Supplementary Information

A backbone design principle for covalent organic frameworks: the impact of weakly interacting units on CO$_2$ adsorption

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SOKENDAI, Hayama 240-0193, Japan

Section A. Methods

Section B. Materials and synthetic procedures

Section C. Elemental analysis

Section D. NMR spectra

Section E. FT IR spectral profiles

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Section A. Methods

Fourier transforms Infrared (FT IR) spectra were recorded on a JASCO model FT IR-6100 infrared spectrometer. Powder X-ray diffraction (PXRD) data were recorded on a Rigaku model RINT Ultima III diffractometer by depositing powder on glass substrate, from $2\theta = 1.5^\circ$ up to $60^\circ$ with $0.02^\circ$ increment. TGA measurements were performed on a Mettler-Toledo model TGA/SDTA851e under N$_2$, by heating to 800 °C at a rate of 10 °C min$^{-1}$. Nitrogen sorption isotherms were measured at 77 K with a Bel Japan Inc. model BELSORP-mini II analyzer. Before measurement, the samples were degassed in vacuum at 120 °C for more than 10 h. By using the non-local density functional theory (NLDFT) model, the pore volume was derived from the sorption curve.

The isosteric heat of adsorption, $Q_{st}$, defined as $Q_{st} = RT^2 \left( \frac{\partial\ln p}{\partial T} \right)_q$, was determined using the pure component isotherm fits using the Clausius-Clapeyron equation. $R$ is the gas constant, 8.314 J mol$^{-1}$ K$^{-1}$.

The crystalline structures were determined using the density-functional tight-binding (DFTB+) method including Lennard-Jones (LJ) dispersion. The calculations were carried out with the DFTB+ program package version 1.2.$^1$ DFTB is an approximate density functional theory method based on the tight binding approach and utilizes an optimized minimal LCAO Slater-type all-valence basis set in combination with a two-center approximation for Hamiltonian matrix elements. The Coulombic interaction between partial atomic charges was determined using the self-consistent charge (SCC) formalism. Lennard-Jones type dispersion was employed in all calculations to describe van der Waals (vdW) and $\pi$-stacking interactions. The lattice dimensions were optimized simultaneously with the geometry. Standard DFTB parameters for X–Y element pair (X, Y = C, S, H and N) interactions were employed from the mio-0-1 set.$^2$
Molecular modeling and Pawley refinement were carried out using Reflex, a software package for crystal determination from XRD pattern, implemented in MS modeling version 4.4 (Accelrys Inc.).\textsuperscript{53} Initially, unit cell dimensions for hexagonal lattices were taken from the DFTB calculation and the space group for hexagonal crystal system were selected as \( P3 \), respectively. We performed Pawley refinement for hexagonal lattice to optimize the lattice parameters iteratively until the \( R_{WP} \) value converges. The pseudo–Voigt profile function was used for whole profile fitting and Berrar–Baldinozzi function was used for asymmetry correction during the refinement processes. The final \( R_{wp} \) and \( R_p \) values were \( R_{WP} = 9.56\% \) and \( R_{P} = 6.56\% \) for TFPB-TAPB-COF, \( R_{WP} = 21.7\% \) and \( R_{P} = 15.08\% \) for TFPA-TAPB-COF, \( R_{WP} = 15.60\% \); \( R_{P} = 12.77\% \) for BTMA-TAPA-COF and \( R_{WP} = 9.90\% \); \( R_{P} = 7.65\% \) for TFPA-TAPA-COF, respectively. The high \( R_{wp} \) and \( R_p \) values of TFPA-TAPB-COF are associated with the unclear shoulder peak at around 6°.
Section B. Materials and synthetic procedures

Mesitylene, 1,4-dioxane and tetrahydrofuran (THF) were purchased from Wako chemicals. Tris(4-aminophenyl)amine (TAPA), 1,3,5-tris(4-aminophenyl)benzene (TAPB), tris(4-formylphenyl)amine (TFPA) and acetic acid were purchased from TCI. 1,3,5-Tris (4-formylphenyl)benzene (TFPB) was synthesized according to a reported method.\textsuperscript{S4} tris(bromoduryl)borane was synthesized according to a reported method.\textsuperscript{S5}

