Supporting Information

for

Efficient natural gas upgrading by a stable Cd-based porous coordination network

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Materials

All chemicals and reagents except 2,4,6-tris (4-pyridyl) pyridine (TPP) were purchased from the commercial suppliers and directly employed without further purification. TPP was synthesized according to a previously reported literature^[1].

Cadmium nitrate tetrahydrate (Cd(NO₃)₂·4H₂O, AR, 99.99%) was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd., 5-tert-butylisophthalic acid (^tBu-IPA, GC, 99.0%) was purchased from Shanghai Macklin Biochemical Technology Co., Ltd, N,N-dimethylformamide (DMF, GC, 99.5%) was purchased from Shanghai Titan Scientific Co., Ltd., acetonitrile (MeCN, AR, 99.5%) was purchased from Guangdong Guanghua Sci-Tech Co., Ltd, and tetrafluoroboric acid (HBF₄, wt. 40%) were purchased from Shanghai Macklin Biochemical Technology Co., Ltd.

Material characterization

Powder X-ray diffraction (PXRD) data were collected at ambient temperature and pressure using a Rigaku-Miniflex-600 diffractometer equipped with Cu Ka radiation ($\lambda = 1.5418$ Å) operated at 40 kV and 15 mA. The data measurement parameters included a radiation range of 20 from to 5-50 degrees, a scan step of 0.02 degree, and scan rate of 20 degree/min. Thermogravimetric analysis (TGA) data were obtained using a TGA-55 Thermogravimetric Analyzer, with test temperatures ranging from room temperature to 800 °C. Throughout the measurement process, the sample was constantly exposed to a nitrogen atmosphere (nitrogen flow rate of 40 mL/min) at a heating rate of 10 °C/min.

X-ray Crystallography data based structural determination

Single crystals of **Cd-TPP-'Bu-IPA** suitable for X-ray analysis were selected directly from the synthesized samples. Single crystals of **Cd-TPP-'Bu-IPA** were collected at 393 K on a Bruker D8 Venture diffractometer equipped with a Ga K α microfocus X-ray generator (λ =1.34139 Å) and Photon II detector. The data were empirically corrected for X-ray adsorption by Sadabs^[2,3] using the Bruker APEX II software suite. The structures were solved by the direct method and refined with the fullmatrix least-squares technique using the SHELXTL program package.^[4] Crystal data and structure determination summary are listed in Supplementary Table 1. The X-ray crystallographic coordinates for the structures reported in this study were deposited at the Cambridge Crystallographic Data Centre (CCDC) under deposition number 2412514 and can be obtained free of charge (http://www.ccdc.cam.ac.uk/data_request/cif).

Single-component gas sorption experiment

All high-purity gases used in the single-component gas sorption experiments were procured commercially, including He (99.999%), N₂ (99.999%), CH₄ (99.99%), C₂H₆ (99.99%), and C₃H₈ (99.99%). Prior to each measurement, approximately 40 mg of the methanol-exchanged **Cd-TPP-**^t**Bu-IPA** samples was degassed under high vacuum at 393 K for 6 h to eliminate impurities from the material pores, ensuring regeneration between every two independent isotherms. A Micromeritics 3Flex instrument was used to collect all sorption isotherms, and when testing N₂ adsorption isotherms, the temperature was controlled at 77 K using a Dewar bottle containing 4 L of liquid N₂.

Calculation of isosteric heat of adsorption (Q_{st}) by Virial equation

Before the calculation of Q_{st} , the gas adsorption isotherms of CH₄, C₂H₆, and C₃H₈ at 273 and 298 K were fitted based on the virial equation^[5]:

$$\ln P = \ln N + \frac{1}{T} \sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i$$

Where *P* is the pressure (kPa), *N* is the amount absorbed in mmol·g⁻¹, *T* is the temperature in K, a_i and b_i are virial coefficients, and *m* and *n* are the coefficients to fit the adsorption isotherm.

