

Supplementary Information

Regulating the Electronic Structure of Covalent Organic Frameworks via Heterocyclic Isomers for Highly Efficient Photocatalytic H₂O₂ Generation

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Table of Contents

Section 1. Materials and Methods	3
Section 2. Supplementary Fig. 1-41	14
Section 3. Supplementary Tables 1-7	43
Section 4. Supplementary References	74

Section 1. Materials and Methods

1.1 Materials

1,2-Dimethoxyethane, thiophene-2-boronic acid pinacol ester, 4,4,5,5-tetramethyl-2-(3-thienyl)-1,3,2-dioxaborolane, 2-furanboronic acid, 3-furanboronic acid, and tetrakis(triphenylphosphine)palladium ($\text{Pd}(\text{PPh}_3)_4$) were purchased from Energy Chemical Co., Ltd. Cerium(IV) sulfate ($\text{Ce}(\text{SO}_4)_2$), 1,3,5-tris(4-aminophenyl)benzene (TAPB), 2,5-dibromoterephthalaldehyde, 5,5-dimethyl-1-pyrroline N-oxide (DMPO), melamine, and p-benzoquinone (p-BQ) were obtained from Shanghai Aladdin Biochemical Technology Co., Ltd. Tert-Butanol (TBA), nitro blue tetrazolium (NBT), and sodium carbonate (Na_2CO_3) were purchased from Shanghai Macklin Biochemical Co., Ltd. Hexane, 1,2-dichlorobenzene (o-DCB), n-butanol (n-BuOH), dimethylformamide (DMF), tetrahydrofuran (THF), and acetic acid (AcOH) were acquired from Lianlong (Tianjin) New Material Technology Co., Ltd. All chemicals were utilized in their purchased form without further purification.

1.2 Characterization

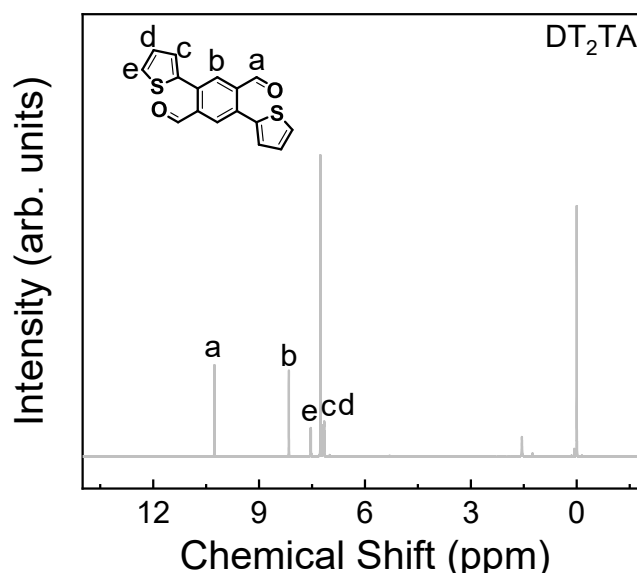
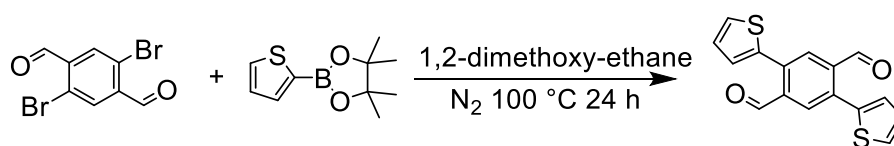
Powder X-ray diffraction (PXRD) measurements were conducted using an X-ray diffraction spectrometer (Ultima IV, Japan), with Cu K α radiation ($\lambda = 1.54 \text{ \AA}$) and operating at 40 kV and 40 mA. X-ray photoelectron spectroscopy (XPS) data were collected using an Axis Supra X-ray photoelectron spectrometer (Shimadzu Corporation, Japan). Fourier transform infrared (FT-IR) spectra were recorded using a Bruker Tensor 27 (TENSOR27, Germany) Fourier transformation infrared spectrometer using KBr pellets. Proton nuclear magnetic resonance (^1H NMR) spectra were acquired on a JNM-ECS 400M spectrometer, while solid-state ^{13}C nuclear magnetic resonance (^{13}C NMR) spectra were carried out on an AVANCE NEO 600 MHz WB FT-NMR spectrometer. Steady state photoluminescence (PL) spectra, time-resolved PL decay curve, and temperature-dependent PL spectra were measured using a Horiba Instruments FL-3

fluorescence spectrometer. Electron paramagnetic resonance (EPR) spectra were obtained on a Bruker ER200DSRC10/12 spectrometer. Transmission electron microscopy (TEM) images were acquired using a Tecnai F30 (FEI Company, USA), and field emission scanning electron microscopy (FESEM) was conducted on a S-4800 (Japan). Optical absorption spectra were recorded using an ultraviolet-visible diffuse reflection spectroscopy (UV-Vis DRS, UV-3600, Shimadzu Corporation, Japan).

1.3 Methods

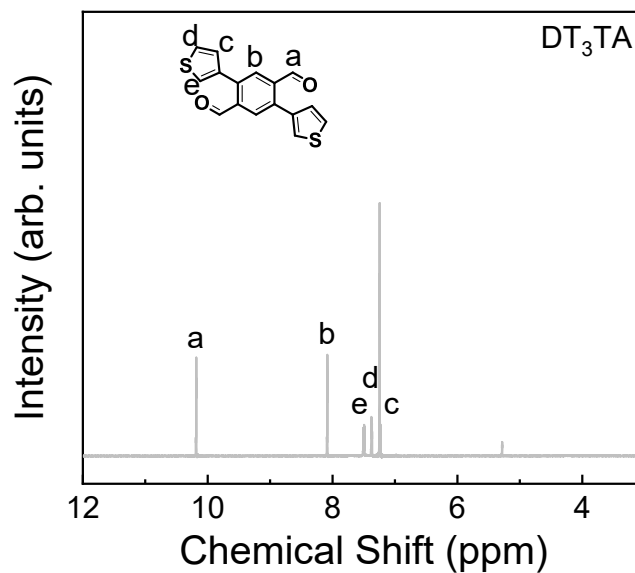
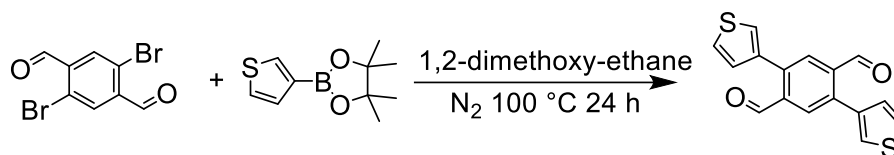
1.3.1 Synthesis of 2,5-di(thiophen-2-yl)terephthalaldehyde

The reaction scheme for the synthesis of 2,5-di(thiophen-2-yl)terephthalaldehyde and its corresponding ^1H NMR spectrum are shown below.



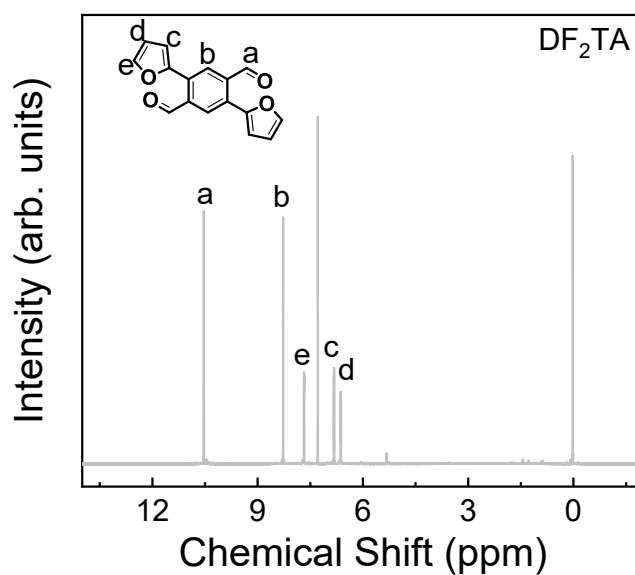
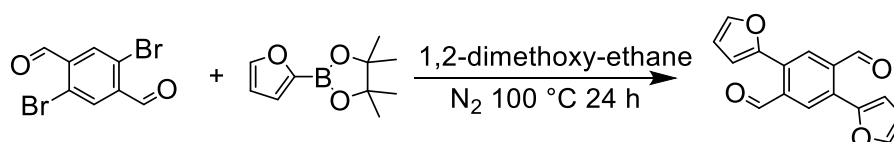
1.3.2 Synthesis of 2,5-di(thiophen-3-yl)terephthalaldehyde

The reaction scheme for the synthesis of 2,5-di(thiophen-3-yl)terephthalaldehyde and its corresponding ^1H NMR spectrum are shown below.



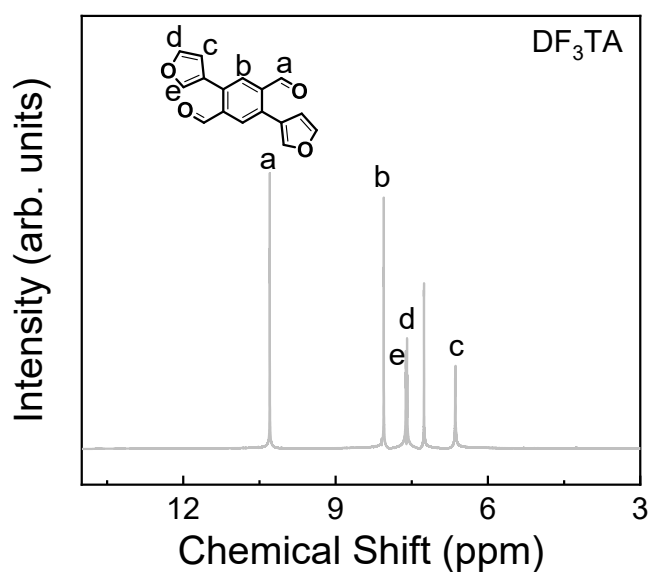
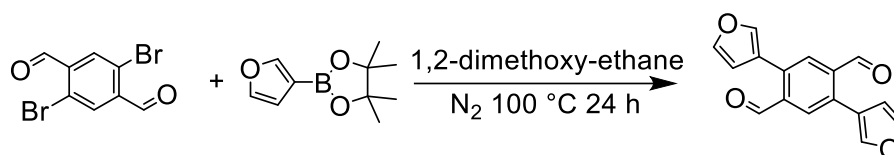
1.3.3 Synthesis of 2,5-di(furan-2-yl)terephthalaldehyde

The reaction scheme for the synthesis of 2,5-di(furan-2-yl)terephthalaldehyde and its corresponding ¹H NMR spectrum are shown below.



1.3.4 Synthesis of 2,5-di(furan-3-yl)terephthalaldehyde

The reaction scheme for the synthesis of 2,5-di(furan-3-yl)terephthalaldehyde and its corresponding ^1H NMR spectrum are shown below.



1.3.5 Synthesis of g-C₃N₄

The g-C₃N₄ was synthesized using a thermo-polymerization method. In this procedure, 5 g of melamine were placed in a crucible and heated at a ramp rate of $10\text{ }^\circ\text{C min}^{-1}$ under air atmospheric conditions. The heating was maintained for 4 h, resulting in the formation of a yellow-colored g-C₃N₄ powder.

1.4 Photocatalytic performance measurement

1.4.1 Photocatalytic H₂O₂ production

Typically, 5 mg of catalyst, 22.5 mL of deionized water, and 2.5 mL of ethanol (EtOH) were added in a 50 mL reaction cell and dispersed using sonication. The suspension was then oxygenated for 20 minutes in the dark. Subsequently, the reaction was irradiated with a 300 W

Xenon lamp (CEL-HXF300-T3, Beijing Zhongjiao Jinyuan Technology Co., Ltd) fitted with a UV cutoff ($\lambda > 420$ nm), while oxygen was continuously bubbled into the cell. Samples were taken every 15 minutes, and 1 mL of liquid was withdrawn and filtered through a 0.22 μm filter to eliminate the photocatalysts before analyzing the H_2O_2 content.

1.4.2 Photocatalytic decomposition of H_2O_2 by COFs

The decomposition of H_2O_2 was conducted using the following procedure: 5 mg of catalyst was dispersed in 25 mL of 1 mmol L^{-1} of H_2O_2 . The mixture was sonicated for 15 minutes and subsequently purged with N_2 for 30 minutes. The suspension was then irradiated using a 300 W Xenon lamp (CEL-HXF300-T3, Beijing Zhongjiao Jinyuan Technology Co., Ltd) with a wavelength of $\lambda > 420$ nm. To assess the concentration of H_2O_2 , 1 mL samples were extracted from the suspension every 15 min and filtrated through a 0.22 μm filter to remove the photocatalyst.

1.4.3 Cycling stability measurement

5 mg of the DT_2TA -TAPB catalyst was dispersed in 25 mL of pure water and irradiated with a 300 W Xenon lamp (light intensity: 100 mW cm^{-2}) under an air atmosphere for 1 h. After the reaction, the catalyst was centrifuged, washed, and dried. The recovered sample was then weighed and reused for the subsequent photocatalytic reaction. This process was repeated five times, with each cycle lasting 1 h, using the recycled photocatalyst.

1.5 H_2O_2 detection method

The quantitative determination of H_2O_2 was performed by the $\text{Ce}(\text{SO}_4)_2$ method. In this method, H_2O_2 reacts with the yellow Ce^{4+} ions to form colorless Ce^{3+} , as illustrated in chemical equation (1). The concentration of Ce^{4+} before and after the reaction can be quantified using UV-vis spectrophotometer, specially by measuring the absorption peak at 316 nm. The concentration of H_2O_2 can then be calculated using chemical equation (2). The 1 mmol L^{-1} solution of

Ce(SO₄)₂ was prepared by dissolving 16.6 mg of Ce(SO₄)₂ in 50 mL of 0.5 mol L⁻¹ sulfuric acid. The concentration of Ce(SO₄)₂ was subsequently measured using UV-vis spectrophotometer, and a linear relationship between Ce⁴⁺ concentration and absorption intensity was established. Utilizing the standard curve, the concentration of H₂O₂ was determined.



$$c(\text{H}_2\text{O}_2) = \frac{1}{2} \Delta c(\text{Ce}^{4+}) \quad (2)$$

1.6 Apparent quantum yield measurement

The apparent quantum yield (AQY) was determined by exposing the samples to a 300 W Xenon lamp, utilizing various band-pass filters (380 nm, 450 nm, 520 nm, 650 nm) for a duration of 1 h. The AQY was subsequently calculated according to the following chemical equation (3).

$$\text{AQY}(\%) = \frac{N_{\text{H}_2\text{O}_2} \times N_A \times h \times c}{A \times P \times T \times \lambda} \times 100 \quad (3)$$

Where $N_{\text{H}_2\text{O}_2}$ is the yield of H₂O₂ (mol); N_A is the Avogadro constant ($6.026 \times 10^{23} \text{ mol}^{-1}$); h is the Planck constant ($6.626 \times 10^{-34} \text{ J s}$); c is the speed of light ($3 \times 10^8 \text{ m s}^{-1}$); A is the irradiation area (cm²); P is the intensity of irradiation light (W cm⁻²); T is the photoreaction time (s); λ is the wavelength of the monochromatic light (nm).

1.7 Electrochemical measurement

1.7.1 Electrochemical impedance spectroscopy (EIS) measurement

EIS measurements were performed using a Gamry electrochemical workstation (Interface 5000E, USA) equipped with a three-electrode cell system. The working electrode was prepared by dispersing 2 mg of catalyst in a mixed solution of 0.9 mL EtOH, 0.1 mL water, and 10 μL Nafion, followed by sonication to ensure uniform dispersion. The resulting suspension was drop-cast onto a fluorine-doped tin oxide (FTO) substrate and allowed to dry at ambient

conditions. A platinum wire served as the counter electrode, while an Ag/AgCl electrode functioned as the reference electrode. The electrolyte solution consisted of 0.5 mol·L⁻¹ Na₂SO₄ solution and 0.1 mol·L⁻¹ K₃[Fe(CN)₆]. EIS measurements were performed in the dark to evaluate the charge transfer resistance (R_{ct}) of the samples. The reference electrode was set to 0 V, and the frequency range was from 100000 Hz to 0.01 Hz.

1.7.2 Tauc plot analysis

The optical band gap energy of the photocatalyst was determined using the Tauc plot method based on the solid-state UV-vis spectrum. The band gap was calculated using the Tauc equation (4):

$$(\alpha h\nu)^{1/n} = A(h\nu - E_g) \quad (4)$$

where α is the absorption coefficient, $h\nu$ is the photon energy, E_g is the band gap energy, and A is a proportionality constant.

The band gap was estimated by plotting $(\alpha h\nu)^{1/n}$ against $h\nu$ and extrapolating the linear portion of the curve which intersected the horizontal axis.

1.7.3 Mott-Schottky measurement

Mott-Schottky measurements were performed using a Gamry electrochemical workstation (Interface 5000E, USA) in a three-electrode cell system. The working electrode was prepared by dispersing 2 mg of catalyst in a solution of 0.9 mL ethanol, 0.1 mL water, and 10 μ L Nafion, followed by sonication to ensure uniform dispersion. The suspension was drop-cast onto an FTO substrate and dried at room temperature. A platinum wire and an Ag/AgCl electrode were used as the counter and reference electrodes, respectively, with 0.5 mol·L⁻¹ Na₂SO₄ solution as the electrolyte. Measurements were carried out at three different frequencies (1000 Hz, 2000 Hz, and 3000 Hz) over a potential range of -1 V to 1 V.

1.7.4 Photocurrent measurement

The experiments were conducted using a CHI660 electrochemical workstation (Shanghai Chenhua Instruments) equipped with a three-electrode system. The working electrode was prepared by dispersing 2 mg of the catalyst in a mixed solution of 0.9 mL ethanol, 0.1 mL deionized water, and 10 μ L of Nafion, followed by sonication to achieve a homogeneous suspension. The resulting suspension was drop-cast onto a fluorine-doped tin oxide (FTO) substrate and naturally dried at room temperature. A platinum wire served as the counter electrode, and an Ag/AgCl electrode was used as the reference electrode, and a 0.5 mol·L⁻¹ Na₂SO₄ aqueous solution as the electrolyte. A 300W Xenon lamp (CEL-HXF300-T3, Beijing Zhongjiao Jinyuan Technology Co., Ltd) with a wavelength of $\lambda > 420$ nm, was used as the light source to illuminate the working electrode. Photocurrent responses were recorded during four continuous "on/off" cycles, each lasting 50-second. During the measurements, the initial voltage was set at 0 V, with a sampling interval of 0.1 second and a sensitivity of 1×10^{-5} A V⁻¹.

1.8 In situ DRIFT measurement

In situ diffuse reflectance infrared fourier transform (in situ DRIFT) spectroscopy was conducted on a React IR15 instruments (METTLER TOLEDO, USA). The catalyst was dispersed in a solution with a volume ratio of water to EtOH ($V_{\text{water}} : V_{\text{EtOH}}=9:1$) and placed in a custom-designed quartz flask. Oxygen was then introduced into the suspension for 30 minutes. Following this, the suspension was irradiated with a 300 W Xenon lamp ($\lambda > 420$ nm) (CEL-HXF300-T3, Beijing Zhongjiao Jinyuan Technology Co. LTD) to initiate H₂O₂ photosynthesis, and the resulting spectrogram was recorded.

1.9 Rotating disk electrode measurement

The number of electrons transferred during oxygen reduction reaction was evaluated using a CHI 760E electrochemical workstation equipped with a three electrodes setup. The working electrode was prepared by dispersing 2.0 mg of catalyst in 1 mL of EtOH and 10 μ L of Nafion

solution, followed by ultrasonic treatment for 30 minutes to obtain a homogeneous suspension. A 6 μL aliquot of this suspension was then drop-coated onto a polished rotating disk electrode (RDE) and dried under an infrared lamp to form a uniform catalyst layer. A platinum wire and an Ag/AgCl electrode served as the counter and reference electrodes, respectively. Linear sweep voltammograms were recorded in an O_2 -saturated 0.1 mol L^{-1} phosphate buffer solution (PBS, pH = 7) at a scan rate of 10 mV s^{-1} and varying rotation speeds. The average number of electrons (n) transferred was calculated using the Koutecky-Levich equation (5-6).

$$\frac{1}{J} = \frac{1}{J_k} + \frac{1}{B\omega^{1/2}} = \frac{1}{J_k} + \frac{1}{J_L} \quad (5)$$

$$B = 0.62nFC_0D_0^{2/3}\nu^{1/6} \quad (6)$$

where J is the measured current density, J_k and J_L are the kinetic and diffusion-limiting current density respectively, ω is the angular velocity (rad s^{-1}), n is transferred electron number, F is Faraday constant (96485 C mol^{-1}), C_0 is the bulk concentration of O_2 ($1.26 \times 10^{-6} \text{ mol cm}^{-3}$), D_0 is the diffusion coefficient of O_2 in 0.1 mol L^{-1} phosphate buffer solution ($2.7 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$), and ν is kinetic viscosity of the electrolyte ($0.01 \text{ cm}^2 \text{ s}^{-1}$), respectively.

1.10 Rotating ring-disk electrode (RRDE) measurement

The oxygen reduction reaction (ORR) activity was evaluated using a rotating ring-disk electrode (RRDE) as the working electrode, which was prepared following the ring-disk electrode (RDE) methodology. The measurements were conducted in a 0.1 M phosphate buffer solution (pH = 7) at a scan rate of 10 mV s^{-1} and a rotation speed of 1600 rpm. To ensure sufficient dissolved O_2 , the electrolyte solution was purged with oxygen for 1 h prior measurements. The potential of the ring electrode was set to 0.6 V (vs. Ag/AgCl reference electrode) to detect the generated H_2O_2 . The selectivity of H_2O_2 was calculated using equation (7):

$$\text{H}_2\text{O}_2 \text{ (%) } = 200 \times \frac{I_r/N}{I_d + I_r/N} \quad (7)$$

Where I_r is the ring current, I_d is the disk current, and N is the collection efficiency (0.37).

