Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information

for

Structural Effect of Carbazole-based Coadsorbents on Cell Performance of Organic Dye-Sensitized Solar Cells

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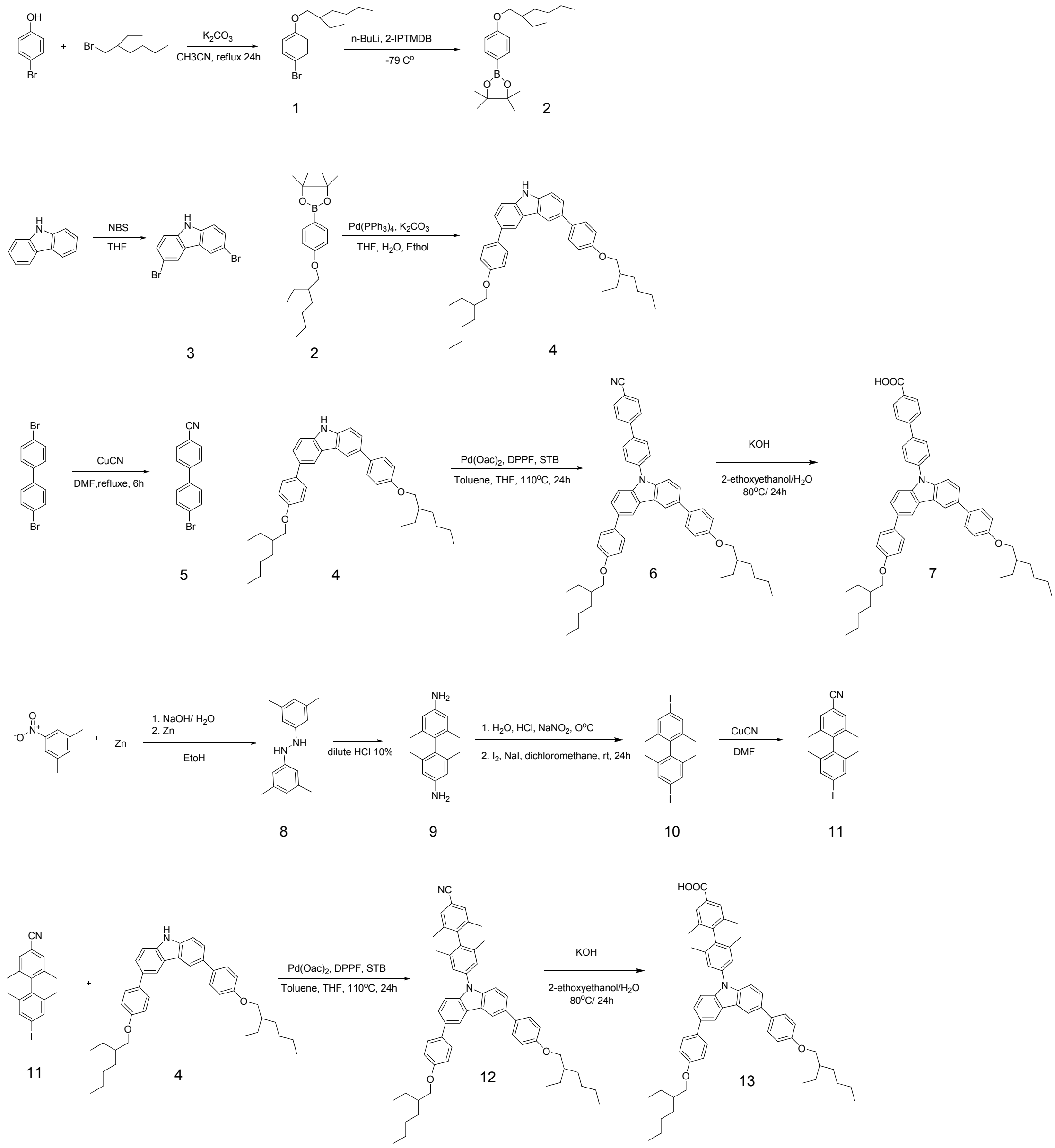
S1. Experimental Section



Scheme S1. Synthetic procedures for coadsorbents.

Materials and Instrumentation:

All reagents and chemicals were purchased from Aldrich. Tetrahydrofuran (THF) was dried over and distilled from a K-Na alloy under a dry nitrogen atmosphere. Toluene was dried over and distilled from Na/benzophenone under a dry nitrogen atmosphere. Other chemicals and reagents were used as received without further purifications. ^{1}H NMR spectroscopy was conducted with a Varian Mercury 300 spectrometer using tetramethylsilane (TMS; $\delta = 0$ ppm) as the internal standard.

1-Bromo-4-(2-ethylhexyloxy)benzene (1)

A mixture of 4-bromophenol (5 g, 28.8 mmol) and K_2CO_3 (9.99 g, 43.2 mmol) in acetonitrile (30 ml) was stirred at room temperature for 1 h. 3-(Bromomethyl)heptane (6.67 g, 34.6 mmol) was added dropwise and stirred at room temperature for 12 h. The reaction mixture was quenched with water and extracted with ethyl acetate. The organic layer was collected and the aqueous layer was washed with ethyl acetate. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (*n*-hexane/DCM = 2/1) to obtain compound 1 (5.52 g, 67%): ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.36 (d, 2H, J = 8.7 Hz, Ar-H), 6.76 (d, 2H, J = 8.7 Hz, Ar-H), 3.80-3.79 (d, 2H, J = 5.7 Hz, CH_2-O), 1.74-1.68 (q, 1H, J = 6.0 Hz, $(CH_2)_3$-H), 1.39-1.37 (m, 8H, -CH_2), 0.95-0.92 (t, 6H, -CH_3).