Based on the virial coefficients $a_0 - a_m$ obtained from the fitted isotherms, the isosteric heat of absorption (Q_{st}) was calculated using the following equation:

$$Q_{st} = -R \sum_{i=0}^{m} a_i N^i$$

 Q_{st} is the coverage-dependent isosteric heat of adsorption and R is the universal gas constant with the value of (8.314 J·K⁻¹·mol⁻¹). The Q_{st} of CH₄, C₂H₆ and C₃H₈ for

Cd-TPP-^t**Bu-IPA** are determined by using the sorption data in the pressure range from 0-100 kPa at 273 K and 298 K.

Ideal Adsorption Solution Theory (IAST) Calculation

The C_2H_6/CH_4 and C_3H_8/CH_4 selectivities in **Cd-TPP-**^t**Bu-IPA** at 298 K were calculated using IAST^[6]. Before this, the single-component gas adsorption isotherms for CH₄, C_2H_6 , and C_3H_8 were fitted using a single-site Langmuir-Freundlich model^[7]:

$$q = q_{A, sat} \frac{(b_A p)^{c_A}}{1 + (b_A p)^{c_A}}$$

Where p (kPa) represents the equilibrium pressure of the bulk gas with the adsorbed phase, q (mmol·g⁻¹) represents the amount of gas uptake, $q_{A,sat}$ (mmol g⁻¹) represents the gas saturation adsorption amount, b_A (kPa⁻¹) represents the affinity coefficient, and c_A represents the deviation from an ideal homogeneous surface site.

The adsorption selectivity of the binary gas mixture was calculated using IAST:

$$S = \frac{X_A / X_B}{Y_A / Y_B}$$

Where *S* is the selectivity of component A over B, X_A and X_B represent the mole fractions of components A and B in the adsorption phase, respectively, *and* Y_A and Y_B represent the mole fractions of components A and B in the bulk phase, respectively.

Dynamic gas breakthrough experiment

All breakthrough curves were obtained using homemade equipment at 298 K and 100 kPa pressure. About 2.3 g of Cd-TPP-^tBu-IPA was packed into a stainless steel column. Before the start of the experiment, the column filled with the samples was continuously purged under a He flow of 10 mL/min at 393 K for 6 h. The total gas flow rates of C_2H_6/CH_4 and C_3H_8/CH_4 (v/v = 50/50), C_2H_6/CH_4 (v/v = 10/90), C_3H_8/CH_4 (v/v = 5/95), and C_3H_8/CH_4 (v/v = 5/10/85) were 5 mL/min. In addition, the outlet gas concentration in the column was continuously measured using a He flow of 10 mL/min at 333 K.

The purity of CH₄ is calculated by the concentration of the gases flowing out of

the packing column. For $C_3H_8/C_2H_6/CH_4$ gas mixture, the purity of CH_4 was calculated using the following equation:

$$P = \frac{C_{CH_4}/C_0 \times F_{CH_4}}{C_{CH_4}/C_0 \times F_{CH_4} + C_{C_2H_6}/C_0 \times F_{C_2H_6} + C_{C_3H_8}/C_0 \times F_{C_3H_8}}$$

Here, P is the purity of CH₄, ${}^{C}C_{2H_6}$, ${}^{C}C_{3H_8}$ is the concentrations of filled column outlet CH₄, C₂H₆ and C₃H₈, respectively. ${}^{C}O$ is the concentration of the inlet gas of the packing column. ${}^{F}C_{H_4}$, ${}^{F}C_{2H_6}$, ${}^{F}C_{3H_8}$ is the flow rate of CH₄, C₂H₆ and C₃H₈ in mL/min.

The calculation of CH_4 purity of C_2H_6/CH_4 and C_3H_8/CH_4 gas mixture uses the same method.