1.11 Isotope labelling experiment

1.11.1 $^{18}\text{O}_2$ isotope labelling experiment

Photocatalyst DT₂TA-TAPB (5 mg) and pure water (H_2^{16}O , 1 mL) were added to a sealed photoreactor with a total volume of 10 mL. To create an oxygen-free environment, the reaction system underwent three vacuum evacuation and nitrogen purging cycles, followed by a final vacuum evacuation. Then, 20 mL of $^{18}\text{O}_2$ was slowly injected into the reactor using a syringe. The reaction proceeded under continuous illumination from a 300 W Xenon lamp for 10 h. After completion, the reaction solution was transferred to a glass bottle preloaded with excess MnO_2 and purged with nitrogen, and the evolved gas was collected and analyzed by gas chromatography-mass spectrometry (GC-MS, GCMS-QP2020).

1.11.2 H_2^{18}O isotope labelling experiment

5 mg of DT₂TA-TAPB catalyst, 2 mg of AgNO_3 , and 1 mL of H_2^{18}O (97%) were added to a sealed 10 mL reactor and ultrasonicated to ensure uniform suspension. To establish an oxygen-free environment, the reaction system was subjected to three vacuum evacuation and nitrogen purging cycles. The reaction was irradiated for 10 h with a 300 W Xenon lamp. Afterward, gas-phase products from the headspace were collected and analyzed by GC-MS. The reaction solution was transferred to a glass bottle containing excess MnO_2 and nitrogen, and the released gases were analyzed using GC-MS.

1.12 Density functional theory calculation

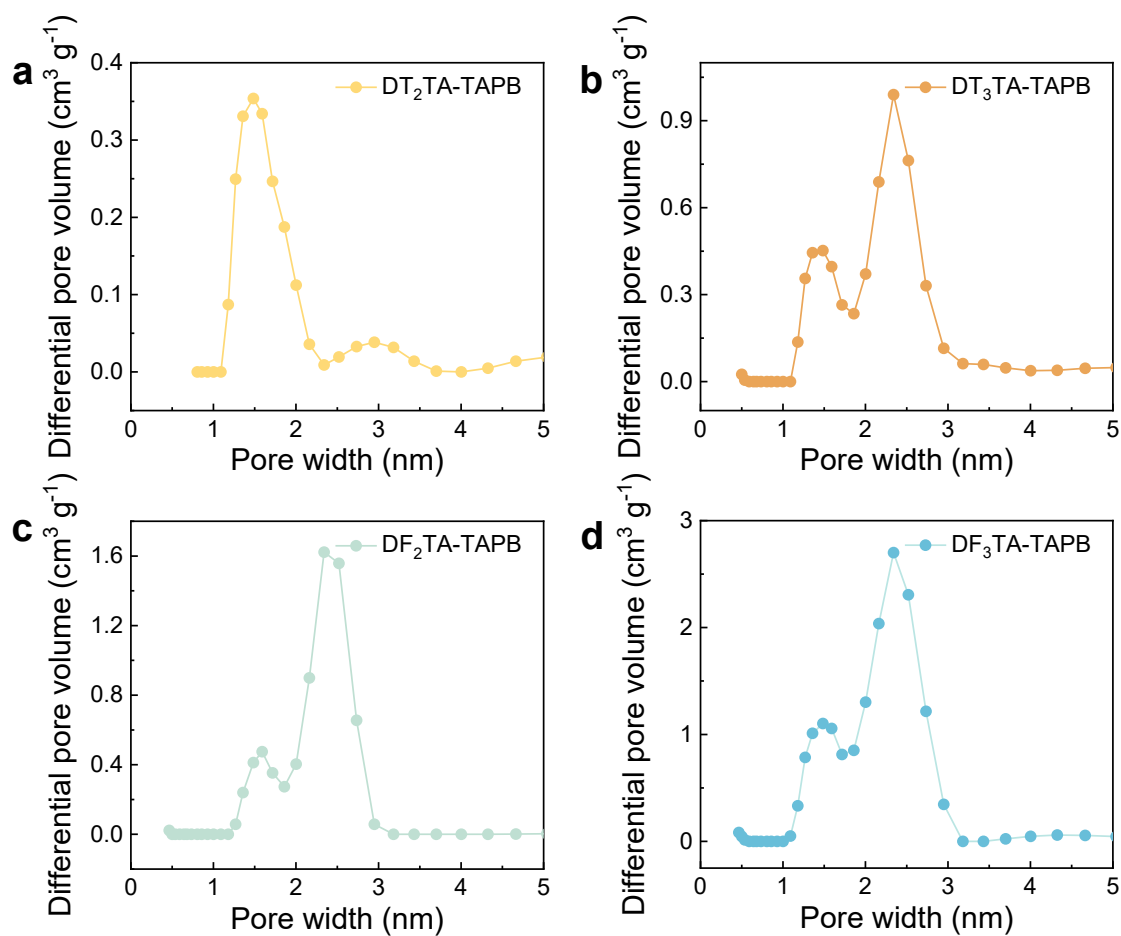
Density functional theory (DFT) calculations were performed using the CP2K/Quickstep

package. Cell parameters were optimized via a hybrid Gaussian and plane-wave approach, employing the Orbital Transformation method for wavefunction optimization. The 1s electrons of H, 2s and 2p electrons of N, C, and O, 3s and 3p electrons of S were explicitly considered as valence electrons. Goedecker–Teter–Hutter (GTH) pseudopotentials and double- ζ valence polarized (DZVP–GTH) basis sets were applied to all elements, with a plane-wave cutoff energy of 400 Ry. The Perdew–Burke–Ernzerhof (PBE) functional was used to describe exchange correlation effects, and all calculations were corrected by Grimme D3 method. The convergence criterion for the maximum force was set to 0.02 eV Å⁻¹. For excited-state calculation, Time-dependent density functional theory (TDDFT) was utilized for static analyses. Hole and electron distribution, including spatial overlap integral (Sr index) calculations and electron-hole spatial separation in the S₁ state, were further analyzed using Multiwfn program^{1,2} and visualized with the VMD software³.

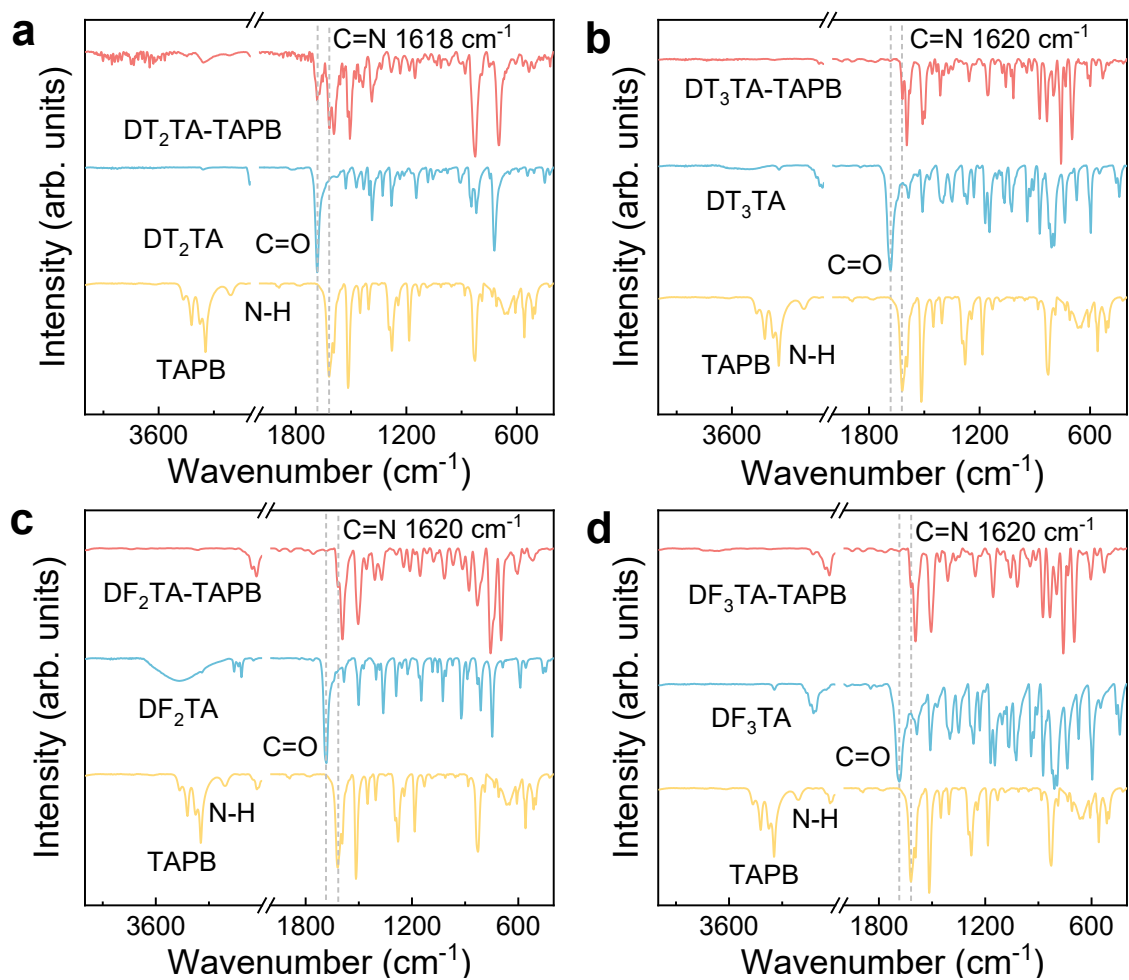
1.13 Single-crystal measurement

Single-crystal X-ray diffraction (SXRD) measurements were performed on a Rigaku XtaLAB Synergy-DW diffractometer equipped with a Cu K α radiation source ($\lambda = 1.5418$ Å). Data acquisition, processing, and reduction were carried out using the CrysAlisPro software suite. The structure was solved using the SHELXT program with intrinsic phasing in Olex2, and refined by least-squares minimisation using the SHELXL package. Detailed crystallographic data for the aldehyde monomers were provided in Supplementary Table 2 and 3.

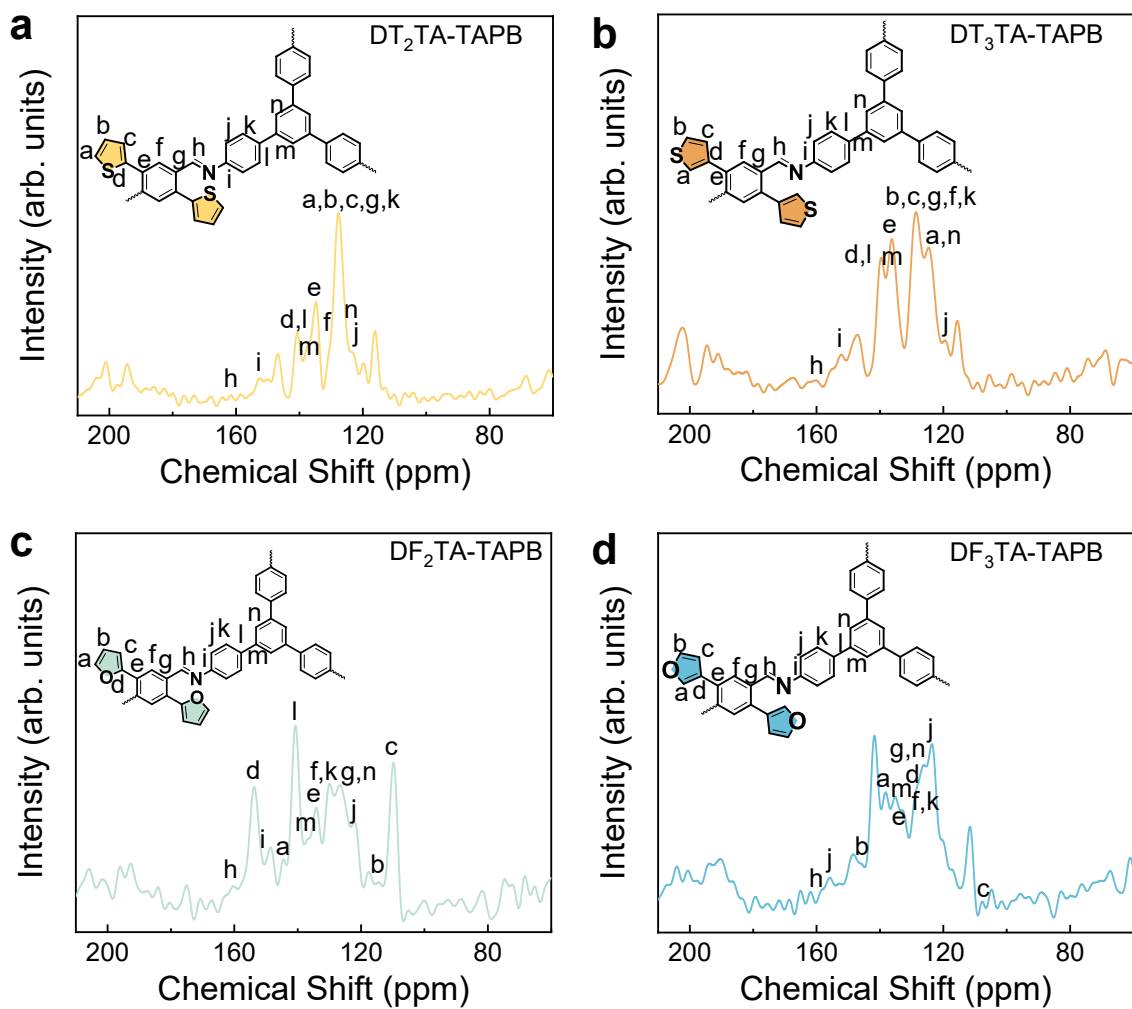
Section 2. Supplementary Fig. 1-41



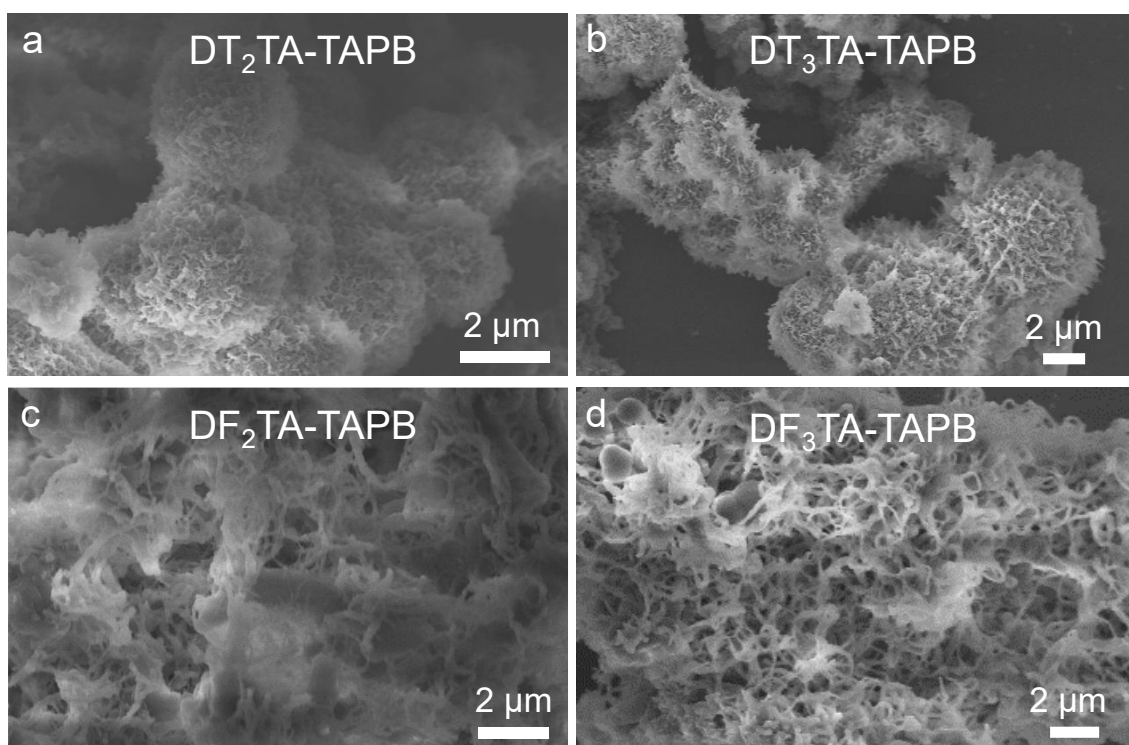
Supplementary Fig. 1. Pore size analysis. Pore size distribution curves of (a) DT₂TA-TAPB, (b) DT₃TA-TAPB, (c) DF₂TA-TAPB, and (d) DF₃TA-TAPB.



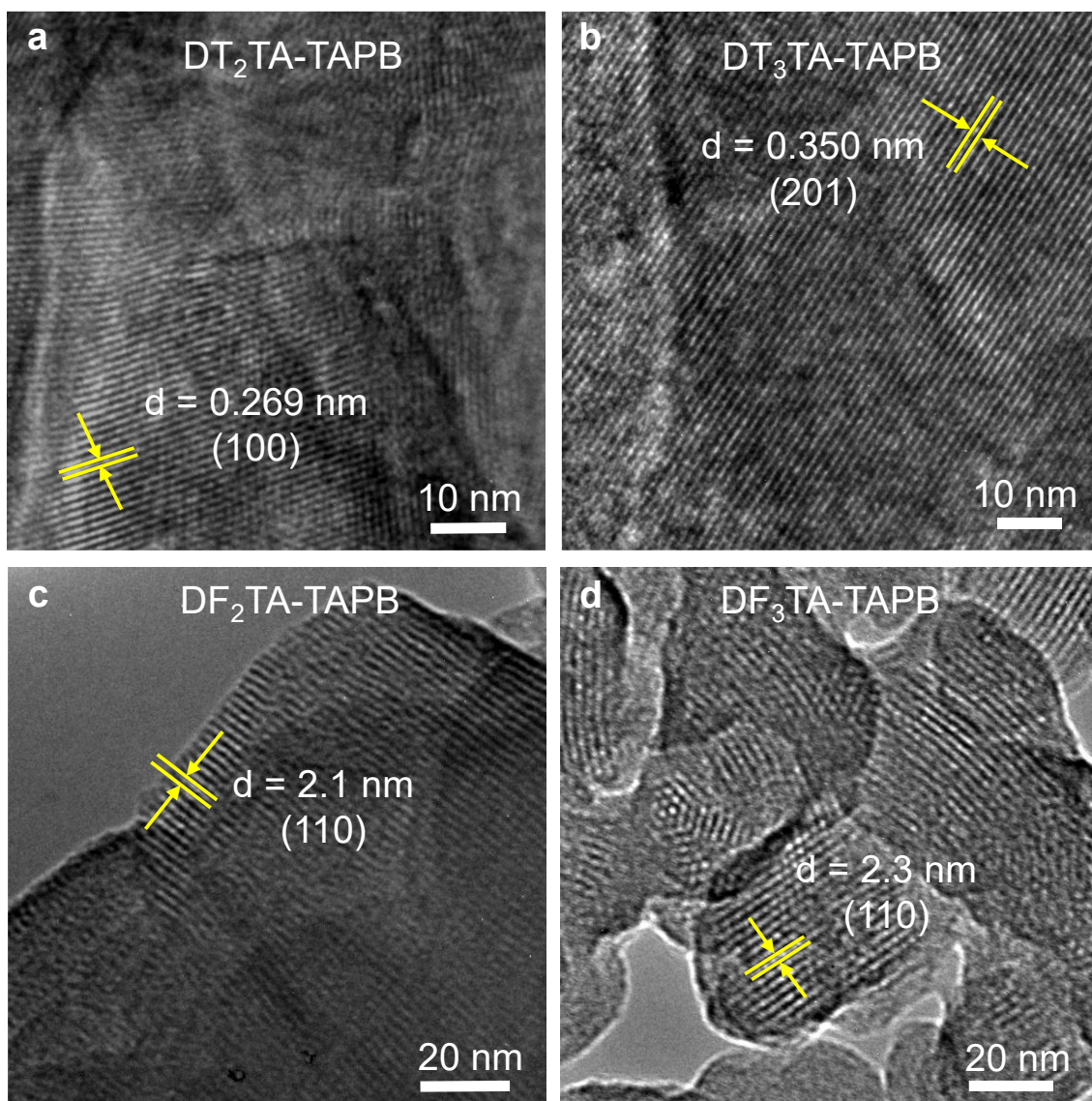
Supplementary Fig. 2. Structural characterization. (a-d) FT-IR spectra of DT₂TA-TAPB, DT₃TA-TAPB, DF₂TA-TAPB, and DF₃TA-TAPB, and corresponding organic building blocks.



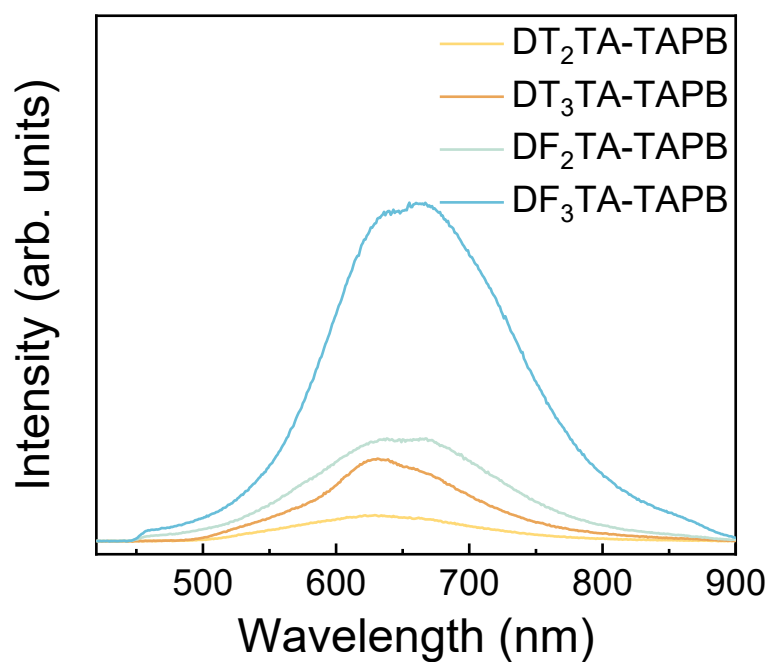
Supplementary Fig. 3. Structural characterization. ^{13}C NMR spectra of (a) $DT_2TA-TAPB$, (b) $DT_3TA-TAPB$, (c) $DF_2TA-TAPB$, and (d) $DF_3TA-TAPB$.