2-(4-(2-Ethylhexyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2)

1-Bromo-4-(2-ethylhexyloxy)benzene (5.52 g, 19.4 mmol) in THF (150 ml) was added dropwise to a solution of *n*-BuLi(1.61 g, 25.2 mmol, 2.5 M in *n*-hexane) at -78°C under nitrogen. The mixture was stirred for 1 h, then 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.32 g, 23.2 mmol) was added dropwise, and the reaction mixture was stirred for another 1 h at −78°C before being stirred overnight at room temperature. The reaction mixture was quenched with water and extracted with ethyl acetate. The organic layer was collected and washed with brine. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (*n*-hexane/DCM = 3/1) to obtain compound 2 (5.9g, 92%): ^1H NMR (300 MHz, $CDCl_3$) δ = 7.73 (d, 2H, *J* = 8.1 Hz, Ar-H), 6.88 (d, 2H, *J* = 8.4 Hz, Ar-H), 3.85 (d, 2H, *J* = 6.0 Hz, CH_2-O), 1.75-1.69 (q, 1H, *J* = 6.0 Hz, $(CH_2)_3$-H), 1.54-1.39 (m, 8H, -CH_2), 0.95-0.87 (t, 6H, -CH_3).

3,6-dibromo-9H-carbazole (3)

9H-carbazole (5g, 29.90 mmol) in THF (50 ml) and a solution of N-bromosuccineiunide (10.64 g, 59.81 mmol) was added dropwise and stirred at room temperature for 4 h. The reaction mixture was quenched with water and extracted with ethyl acetate. The organic layer was collected and the aqueous layer washed with ethyl acetate. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (n-hexane/EtOAc = 4/1) to obtain compound 3 (4.7 g, 80%) ^1H NMR (300 MHz, $CDCl_3$) δ = 8.13 (s, 2H, Ar-H), 7.53 (d, 2H, J = 8.4, Ar-H), 7.32 (d, 2H, J = 8.4 Hz, Ar-H).

3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazole (4)

3,6-dibromo-9H-carbazole (3.0 g, 9.23 mmol) and 2-(4-(2-ethylhexyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6.13 g, 18.46mmol), potassium carbonate (5.10 g, 36.92 mmol), toluene/tetrahydrofuran/H_2O/ethanol (3:1:1:1) 100 ml, tetrakis(triphenylphosphine) palladium($Pd(PPh_3)_4$) (0.76 g, 0.65 mmol) was degassed and charged with nitrogen. The reaction was refluxed for 12 h. The reaction mixture was separated, and the aqueous layer was washed with ethyl acetate. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by flash column chromatography (n-hexane/EtOAc = 3/1) to obtain compound 4 (3.2 g, 60%) ^{1}H NMR (300 MHz, CDCl) δ = 8.27 (d, 2H, Ar-H), 7.65 (m, 6H, Ar-H), 7.49 (d, 2H, J = 8.7 Hz, Ar-H), 7.03 (d, 2H, J = 8.4 Hz, Ar-H), 3.90 (d, 4H, J = 9.0 Hz, CH2-O), 1.68 (q, 2H, (CH2)3-H), 1.44-1.30 (m, 16H, -CH2), 0.92-0.87 (t, 12H, -CH3).

4'-Bromobiphenyl-4-carbonitrile (5)

4,4'-Dibromobiphenyl (15 g, 48.08 mmol) and 4.31 g (48.08 mmol) of CuCN (CAUTION, keep away from water) were combined in a round bottom flask with 30 mL of DMF. The mixture was put under N_2 and refluxed for 12 h and left to cool overnight. The DMF was distilled off under vacuum and after cooling, chloroform with a few drops of triethylamine was added. The solid was washed thoroughly with multiple aliquots of chloroform. The combined fractions were then passed through a silica plug and dried to yield a crude solid. The residue was purified by flash column chromatography (n-hexane/chloroform = 1/1) to obtain compound 5 (4.4 g, 35%): ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.74 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.66-7.59 (m, 4H, Ar-H), 7.46 (d, 2H, *J* = 8.7 Hz, Ar-H).

