-4.780509	-0.570389
52	6	0	-7.029724	-5.195600	-0.423016
53	8	0	-4.994715	-4.252456	-0.234538
54	6	0	-9.311452	-5.638747	-0.653087
55	6	0	-9.022288	-6.950121	-0.581881
56	6	0	-7.753268	-7.373799	-0.433085
57	6	0	-6.733666	-6.500442	-0.350557
58	8	0	-9.305992	-2.749486	-0.742664
59	8	0	5.010611	4.274907	-0.207492
60	6	0	-6.629027	1.397822	-0.574645
61	6	0	-5.811742	2.634718	-0.135124
62	6	0	-4.312272	2.348653	-0.389469
63	6	0	-6.312096	3.957119	-0.663714
64	6	0	-6.734433	4.788196	0.301676
65	6	0	-6.588901	4.195291	1.495786
66	6	0	-6.069425	2.969516	1.324106
67	6	0	-6.359244	4.332084	-1.949704
68	6	0	-6.829290	5.549447	-2.278425
69	6	0	-7.252513	6.370274	-1.298029
70	6	0	-7.209466	6.002309	-0.006605
71	6	0	-6.877036	4.647455	2.723532
72	6	0	-6.635898	3.850452	3.777472
73	6	0	-6.113993	2.618684	3.624198
74	6	0	-5.831635	2.181636	2.383256
75	6	0	-6.891178	5.975843	-3.726462
76	6	0	-5.859002	1.750624	4.834097
77	1	0	7.590970	1.119141	0.402406
78	1	0	10.385847	5.325574	0.031981
79	1	0	9.879144	7.697945	-0.329098
80	1	0	7.579802	8.449251	-0.596380
81	1	0	5.723400	6.857939	-0.508806
82	1	0	6.971307	-1.271475	1.689639
83	1	0	7.501069	-1.220782	-0.054934
84	1	0	3.656161	-2.813693	-0.155998
85	1	0	3.980445	-2.500370	1.614232
86	1	0	7.525728	-6.763420	0.051075
87	1	0	7.601912	-7.091815	2.456442
88	1	0	5.987829	-3.221676	3.072956
89	1	0	5.407097	-1.495610	-2.188162
90	1	0	6.853623	-4.883376	-4.280189
91	1	0	7.275092	-6.027202	-2.186154
92	1	0	6.236268	-6.299333	4.672762
93	1	0	7.911830	-5.621496	4.712439
94	1	0	6.496761	-4.550649	4.984604
95	1	0	6.388757	-1.437093	-4.685095
96	1	0	6.165303	-2.994968	-5.547073
97	1	0	4.752869	-2.201145	-4.770267
98	1	0	1.506486	2.208956	-0.088753
99	1	0	-1.506512	-2.154648	0.076690
100	1	0	-7.575917	-1.062233	-0.617488
101	1	0	-10.350361	-5.293859	-0.774869
102	1	0	-9.838746	-7.689177	-0.646471
103	1	0	-7.544683	-8.455772	-0.377825
104	1	0	-5.698653	-6.856782	-0.228600
105	1	0	-7.523222	1.220343	0.061456
106	1	0	-6.926783	1.465518	-1.646111
107	1	0	-4.006311	2.671801	-1.410887
108	1	0	-3.662982	2.821321	0.378597
109	1	0	-6.009145	3.639719	-2.731175
110	1	0	-7.642233	7.369908	-1.553055
111	1	0	-7.560776	6.695332	0.774106
112	1	0	-7.303568	5.650713	2.880102
113	1	0	-6.870865	4.216083	4.791123
114	1	0	-5.404978	1.178430	2.232524
115	1	0	-5.902047	6.377318	-4.044298
116	1	0	-7.152252	5.121260	-4.390713
117	1	0	-7.657246	6.764905	-3.898630
118	1	0	-6.784229	1.652828	5.446472
119	1	0	-5.532635	0.721989	4.562546
120	1	0	-5.061836	2.201922	5.467735

Optimized structure of **TT-T-ID**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.892473	0.894382	0.040122
2	6	0	-3.124931	1.446452	0.036043
3	6	0	-3.434511	2.750930	0.041138
4	16	0	-4.368799	0.666884	0.025199
5	6	0	-5.381074	1.724337	0.020711
6	6	0	-4.761873	2.920649	0.033404
7	6	0	-6.721321	1.577790	0.006172
8	6	0	-7.597295	0.547197	-0.012510
9	6	0	-8.944577	0.800997	-0.022691
10	6	0	-9.546603	-0.410023	-0.041689

11	6	0	-8.615989	-1.362850	-0.043143
12	6	0	-7.379471	-0.805026	-0.025184
13	6	0	-10.854552	-0.696433	-0.057676
14	6	0	-11.199517	-1.996039	-0.075520
15	6	0	-10.262267	-2.962254	-0.077218
16	6	0	-8.951725	-2.660045	-0.060928
17	8	0	-9.525561	1.866007	-0.016710
18	6	0	7.379250	0.805177	-0.024875
19	6	0	-5.410341	4.280893	0.036212
20	16	0	-0.651541	1.707148	0.045221
21	6	0	0.293762	0.595953	0.043692
22	6	0	-0.293592	-0.596411	0.043067
23	6	0	-1.616464	-0.428201	0.040096
24	6	0	1.616539	0.427822	0.041193
25	6	0	1.892656	-0.894726	0.040302
26	16	0	0.651646	-1.707612	0.044168
27	6	0	3.125079	-1.446746	0.036418
28	6	0	3.434730	-2.751233	0.040542
29	16	0	4.368835	-0.667112	0.026862
30	6	0	5.381335	-1.724500	0.021500
31	6	0	4.762149	-2.920886	0.033151
32	6	0	6.721495	-1.577783	0.007106
33	6	0	7.597250	-0.547066	-0.011794
34	6	0	8.944575	-0.800652	-0.021895
35	6	0	9.546472	0.410466	-0.041579
36	6	0	8.615692	1.363118	-0.043325
37	8	0	6.372637	1.478755	-0.023455
38	6	0	10.854434	0.697007	-0.057823
39	6	0	11.199128	1.996673	-0.076483
40	6	0	10.261703	2.962725	-0.078494
41	6	0	8.951282	2.660388	-0.061888
42	8	0	9.525773	-1.865593	-0.015558
43	8	0	-6.372882	-1.478746	-0.023351
44	6	0	5.410675	-4.280991	0.034406
45	1	0	-2.722520	3.588150	0.050129
46	1	0	-7.226555	2.559732	0.009393
47	1	0	-11.622828	0.092751	-0.056549
48	1	0	-12.267256	-2.273205	-0.089211
49	1	0	-10.573391	-4.020656	-0.092254
50	1	0	-8.192975	-3.458412	-0.062660
51	1	0	-6.047265	4.413136	0.940049
52	1	0	-4.654417	5.097757	0.048751
53	1	0	-6.030772	4.425100	-0.877109
54	1	0	-2.337910	-1.257498	0.037481
55	1	0	2.337962	1.257149	0.039571
56	1	0	2.722894	-3.588530	0.048439
57	1	0	7.226808	-2.559699	0.010261
58	1	0	11.622844	-0.092088	-0.056360
59	1	0	12.266852	2.273959	-0.090491
60	1	0	10.572739	4.021211	-0.094314
61	1	0	8.192426	3.458635	-0.063923
62	1	0	6.047394	-4.414364	0.938214
63	1	0	4.654863	-5.097966	0.045620
64	1	0	6.031334	-4.424044	-0.879007