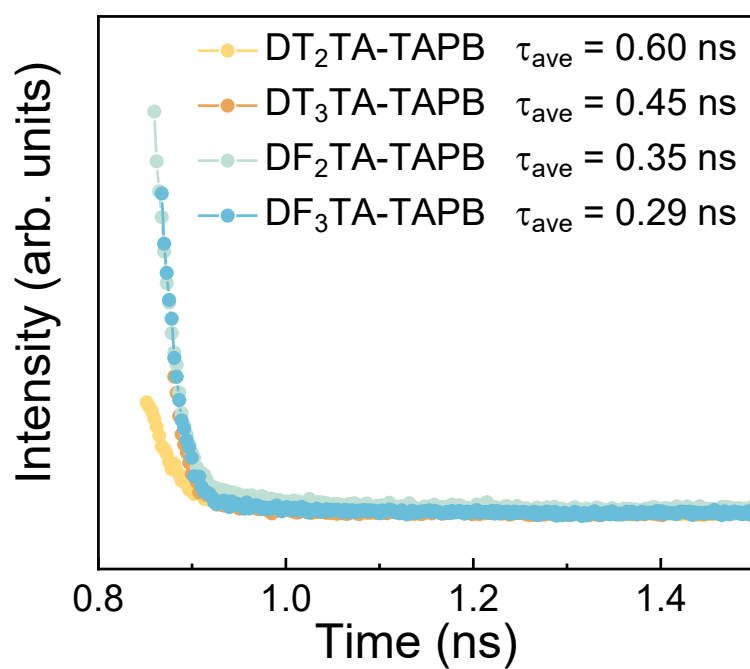
Supplementary Fig. 4. Morphological characterization of COFs. SEM image of (a) DT₂TA-TAPB, (b) DT₃TA-TAPB, (c) DF₂TA-TAPB, and (d) DF₃TA-TAPB.



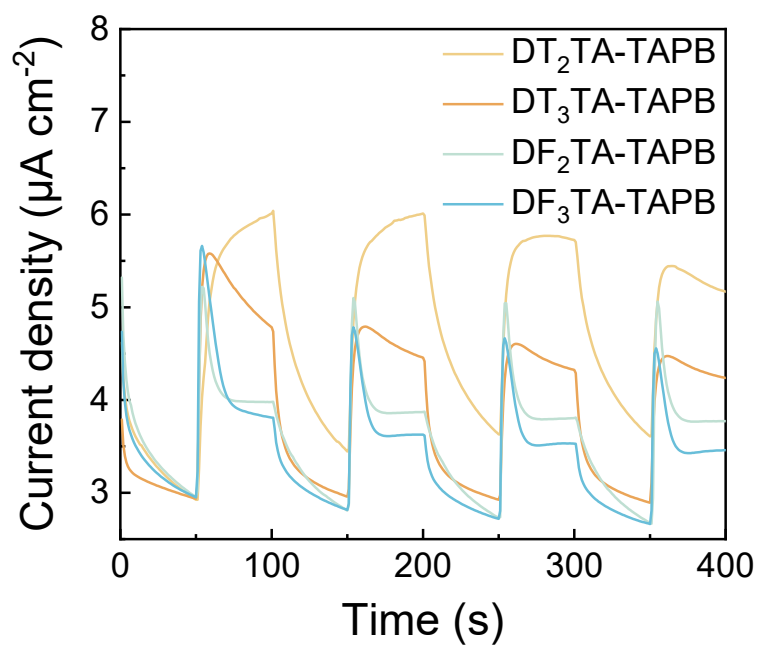
Supplementary Fig. 5. Structural characterization of the COFs. TEM image of (a) DT₂TA-TAPB, (b) DT₃TA-TAPB, (c) DF₂TA-TAPB, and (d) DF₃TA-TAPB.



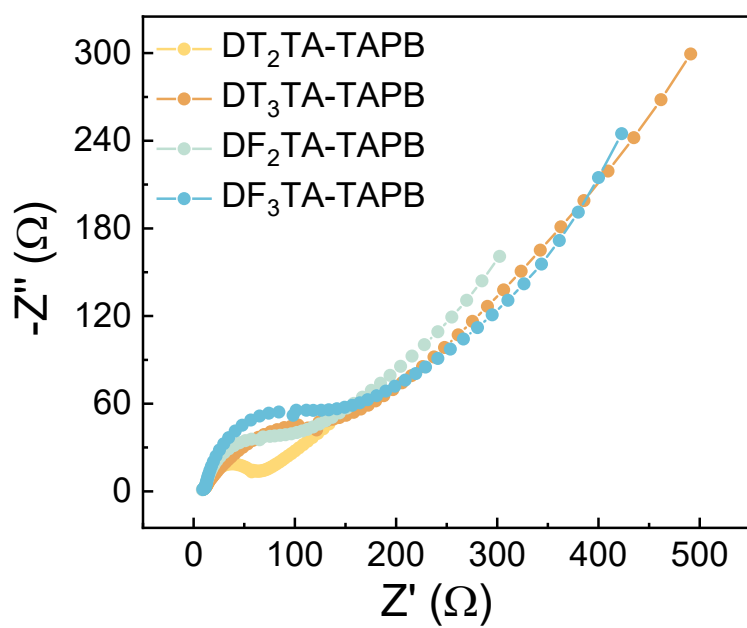
Supplementary Fig. 6. Optical emission properties of the COFs. Steady-state PL spectra of the COFs (excitation wavelength was 400 nm).



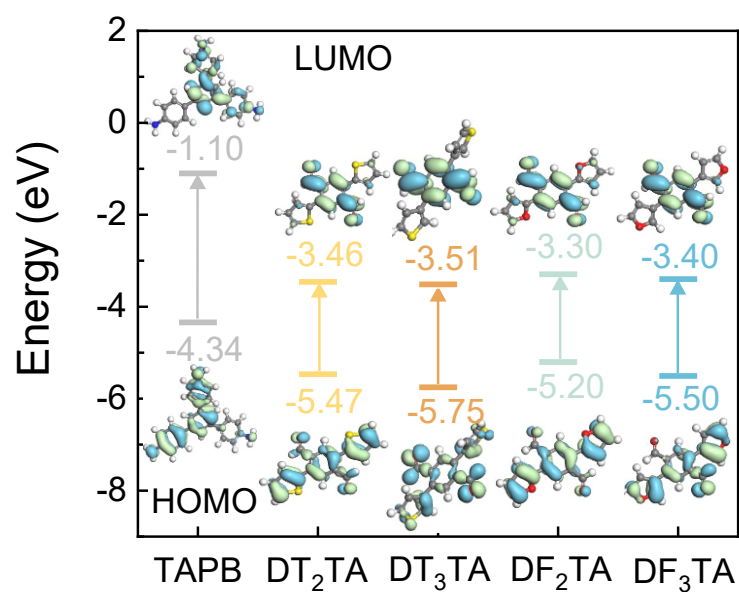
Supplementary Fig. 7. Investigation of excited-state lifetimes. TR-PL decay curves of the COFs.



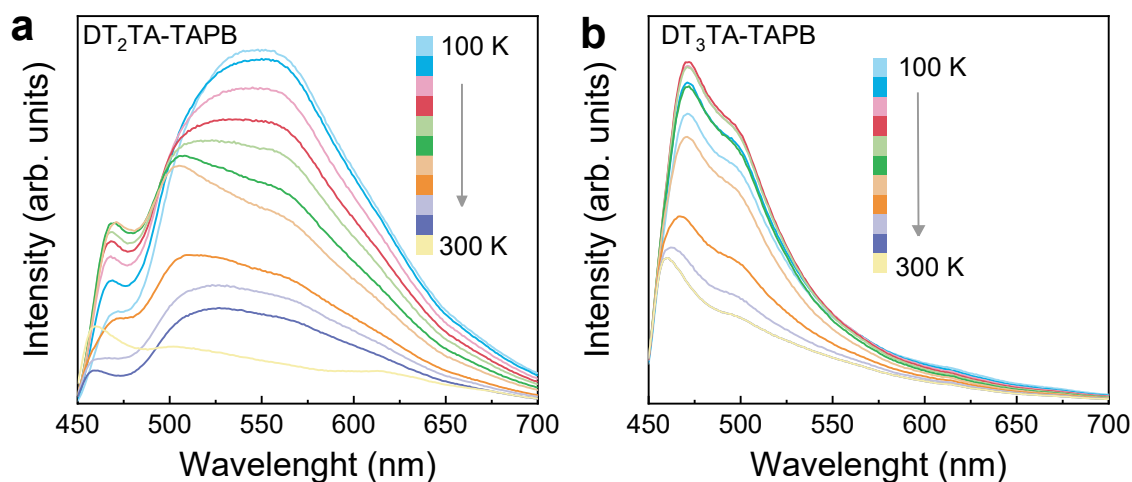
Supplementary Fig. 8. Evaluation of photoresponse behavior. Transient photocurrent responses of the COFs under illumination.



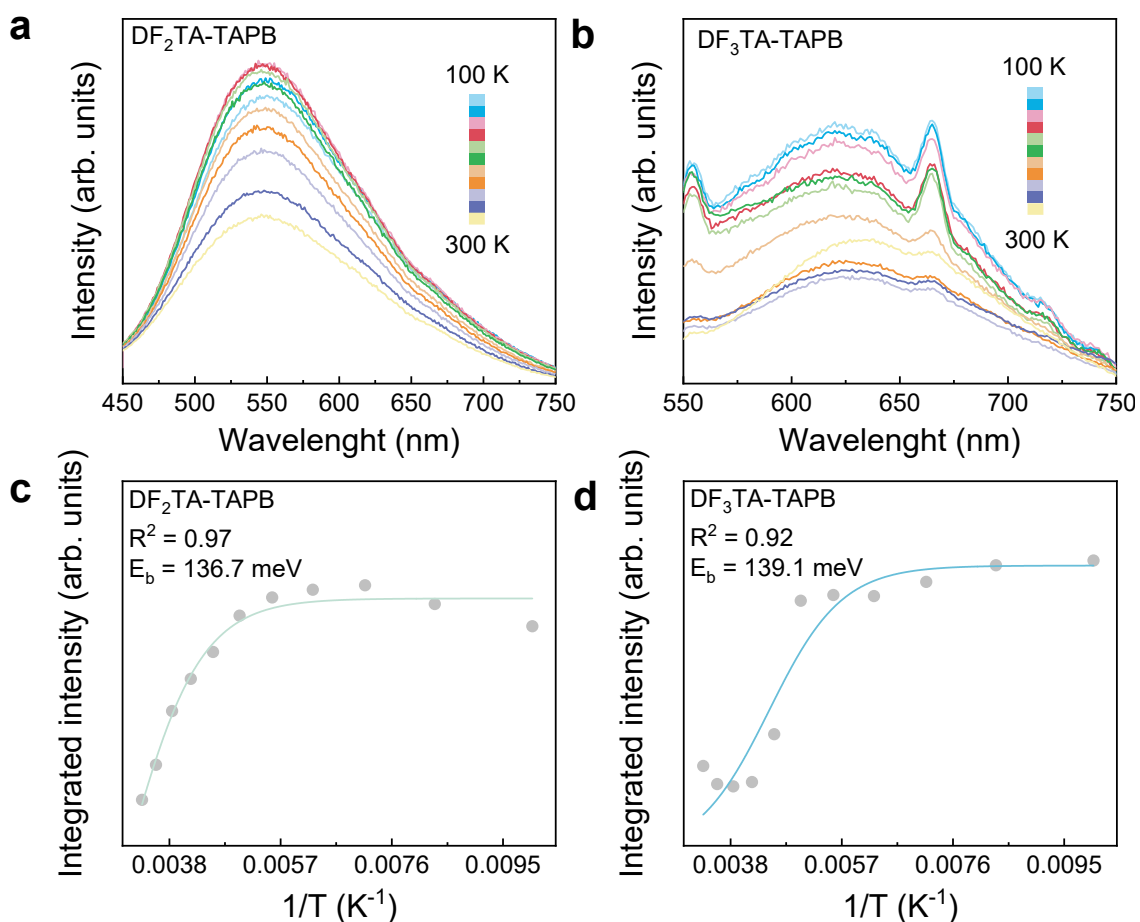
Supplementary Fig. 9. Charge transfer analysis. EIS spectra of the COFs.



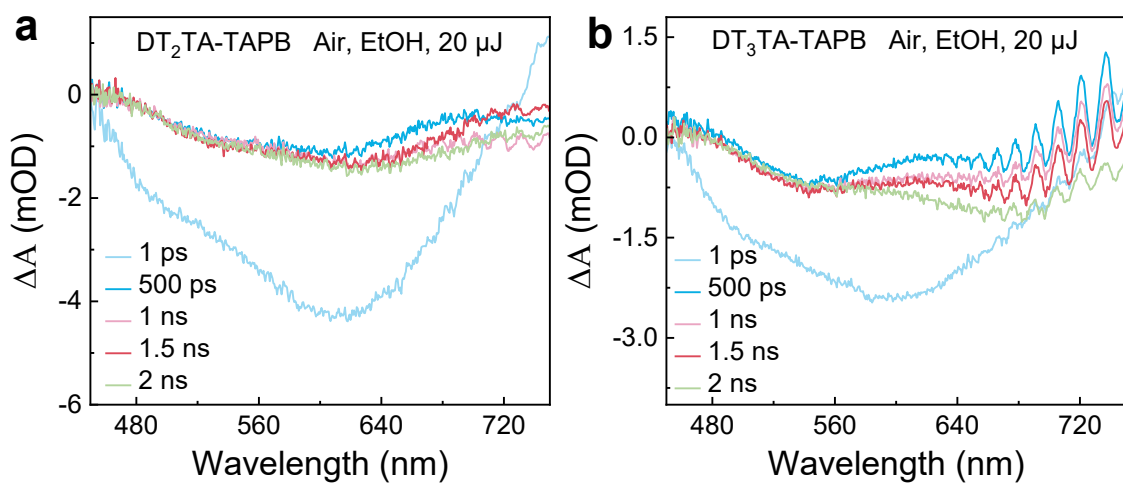
Supplementary Fig. 10. Electronic structure and charge distribution of the building blocks. HOMO and LUMO energy level diagrams of the building blocks and the corresponding charge density distributions.



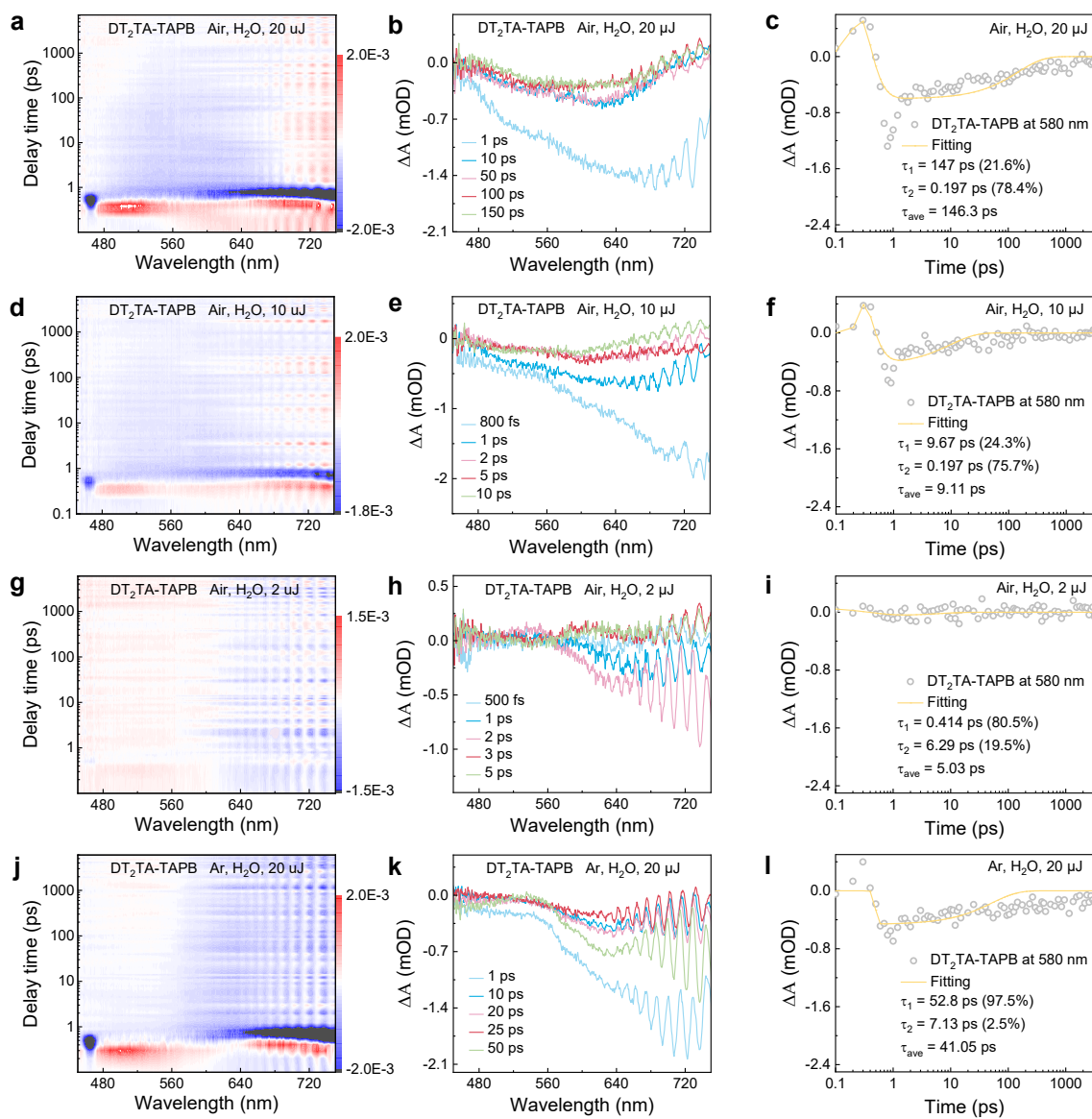
Supplementary Fig. 11. Temperature-dependent PL behavior of COFs. Temperature-dependent PL spectra under 400 nm excitation for (a) DT₂TA-TAPB and (b) DT₃TA-TAPB.



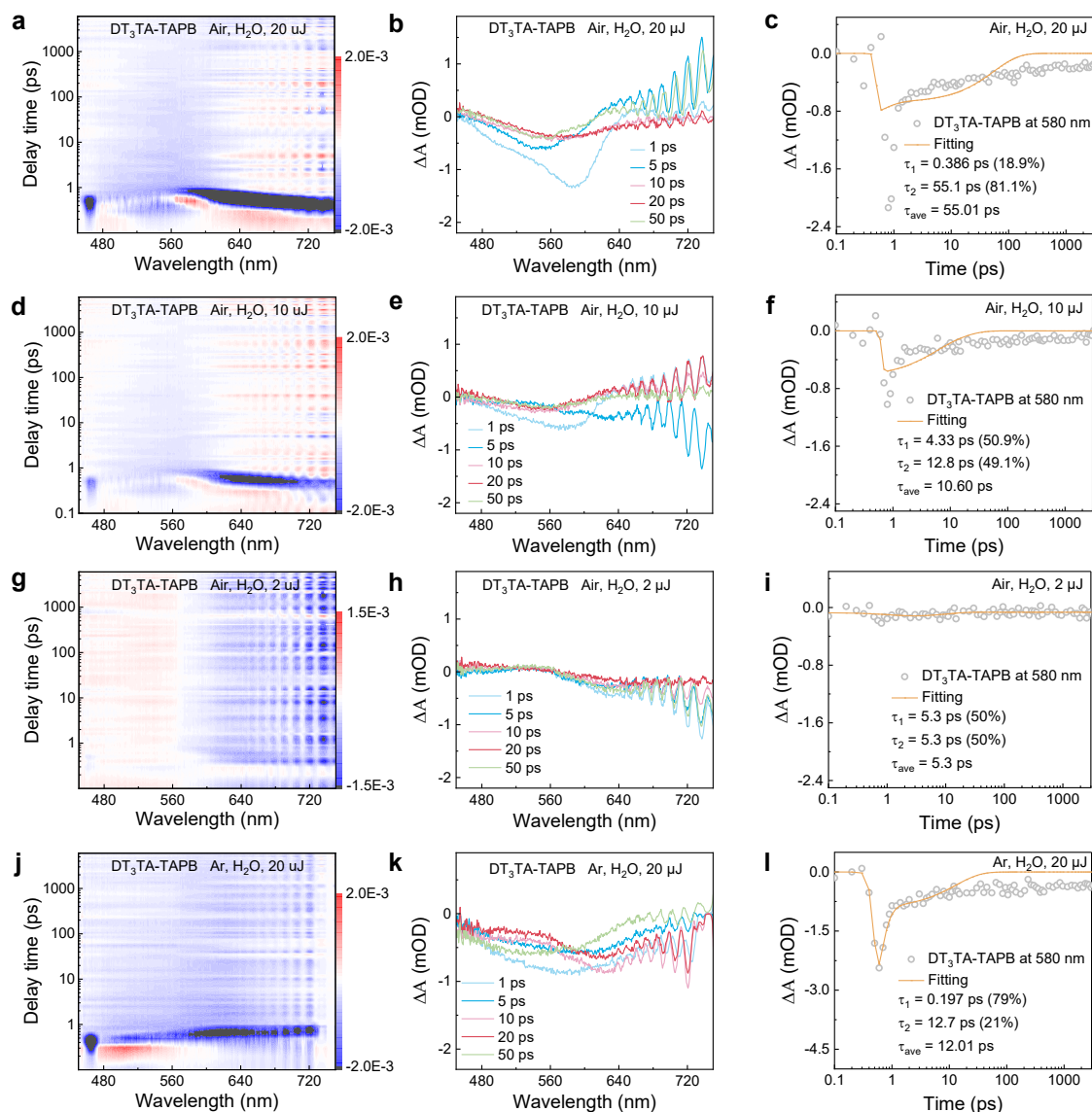
Supplementary Fig. 12. Investigation of exciton binding energy of DF₂TA-TAPB and DF₃TA-TAPB. Temperature-dependent PL spectra under 400 nm excitation for (a) DF₂TA-TAPB and (b) DF₃TA-TAPB. Arrhenius fitting curves for (c) DF₂TA-TAPB and (d) DF₃TA-TAPB.