4'-(3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazol-9-yl)biphenyl-4-carbonitrile (6)

4'-Bromobiphenyl-4-carbonitrile (2.0 g, 7.75 mmol), 3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazole (4.46 g, 7.75 mmol), $Pd(OAc)_2$ (0.17 g, 0.77 mmol), 1,1'- Bis(diphenylphosphino) ferrocene (0.43 g, 0.77 mmol), sodium *t*-butoxide (2.21 g, 23.02 mmol) and toluene/tetrahydrofuran (9:1; 100 ml) was degassed and charged with nitrogen. The reaction was refluxed for 12 h. The reaction mixture was separated and the aqueous layer washed with ethyl acetate. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (n-hexane/EtOAc = 5/1) to obtain compound 6 (3.5 g, 60%): ^{1}H NMR (300 MHz, DMSO) δ = 8.65 (s, 2H, Ar-H), 8.08(m, 4H, Ar-H), 8.04 (d, 2H, J = 8.7 Hz, Ar-H), 7.82 (d, 6H, J = 8.7 , J 3.0 Hz, J 3.0 Hz, Ar-H), 7.68 (d, 2H, J = 8.7 Hz, Ar-H), 7.52 (d, 2H, J = 8.7 Hz, Ar-H), 7.07(d, 4H, J = 9 Hz, Ar-H),3.90 (d, 4H, J = 8.7 Hz, CH2-O), 1.80-1.56 (q, 2H, J = 6.3 Hz, (CH2)3-H), 1.56-1.45 (m, 16H, -CH2), 0.99-0.92 (t, 12H, -CH3).

4'-(3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazol-9-yl)biphenyl-4-carboxylic acid (7)

4'-(3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazol-9-yl)biphenyl-4-carbonitrile (3.5 g, 4.65 mmol) and potassium hydroxide (1.86 g, 46.48 mmol) in 2-ethoxyethanol/H_2O (2:1; 300 ml) was stirred at 80°C for 24 h . The reaction mixture was allowed to cool at room temperature and then acidified with 2 M HCl solution until the pH 3. After it was poured into water and extracted with ethyl acetate. The combined organic layer was washed with brine and then dried over anhydrous MgSO4, filtered and concentrated in vacuo. The residue was purified by flash column chromatography (n-hexane/EtOAc = 2/1) to obtain compound 7 (3.5 g, 90%): ^{1}H NMR (300 MHz, DMSO) δ = 8.65 (s, 2H, Ar-H), 8.08(m, 4H, Ar-H), 8.04 (d, 2H, J = 8.7 Hz, Ar-H), 7.82 (d, 6H, J = 8.7 , J 3.0 Hz, J 3.0 Hz, Ar-H), 7.68 (d, 2H, J = 8.7 Hz, Ar-H), 7.52 (d, 2H, J = 8.7 Hz, Ar-H), 7.07(d, 4H, J = 9 Hz, Ar-H),3.90 (d, 4H, J = 8.7 Hz, CH2-O), 1.80-1.56 (q, 2H, J = 6.3 Hz, (CH2)3-H), 1.56-1.45 (m, 16H, -CH2), 0.99-0.92 (t, 12H, -CH3); FT-IR (KBr) [cm-1] 1700 (carboxylic acid, -C=O), 3150-3700 (carboxylic acid-OH). MS (FAB) m/z 772.02[M+].

1,2-bis(3,5-dimethylphenyl)hydrazine (8)

A suspension of 3,5-dimethylnitrobenzene (10.00 g, 66.20 mmol) and zinc powder (25.0 g, 0.382 mol, 5.8 equiv.) in EtOH (40 mL) was heated at reflux under an inert gas. Then the heating source was removed, and a solution of NaOH (15.0 g, 0.375 mol, 5.7 equiv.) in water (50 mL) was added dropwise to the reaction mixture at such a rate that the solution boiled vigorously. After addition of about a third of the base, heating was needed to maintain a steady reflux. After all of the base had been added, heating was continued at reflux for 4 h, and more zinc powder (10.0 g, 0.153 mol, 2.3 equiv.) was added in portions over this period of time. The hot suspension was filtered through Celite and washed with hot EtOH (60 mL) into a mixture of AcOH (150 mL, 30%) and sodium bisulfite (1.0 g, 9.6 mmol, 0.15 equiv.). The slurry was cooled to 10 °C, and the solid was filtered off. Recrystallization from hot heptane (80 mL) afforded 1,2- bis(3,5-dimethylphenyl)hydrazine (3.96 g, 16.48 mmol, 50 %) as long white needles. M.p. 119–123 °C. TLC: Rf = 0.77 (ethyl acetate/ hexane, 2:1). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.24 (s, 12 H), 5.46 (s, 2 H), 6.52 (s, 6 H).

2,2',6,6'-tetramethylbiphenyl-4,4'-diamine (9)

Diluted HCl (175 mL, 10%)was degassed with nitrogen for 30 min. Then 1,2-bis(3,5-dimethylphenyl) hydrazine (3.70 g, 15.4 mmol) was added, and the reaction mixture was heated at reflux. After 2 h, TLC showed full conversion of the starting material. The solution was cooled to room temperature, and NaOH was added until pH = 10. The product was extracted with t-BME (3X60 mL), and the combined organic phases were washed with brine and dried with $MgSO_4$. After evaporation of the solvent, the residue was recrystallized from benzene/ hexane to obtain 2,2',6,6'-tetramethylbiphenyl-4,4'-diamine (2.87 g, 11.90 mmol, 77%) as a pink powder. For further purification, the free base was recrystallized several times from EtOH/water; however, traces of isomeric impurities remained in the sample. M.p. 163–165 °C. TLC: Rf = 0.47 (ethyl acetate/hexane, 2:1). 1H NMR (300 MHz, CDCl3): δ = 1.82 (s, 12 H), 3.52 (br. s, 4 H), 6.48(s, 4 H).