Synthesis of 4,4',4"-boranetriyltris(2,3,5,6-tetramethylbenzaldehyde) (BTMA). To an anhydrous THF solution (40 mL) of tris(bromoduryl)borane (1 g, 1.6 mmol) was added dropwise with a pentane solution of t-BuLi (1.5 M, 5 mL, 7.5 mmol) at −78 °C. The mixture was stirred for 2 h and anhydrous DMF (5 mL) was added at −78 °C. The mixture was warmed up to room temperature over 1 h and stirred overnight. The mixture was charged with concentrated HCl and stirred for 1 h. After addition of water (100 mL), the mixture was extracted with CH\textsubscript{2}Cl\textsubscript{2} (100 mL x 3). The extract was combined and washed with brine and water, dried over anhydrous MgSO\textsubscript{4}, and concentrated under reduced pressure. The crude product was purified by column chromatography using a mixture of CH\textsubscript{2}Cl\textsubscript{2} and hexane (1:1 to 3:1) as eluent to obtain the product 4,4',4"-boranetriyltris(2,3,5,6-tetramethylbenzaldehyde) as a white solid (220 mg, 27% yield). \textsuperscript{1}HNMR (CDCl\textsubscript{3}): 10.64 (s, 3H), 2.28 (s, 18H) and 1.97 (s, 18H).

**TFPB-TAPB-COF.** A mesitylene/1,4-dioxane (0.9 mL/0.1 mL) mixture of TFPB (0.048 mmol, 18.9 mg) and TAPB (0.048 mmol, 17 mg) in the presence of acetic acid (6 M, 0.1 mL) in a Pyrex tube (10 mL) was degassed by three freeze-pump-thaw cycles. The tube was sealed off by flame sand heated at 120 °C for 3 days. The precipitate was collected via centrifuge, washed with THF for 6 times. The powder was dried at 120 °C under vacuum overnight to give the corresponding TFPB-TAPB-COF in 87% isolated yield.

**TFPA-TAPB-COF.** A mesitylene/1,4-dioxane (0.5 mL/0.5 mL) mixture of TFPA (0.048 mmol, 15.94 mg) and TAPB (0.048 mmol, 17 mg) in the presence of acetic acid (6 M, 0.1 mL) in a
Pyrex tube (10 mL) was degassed by three freeze-pump-thaw cycles. The tube was sealed off by flame and heated at 120 °C for 3 days. The precipitate was collected via centrifuge, washed with THF for 6 times. The powder was dried at 120 °C under vacuum overnight to give the corresponding TFPA-TAPB-COF in 84% isolated yield.

**BTMA-TAPA-COF.** An o-DCB/n-BuOH (0.5 mL/0.5 mL) mixture of TAPA (17.8 mg, 0.0617 mmol) and BTMA (30.37 mg, 0.0617 mmol) in the presence of acetic acid (6 M, 0.1 mL) in a Pyrex tube (10 mL) was degassed by three freeze-pump-thaw cycles. The tube was sealed off by flame and heated at 120 °C for 3 days. The precipitate was collected via centrifuge, washed with THF for 6 times. The powder was dried at 120 °C under vacuum overnight to give the corresponding BTMA-TAPA-COF in 78% isolated yield.