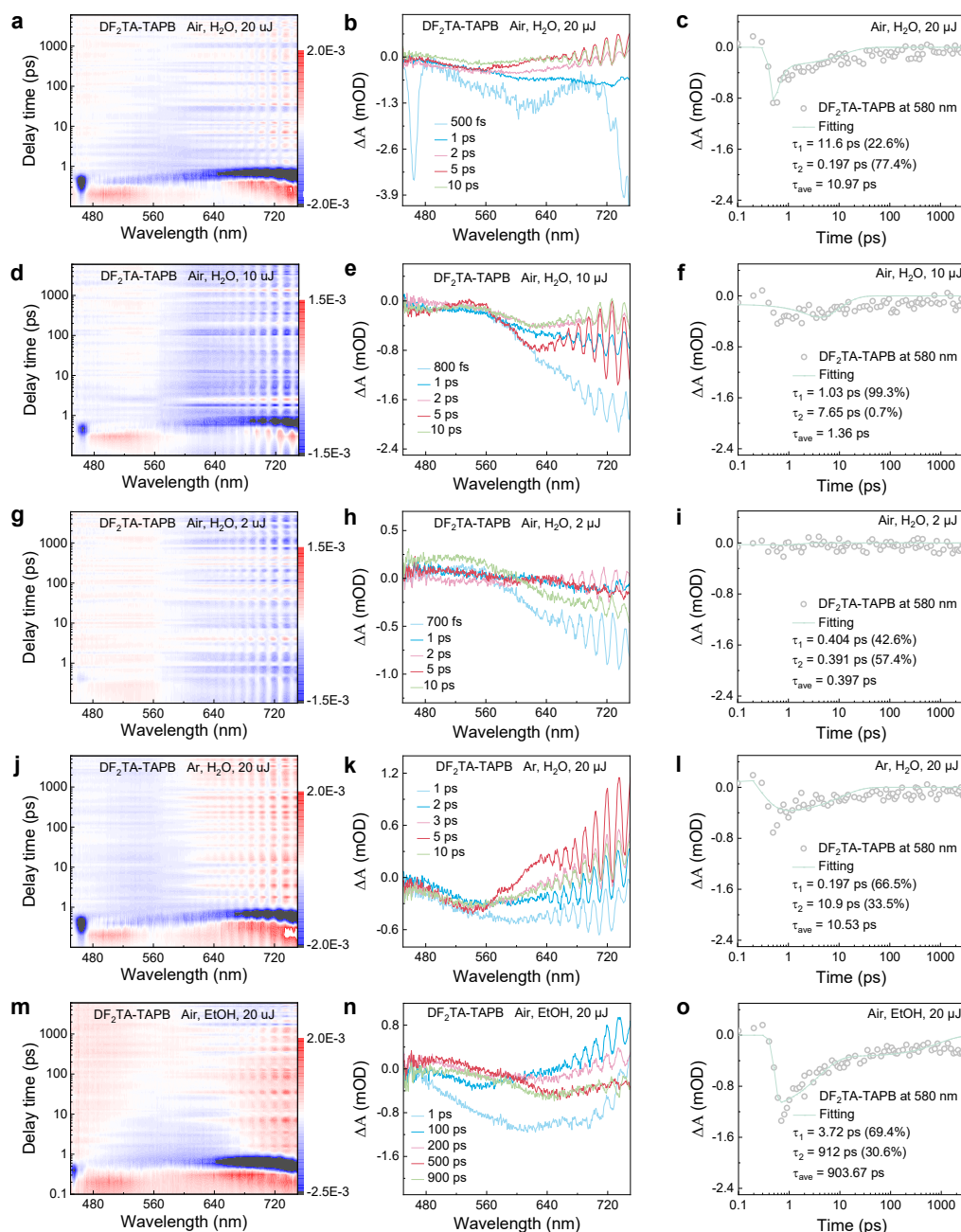
Supplementary Fig. 13. Transient absorption spectra. Transient absorption spectra of (a) DT₂TA-TAPB and (b) DT₃TA-TAPB at different delay times.



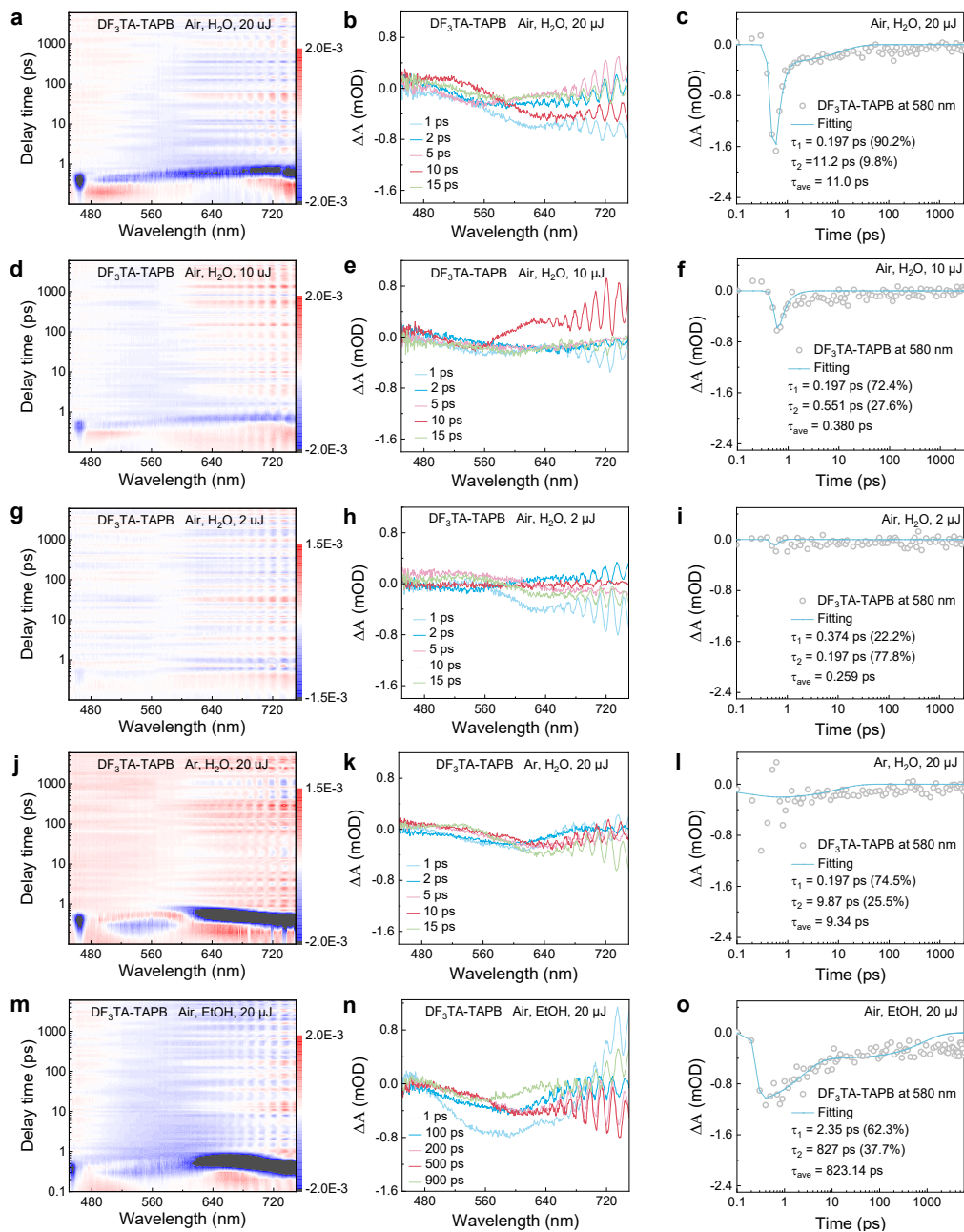
Supplementary Fig. 14. Femtosecond transient absorption spectra of DT₂TA-TAPB under various experimental conditions, including pseudo-color plots, fs-TA spectra, and decay curves. (a-c) Measurements conducted in air-saturated pure water with a pump pulse of 20 μ J. (d-f) Measurements conducted in air-saturated pure water with a pump pulse of 10 μ J. (g-i) Measurements conducted in air-saturated pure water with a pump pulse of 2 μ J. (j-l) Measurements conducted in Ar-saturated pure water with a pump pulse of 20 μ J.



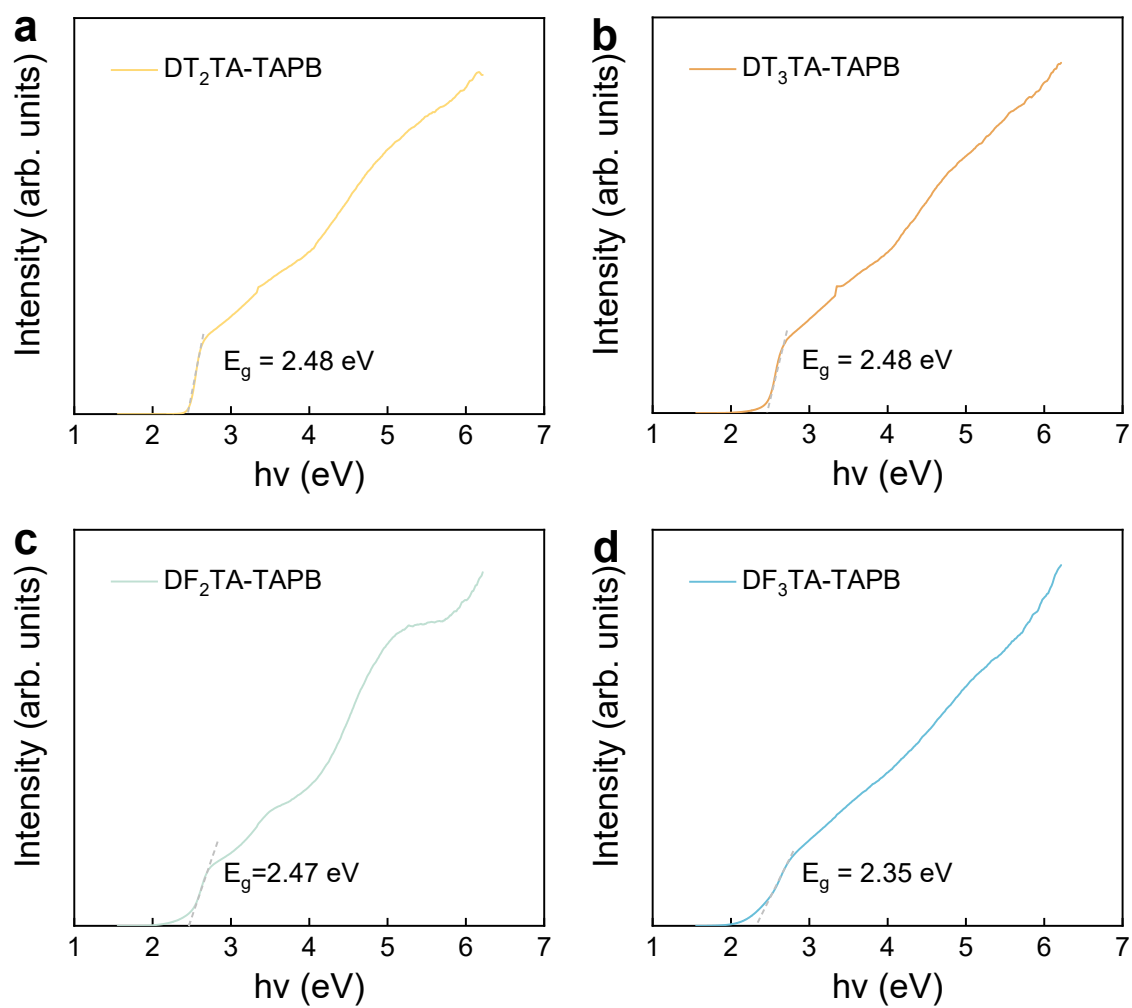
Supplementary Fig. 15. Femtosecond transient absorption spectra of DT₃TA-TAPB under various experimental conditions, including pseudo-color plots, fs-TA spectra, and decay curves. (a-c) Measurements conducted in air-saturated pure water with a pump pulse of 20 μ J. (d-f) Measurements conducted in air-saturated pure water with a pump pulse of 10 μ J. (g-i) Measurements conducted in air-saturated pure water with a pump pulse of 2 μ J. (j-l) Measurements conducted in Ar-saturated pure water with a pump pulse of 20 μ J.



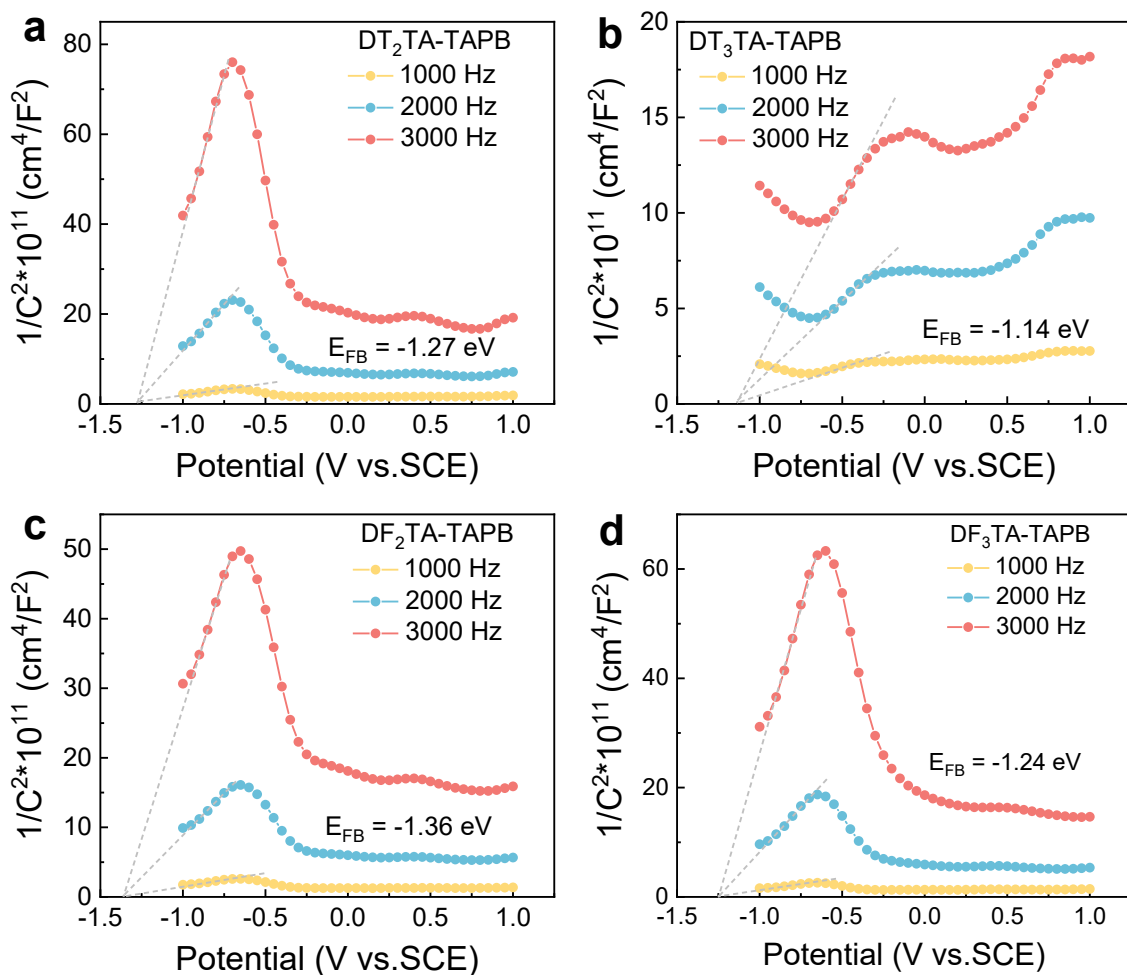
Supplementary Fig. 16. Femtosecond transient absorption spectra of DF₂TA-TAPB under various experimental conditions, including pseudo-color plots, fs-TA spectra, and decay curves. (a-c) Measurements conducted in air-saturated pure water with a pump pulse of 20 μJ. (d-f) Measurements conducted in air-saturated pure water with a pump pulse of 10 μJ. (g-i) Measurements conducted in air-saturated pure water with a pump pulse of 2 μJ. (j-l) Measurements conducted in Ar-saturated pure water with a pump pulse of 20 μJ. (m-o) Measurements conducted in air-saturated ethanol with a pump pulse of 20 μJ.



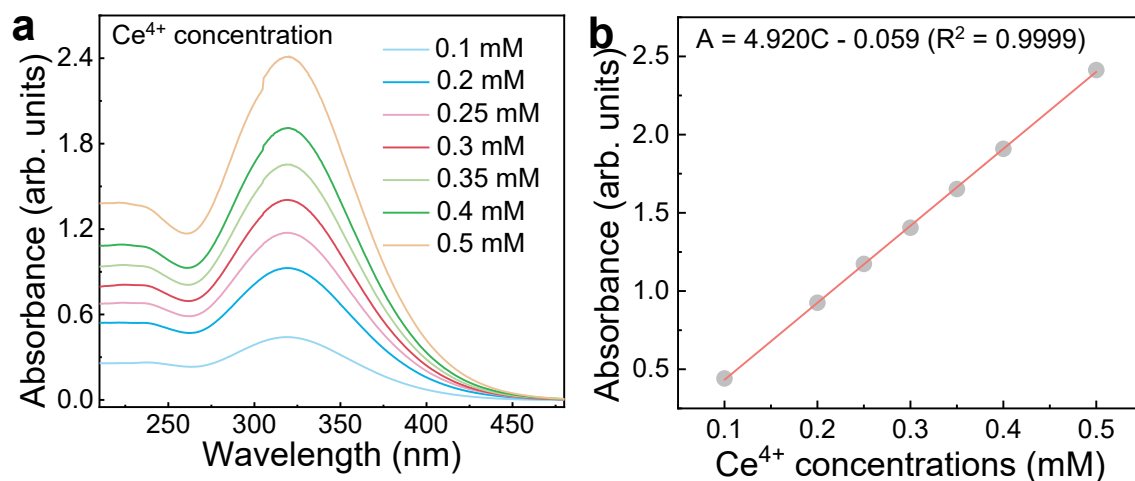
Supplementary Fig. 17. Femtosecond transient absorption spectra of DF₃TA-TAPB under various experimental conditions, including pseudo-color plots, fs-TA spectra, and decay curves. (a-c) Measurements conducted in air-saturated pure water with a pump pulse of 20 μ J. (d-f) Measurements conducted in air-saturated pure water with a pump pulse of 10 μ J. (g-i) Measurements conducted in air-saturated pure water with a pump pulse of 2 μ J. (j-l) Measurements conducted in Ar-saturated pure water with a pump pulse of 20 μ J. (m-o) Measurements conducted in air-saturated ethanol with a pump pulse of 20 μ J.



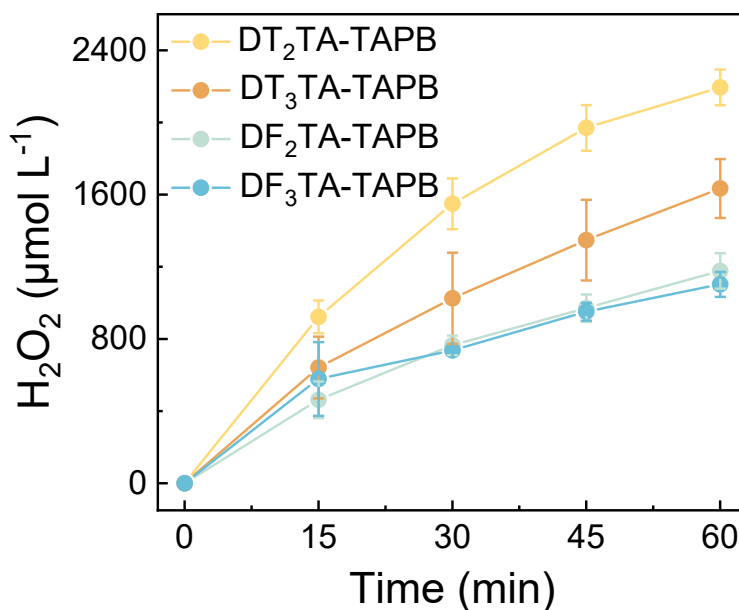
Supplementary Fig. 18. Determination of optical band gap. (a-d) Tauc plots of the COFs.



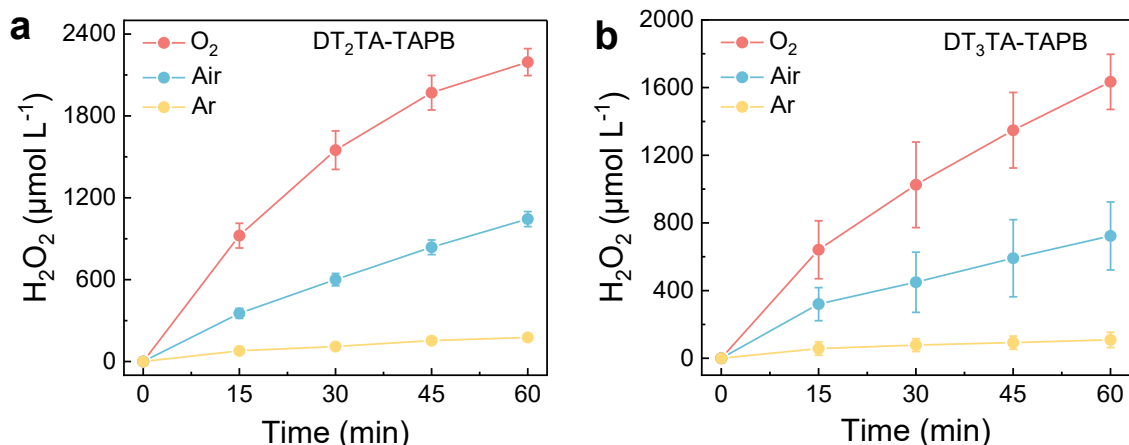
Supplementary Fig. 19. Determination of conduction band position. Mott-Schottky plots of (a) DT₂TA-TAPB, (b) DT₃TA-TAPB, (c) DF₂TA-TAPB, and (d) DF₃TA-TAPB.



Supplementary Fig. 20. Detection of H_2O_2 by cerium sulfate method. (a) UV-vis absorption spectra of Ce^{4+} solutions with different concentrations. (b) The linear relationship between Ce^{4+} concentration and absorption intensity.