4,4'-diiodo-2,2',6,6'-tetramethylbiphenyl (10)

A solution of $NaNO_2$ (600 mg, 8.70 mmol, 2.2 equiv.) in water (2.0 mL) was added to a suspension of 2,2',6,6'-tetramethylbiphenyl-4,4'-diamine (18; 0.93 g, 3.87 mmol) in water (15 mL) and H_2SO_4 (8 mL, 0.142 mol, 36.4 equiv., 95%) at 4 °C. After stirring at this temperature for another 30 min, all the starting materials had dissolved, and the reaction mixture was transferred to a cold solution of I_2 (2.70 g, 10.64 mmol, 2.8 equiv.) and NaI (2.70 g, 18.00 mmol, 4.7 equiv.) in water (5 mL). After 20 min, more water (20 mL) and CH_2Cl_2 (50 mL) were added to dissolve the reaction components again. After stirring at room temperature overnight, sodium thiosulfate (2.00 g, 12.7 mmol, 3.3 equiv.) was added, and the reaction mixture was stirred for 10 min. The black precipitate was filtered off and the phases separated. The aqueous phase was extracted with $CHCl_3$ (2x30 mL), and the combined organic layers were washed again with a thiosulfate solution (25 mL, 10%) and brine. After drying with $MgSO_4$ and evaporation of the solvent, flash chromatography was performed to obtain 4,4'-diiodo-2,2',6,6'-tetramethylbiphenyl (908 mg, 1.97 mmol, 51%) as bright-yellow crystals. M.p. 196 °C. TLC: Rf = 0.52 (hexane). 1H NMR (300 MHz, CDCl3): δ = 1.83 (s, 12 H), 7.48 (s, 4 H).

4'-iodo-2,2',6,6'-tetramethylbiphenyl-4-carbonitrile (11)

The preparation method was the same as that of 5, 1H NMR (300 MHz, CDCl3) δ = 7.51 (s, 2H, Ar-H), 7.43 (s, 2H, Ar-H).

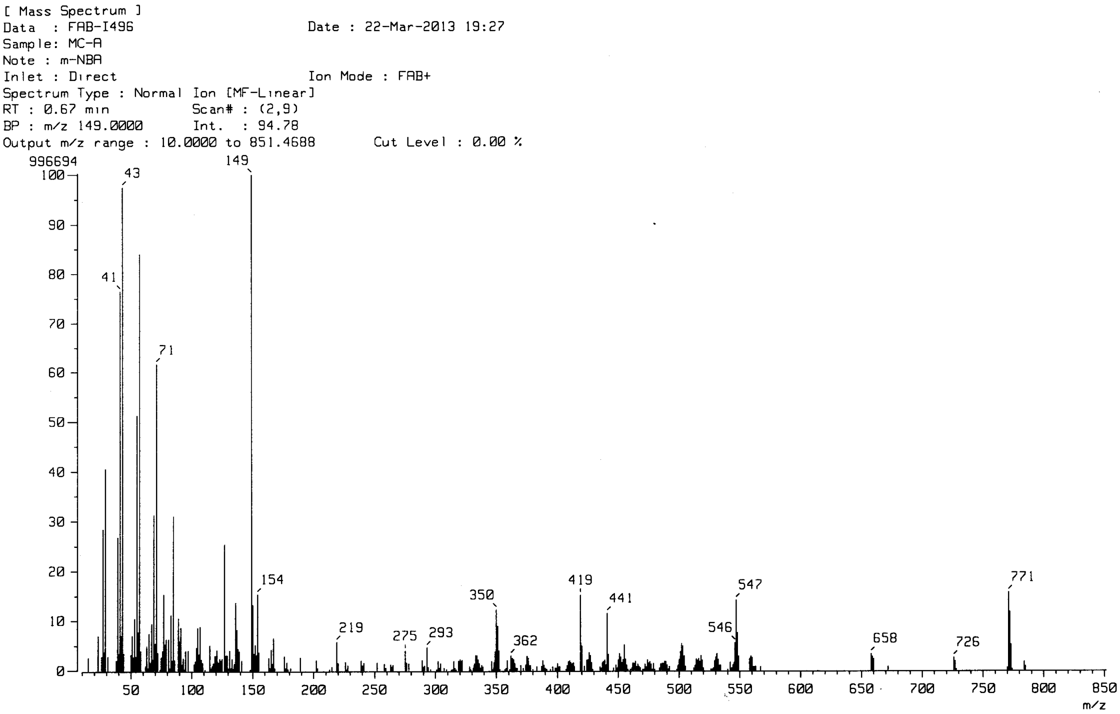
4'-(3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazol-9-yl)-2,2',6,6'-tetramethylbiphenyl-4-carbonitrile (12)

The preparation method was the same as that of **6,** ^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.34 (s, 2H, Ar-H), 7.66(d, 8H, J = 8.4, Ar-H), 7.53 (d, 4H, Ar-H), 7.40 (d, 2H, Ar-H), 7.04 (d, 4H, J

= 8.4 Hz, Ar-H), ,3.90 (d, 4H, J = 8.7 Hz, CH_2-O), 1.80-1.56 (q, 2H, J = 6.3 Hz, $(CH_2)_3$-H), 1.56-1.45 (m, 16H, -CH_2), 0.99-0.92 (t, 12H, -CH_3).