 CH_4 productivity was obtained from the breakthrough curve of CH_4 and calculated using the following equation:

$$Q_{CH_4} = \frac{\int_{t_1}^{t_2} \frac{C_t}{C_0} dt \times F_{CH_4}}{V_m}$$

Where t_1 is the per gram CH₄ eluted time in min/g, t_2 is the per gram C₂H₆ eluted time in min/g, C_0 is the CH₄ concentration in the mixed gas, C_t is the CH₄ concentration in the outlet gas, ${}^{F}_{CH_4}$ is the flow rate of CH₄ in mL/min, and V_m is the molar volume of the gas.

Grand Canonical Monte Carlo (GCMC) simulation

The GCMC simulations were performed using the Material Studio software package, and the simulation models of the adsorption sites of CH_4 , C_2H_6 , and C_3H_8 were obtained using the sorption module from the GCMC simulations. Both the host framework and guest molecules were considered rigid bodies. The simulation box consists of a 2 × 2 × 2 supercell. Additionally, a standard universal force field was used to describe interatomic interactions ^[8].

Before the GCMC simulations, a simulation model of the Cd–TPP-^tBu-IPA framework was built from the crystal data (CCDC NO. 2412514). The loading,

equilibration, and production steps were all set to 2.0×10^7 . Saturation uptakes were simulated at 298 K using the fixed pressure task, which included 1.0×10^5 equilibration steps followed by 2.0×10^7 production steps to calculate the ensemble averages. The beneficial adsorption sites were modeled using the locate task with one guest molecule, and the fixed loading task was utilized to evaluate the binding energy at 298 K.

Stability Testing Methods

To evaluate thermal stability, the as-synthesized samples were placed in a hightemperature oven under an ambient air atmosphere. The samples were heated successively to 25, 50, 100, 150, 200, 250, 300, 350, and 400 °C at a constant heating rate of 10 °C/min and were maintained at each temperature for 30 minutes. Subsequently, PXRD patterns were recorded after each temperature step to assess the structural stability of the materials.

To evaluate solvent stability, the as-synthesized samples were soaked in various organic solvents and aqueous solutions (acidic, basic, and neutral) for 1 day and 3 days, followed by characterization via PXRD measurements, N_2 adsorption at 77 K and C_2H_6 adsorption at 298 K.

The moisture stability of **Cd-TPP-'Bu-IPA** was evaluated through controlled accelerated aging tests by exposing the samples under simulated humid air conditions (40 °C, 75% relative humidity) for a certain time in a sealed two-layer desiccator. The samples and a supersaturated aqueous sodium chloride (NaCl) solution were first placed in an enclosed desiccator, which was subsequently placed in an oven held at 40 °C to maintain the target humidity level. The time frame used for our studies was 1 h, 3 h, 5 h, 12 h, 1 d, 3 d, and 7 d. Once the sample was subjected to the desired amount of time, it was removed from the desiccator and characterized in order to detect if the sample had been affected by exposure to humidity. The moisture stability of the samples was determined by PXRD measurements, N₂ sorption measurements at 77 K, and C_2H_6 gas sorption measurements at 298 K, in which structural integrity was quantified through PXRD patterns, while bulk porosity and chemical stability was quantified through N₂ physisorption at 77 K and C_2H_6 gas sorption at 298 K.



Figure S1. Local coordination environments of Cd²⁺, ^tBu-IPA^{2-,} and TPP ligands in Cd-TPP-^tBu-IPA.



Figure S2. TG curves of Cd-TPP-^tBu-IPA.



Figure S3. BET fitting for 77 K N_2 for Cd-TPP-^tBu-IPA.



Figure S4. Single-component CH_4 , C_2H_{6} , and C_3H_8 adsorption isotherms of Cd-TPP-^tBu-IPA at 273 K.



Figure S6. Comparison of the zero-coverage isosteric heat of adsorption (Q_{st}) for C_2H_6 and C_3H_8 between Cd-TPP-^tBu-IPA and other reported materials.



Figure S7. Langmuir-Freundlich (L-F) fitting of CH_4 (a), C_2H_6 (b), C_3H_8 (c) adsorption data and fitting parameters (d) at 298 K for **Cd-TPP-^tBu-IPA**.