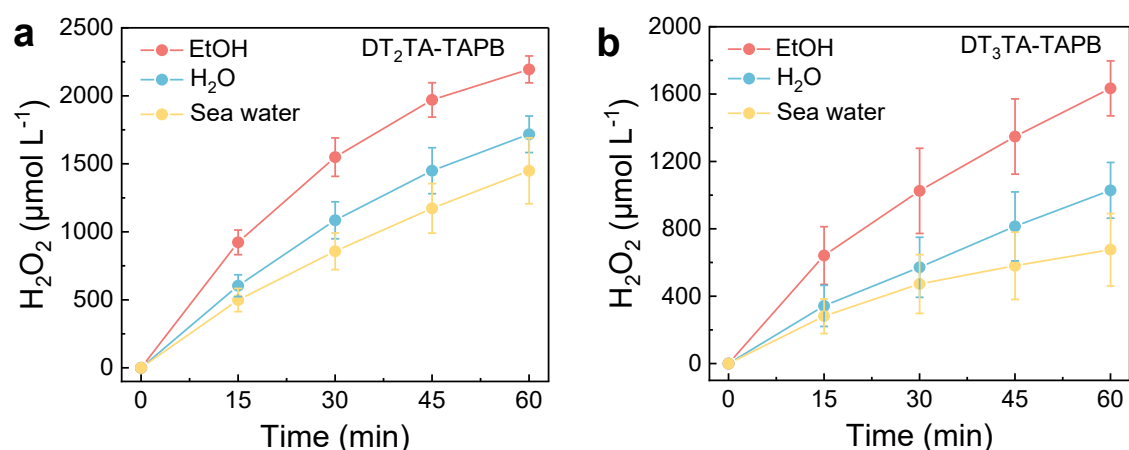


Supplementary Fig. 21. Evaluation of H_2O_2 generation by various COFs. Time-dependent H_2O_2 production curves for different photocatalysts under visible light irradiation. Reaction condition: 300 W Xenon lamp ($\lambda > 420$ nm), 10% EtOH solution. Error bars indicate the standard deviations of four replicate measurements.



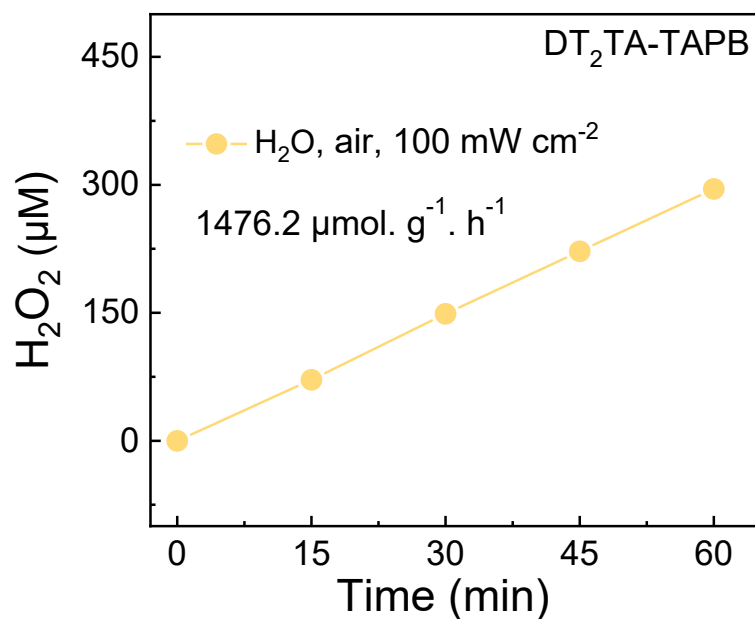
Supplementary Fig. 22. Evaluation of H₂O₂ generation under different atmospheres.

Time-dependent H₂O₂ production curves for (a) DT₂TA-TAPB and (b) DT₃TA-TAPB under various atmosphere. Error bars represent the standard deviations of four replicate measurements.



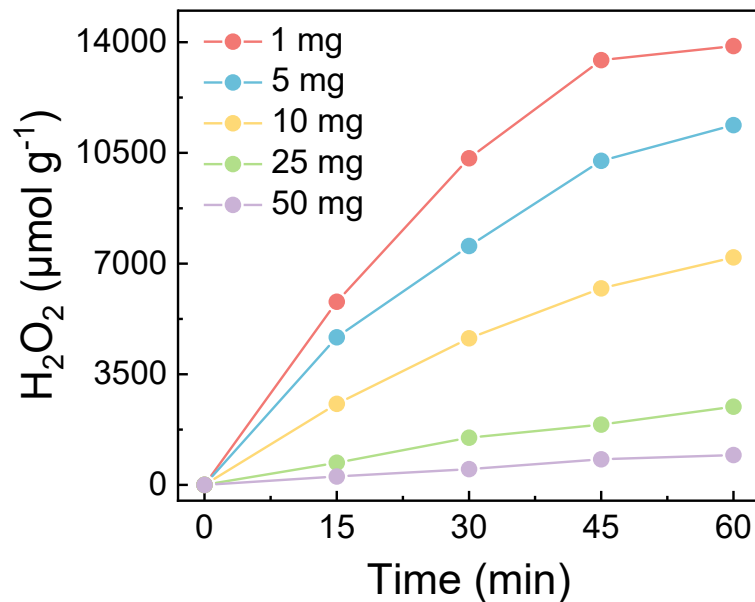
Supplementary Fig. 23. Evaluation of H₂O₂ generation under different reaction systems.

Time-dependent H₂O₂ production curves for (a) DT₂TA-TAPB and (b) DT₃TA-TAPB in 10% EtOH, pure water, and seawater. Error bars represent the standard deviations of four replicate measurements. Error bars indicate the standard deviations of four replicate measurements.

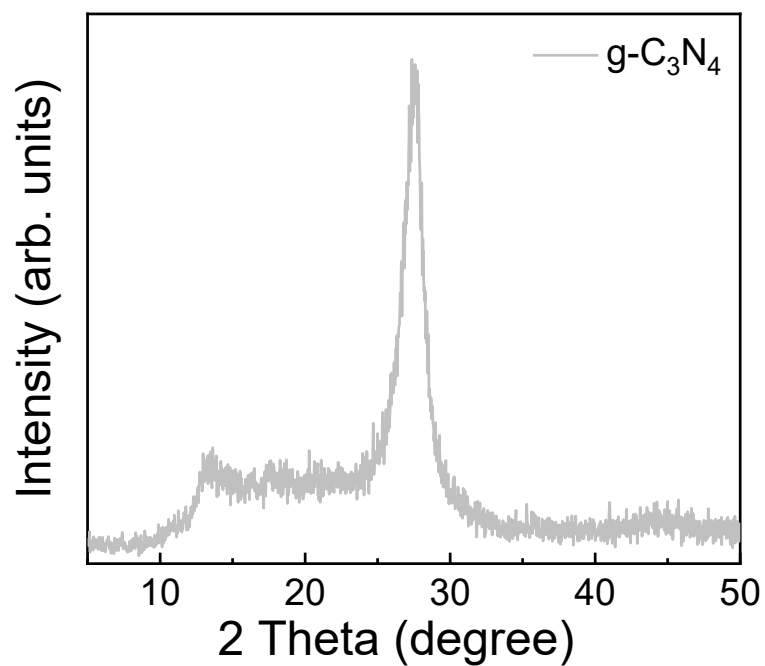


Supplementary Fig. 24. Measurement of H₂O₂ yield under simulated natural conditions.

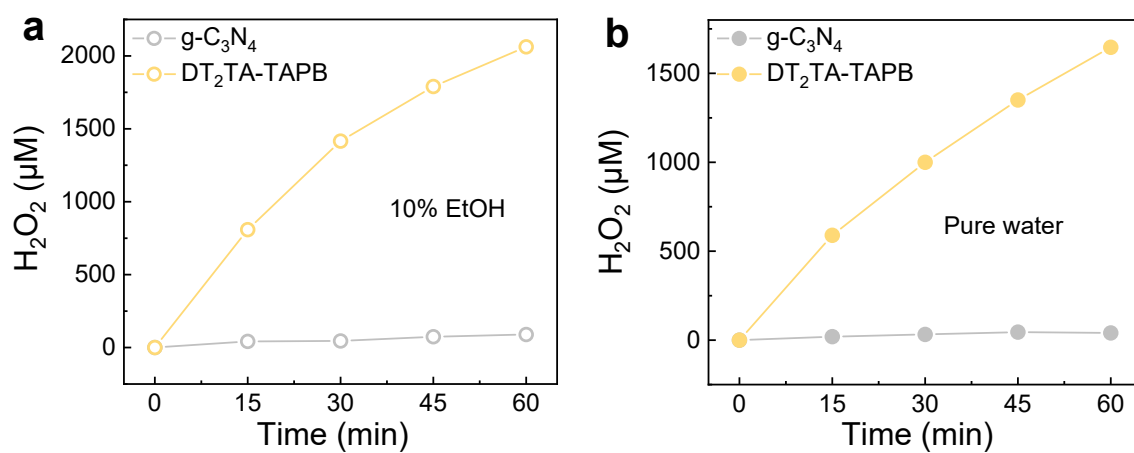
Photocatalytic H₂O₂ yield of DT₂TA-TAPB in pure water, air atmosphere, and light intensity 100 mW cm⁻².



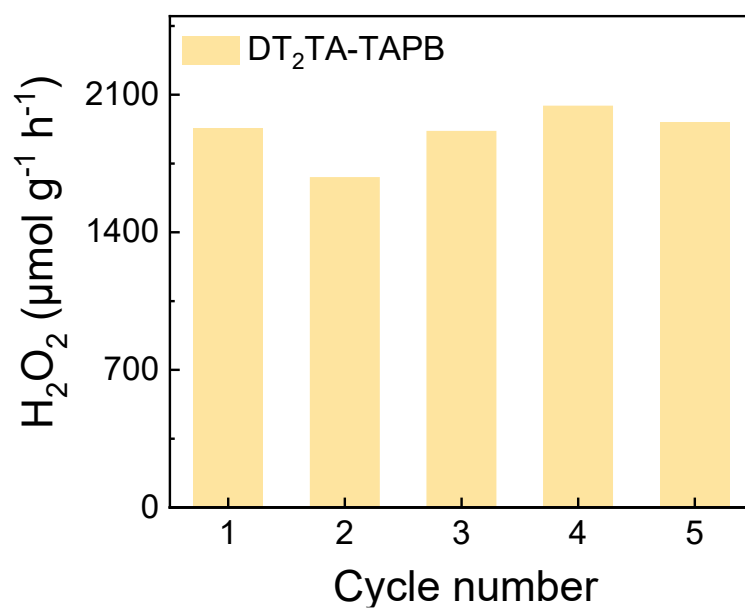
Supplementary Fig. 25. Effect of catalyst amount on H₂O₂ yield. Time-dependent photocatalytic H₂O₂ generation curves of DT₂TA-TAPB with different catalyst dosages (water: EtOH = 9:1; O₂ atmosphere; λ > 420 nm).



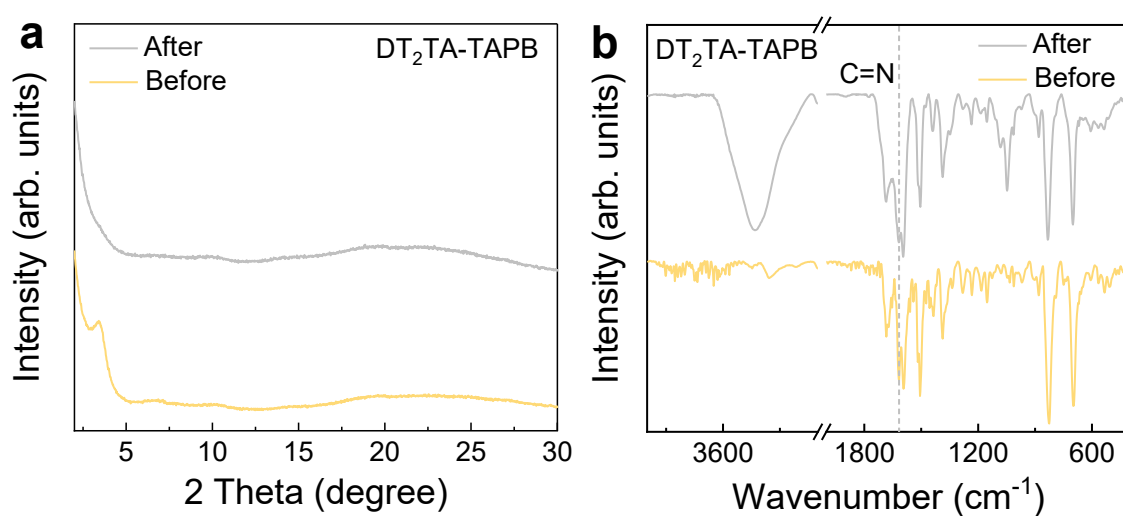
Supplementary Fig. 26. Structure of g-C₃N₄. PXRD pattern of g-C₃N₄.



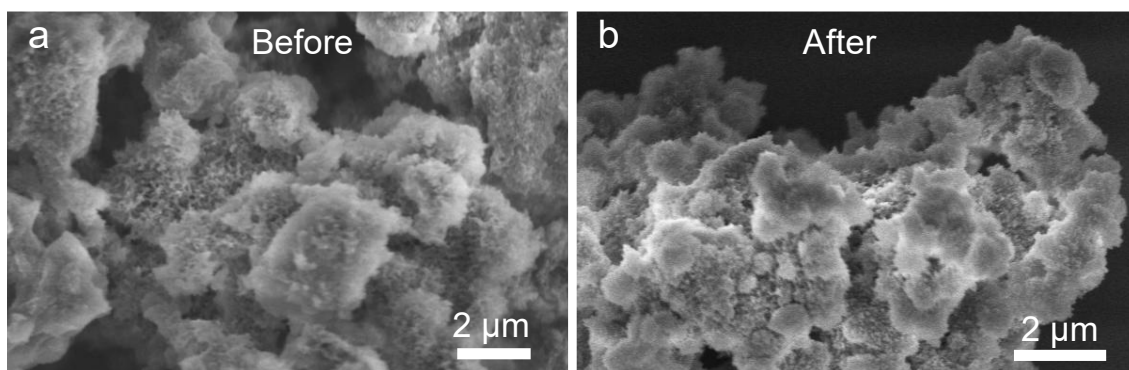
Supplementary Fig. 27. Comparison of H₂O₂ production performance between DT₂TA-TAPB and g-C₃N₄. (a-b) Performance comparison of DT₂TA-TAPB and g-C₃N₄ photocatalytic H₂O₂ production in 10% EtOH and pure water, respectively.



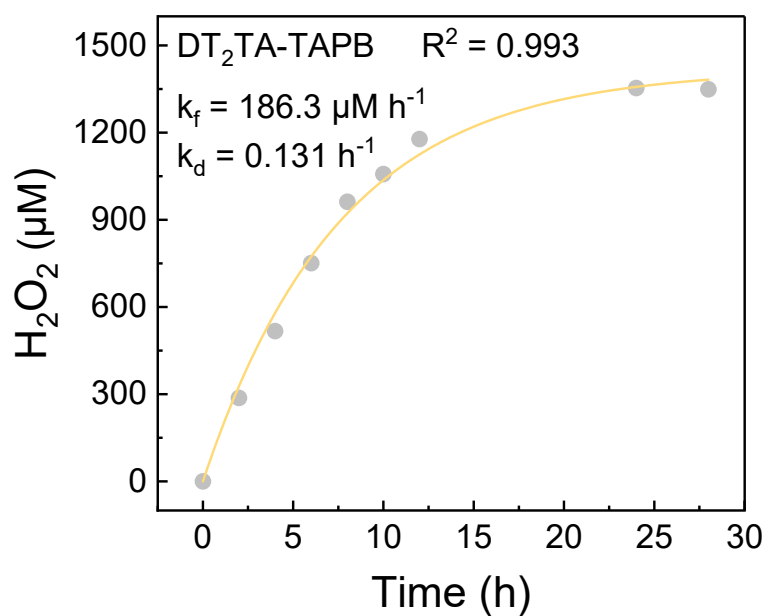
Supplementary Fig. 28. Cycling stability test. Cyclic stability experiment of DT₂TA-TAPB photocatalytic H₂O₂ production. Reaction conditions: air atmosphere, pure water, 300 W Xenon lamp (light intensity: 100 mW cm⁻²).



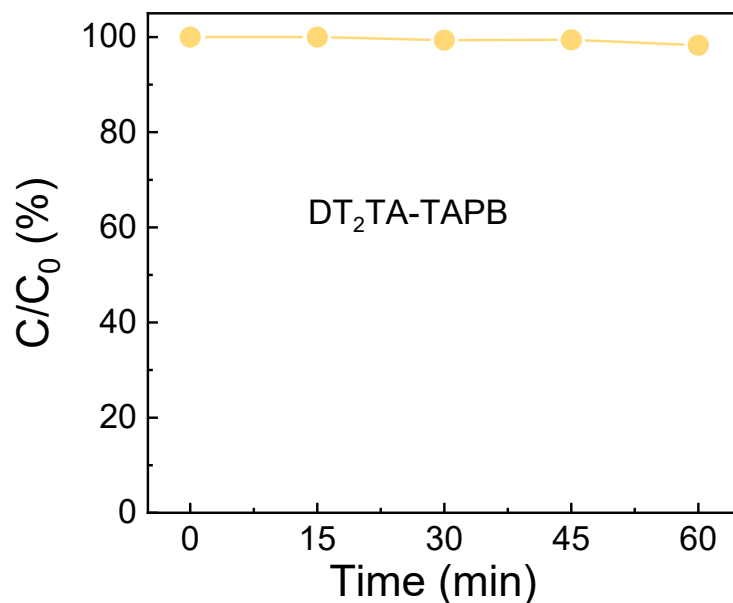
Supplementary Fig. 29. Structural changes before and after reaction. (a) PXRD patterns and (b) FT-IR spectra of DT₂TA-TAPB before and after the photocatalytic reaction.



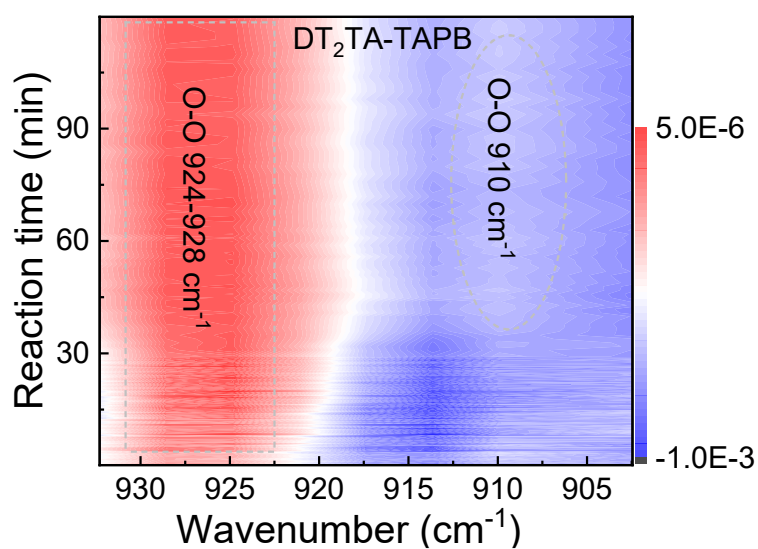
Supplementary Fig. 30. Morphological changes before and after reaction. (a-b) SEM images of DT₂TA-TAPB before and after the photocatalytic reaction.



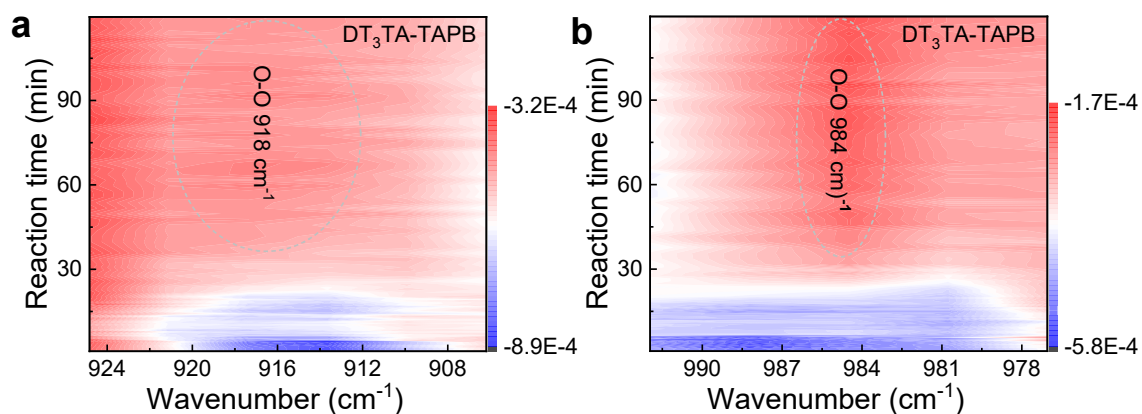
Supplementary Fig. 31. Kinetic analysis of H₂O₂ formation and decomposition. H₂O₂ formation and decomposition rate constant.



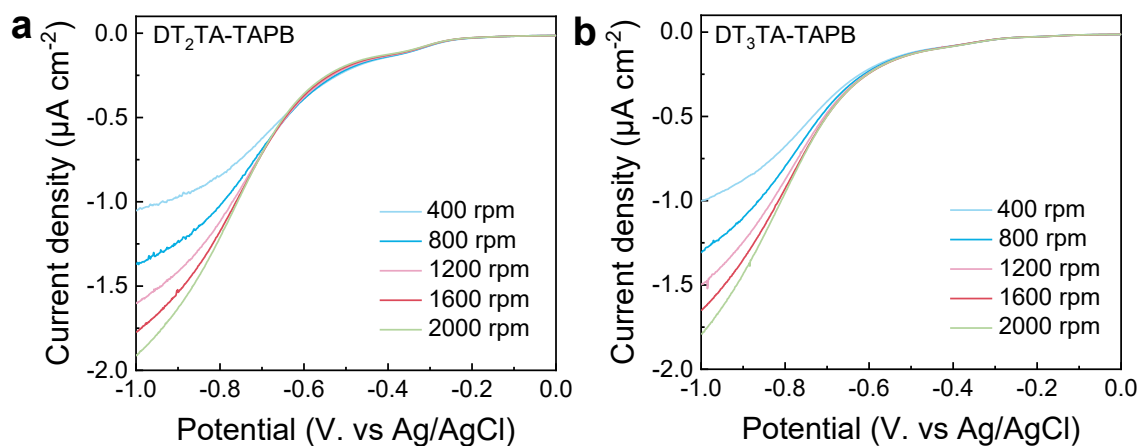
Supplementary Fig. 32. Photocatalytic decomposition of H₂O₂. Photocatalytic decomposition of H₂O₂ under visible light irradiation over DT₂TA-TAPB. Reaction conditions: [H₂O₂] = 1 mM, Ar atmosphere.