4'-(3,6-bis(4-(2-ethylhexyloxy)phenyl)-9H-carbazol-9-yl)-2,2',6,6'-tetramethylbiphenyl-4-carboxylic acid (13)

The preparation method was the same as that of **7,** ^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.34 (s, 2H, Ar-H), 7.66(d, 8H, J = 8.4, Ar-H), 7.53 (d, 4H, Ar-H), 7.40 (d, 2H, Ar-H), 7.04 (d, 4H, J = 8.4 Hz, Ar-H), ,3.90 (d, 4H, J = 8.7 Hz, CH_2-O), 1.80-1.56 (q, 2H, J = 6.3 Hz, $(CH_2)_3$-H), 1.56-1.45 (m, 16H, -CH_2), 0.99-0.92 (t, 12H, -CH_3); FT-IR (KBr) [cm-1] 1700 (carboxylic acid, -C=O), 3150-3700 (carboxylic acid-OH). MS (TOF) m/z 828.13[M+].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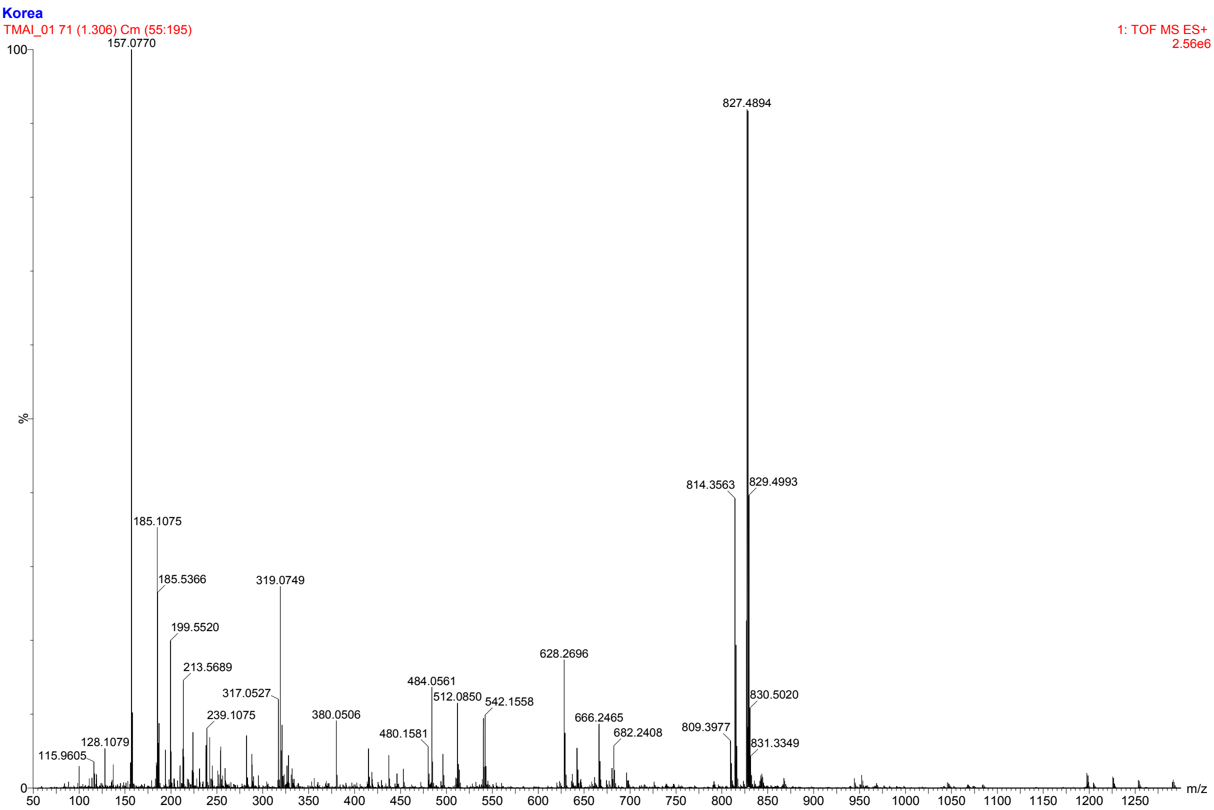
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%
m/z

Fabrication of the dye-sensitized solar cells

FTO (luorine doped tin oxide) plates were cleaned in detergent solution, water and ethanol in an ultrasonic bath. The FTO substrates were immersed in 40 mM aqueous $TiCl_4$ solution at 70 °C for 30 min and washed with water and ethanol. A TiO_2 colloidal paste (Solaronix, Ti-Nanoxide T/SP) was screen-printed onto FTO/glass and sintered at 500 °C for 30 min in air. The thickness of the transparent layer was measured using an Alpha-step 250 surface profilometer (Tencor Instruments, San Jose, CA), and a paste for the scattering layer containing 500-nm-sized anatase particles (ENB Korea, STP-500N) was deposited by doctor blade printing and then dried for 2 h at 25°C. The TiO_2 electrodes were sintered at 500°C for 30 min. The resulting TiO_2 photoanode was immersed in a THF/ethanol (v/v, 2/1) solution containing 2×10^{-4} M of FP porphyrin dye and kept at room temperature for 12 h. Counter electrodes were prepared by coating with a drop of H_2PtCl_6 solution (2 mg of Pt in 1 mL of ethanol) on an FTO plate and heating at 400°C for 15 min. The dye-adsorbed TiO_2 photoanodes were assembled with Pt-coated FTO using a thermal adhesive film (60-μm thick Surlyn, Du-Pont) as a spacer to produce a sandwich-type cell. Electrolyte solution was introduced through a drilled hole on the CEs via vacuum backfilling. The hole was sealed with cover glass using Surlyn.