Figure S8. Dynamic breakthrough curves of Cd-TPP-^tBu-IPA for C_2H_6/CH_4 (v/v = 10/90) gas mixtures at 298 K and 100 kPa.



Figure S9. Concentrations of C_2H_6 and CH_4 in the C_2H_6/CH_4 (v/v = 10/90) gas mixture of Cd-TPP-^tBu-IPA.



Figure S10. Dynamic breakthrough curves of Cd-TPP-^tBu-IPA for C_3H_8/CH_4 (v/v = 5/95) gas mixtures at 298 K and 100 kPa.



Figure S11. Concentrations of C_3H_8 and CH_4 in the outlet C_3H_8/CH_4 (v/v = 5/95) gas mixture of Cd-TPP-^tBu-IPA.



Figure S12. Dynamic breakthrough curves of Cd-TPP-^tBu-IPA for C_2H_6/CH_4 (v/v = 50/50) gas mixtures at 298 K and 100 kPa.



Figure S13. Concentrations of C_2H_6 and CH_4 in the C_2H_6/CH_4 (v/v = 50/50) gas mixture of Cd-TPP-^tBu-IPA.



Figure S14. Dynamic breakthrough curves of Cd-TPP-^tBu-IPA for C_3H_8/CH_4 (v/v = 50/50) gas mixtures at 298 K and 100 kPa.



Figure S15. Concentrations of C_3H_8 and CH_4 in the C_3H_8/CH_4 (v/v = 50/50) gas mixture of Cd-TPP-^tBu-IPA.



Figure S16. Concentrations of C_3H_8 , C_2H_{6} , and CH_4 in the outlet $C_3H_8/C_2H_6/CH_4$ (v/v/v = 5/10/85) gas mixture of **Cd-TPP-^tBu-IPA** during the breakthrough time.



Figure S17. The integrated areas of (a) 99.9% and (b) 95% CH₄ purity in Cd-TPP-^tBu-IPA during $C_3H_8/C_2H_6/CH_4$ (v/v/v = 5/10/85) ternary breakthrough experiment at 298 K and 100 kPa.

The corresponding CH₄ productivity values were calculated as:

$$Q_{CH_4}(99.9\%) = \frac{60.54163 \times 4.25}{22.4} = 11.49 \ mmol \cdot g^{-1}$$
$$Q_{CH_4}(95\%) = \frac{63.19403 \times 4.25}{22.4} = 11.99 \ mmol \cdot g^{-1}$$



Figure S18. Concentrations of C_3H_8 , C_2H_6 , and CH_4 in the outlet $C_3H_8/C_2H_6/CH_4$ (v/v/v = 5/10/85) gas mixture of **Cd-TPP-^tBu-IPA** during the regeneration time.



Figure S19. The integrated areas of 99.5% C_3H_8 purity in **Cd-TPP-**^t**Bu-IPA** during $C_3H_8/C_2H_6/CH_4$ (v/v/v = 5/10/85) during the desorption process at 298 K and 100 kPa.

The productivity of C₃H₈ (>99.5%) was calculated as:

$$Q_{C_3H_8} = \frac{\int_{t_1}^{t_2} \frac{C_t}{C_0} dt \times F_{C_3H_8}}{V_m} = \frac{50.93431 \times 0.25}{22.4} = 0.57 \, mmol \cdot g^{-1}$$

The recovery of C_3H_8 (>99.5%) was calculated as:

$$Rec_{C_{3}H_{8}}(\%) = \frac{Q_{C_{3}H_{8}}}{F_{feed, C_{3}H_{8}}} \times 100\% = \frac{Q_{C_{3}H_{8}}}{t_{3} \times F_{C_{3}H_{8}}/V_{m}} \times 100\%$$
$$= \frac{0.57}{230.0 \times 0.25/22.4} \times 100\% = 22.21\%$$

Here, t_1 , t_2 , t_3 are the per gram C₃H₈ eluted time in min/g, specifically 256.3 min/g, 301.2 min/g, and 230.0 min/g, respectively. C_0 is the C₃H₈ concentration in the mixed gas, C_t is the C₃H₈ concentration in the outlet gas, ${}^{F}C_{3}H_{8}$ is the flow rate of C₃H₈ in mL/min, ${}^{F}feed$, $C_{3}H_{8}$ is the feed quantity of C₃H₈ in mmol·g⁻¹, and V_m is the molar volume of the gas.