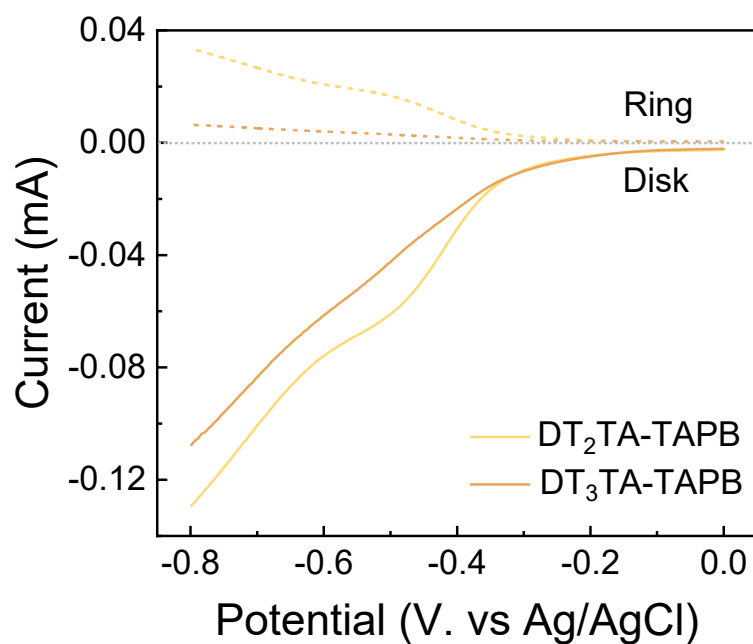
Supplementary Fig. 33. Investigation of intermediates in O₂ reduction to H₂O₂. In situ DRIFT spectra of DT₂TA-TAPB.



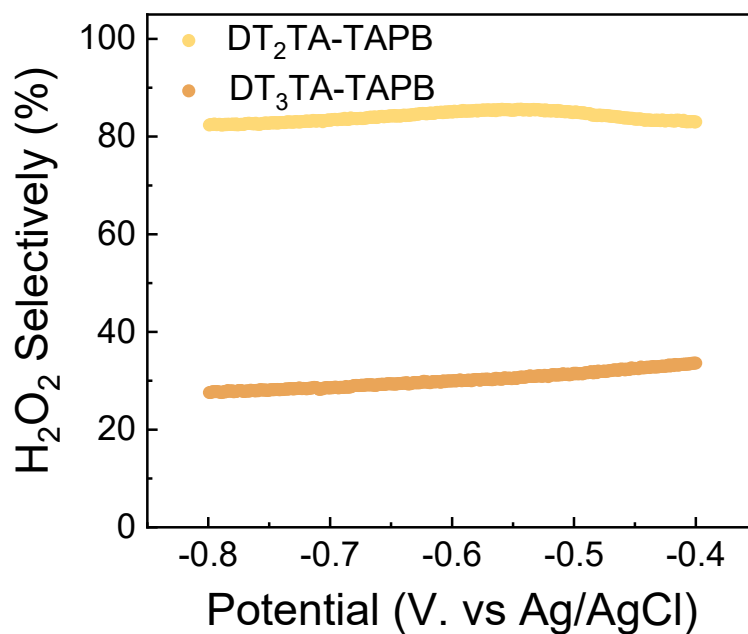
Supplementary Fig. 34. Investigation of intermediates in O₂ reduction to H₂O₂ over DT₃TA-TAPB. (a-b) In situ DRIFT spectra of DT₃TA-TAPB.



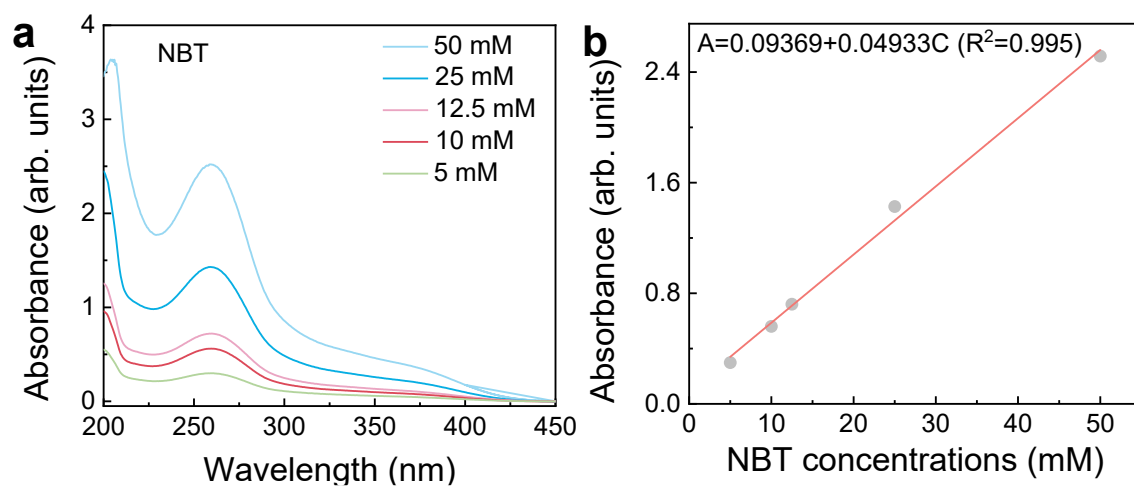
Supplementary Fig. 35. LSV curves at various rotation speeds. (a-b) Linear sweep voltammetry curves of DT₂TA-TAPB and DT₃TA-TAPB on a rotating disk electrode at different rotational speeds.



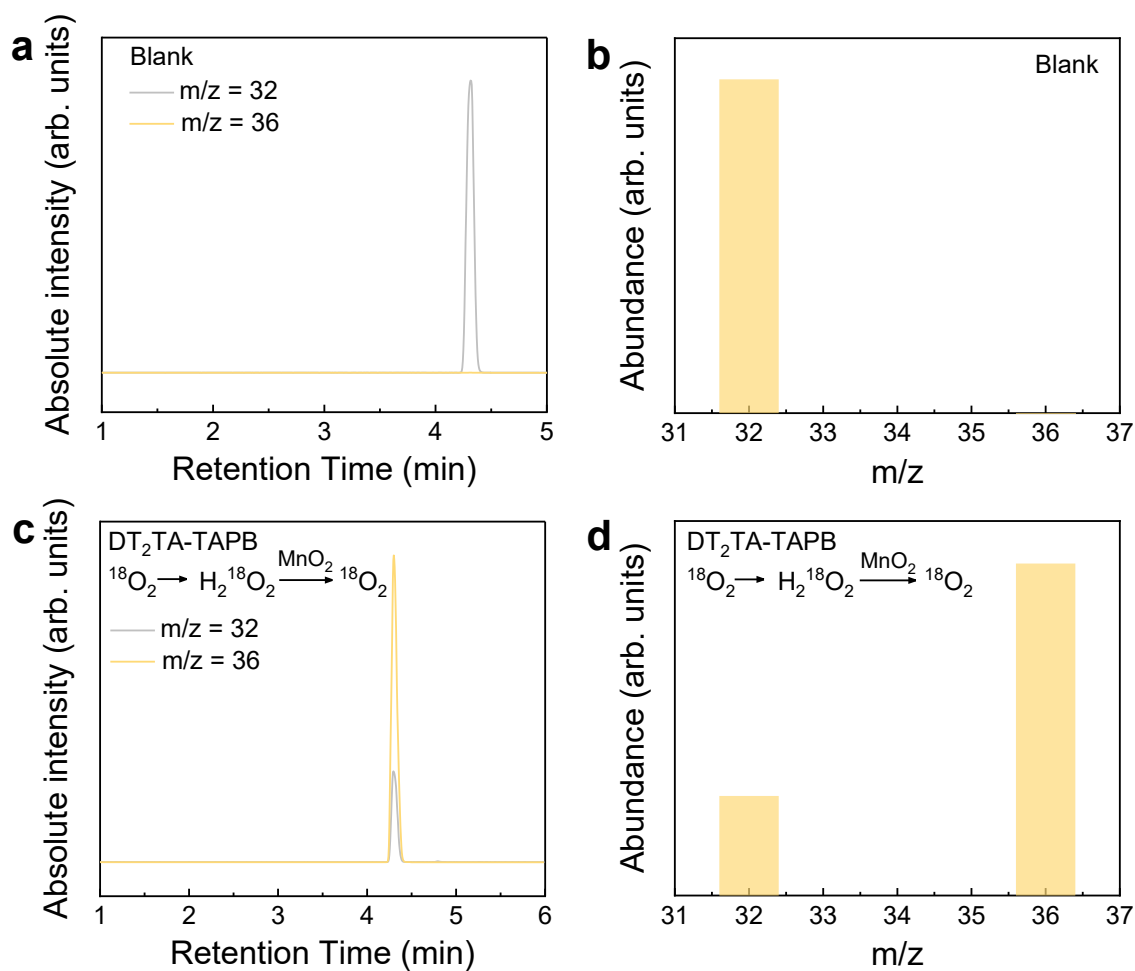
Supplementary Fig. 36. RRDE curves at 1600 rpm in O₂-saturated electrolyte. RRDE curves of DT₂TA-TAPB and DT₃TA-TAPB measured at 1600 rpm in O₂-saturated 0.1 M phosphate buffer (pH = 7) electrolyte.



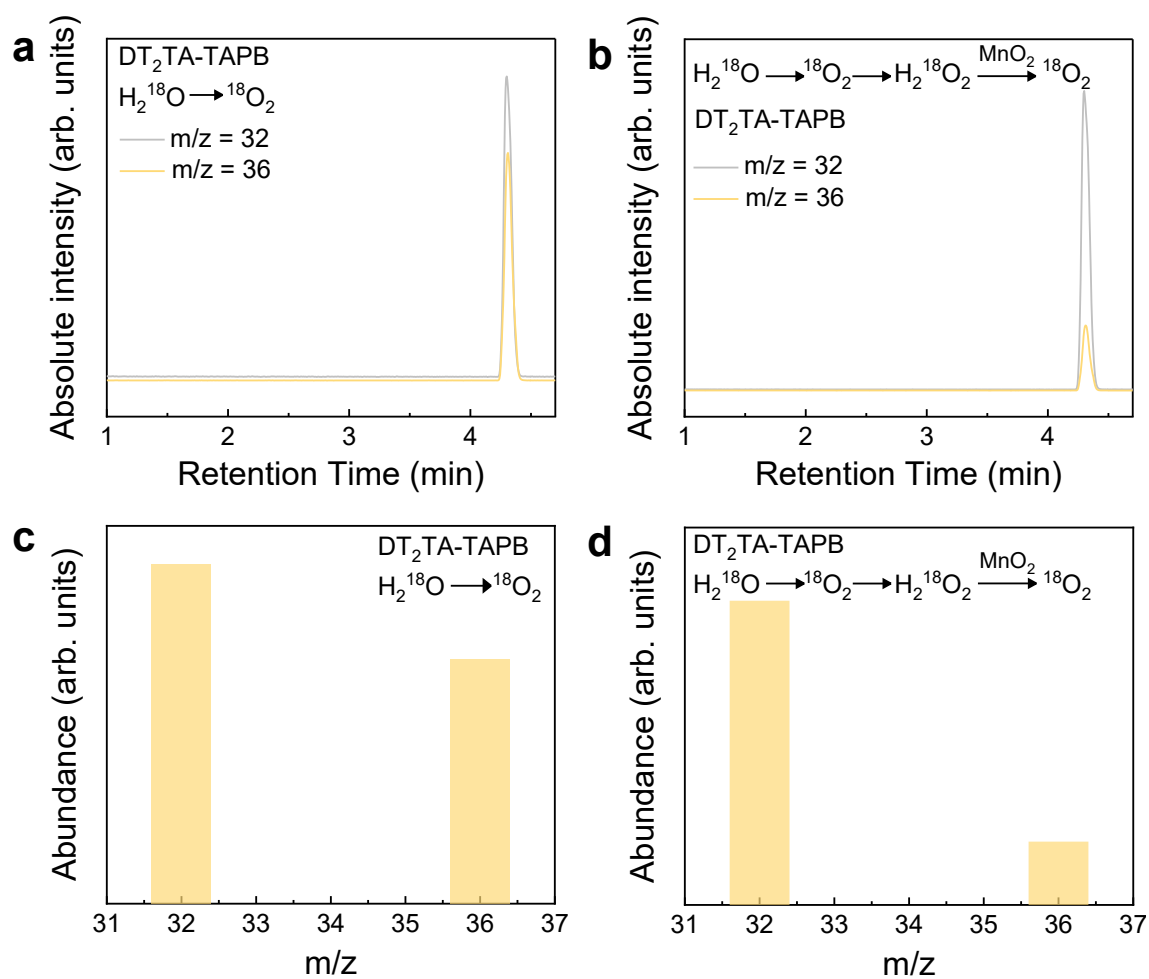
Supplementary Fig. 37. Investigation of selectivity in O₂ reduction. Calculated H₂O₂ selectivity of DT₂TA-TAPB and DT₃TA-TAPB based on RRDE measurements.



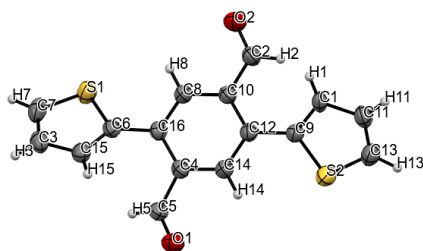
Supplementary Fig. 38. Quantitative detection of superoxide radicals by NBT. (a) UV-vis absorption spectra of different concentrations of NBT. (b) The linear relationship between NBT concentration and absorption intensity.



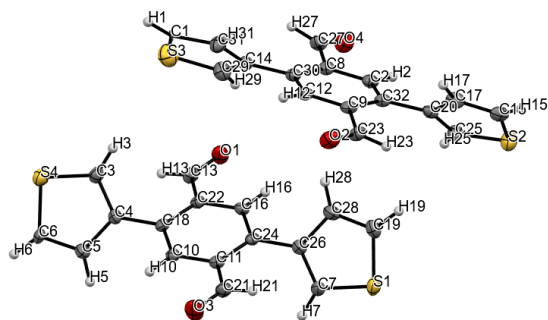
Supplementary Fig. 39. Investigation of the O₂ reduction mechanism using ¹⁸O-labeled O₂. (a-b) Chromatograms and mass spectra of the blank sample. (c-d) Chromatograms and mass spectra of ¹⁸O-labeled oxygen molecules used to probe the source of H₂O₂ generation over DT₂TA-TAPB.



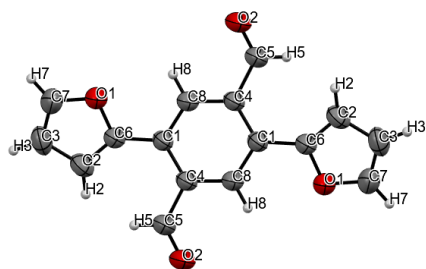
Supplementary Fig. 40. Investigation of the O₂ reduction mechanism using ¹⁸O-labeled H₂O. (a-b) Chromatograms of ¹⁸O-labeled H₂O used to probe the origin of H₂O₂ generation over DT₂TA-TAPB. (c-d) Mass spectra of ¹⁸O-labeled H₂O tracing the source of H₂O₂ formation over DT₂TA-TAPB.



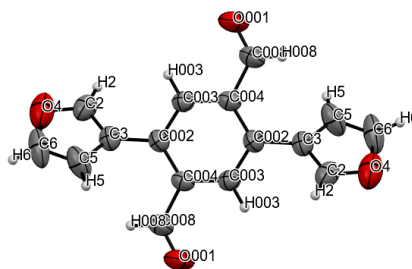
DT₂TA (CCDC: 2323749)



DT₃TA (CCDC: 2323748)



DF₂TA (CCDC: 2339826)



DF₃TA (CCDC: 2323750)

Supplementary Fig. 41. Structure of aldehyde monomers. Single crystal structures of DT₂TA, DT₃TA, DF₂TA, and DF₃TA.

Section 3. Supplementary Tables 1-7

Supplementary Table 1. Comparison of photocatalytic H₂O₂ production by reported COF-based photocatalysts.

Samples	Reaction condition	H ₂ O ₂ yield rate ($\mu\text{mol g}^{-1} \text{ h}^{-1}$)	Reference
DT₂TA-TAPB	$\lambda > 420 \text{ nm}$, H ₂ O : EtOH (9:1)	10972	This work
	$\lambda > 420 \text{ nm}$, pure water	8587	
TAPT-TFPA	1.5 G solar intensity,	2143	4
COFs@Pd ICs	H ₂ O:EtOH (9:1)		
CoPc-BTM-COF	$\lambda > 400 \text{ nm}$, H ₂ O : EtOH (9:1)	2096	5
TF ₅₀ -COF	$\lambda > 400 \text{ nm}$, H ₂ O : EtOH (9:1)	1739	6
EBA-COF	420 nm, H ₂ O : EtOH (9:1)	1830	7
DCMR-1NH	420-700nm, H ₂ O : IPA (10:1)	3904	8
Py-Da-COF	$\lambda > 420 \text{ nm}$, H ₂ O : EtOH (9:1)	682	9
FS-COF	$\lambda > 420 \text{ nm}$, pure water	3904	10
TpDz	$\lambda > 420 \text{ nm}$, pure water	7327	11
DETH-COF	$\lambda > 420 \text{ nm}$, pure water	1665	12
TTF-BT-COF	$\lambda > 420 \text{ nm}$, pure water	2760	13
Bpt-CTF	$\lambda = 350\text{-}780 \text{ nm}$, pure water	3268	14
AP-TfpBpy	$\lambda > 300 \text{ nm}$, pure water	3940	15
TaptBtt	$\lambda > 420 \text{ nm}$, pure water	1407	16
TZ-COF	$\lambda > 420 \text{ nm}$, pure water	268	17

Supplementary Table 2. Single crystal data of DT₂TA and DT₃TA.

Name	DT ₂ TA	DT ₃ TA
Formula	C ₁₆ H ₁₀ O ₂ S ₂	C ₃₂ H ₂₀ O ₄ S ₄
CCDC Deposition Number	2323749	2323748
Formula weight	298.36	596.72
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /c	P2 ₁
Temperature/K	302.49(10)	150.00(10)
a/Å	10.53950(10)	8.91610(10)
b/Å	7.62970(10)	16.69800(10)
c/Å	17.2813(2)	9.02220(10)
$\alpha/^\circ$	90	90
$\beta/^\circ$	102.6980(10)	91.9050(10)
$\gamma/^\circ$	90	90
F (000)	616.0	272.0
ρ_{calc} , g/cm ³	1.462	1.476
Volume/Å ³	1355.66(3)	1342.49(2)
Z	4	2
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ = 0.0463	R ₁ = 0.0411
	wR ₂ = 0.1349	wR ₂ = 0.1214
Final R indexes [all data]	R ₁ = 0.0478	R ₁ = 0.0414
	wR ₂ = 0.1366	wR ₂ = 0.1217

Supplementary Table 3. Single crystal data of DF₂TA and DF₃TA.