Photovoltaic measurements of the solar cells

Photoelectrochemical data were measured using a 1000 W xenon light source (Oriel, 91193) that was focused to give 100 mW cm^{-2}, which is the equivalent of one sun at Air Mass (AM) 1.5G at the surface of the test cell. The light intensity was adjusted with a Si solar cell that was doubled-checked with an NREL calibrated Si solar cell (PV Measurement Inc.). The applied potential and measured cell currents were measured using a Keithley model 2400 digital source meter. The current-voltage characteristics of the cell under these conditions were determined by biasing the cell externally and measuring the generated photocurrent. This process was fully automated using the Wavemetrics software. The measurement-settling time between applying a voltage and measuring a current for the *J–V* characterization of DSSCs was fixed at 40 ms.

Characterization

^{1}H-NMR spectra were recorded at room temperature with a Varian Oxford 300 spectrometer and chemical shifts were reported in ppm units with tetramethylsilane as the internal standard. Mass spectra were obtained with a JEOL JMS-700 spectrometer in EI mode. The electrospray ionization (ESI) source was coupled to a hybrid quadrupole orthogonal time-of-flight (Q-TOF) mass spectrometer (SYNAPT G2, Waters, MS Technologies, Manchester, U.K.) was used to mass spectra acquirement in positive- and negative-ion mode. A capillary and cone voltage of ± 3.0kV and 30 V, and capillary temperature of 120 °C were used for both polarities, respectively. The desolvation source conditions were as follows; for the desolvation gas 800 L/h was used and the desolvation temperature was kept at 600 °C. Data acquisition took place over the mass range of m/z 50 to m/z 1200 for MS modes. The sample was introduced into the ESI source at a constant flow rate of 20 µl/min by using an external syringe pump (HARVARD 11Plus, Holliston, MA, USA). UV-vis absorption spectra of dye-loaded films were recorded with a Shimadzu UV-2401PC spectrophotometer.

Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS)

All electrochemical measurements were carried out with a *VersaSTAT* 3, AMETEK connected to a potentiostat under dark conditions at room temperature. Cyclic voltammetry

(CV) measurements were carried out using a typical three-electrode electrochemical cell in a solution with 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as the supporting electrolyte in water-free THF at a scan rate of 50 mV s^{-1} at room temperature, which was degassed with argon gas for 10 min prior to the scan. A Pt rod with a diameter of 0.2 mm was used as the working electrode, a Pt wire as the counter electrode and an Ag/AgCl electrode saturated with KCl as the reference electrode. The electrical potential of the reference electrode was calibrated with the Fc/Fc^+ couple, and all potentials mentioned in this study were against the normal hydrogen electrode (NHE). The potential level of the HOMO with respect to the NHE was determined by: $E_{HOMO} = E_{ox} - E_{Fc/Fc^+} + 0.67$ V. The impedance spectra were acquired in the frequency range from 10^6 Hz to 0.1 Hz, and the AC modulation voltage amplitude was 10 mV. Electrochemical impedance data analysis was processed using the Zplot/Zview2 software.