**TFPA-TAPA-COF.** A mesitylene/1,4-dioxane (0.5 mL/0.5 mL) mixture of TAPA (0.049 mmol, 14.1 mg) and TFPA (0.048 mmol, 15.94 mg) in the presence of acetic acid (6 M, 0.1 mL) in a Pyrex tube (10 mL) was degassed by three freeze-pump-thaw cycles. The tube was sealed off by flame and heated at 120 °C for 3 days. The precipitate was collected via centrifuge, washed with THF for 6 times. The powder was dried at 120 °C under vacuum overnight to give the corresponding TFPA-TAPA-COF in 85% isolated yield.
Section C. Elemental analysis

**Table S1.** Elemental analysis results of TFPB-TAPB-COF, TFPA-TAPB-COF, BTMA-TAPA-COF and TFPA-TAPA-COF

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Section D. NMR spectra

Figure S1. $^1$HNMR of 4,4',4''-boranetriyltris(2,3,5,6-tetramethylbenzaldehyde, BTMA) (CDCl$_3$)

Figure S2. $^{13}$C NMR of 4,4',4''-boranetriyltris(2,3,5,6-tetramethylbenzaldehyde, BTMA) (CDCl$_3$)
Section E. IR spectroscopy

Figure S3. FT-IR spectra of TFPB-TAPB-COF (black), TFPA-TAPB-COF (blue), BTMA-TAPA-COF (purple) and TFPA-TAPA-COF (red).
Section F. Thermal gravimetric analysis

**Figure S4.** TGA curve of TFPB-TAPB-COF (black curves), TFPA-TAPB-COF (blue curves), BTMA-TAPA-COF (purple curves) and TFPA-TAPA-COF (red curves).
Figure S5. PXRD assignments of (A) TFPB-TAPB-COF, (B) TFPA-TAPB-COF, (C) BTMA-TAPA-COF and (D) TFPA-TAPA-COF. The originality of the shoulder peak around 6° in (B) is unclear.
Section H. Nitrogen adsorption isotherm

**Figure S6.** Nitrogen adsorption isotherm curves of TFPB-TAPB-COF (black curve), TFPA-TAPB-COF (blue curve), BTMA-TAPA-COF (purple curve) and TFPA-TAPA-COF (red curve) at (A) 273 K and (B) 298 K.
Section I. Cycling performance of CO$_2$ capture capacity

Figure S7. CO$_2$ uptake cycling performance of TFPA-TAPA-COF at 273 K.
Section J. Atomistic coordinates

Table S2. Atomistic coordinates for the AA-stacking mode of TFPB-TAPB-COF optimized by using DFTB+ method. Space group: $P3; a = 26.0324 \, \text{Å}, b = 26.0324 \, \text{Å},$ and $c = 3.6329 \, \text{Å}$.

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Table S3. Atomistic coordinates for the refined unit cell parameters for TFPB-TAPB-COF via Pawley refinement. Space group: $P3; a = 26.0077 \text{ Å}, b = 26.0077 \text{ Å},$ and $c = 3.6347 \text{ Å}.$

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Table S4. Atomistic coordinates for the AB-stacking mode of TFPB-TAPB-COF optimized by using DFTB+ method. Space group: \( P3; \ a = 25.9516 \, \text{Å}, \ b = 25.9516 \, \text{Å}, \) and \( c = 6.3891 \, \text{Å} \).

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Table S6. Atomistic coordinates for the refined unit cell parameters for TFPA-TAPB-COF via Pawley refinement. Space group: *P*3; *a* = 23.4694 Å, *b* = 23.4694 Å, and *c* = 3.8935 Å.

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**Table S9.** Atomistic coordinates for the refined unit cell parameters for TFPA-TAPA-COF via Pawley refinement. Space group: $P3; \ a = 20.0691\ \diameter, \ b = 20.0691\ \diameter, \text{and} \ c = 4.1936\diameter$.

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Table S10. Atomistic coordinates for the AB-stacking mode of TFPA-TAPA-COF optimized by using DFTB+ method. Space group: $P3$; $a = 20.8778$ Å, $b = 20.8778$ Å, and $c = 7.7734$ Å.

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Table S13. Atomistic coordinates for the AB-stacking mode of BTMA-TAPA-COF optimized by using DFTB+ method. Space group: $P3$; $a = 20.878$ Å, $b = 20.8778$ Å, and $c = 7.7734$ Å.

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Section K. Supporting references