Name	DF ₂ TA	DF ₃ TA
Formula	C ₈ H ₅ O ₂	C ₁₆ H ₁₀ O ₄
CCDC Deposition Number	2339826	2323750
Formula weight	133.12	264.22
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /c	P2 ₁ /n
Temperature/K	291.9(7)	300.56(10)
a/Å	3.86971(18)	12.2699(2)
b/Å	17.5555(8)	3.93519(8)
c/Å	9.1719(4)	12.9934(2)
α /°	90	90
β /°	101.218(5)	95.9334(18)
γ /°	90	90
F(000)	276.0	272.0
ρ_{calc} , g/cm ³	1.447	1.406
Volume/Å ³	611.19(5)	624.01(2)
Z	4	2
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ = 0.0469	R ₁ = 0.0727
	wR ₂ = 0.1357	wR ₂ = 0.2274
Final R indexes [all data]	R ₁ = 0.0526	R ₁ = 0.0779
	wR ₂ = 0.1410	wR ₂ = 0.2348

Supplementary Table 4. Atomic coordinates of the optimized computational models of DT₂TA-TAPB used in electronic structure calculations.

		x	y	z	Occupancy	U
C1	C	0.47086	0.45501	0.56163	1.000	0.000
C2	C	0.54498	0.01594	0.56981	1.000	0.000
C3	C	0.98409	0.52907	0.55955	1.000	0.000
C4	C	0.52918	0.54509	0.56268	1.000	0.000
C5	C	0.45489	0.98416	0.57174	1.000	0.000
C6	C	0.01592	0.47081	0.55949	1.000	0.000
C7	C	0.45655	0.48462	0.54350	1.000	0.000
C8	C	0.51538	0.97206	0.54506	1.000	0.000
C9	C	0.02803	0.54343	0.54172	1.000	0.000
C10	C	0.54350	0.51548	0.54441	1.000	0.000
C11	C	0.48450	0.02812	0.56145	1.000	0.000
C12	C	0.97198	0.45646	0.54213	1.000	0.000
C13	C	0.48447	0.52873	0.54702	1.000	0.000
C14	C	0.47126	0.95586	0.54922	1.000	0.000
C15	C	0.04425	0.51553	0.54498	1.000	0.000
C16	C	0.51558	0.47137	0.54692	1.000	0.000
C17	C	0.52860	0.04431	0.56351	1.000	0.000
C18	C	0.95576	0.48435	0.54538	1.000	0.000
C19	C	0.46483	0.55617	0.52011	1.000	0.000
C20	C	0.44384	0.90880	0.51954	1.000	0.000
C21	C	0.09134	0.53521	0.51882	1.000	0.000

C22	C	0.53522	0.44393	0.52014	1.000	0.000
C23	C	0.55609	0.09140	0.54042	1.000	0.000
C24	C	0.90867	0.46468	0.51938	1.000	0.000
C25	C	0.43391	0.59411	0.70624	1.000	0.000
C26	C	0.40596	0.83991	0.70483	1.000	0.000
C27	C	0.16019	0.56624	0.70535	1.000	0.000
C28	C	0.56621	0.40607	0.70712	1.000	0.000
C29	C	0.59403	0.16020	0.72639	1.000	0.000
C30	C	0.83983	0.43368	0.70685	1.000	0.000
C31	C	0.44948	0.62366	0.43829	1.000	0.000
C32	C	0.37641	0.82590	0.43679	1.000	0.000
C33	C	0.17421	0.55069	0.43748	1.000	0.000
C34	C	0.55067	0.37648	0.43940	1.000	0.000
C35	C	0.62362	0.17410	0.45872	1.000	0.000
C36	C	0.82576	0.44916	0.43895	1.000	0.000
C37	C	0.42172	0.63528	0.26253	1.000	0.000
C38	C	0.36487	0.78654	0.26086	1.000	0.000
C39	C	0.21358	0.57847	0.26171	1.000	0.000
C40	C	0.57846	0.36486	0.26413	1.000	0.000
C41	C	0.63529	0.21345	0.28255	1.000	0.000
C42	C	0.78640	0.42132	0.26324	1.000	0.000
C43	C	0.38327	0.62681	0.44402	1.000	0.000
C44	C	0.37336	0.75659	0.44253	1.000	0.000
C45	C	0.24355	0.61690	0.44339	1.000	0.000
C46	C	0.61686	0.37332	0.44635	1.000	0.000

C47	C	0.62672	0.24344	0.46247	1.000	0.000
C48	C	0.75645	0.38291	0.44557	1.000	0.000
C49	C	0.36920	0.59846	0.72182	1.000	0.000
C50	C	0.40169	0.77088	0.72040	1.000	0.000
C51	C	0.22925	0.63095	0.72111	1.000	0.000
C52	C	0.63090	0.40170	0.72380	1.000	0.000
C53	C	0.59835	0.22925	0.74015	1.000	0.000
C54	C	0.77079	0.36895	0.72373	1.000	0.000
C55	C	0.39795	0.58886	0.91005	1.000	0.000
C56	C	0.41125	0.80922	0.90859	1.000	0.000
C57	C	0.19089	0.60220	0.90923	1.000	0.000
C58	C	0.60217	0.41137	0.91117	1.000	0.000
C59	C	0.58883	0.19097	0.92962	1.000	0.000
C60	C	0.80918	0.39773	0.91121	1.000	0.000
C61	C	0.35751	0.64568	0.32006	1.000	0.000
C62	C	0.35447	0.71193	0.31910	1.000	0.000
C63	C	0.28821	0.64265	0.31990	1.000	0.000
C64	C	0.64251	0.35418	0.32536	1.000	0.000
C65	C	0.64544	0.28788	0.33420	1.000	0.000
C66	C	0.71174	0.35712	0.32381	1.000	0.000
C67	C	0.31276	0.62231	0.31257	1.000	0.000
C68	C	0.37784	0.69056	0.31159	1.000	0.000
C69	C	0.30959	0.68739	0.31155	1.000	0.000
C70	C	0.68723	0.37750	0.31388	1.000	0.000
C71	C	0.62211	0.30929	0.32462	1.000	0.000

C72	C	0.69031	0.31236	0.32152	1.000	0.000
C73	C	0.44010	0.40958	0.63207	1.000	0.000
C74	C	0.59041	0.03056	0.63902	1.000	0.000
C75	C	0.96939	0.55984	0.62859	1.000	0.000
C76	C	0.55995	0.59052	0.63344	1.000	0.000
C77	C	0.40937	0.96938	0.64008	1.000	0.000
C78	C	0.03064	0.44005	0.62832	1.000	0.000
C79	C	0.03507	0.37253	0.65279	1.000	0.000
C80	C	0.62747	0.66246	0.65920	1.000	0.000
C81	C	0.33743	0.96498	0.66313	1.000	0.000
C82	C	0.96507	0.62741	0.65337	1.000	0.000
C83	C	0.37261	0.33761	0.65803	1.000	0.000
C84	C	0.66235	0.03497	0.66382	1.000	0.000
C85	C	0.05975	0.40223	0.90313	1.000	0.000
C86	C	0.59772	0.65739	0.90933	1.000	0.000
C87	C	0.34235	0.94025	0.91343	1.000	0.000
C88	C	0.94036	0.59771	0.90364	1.000	0.000
C89	C	0.40236	0.34272	0.90818	1.000	0.000
C90	C	0.65734	0.05968	0.91395	1.000	0.000
C91	C	0.05799	0.44075	0.88215	1.000	0.000
C92	C	0.55919	0.61712	0.88747	1.000	0.000
C93	C	0.38265	0.94202	0.89345	1.000	0.000
C94	C	0.94205	0.55916	0.88242	1.000	0.000
C95	C	0.44087	0.38300	0.88620	1.000	0.000
C96	C	0.61706	0.05793	0.89283	1.000	0.000

N1	N	0.45409	0.56994	0.80133	1.000	0.000
N2	N	0.43005	0.88423	0.80048	1.000	0.000
N3	N	0.11583	0.54601	0.80031	1.000	0.000
N4	N	0.54599	0.43021	0.80151	1.000	0.000
N5	N	0.56982	0.11586	0.82210	1.000	0.000
N6	N	0.88421	0.45392	0.80099	1.000	0.000
H1	H	0.29610	0.58717	0.34699	1.000	0.000
H2	H	0.41299	0.70905	0.34516	1.000	0.000
H3	H	0.29111	0.70406	0.34511	1.000	0.000
H4	H	0.70397	0.41270	0.34299	1.000	0.000
H5	H	0.58702	0.29094	0.36254	1.000	0.000
H6	H	0.70881	0.29574	0.35640	1.000	0.000
H7	H	0.47883	0.62995	0.29482	1.000	0.000
H8	H	0.37008	0.84894	0.29342	1.000	0.000
H9	H	0.15117	0.52133	0.29399	1.000	0.000
H10	H	0.52132	0.37015	0.29574	1.000	0.000
H11	H	0.62995	0.15101	0.31624	1.000	0.000
H12	H	0.84879	0.47848	0.29494	1.000	0.000
H13	H	0.43544	0.66159	0.06197	1.000	0.000
H14	H	0.33855	0.77391	0.06037	1.000	0.000
H15	H	0.22619	0.56475	0.06126	1.000	0.000
H16	H	0.56478	0.33855	0.06357	1.000	0.000
H17	H	0.66159	0.22600	0.08196	1.000	0.000
H18	H	0.77376	0.43500	0.06280	1.000	0.000
H19	H	0.33827	0.58904	0.84803	1.000	0.000

H20	H	0.41110	0.74937	0.84684	1.000	0.000
H21	H	0.25075	0.66187	0.84755	1.000	0.000
H22	H	0.66175	0.41098	0.85120	1.000	0.000
H23	H	0.58860	0.25062	0.86383	1.000	0.000
H24	H	0.74921	0.33816	0.85171	1.000	0.000
H25	H	0.38432	0.56261	1.11087	1.000	0.000
H26	H	0.43752	0.82188	1.10932	1.000	0.000
H27	H	0.17827	0.61582	1.11016	1.000	0.000
H28	H	0.61576	0.43759	1.11227	1.000	0.000
H29	H	0.56260	0.17841	1.13068	1.000	0.000
H30	H	0.82185	0.38413	1.11188	1.000	0.000
H31	H	0.89459	0.45770	0.21535	1.000	0.000
H32	H	0.54221	0.43685	0.21602	1.000	0.000
H33	H	0.56326	0.10556	0.23680	1.000	0.000
H34	H	0.10543	0.54221	0.21488	1.000	0.000
H35	H	0.45786	0.56328	0.21606	1.000	0.000
H36	H	0.43677	0.89476	0.21531	1.000	0.000
H37	H	0.42167	0.47258	0.54656	1.000	0.000
H38	H	0.52743	0.94923	0.54196	1.000	0.000
H39	H	0.05083	0.57831	0.54500	1.000	0.000
H40	H	0.57838	0.52753	0.54822	1.000	0.000
H41	H	0.47245	0.05094	0.57173	1.000	0.000
H42	H	0.94918	0.42157	0.54597	1.000	0.000
H43	H	0.03127	0.34096	0.59493	1.000	0.000
H44	H	0.65904	0.69026	0.60180	1.000	0.000

H45	H	0.30967	0.96879	0.60441	1.000	0.000
H46	H	0.96889	0.65899	0.59556	1.000	0.000
H47	H	0.34104	0.30980	0.60077	1.000	0.000
H48	H	0.69013	0.03119	0.60593	1.000	0.000
H49	H	0.07825	0.39717	1.11457	1.000	0.000
H50	H	0.60270	0.68095	1.12065	1.000	0.000
H51	H	0.31876	0.92180	1.12483	1.000	0.000
H52	H	0.92184	0.60278	1.11496	1.000	0.000
H53	H	0.39741	0.31918	1.11956	1.000	0.000
H54	H	0.68092	0.07822	1.12521	1.000	0.000
H55	H	0.07184	0.46527	0.09405	1.000	0.000
H56	H	0.53464	0.60643	0.09910	1.000	0.000
H57	H	0.39319	0.92807	0.10551	1.000	0.000
H58	H	0.92818	0.53464	0.09431	1.000	0.000
H59	H	0.46542	0.39374	0.09789	1.000	0.000
H60	H	0.60641	0.07179	0.10467	1.000	0.000
S1	S	0.01291	0.39365	0.37631	1.000	0.000
S2	S	0.60641	0.61926	0.38219	1.000	0.000
S3	S	0.38077	0.98711	0.38718	1.000	0.000
S4	S	0.98716	0.60625	0.37669	1.000	0.000
S5	S	0.39363	0.38081	0.38091	1.000	0.000
S6	S	0.61911	0.01284	0.38706	1.000	0.000

Supplementary Table 5. Atomic coordinates of the optimized computational models of DT₃TA-TAPB used in electronic structure calculations.

		x	y	z	Occupancy	U
C1	C	0.47075	0.45675	0.54436	1.000	0.000
C2	C	0.54345	0.01392	0.52177	1.000	0.000
C3	C	0.98519	0.52872	0.52354	1.000	0.000
C4	C	0.53195	0.54598	0.53872	1.000	0.000
C5	C	0.45423	0.98593	0.51759	1.000	0.000
C6	C	0.01496	0.46888	0.51786	1.000	0.000
C7	C	0.45839	0.48781	0.51347	1.000	0.000
C8	C	0.51238	0.97049	0.49113	1.000	0.000
C9	C	0.02882	0.54195	0.49266	1.000	0.000
C10	C	0.54436	0.51486	0.52065	1.000	0.000
C11	C	0.48536	0.02944	0.49906	1.000	0.000
C12	C	0.97123	0.45560	0.49929	1.000	0.000
C13	C	0.48762	0.53170	0.52205	1.000	0.000
C14	C	0.46850	0.95588	0.50060	1.000	0.000
C15	C	0.04430	0.51340	0.50133	1.000	0.000
C16	C	0.51511	0.47100	0.53499	1.000	0.000
C17	C	0.52920	0.04402	0.51299	1.000	0.000
C18	C	0.95579	0.48416	0.51380	1.000	0.000
C19	C	0.46885	0.56005	0.49655	1.000	0.000
C20	C	0.44014	0.90878	0.47593	1.000	0.000
C21	C	0.09148	0.53288	0.47613	1.000	0.000

C22	C	0.53372	0.44248	0.51675	1.000	0.000
C23	C	0.55766	0.09115	0.49553	1.000	0.000
C24	C	0.90860	0.46483	0.49591	1.000	0.000
C25	C	0.43732	0.59749	0.68135	1.000	0.000
C26	C	0.40285	0.83984	0.66386	1.000	0.000
C27	C	0.16042	0.56435	0.66343	1.000	0.000
C28	C	0.56456	0.40449	0.70324	1.000	0.000
C29	C	0.59534	0.15994	0.68489	1.000	0.000
C30	C	0.83982	0.43401	0.68529	1.000	0.000
C31	C	0.45239	0.62696	0.41280	1.000	0.000
C32	C	0.37340	0.82521	0.39534	1.000	0.000
C33	C	0.17473	0.54913	0.39537	1.000	0.000
C34	C	0.54916	0.37499	0.43497	1.000	0.000
C35	C	0.62485	0.17431	0.41674	1.000	0.000
C36	C	0.82575	0.44954	0.41764	1.000	0.000
C37	C	0.42409	0.63791	0.23725	1.000	0.000
C38	C	0.36271	0.78599	0.22047	1.000	0.000
C39	C	0.21415	0.57714	0.22100	1.000	0.000
C40	C	0.57709	0.36355	0.25959	1.000	0.000
C41	C	0.63598	0.21363	0.24182	1.000	0.000
C42	C	0.78623	0.42186	0.24366	1.000	0.000
C43	C	0.38534	0.62868	0.41800	1.000	0.000
C44	C	0.37206	0.75665	0.40310	1.000	0.000
C45	C	0.24389	0.61563	0.40353	1.000	0.000
C46	C	0.61571	0.37233	0.44023	1.000	0.000

C47	C	0.62707	0.24327	0.42445	1.000	0.000
C48	C	0.75626	0.38347	0.42589	1.000	0.000
C49	C	0.37176	0.60034	0.69572	1.000	0.000
C50	C	0.40033	0.77162	0.68125	1.000	0.000
C51	C	0.22922	0.62936	0.68087	1.000	0.000
C52	C	0.62959	0.40070	0.71785	1.000	0.000
C53	C	0.59879	0.22859	0.70266	1.000	0.000
C54	C	0.77068	0.36946	0.70309	1.000	0.000
C55	C	0.40108	0.59156	0.88486	1.000	0.000
C56	C	0.40898	0.80974	0.86878	1.000	0.000
C57	C	0.19088	0.60040	0.86785	1.000	0.000
C58	C	0.60061	0.40996	0.90682	1.000	0.000
C59	C	0.58964	0.19030	0.88986	1.000	0.000
C60	C	0.80915	0.39814	0.88984	1.000	0.000
C61	C	0.35878	0.64660	0.29136	1.000	0.000
C62	C	0.35409	0.71198	0.28188	1.000	0.000
C63	C	0.28870	0.64191	0.28330	1.000	0.000
C64	C	0.64180	0.35390	0.31354	1.000	0.000
C65	C	0.64554	0.28801	0.30355	1.000	0.000
C66	C	0.71144	0.35762	0.30546	1.000	0.000
C67	C	0.31403	0.62241	0.28214	1.000	0.000
C68	C	0.37826	0.69142	0.27932	1.000	0.000
C69	C	0.30927	0.68662	0.27200	1.000	0.000
C70	C	0.68656	0.37762	0.30439	1.000	0.000
C71	C	0.62182	0.30905	0.30117	1.000	0.000

C72	C	0.69039	0.31289	0.29388	1.000	0.000
C73	C	0.43752	0.41378	0.66131	1.000	0.000
C74	C	0.58645	0.02371	0.63827	1.000	0.000
C75	C	0.97456	0.56132	0.64048	1.000	0.000
C76	C	0.56514	0.58917	0.65269	1.000	0.000
C77	C	0.41110	0.97600	0.63225	1.000	0.000
C78	C	0.02582	0.43630	0.63188	1.000	0.000
C79	C	0.01173	0.39478	0.45637	1.000	0.000
C80	C	0.60678	0.61598	0.47707	1.000	0.000
C81	C	0.38435	0.99091	0.45676	1.000	0.000
C82	C	0.98858	0.60286	0.46551	1.000	0.000
C83	C	0.39585	0.38692	0.48623	1.000	0.000
C84	C	0.61338	0.00898	0.46316	1.000	0.000
C85	C	0.04187	0.40203	1.10320	1.000	0.000
C86	C	0.60012	0.63930	1.12384	1.000	0.000
C87	C	0.36101	0.96092	1.10351	1.000	0.000
C88	C	0.95841	0.59546	1.11236	1.000	0.000
C89	C	0.40262	0.36370	1.13305	1.000	0.000
C90	C	0.63656	0.03898	1.11003	1.000	0.000
C91	C	0.04784	0.44109	0.94000	1.000	0.000
C92	C	0.56076	0.60672	0.96052	1.000	0.000
C93	C	0.39352	0.95405	0.93996	1.000	0.000
C94	C	0.95254	0.55644	0.94885	1.000	0.000
C95	C	0.44196	0.39631	0.96944	1.000	0.000
C96	C	0.60388	0.04561	0.94654	1.000	0.000

N1	N	0.45813	0.57388	0.77738	1.000	0.000
N2	N	0.42638	0.88432	0.75725	1.000	0.000
N3	N	0.11598	0.54376	0.75728	1.000	0.000
N4	N	0.54421	0.42857	0.79855	1.000	0.000
N5	N	0.57142	0.11547	0.77781	1.000	0.000
N6	N	0.88427	0.45417	0.77814	1.000	0.000
H1	H	0.48191	0.63379	0.26924	1.000	0.000
H2	H	0.36657	0.84781	0.25022	1.000	0.000
H3	H	0.15191	0.51972	0.25107	1.000	0.000
H4	H	0.51973	0.36849	0.29151	1.000	0.000
H5	H	0.63141	0.15150	0.27197	1.000	0.000
H6	H	0.84879	0.47884	0.27316	1.000	0.000
H7	H	0.43748	0.66427	0.03713	1.000	0.000
H8	H	0.33632	0.77280	0.02048	1.000	0.000
H9	H	0.22693	0.56358	0.02053	1.000	0.000
H10	H	0.56345	0.33720	0.05931	1.000	0.000
H11	H	0.66234	0.22655	0.04166	1.000	0.000
H12	H	0.77368	0.43560	0.04285	1.000	0.000
H13	H	0.34060	0.59007	0.82084	1.000	0.000
H14	H	0.41032	0.75065	0.80967	1.000	0.000
H15	H	0.25052	0.66022	0.80896	1.000	0.000
H16	H	0.66068	0.41059	0.84300	1.000	0.000
H17	H	0.58923	0.24987	0.83141	1.000	0.000
H18	H	0.74916	0.33866	0.83107	1.000	0.000
H19	H	0.38776	0.56525	1.08530	1.000	0.000

H20	H	0.43530	0.82293	1.06908	1.000	0.000
H21	H	0.17810	0.61387	1.06885	1.000	0.000
H22	H	0.61418	0.43623	1.10754	1.000	0.000
H23	H	0.56334	0.17738	1.09030	1.000	0.000
H24	H	0.82168	0.38447	1.09127	1.000	0.000
H25	H	0.89435	0.45778	0.19198	1.000	0.000
H26	H	0.54071	0.43522	0.21286	1.000	0.000
H27	H	0.56487	0.10540	0.19163	1.000	0.000
H28	H	0.10559	0.53999	0.17150	1.000	0.000
H29	H	0.46182	0.56713	0.19194	1.000	0.000
H30	H	0.43308	0.89467	0.17122	1.000	0.000
H31	H	0.42382	0.47723	0.51116	1.000	0.000
H32	H	0.52293	0.94648	0.48827	1.000	0.000
H33	H	0.05229	0.57667	0.49041	1.000	0.000
H34	H	0.57893	0.52545	0.52431	1.000	0.000
H35	H	0.47480	0.05345	0.50304	1.000	0.000
H36	H	0.94776	0.42088	0.50273	1.000	0.000
H37	H	-0.02100	0.38001	0.34767	1.000	0.000
H38	H	0.62099	0.59750	0.36831	1.000	0.000
H39	H	0.40285	1.02359	0.34788	1.000	0.000
H40	H	1.02132	0.61775	0.35699	1.000	0.000
H41	H	0.38155	0.40531	0.37758	1.000	0.000
H42	H	0.59504	-0.02372	0.35456	1.000	0.000
H43	H	0.07114	0.40375	1.21138	1.000	0.000
H44	H	0.59905	0.66719	1.23214	1.000	0.000

H45	H	0.33310	0.93200	1.21192	1.000	0.000
H46	H	0.92908	0.59360	1.22042	1.000	0.000
H47	H	0.40379	0.33585	1.24105	1.000	0.000
H48	H	0.66436	0.06804	1.21803	1.000	0.000
H49	H	0.06013	0.47059	0.09294	1.000	0.000
H50	H	0.53119	0.59004	0.11338	1.000	0.000
H51	H	0.41014	0.94106	0.09243	1.000	0.000
H52	H	0.94019	0.52688	0.10092	1.000	0.000
H53	H	0.47158	0.41298	0.12149	1.000	0.000
H54	H	0.58711	0.05844	0.09876	1.000	0.000
H55	H	0.29798	0.58732	0.31883	1.000	0.000
H56	H	0.41337	0.71059	0.31351	1.000	0.000
H57	H	0.29013	0.70267	0.30050	1.000	0.000
H58	H	0.70300	0.41272	0.34156	1.000	0.000
H59	H	0.58669	0.29024	0.33528	1.000	0.000
H60	H	0.70916	0.29647	0.32263	1.000	0.000
S1	S	0.01635	0.36033	0.77860	1.000	0.000
S2	S	0.64171	0.65472	0.79929	1.000	0.000
S3	S	0.34563	0.98713	0.77898	1.000	0.000
S4	S	0.98377	0.63719	0.78781	1.000	0.000
S5	S	0.36100	0.34815	0.80855	1.000	0.000
S6	S	0.65221	0.01301	0.78545	1.000	0.000

Supplementary Table 6. Atomic coordinates of the optimized computational models of DF₂TA-TAPB used in electronic structure calculations.

		x	y	z	Occupancy	U
C1	C	0.46894	0.45494	0.80832	1.000	0.000
C2	C	0.54322	0.01494	0.80387	1.000	0.000
C3	C	0.98467	0.53094	0.82260	1.000	0.000
C4	C	0.52903	0.54403	0.82470	1.000	0.000
C5	C	0.45355	0.98446	0.80171	1.000	0.000
C6	C	0.01475	0.47196	0.77369	1.000	0.000
C7	C	0.45578	0.48519	0.84232	1.000	0.000
C8	C	0.51334	0.97137	0.83385	1.000	0.000
C9	C	0.02817	0.54431	0.85684	1.000	0.000
C10	C	0.54221	0.51363	0.83764	1.000	0.000
C11	C	0.48347	0.02820	0.81646	1.000	0.000
C12	C	0.97105	0.45812	0.78750	1.000	0.000
C13	C	0.48485	0.52917	0.84276	1.000	0.000
C14	C	0.46922	0.95579	0.82529	1.000	0.000
C15	C	0.04368	0.51583	0.82516	1.000	0.000
C16	C	0.51314	0.46968	0.82068	1.000	0.000
C17	C	0.52763	0.04377	0.81026	1.000	0.000
C18	C	0.95565	0.48670	0.80510	1.000	0.000
C19	C	0.46583	0.55705	0.80800	1.000	0.000
C20	C	0.44211	0.90879	0.78829	1.000	0.000
C21	C	0.09065	0.53524	0.78907	1.000	0.000