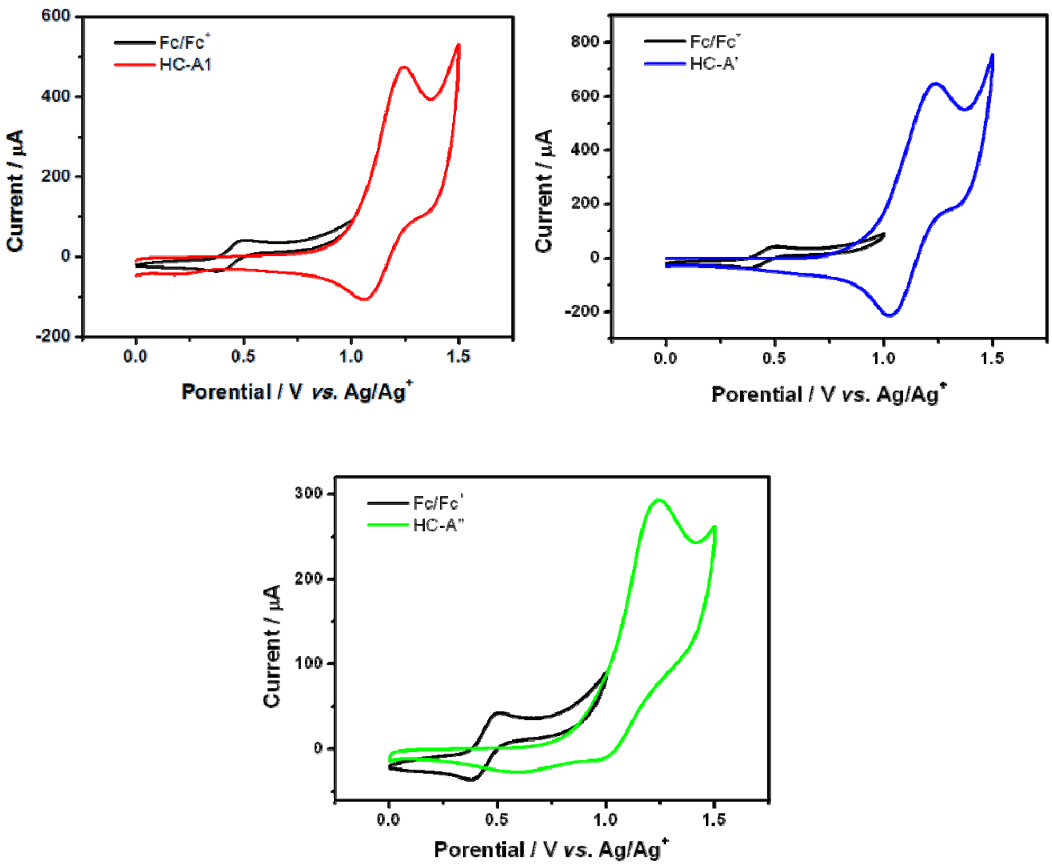

Figure S1. Cyclic voltammograms of **HC-A1**, **HC-A′** and **HC-A″** in water-free ACN containing 0.1 M $TBAPF_6$ at a scan rate of 50 mV s^{-1} under room temperature.

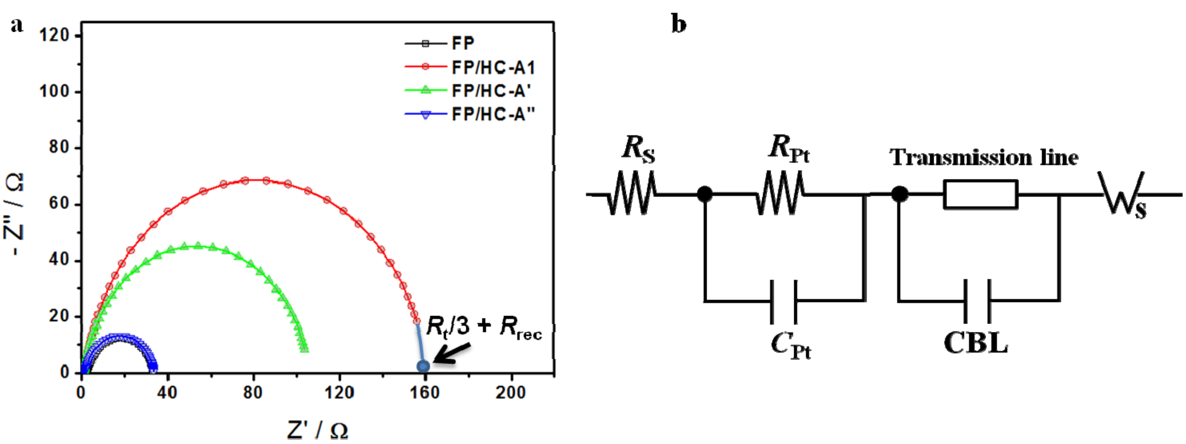

Figure S2. (a) Fitted curves from the EIS spectra of the DSSCs shown in **Figure 4a**. (b) The transmission line equivalent circuit model to evaluate the charge transfer and recombination resistance.