Figure S20. Concentrations of C_3H_8 , C_2H_6 , and CH_4 in the outlet $C_3H_8/C_2H_6/CH_4$ (v/v/v = 33/33/33) gas mixture of **Cd-TPP-**^t**Bu-IPA** during the breakthrough time.



Figure S21. The integrated areas of (a) 99.9% and (b) 95% CH₄ purity in Cd-TPP-^tBu-IPA during $C_3H_8/C_2H_6/CH_4$ (v/v/v = 33/33/33) ternary breakthrough experiment at 298 K and 100 kPa.

The corresponding CH₄ productivity values were calculated as: $Q_{CH_4}(99.9\%) = \frac{50.95028 \times 1.67}{22.4} = 3.80 \text{ mmol} \cdot g^{-1}$ $Q_{CH_4}(95\%) = \frac{52.72122 \times 1.67}{22.4} = 3.93 \text{ mmol} \cdot g^{-1}$



Figure S22. PXRD patterns of Cd-TPP-^tBu-IPA after gas adsorption and breakthrough tests.



Figure S23. VT-PXRD patterns of Cd-TPP-^tBu-IPA under air atmosphere.



Figure S24. PXRD patterns of as-synthesized **Cd-TPP-**^t**Bu-IPA** after soaking in common solvents for 1 d (DCM refers to dichloromethane, EtOH refers to ethanol).



Figure S25. PXRD patterns of as-synthesized Cd-TPP-^tBu-IPA after soaking in common solvents for 3 d.



Figure S26. Comparison of (a) N_2 adsorption at 77 K and (b) C_2H_6 adsorption capacity at 298 K and 100 kPa for **Cd-TPP-**^t**Bu-IPA** after soaking in common solvents for 1 d (n_0 , N_2 or C_2H_6 uptake for as-synthesized samples; n, N_2 or C_2H_6 uptake for processed samples).



Figure S27. Comparison of (a) N_2 adsorption at 77 K and (b) C_2H_6 adsorption capacity at 298 K and 100 kPa for **Cd-TPP-**^t**Bu-IPA** after soaking in common solvents for 3 d (n_0 , N_2 or C_2H_6 uptake for as-synthesized samples; n, N_2 or C_2H_6 uptake for processed samples).



Figure S28. PXRD patterns of as-synthesized **Cd-TPP-'Bu-IPA** after exposed to a relative humidity of 75% for a certain time.



Figure S29. Comparison of (a) N_2 adsorption at 77 K and (b) C_2H_6 adsorption capacity at 298 K and 100 kPa for **Cd-TPP-'Bu-IPA** after being exposed to a relative humidity of 75% for a certain time (n_0 , N_2 or C_2H_6 uptake for as-synthesized samples; n, N_2 or C_2H_6 uptake for processed samples).



Figure S30. PXRD patterns (a) and picture (b) of up-scaled synthesis of Cd-TPP-^tBu-IPA.

Identification code	Cd-TPP- ^t Bu-IPA
Formula	$C_{25.3}H_{22}CdN_{2.67}O_4$
Formula weight	539.68
Temperature, K	393
Crystal system	Trigonal
Space group	$R\overline{3}$
a, Å	27.7586(5)
b, Å	27.7586(5)
c, Å	21.8927(5)
α, °	90
β, °	90
γ, °	120
Z	18
V, Å ³	14609.2(6)
D_c , g cm ⁻³	1.104
μ, mm ⁻¹	5.602
F(000)	4903.3
R ₁ (all data)	0.0678
wR_2 (all data)	0.1892
GOF	1.057
CCDC No.	2412514

 Table S1. Crystal data and refinement parameters of Cd-TPP-'Bu-IPA.