C22	C	0.53230	0.44201	0.77036	1.000	0.000
C23	C	0.55520	0.09071	0.76625	1.000	0.000
C24	C	0.90874	0.46731	0.76325	1.000	0.000
C25	C	0.43422	0.59445	0.99000	1.000	0.000
C26	C	0.40553	0.83966	0.97040	1.000	0.000
C27	C	0.15980	0.56674	0.97161	1.000	0.000
C28	C	0.56478	0.40509	0.94651	1.000	0.000
C29	C	0.59310	0.15996	0.94643	1.000	0.000
C30	C	0.83957	0.43504	0.94492	1.000	0.000
C31	C	0.44937	0.62369	0.71964	1.000	0.000
C32	C	0.37632	0.82530	0.69979	1.000	0.000
C33	C	0.17380	0.55149	0.70135	1.000	0.000
C34	C	0.54981	0.37589	0.67577	1.000	0.000
C35	C	0.62228	0.17391	0.67561	1.000	0.000
C36	C	0.82524	0.44993	0.67433	1.000	0.000
C37	C	0.42135	0.63492	0.54294	1.000	0.000
C38	C	0.36531	0.78608	0.52352	1.000	0.000
C39	C	0.21327	0.57915	0.52597	1.000	0.000
C40	C	0.57801	0.36489	0.49868	1.000	0.000
C41	C	0.63406	0.21337	0.49985	1.000	0.000
C42	C	0.78598	0.42172	0.49809	1.000	0.000
C43	C	0.38289	0.62629	0.72509	1.000	0.000
C44	C	0.37382	0.75632	0.70823	1.000	0.000
C45	C	0.24342	0.61727	0.71030	1.000	0.000
C46	C	0.61640	0.37343	0.68221	1.000	0.000

C47	C	0.62604	0.24355	0.68351	1.000	0.000
C48	C	0.75618	0.38334	0.68196	1.000	0.000
C49	C	0.36899	0.59800	1.00308	1.000	0.000
C50	C	0.40207	0.77089	0.98653	1.000	0.000
C51	C	0.22913	0.63132	0.98795	1.000	0.000
C52	C	0.63016	0.40171	0.96027	1.000	0.000
C53	C	0.59774	0.22926	0.96144	1.000	0.000
C54	C	0.77080	0.36968	0.96004	1.000	0.000
C55	C	0.39809	0.58900	1.19362	1.000	0.000
C56	C	0.41120	0.80916	1.17465	1.000	0.000
C57	C	0.19072	0.60263	1.17617	1.000	0.000
C58	C	0.60104	0.41077	1.14952	1.000	0.000
C59	C	0.58815	0.19093	1.15066	1.000	0.000
C60	C	0.80902	0.39885	1.14877	1.000	0.000
C61	C	0.35722	0.64508	0.59790	1.000	0.000
C62	C	0.35476	0.71157	0.58784	1.000	0.000
C63	C	0.28824	0.64261	0.59007	1.000	0.000
C64	C	0.64223	0.35457	0.55962	1.000	0.000
C65	C	0.64515	0.28826	0.56062	1.000	0.000
C66	C	0.71146	0.35749	0.56005	1.000	0.000
C67	C	0.31249	0.62195	0.58883	1.000	0.000
C68	C	0.37786	0.68995	0.58523	1.000	0.000
C69	C	0.30988	0.68731	0.57827	1.000	0.000
C70	C	0.68696	0.37788	0.55181	1.000	0.000
C71	C	0.62185	0.30969	0.55208	1.000	0.000

C72	C	0.69004	0.31274	0.55290	1.000	0.000
C73	C	0.43547	0.41023	0.69388	1.000	0.000
C74	C	0.58852	0.02708	0.69538	1.000	0.000
C75	C	0.97293	0.56451	0.72021	1.000	0.000
C76	C	0.56221	0.58919	0.71651	1.000	0.000
C77	C	0.40797	0.97134	0.69375	1.000	0.000
C78	C	0.02713	0.43971	0.64978	1.000	0.000
C79	C	0.02218	0.40949	0.07380	1.000	0.000
C80	C	0.59189	0.61426	0.13571	1.000	0.000
C81	C	0.38209	0.97466	0.11304	1.000	0.000
C82	C	0.97744	0.59382	0.13629	1.000	0.000
C83	C	0.40541	0.38550	0.11479	1.000	0.000
C84	C	0.61378	0.02282	0.11420	1.000	0.000
C85	C	0.06451	0.42497	0.22302	1.000	0.000
C86	C	0.57584	0.64079	0.28489	1.000	0.000
C87	C	0.35685	0.93188	0.26227	1.000	0.000
C88	C	0.93472	0.57745	0.28487	1.000	0.000
C89	C	0.42090	0.35851	0.26223	1.000	0.000
C90	C	0.63986	0.06550	0.26272	1.000	0.000
C91	C	0.06839	0.44772	0.52780	1.000	0.000
C92	C	0.55383	0.62226	0.59313	1.000	0.000
C93	C	0.37588	0.92939	0.57101	1.000	0.000
C94	C	0.93139	0.55588	0.59538	1.000	0.000
C95	C	0.44338	0.37692	0.56889	1.000	0.000
C96	C	0.62124	0.06868	0.57144	1.000	0.000

N97	N	0.45484	0.57081	1.08809	1.000	0.000
N98	N	0.42871	0.88396	1.06785	1.000	0.000
N99	N	0.11551	0.54636	1.06838	1.000	0.000
N100	N	0.54376	0.42826	1.04736	1.000	0.000
N101	N	0.56918	0.11570	1.04470	1.000	0.000
N102	N	0.88388	0.45603	1.04289	1.000	0.000
H103	H	0.29560	0.58684	0.62650	1.000	0.000
H104	H	0.41300	0.70831	0.62012	1.000	0.000
H105	H	0.29157	0.70421	0.60737	1.000	0.000
H106	H	0.70365	0.41304	0.58508	1.000	0.000
H017	H	0.58670	0.29124	0.58539	1.000	0.000
H108	H	0.70851	0.29606	0.58684	1.000	0.000
H109	H	0.47813	0.62934	0.57086	1.000	0.000
H110	H	0.37052	0.84824	0.54987	1.000	0.000
H111	H	0.15056	0.52300	0.55054	1.000	0.000
H112	H	0.52085	0.36992	0.52807	1.000	0.000
H113	H	0.62753	0.15061	0.52531	1.000	0.000
H114	H	0.84822	0.47876	0.52527	1.000	0.000
H115	H	0.43496	0.66137	0.34361	1.000	0.000
H116	H	0.33888	0.77315	0.32404	1.000	0.000
H117	H	0.22583	0.56528	0.32650	1.000	0.000
H118	H	0.56444	0.33841	0.29952	1.000	0.000
H119	H	0.66053	0.22593	0.30063	1.000	0.000
H120	H	0.77305	0.43524	0.29874	1.000	0.000
H121	H	0.33790	0.58819	1.12809	1.000	0.000

H122	H	0.41134	0.74943	1.11629	1.000	0.000
H123	H	0.25086	0.66202	1.11681	1.000	0.000
H124	H	0.66105	0.41122	1.08780	1.000	0.000
H125	H	0.58853	0.25087	1.08885	1.000	0.000
H24	H	0.74945	0.33884	1.08860	1.000	0.000
H25	H	0.38461	0.56259	1.39309	1.000	0.000
H26	H	0.43763	0.82220	1.37392	1.000	0.000
H27	H	0.17809	0.61638	1.37591	1.000	0.000
H28	H	0.61448	0.43721	1.34866	1.000	0.000
H29	H	0.56175	0.17831	1.35013	1.000	0.000
H30	H	0.82203	0.38543	1.34808	1.000	0.000
H31	H	0.89499	0.46035	0.45798	1.000	0.000
H32	H	0.53910	0.43528	0.46386	1.000	0.000
H33	H	0.56220	0.10439	0.46045	1.000	0.000
H34	H	0.10444	0.54196	0.48359	1.000	0.000
H35	H	0.45904	0.56412	0.50302	1.000	0.000
H36	H	0.43529	0.89500	0.48298	1.000	0.000
H37	H	0.42133	0.47453	0.83508	1.000	0.000
H38	H	0.52451	0.94797	0.83120	1.000	0.000
H39	H	0.05158	0.57881	0.87588	1.000	0.000
H40	H	0.57667	0.52438	0.82532	1.000	0.000
H41	H	0.47224	0.05152	0.79944	1.000	0.000
H42	H	0.94772	0.42385	0.74975	1.000	0.000
H43	H	0.00333	0.37683	-0.03957	1.000	0.000
H44	H	0.62479	0.62892	0.02581	1.000	0.000

H45	H	0.36624	0.99177	0.00304	1.000	0.000
H46	H	0.99534	0.62688	0.02903	1.000	0.000
H47	H	0.37263	0.37149	0.00329	1.000	0.000
H48	H	0.62893	0.00503	0.00422	1.000	0.000
H49	H	0.09136	0.42387	0.09808	1.000	0.000
H50	H	0.57631	0.66843	0.16047	1.000	0.000
H51	H	0.32978	0.90407	0.13862	1.000	0.000
H52	H	0.90739	0.57748	0.15975	1.000	0.000
H53	H	0.42013	0.33087	0.13465	1.000	0.000
H54	H	0.66719	0.09292	0.13759	1.000	0.000
H55	H	0.09759	0.46264	-0.31319	1.000	0.000
H56	H	0.53890	0.63659	-0.24930	1.000	0.000
H57	H	0.36248	0.90023	-0.27069	1.000	0.000
H58	H	0.90201	0.54078	-0.24868	1.000	0.000
H59	H	0.45858	0.36265	-0.27572	1.000	0.000
H60	H	0.63516	0.09798	-0.27160	1.000	0.000
O1	O	-0.00020	0.41635	0.35544	1.000	0.000
O2	O	0.58586	0.58560	0.42088	1.000	0.000
O3	O	0.41016	0.99812	0.39930	1.000	0.000
O4	O	1.00019	0.58812	0.42280	1.000	0.000
O5	O	0.41195	0.41434	0.39974	1.000	0.000
O6	O	0.58545	-0.00015	0.40047	1.000	0.000

Supplementary Table 7. Atomic coordinates of the optimized computational models of DF₃TA-TAPB used in electronic structure calculations.

		x	y	z	Occupancy	U
C1	C	0.48360	0.45692	0.63736	1.000	0.000
C2	C	0.54308	0.02668	0.63736	1.000	0.000
C3	C	0.97332	0.51640	0.63736	1.000	0.000
C4	C	0.51640	0.54308	0.63736	1.000	0.000
C5	C	0.45692	0.97332	0.63736	1.000	0.000
C6	C	0.02668	0.48360	0.63736	1.000	0.000
C7	C	0.45686	0.47275	0.63754	1.000	0.000
C8	C	0.52725	0.98411	0.63754	1.000	0.000
C9	C	0.01589	0.54314	0.63754	1.000	0.000
C10	C	0.54314	0.52725	0.63754	1.000	0.000
C11	C	0.47275	0.01589	0.63754	1.000	0.000
C12	C	0.98411	0.45686	0.63754	1.000	0.000
C13	C	0.47258	0.51558	0.62034	1.000	0.000
C14	C	0.48442	0.95700	0.62034	1.000	0.000
C15	C	0.04300	0.52742	0.62034	1.000	0.000
C16	C	0.52742	0.48442	0.62034	1.000	0.000
C17	C	0.51558	0.04300	0.62034	1.000	0.000
C18	C	0.95700	0.47258	0.62034	1.000	0.000
C19	C	0.44401	0.53157	0.56370	1.000	0.000
C20	C	0.46843	0.91244	0.56370	1.000	0.000
C21	C	0.08756	0.55599	0.56370	1.000	0.000

C22	C	0.55599	0.46843	0.56370	1.000	0.000
C23	C	0.53157	0.08756	0.56370	1.000	0.000
C24	C	0.91244	0.44401	0.56370	1.000	0.000
C25	C	0.43028	0.58838	0.59483	1.000	0.000
C26	C	0.41162	0.84190	0.59483	1.000	0.000
C27	C	0.15810	0.56972	0.59483	1.000	0.000
C28	C	0.56972	0.41162	0.59483	1.000	0.000
C29	C	0.58838	0.15810	0.59483	1.000	0.000
C30	C	0.84190	0.43028	0.59483	1.000	0.000
C31	C	0.44980	0.63171	0.56947	1.000	0.000
C32	C	0.36829	0.81809	0.56947	1.000	0.000
C33	C	0.18191	0.55020	0.56947	1.000	0.000
C34	C	0.55020	0.36829	0.56947	1.000	0.000
C35	C	0.63171	0.18191	0.56947	1.000	0.000
C36	C	0.81809	0.44980	0.56947	1.000	0.000
C37	C	0.42633	0.65093	0.54494	1.000	0.000
C38	C	0.34907	0.77540	0.54494	1.000	0.000
C39	C	0.22460	0.57367	0.54494	1.000	0.000
C40	C	0.57367	0.34907	0.54494	1.000	0.000
C41	C	0.65093	0.22460	0.54494	1.000	0.000
C42	C	0.77540	0.42633	0.54494	1.000	0.000
C43	C	0.38298	0.62738	0.54506	1.000	0.000
C44	C	0.37262	0.75560	0.54506	1.000	0.000
C45	C	0.24440	0.61702	0.54506	1.000	0.000
C46	C	0.61702	0.37262	0.54506	1.000	0.000

C47	C	0.62738	0.24440	0.54506	1.000	0.000
C48	C	0.75560	0.38298	0.54506	1.000	0.000
C49	C	0.36374	0.58416	0.57752	1.000	0.000
C50	C	0.41584	0.77958	0.57752	1.000	0.000
C51	C	0.22042	0.63626	0.57752	1.000	0.000
C52	C	0.63626	0.41584	0.57752	1.000	0.000
C53	C	0.58416	0.22042	0.57752	1.000	0.000
C54	C	0.77958	0.36374	0.57752	1.000	0.000
C55	C	0.38724	0.56504	0.60530	1.000	0.000
C56	C	0.43496	0.82220	0.60530	1.000	0.000
C57	C	0.17780	0.61276	0.60530	1.000	0.000
C58	C	0.61276	0.43496	0.60530	1.000	0.000
C59	C	0.56504	0.17780	0.60530	1.000	0.000
C60	C	0.82220	0.38724	0.60530	1.000	0.000
C61	C	0.35739	0.64724	0.53045	1.000	0.000
C62	C	0.35276	0.71015	0.53045	1.000	0.000
C63	C	0.28985	0.64261	0.53045	1.000	0.000
C64	C	0.64261	0.35276	0.53045	1.000	0.000
C65	C	0.64724	0.28985	0.53045	1.000	0.000
C66	C	0.71015	0.35739	0.53045	1.000	0.000
C67	C	0.31441	0.62331	0.52922	1.000	0.000
C68	C	0.37669	0.69110	0.52922	1.000	0.000
C69	C	0.30890	0.68559	0.52922	1.000	0.000
C70	C	0.68559	0.37669	0.52922	1.000	0.000
C71	C	0.62331	0.30890	0.52922	1.000	0.000

C72	C	0.69110	0.31441	0.52922	1.000	0.000
C73	C	0.47013	0.42066	0.65129	1.000	0.000
C74	C	0.57934	0.04947	0.65129	1.000	0.000
C75	C	0.95053	0.52987	0.65129	1.000	0.000
C76	C	0.52987	0.57934	0.65129	1.000	0.000
C77	C	0.42066	0.95053	0.65129	1.000	0.000
C78	C	0.04947	0.47013	0.65129	1.000	0.000
C79	C	0.04369	0.42985	0.44703	1.000	0.000
C80	C	0.57015	0.61384	0.44703	1.000	0.000
C81	C	0.38616	0.95631	0.44703	1.000	0.000
C82	C	0.95631	0.57015	0.44703	1.000	0.000
C83	C	0.42985	0.38616	0.44703	1.000	0.000
C84	C	0.61384	0.04369	0.44703	1.000	0.000
C85	C	0.11163	0.46043	0.81334	1.000	0.000
C86	C	0.53957	0.65120	0.81334	1.000	0.000
C87	C	0.34880	0.88837	0.81334	1.000	0.000
C88	C	0.88837	0.53957	0.81334	1.000	0.000
C89	C	0.46043	0.34880	0.81334	1.000	0.000
C90	C	0.65120	0.11163	0.81334	1.000	0.000
C91	C	0.09147	0.48903	0.87769	1.000	0.000
C92	C	0.51097	0.60244	0.87769	1.000	0.000
C93	C	0.39756	0.90853	0.87769	1.000	0.000
C94	C	0.90853	0.51097	0.87769	1.000	0.000
C95	C	0.48903	0.39756	0.87769	1.000	0.000
C96	C	0.60244	0.09147	0.87769	1.000	0.000

N1	N	0.45504	0.56947	0.63635	1.000	0.000
N2	N	0.43053	0.88557	0.63635	1.000	0.000
N3	N	0.11443	0.54496	0.63635	1.000	0.000
N4	N	0.54496	0.43053	0.63635	1.000	0.000
N5	N	0.56947	0.11443	0.63635	1.000	0.000
N6	N	0.88557	0.45504	0.63635	1.000	0.000
H1	H	0.48643	0.65188	0.56905	1.000	0.000
H2	H	0.34812	0.83455	0.56905	1.000	0.000
H3	H	0.16545	0.51357	0.56905	1.000	0.000
H4	H	0.51357	0.34812	0.56905	1.000	0.000
H5	H	0.65188	0.16545	0.56905	1.000	0.000
H6	H	0.83455	0.48643	0.56905	1.000	0.000
H7	H	0.44287	0.68749	0.52368	1.000	0.000
H8	H	0.31251	0.75538	0.52368	1.000	0.000
H9	H	0.24462	0.55713	0.52368	1.000	0.000
H10	H	0.55713	0.31251	0.52368	1.000	0.000
H11	H	0.68749	0.24462	0.52368	1.000	0.000
H12	H	0.75538	0.44287	0.52368	1.000	0.000
H13	H	0.32712	0.56381	0.58125	1.000	0.000
H14	H	0.43619	0.76331	0.58125	1.000	0.000
H15	H	0.23669	0.67288	0.58125	1.000	0.000
H16	H	0.67288	0.43619	0.58125	1.000	0.000
H17	H	0.56381	0.23669	0.58125	1.000	0.000
H18	H	0.76331	0.32712	0.58125	1.000	0.000
H19	H	0.37056	0.52859	0.63817	1.000	0.000

H20	H	0.47141	0.84197	0.63817	1.000	0.000
H21	H	0.15803	0.62944	0.63817	1.000	0.000
H22	H	0.62944	0.47141	0.63817	1.000	0.000
H23	H	0.52859	0.15803	0.63817	1.000	0.000
H24	H	0.84197	0.37056	0.63817	1.000	0.000
H25	H	0.90085	0.41032	0.44970	1.000	0.000
H26	H	0.58968	0.49053	0.44970	1.000	0.000
H27	H	0.50947	0.09915	0.44970	1.000	0.000
H28	H	0.09915	0.58968	0.44970	1.000	0.000
H29	H	0.41032	0.50947	0.44970	1.000	0.000
H30	H	0.49053	0.90085	0.44970	1.000	0.000
H31	H	0.42060	0.44999	0.65229	1.000	0.000
H32	H	0.55001	0.97061	0.65229	1.000	0.000
H33	H	0.02939	0.57940	0.65229	1.000	0.000
H34	H	0.57940	0.55001	0.65229	1.000	0.000
H35	H	0.44999	0.02939	0.65229	1.000	0.000
H36	H	0.97061	0.42060	0.65229	1.000	0.000
H37	H	0.01757	0.40617	0.25138	1.000	0.000
H38	H	0.59383	0.61140	0.25138	1.000	0.000
H39	H	0.38860	0.98243	0.25138	1.000	0.000
H40	H	0.98243	0.59383	0.25138	1.000	0.000
H41	H	0.40617	0.38860	0.25138	1.000	0.000
H42	H	0.61140	0.01757	0.25138	1.000	0.000
H43	H	0.14231	0.46231	0.92394	1.000	0.000
H44	H	0.53769	0.68000	0.92394	1.000	0.000

H45	H	0.32000	0.85769	0.92394	1.000	0.000
H46	H	0.85769	0.53769	0.92394	1.000	0.000
H47	H	0.46231	0.32000	0.92394	1.000	0.000
H48	H	0.68000	0.14231	0.92394	1.000	0.000
H49	H	0.10812	0.51831	0.06752	1.000	0.000
H50	H	0.48169	0.58981	0.06752	1.000	0.000
H51	H	0.41019	0.89188	0.06752	1.000	0.000
H52	H	0.89188	0.48169	0.06752	1.000	0.000
H53	H	0.51831	0.41019	0.06752	1.000	0.000
H54	H	0.58981	0.10812	0.06752	1.000	0.000
H55	H	0.29818	0.58669	0.52714	1.000	0.000
H56	H	0.41331	0.71149	0.52714	1.000	0.000
H57	H	0.28851	0.70182	0.52714	1.000	0.000
H58	H	0.70182	0.41331	0.52714	1.000	0.000
H59	H	0.58669	0.28851	0.52714	1.000	0.000
H60	H	0.71149	0.29818	0.52714	1.000	0.000
O1	O	0.08210	0.42385	0.54718	1.000	0.000
O2	O	0.57615	0.65825	0.54718	1.000	0.000
O3	O	0.34175	0.91790	0.54718	1.000	0.000
O4	O	0.91790	0.57615	0.54718	1.000	0.000
O5	O	0.42385	0.34175	0.54718	1.000	0.000
O6	O	0.65825	0.08210	0.54718	1.000	0.000

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Section 4. Supplementary References

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