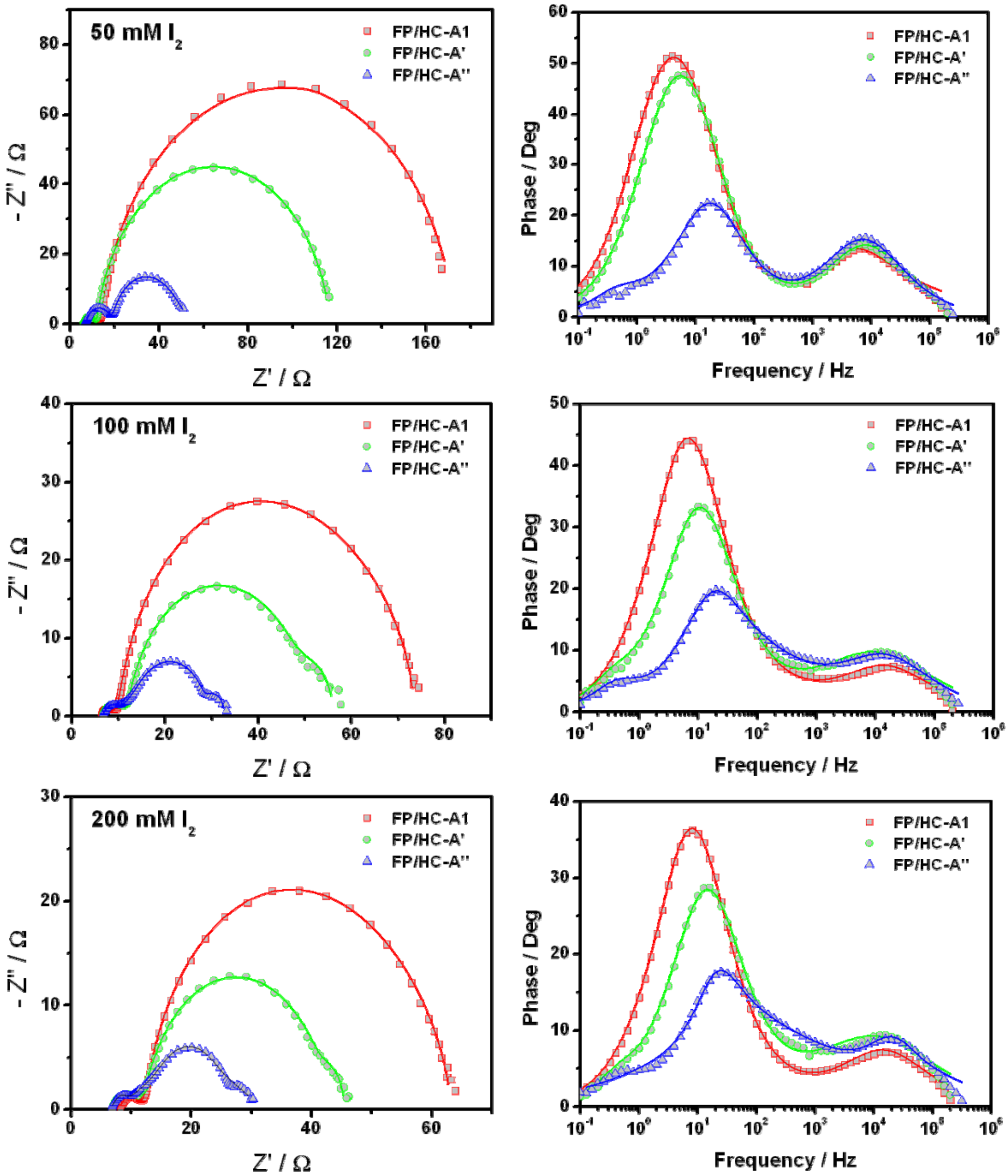

Fig S3. Nyquist and Bode phase plots for the DSSCs with the different coadsorbents as a function of I_2 concentration at a forward bias of −0.65 V under dark conditions. Solid lines are fitted lines.

Table S1 Major contributions to those transitions with the oscillator strength greater than 0.1 obtained from the DFT calculations: the absorption wavelength (λ), oscillation strength (f), the character of the transition, % contribution of a particular molecular transition. See labels in Fig S4 for nature of transition.

	λ(nm)	f	Character (%)
HC-A1	395.2	0.2762	HOMO->LUMO (99%)
	293.5	0.8703	H-1->L+1 (43%), HOMO->L+3 (45%)
	291.4	0.20	H-3->LUMO (96%)
	263.4	0.4245	H-3->L+1 (32%), H-1->L+3 (27%), HOMO->L+4 (-23%)
	260.0	0.5481	H-3->L+1 (36%), H-2->L+1 (25%), H-1->L+3 (-14%)
	259.4	0.5265	H-9->LUMO (-11%), H-3->L+1 (-24%), H-2->L+1 (37%)
	259.0	0.1324	H-9->LUMO (77%), H-2->L+1 (13%)
	229.6	0.125	H-7->LUMO (56%) H-10->LUMO (-7%), H-8->LUMO (-6%), H-8->L+2 (-2%), H-4->L+1 (8%), H-2->L+4 (-4%), H-2->L+5 (-3%), H-1->L+7 (-2%)
HC-A′	431.0	0.3023	HOMO->LUMO (99%)
	314.1	0.4433	H-3->LUMO (82%) HOMO->L+3 (-6%), HOMO->L+5 (8%)
	311.9	0.1120	H-1->L+1 (38%), HOMO->L+4 (56%)
	280.6	0.2683	H-10->LUMO (-19%), H-9->LUMO (-14%), H-8->LUMO (10%), H-4->LUMO (34%)
	273.5	0.311	H-1->L+4 (31%), HOMO->L+7 (-22%), HOMO->L+8 (17%)
	271.1	0.3293	H-10->LUMO (11%), H-9->LUMO (10%), H-4->LUMO (37%), HOMO->L+8 (20%)
	262.1	0.6187	H-2->L+1 (69%)
	260.1	0.1393	H-1->L+4 (-19%), HOMO->L+6 (13%), HOMO->L+8 (31%)
	255.3	0.1016	H-7->LUMO (58%), H-2->L+2 (-21%)
HC-A″	330.8	0.4433	HOMO->L+2 (98%)
	313.3	0.1589	H-1->L+1 (33%), HOMO->L+3 (41%), HOMO->L+4 (-23%)
	301.1	0.7497	H-1->L+1 (46%), H-1->L+2 (17%), HOMO->L+3 (-20%), HOMO->L+4 (10%)
	274.7	0.1104	H-1->L+3 (18%), H-1->L+4 (-10%), HOMO->L+7 (-12%), HOMO->L+8 (48%)
	266.0	0.1453	H-1->L+4 (70%)

	265.9	0.3865	H-3->L+1 (-11%), H-1->L+3 (39%), HOMO->L+6 (-15%), HOMO->L+8 (-19%)
	262.8	0.7282	H-2->L+1 (42%), H-2->L+2 (-39%)
	262.3	0.295	H-3->L+1 (75%)
	260.8	0.1316	H-2->L+1 (37%), H-2->L+2 (47%)
	235.1	0.1849	H-11->LUMO (13%), H-10->LUMO (-21%), H-7->LUMO (22%), H-3->L+3 (-11%), H-3->L+4 (-15%)