Materials	$\begin{array}{c} C_2H_6\\ (kJ\cdot mol^{-1})\end{array}$	C_3H_8 (kJ·mol ⁻¹)	Ref.
Cd-TPP- ^t Bu-IPA	-35.56	-47.67	This Work
ZUL-C2	-45	-75	[10]
Ni(TMBDC)(DABCO) _{0.5}	-36	-59	[11]
BSF-2	-32.8	-39.7	[9]
MIL-160	-28	-35	[13]
Zn-BPA-SA	-18.5	-33.5	[19]
Fe-pyz	-51.45	-32.41	[16]
CMOM-7	-27.9	-31.2	[23]
MIL-101-Fe-NH ₂	-24.6	-28.3	[18]
MIL-142A	-25.5	-26.6	[22]
Zn(BDC)(TED) _{0.5}	-21	-25.1	[15]

Table S2. Comparison of the zero-coverage isosteric heat of adsorption (Q_{st}) for C_2H_6 and C_3H_8 among some reported materials.

Table S3. Comparison of the IAST selectivity towards gas mixtures of C_2H_6/CH_4 (v/v = 50/50) and C_3H_8/CH_4 (v/v = 50/50) of some reported materials at 298 K and 100 kPa.

Materials	C ₂ H ₆ /CH ₄ selectivity	C ₃ H ₈ /CH ₄ selectivity	Ref.
Cd-TPP- ^t Bu-IPA	24.4	271.1	This Work
BSF-2	53	2609	[9]
ZUL-C2	82ª	741 ^b	[10]
Ni(TMBDC)(DABCO) _{0.5}	29 ^a	274 ^b	[11]
$DMOF-(CF_3)_2$	15.1ª	196.9 ^b	[12]
MIL-160	20ª	174 ^b	[13]
NUM-18a	19.7	109.0	[14]
Zn(BDC)(TED) _{0.5}	9.7ª	96 ^b	[15]
Fe-pyz	23	89	[16]
iso-MOF-4	8.5	80	[17]
MIL-101-Fe-NH ₂	11.6 ^a	42.5 ^b	[18]
Zn-BPA-SA	10.5	40.6	[19]

^a IAST selectivity calculated using ideal adsorption solution theory under the condition $C_2H_6/CH_4 = 10/85$.

^b IAST selectivity calculated using ideal adsorption solution theory under the condition $C_3H_8/CH_4 = 5/85$.

Materials	CH ₄ productivity (mmol·g ⁻¹)	Ref.
Cd-TPP- ^t Bu-IPA	11.49	This Work
Ni(TMBDC)(DABCO) _{0.5}	13.28	[11]
ZUL-C2	11.4	[10]
$Zn(NDC)(TED)_{0.5}$	10.07	[15]
Fe-pyz	8.54	[16]
SNNU-Bai69	6	[20]
Ni(3-aia)(2-atp) _{0.5}	4.4	[21]
MIL-142A	3.8	[22]
BSF-2	3.1	[9]
CMOM-7	3.04	[23]
UiO-66-Naph	2.25	[24]
LIFM-W2	1.02	[25]

Table S4. Comparison of Cd-TPP-^tBu-IPA with other materials on CH₄ productivity for $C_3H_8/C_2H_6/CH_4$ (5/10/85, v/v/v).

C ₃ H ₈ /C ₂ H ₆ /CH ₄ (v/v/v)	CH ₄ purity	CH ₄ productivity (mmol·g ⁻¹)
5/10/85	99.9%	11.49
	95%	11.99
33/33/33	99.9%	3.80
	95%	3.93

Table S5. CH_4 productivity corresponding to different purity levels during the $C_3H_8/C_2H_6/CH_4$ ternary breakthrough experiments.

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