

Supplementary Information

Isomers recognition by dynamic guest-adaptive ligand rotation in a metal-organic framework with local flexibility

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1. Materials and Methods

Materials and reagents

All chemicals were used directly without further purification. *N, N*-dimethylformamide (DMF) and methanol were bought from Tianjin Damao Chemical Reagent Factory. PX, MX, and OX were purchased from Tianjin Guangfu Fine Chemical Industry Research Institute. EB was obtained from Alfa Aesar (China) Chemicals Co., Ltd. *N*-propylbenzene (N-PB), and ethyltoluene isomers including *p*-ethyltoluene (P-ET), *m*-ethyltoluene (M-ET) and *o*-ethyltoluene (O-ET) were purchased from Aladdin Co. Ltd (Shanghai, China). 1,4-diazabicyclo [2.2.2] octane (TED) and 1,4-benzenedicarboxylic acid (H₂BDC) were procured from Shanghai Bepharma Science & Technology Co., Ltd. Nickel (II) chloride hexahydrate (NiCl₂·6H₂O) was purchased from Fuchen (Tianjin) Chemical Reagent Co., Ltd. 9,10-anthracenedicarboxylic acid (H₂ADC) was obtained from Shanghai Tengsai Biotechnology Co., Ltd. Chloroform-*d* (deuteriochloroform, CDCl₃) was purchased from J&K Scientific Ltd.

Methods

Pawley refinements were performed on the Reflex module of Materials Studio, using 2 theta data from 5° to 50°. The integrated intensities were extracted with the Pseudo-Voigt profile and the Finger-Cox-Jephcoat method was used to correct the peak asymmetry. For all structures, the unit cell parameters *a*, *b*, *c*, FWHM parameters, *U*, *V*, *W*, profile parameters *NA*, *NB*, and zero point were refined. The background was also refined with 20th order polynomial.

The Hirshfeld surface was calculated through the program Crystal Explorer¹, and it was constructed on the basis of the calculated electron distribution as the sum of spherical atom electron densities.^{2,3} The Hirshfeld surface is implicitly defined by the equation $w(r)$:

$$w(r) = \sum_{i \in molecule} \rho_i(r) / \sum_{i \in crystal} \rho_i(r) \quad (S1)$$

Where $\rho_i(r)$ is a spherically-averaged atomic electron density located at the i th nucleus.

Calculation of Thermodynamic Parameters.

The adsorption enthalpy and adsorption entropy of the analytes on the stationary phase were determined by gas chromatography and calculated by van't Hoff formula:

$$\ln k' = \frac{\Delta H}{RT} + \frac{\Delta S}{R} + \ln \Phi \quad (S2)$$

Here, k' was the retention factor, R was the gas constant, T was the absolute temperature, Φ was the phase ratio, V_s was volume of the stationary phase, and V_m was the mobile phase.

It was worthy nothing that V_s was calculated from the thickness of stationary phase on the capillary column according to SEM images, while V_m was calculated from the column internal volume subtract the V_s . Then, we could calculate Φ according to the following equation. Finally, we obtained the $\ln \Phi$ for Ni(ADC)(TED)_{0.5} columns were -0.874.

$$\Phi = \frac{V_s}{V_m} \quad (S3)$$

k' was obtained based on:

$$k' = \frac{t - t_0}{t_0} \quad (S4)$$

2. Supplementary Figures

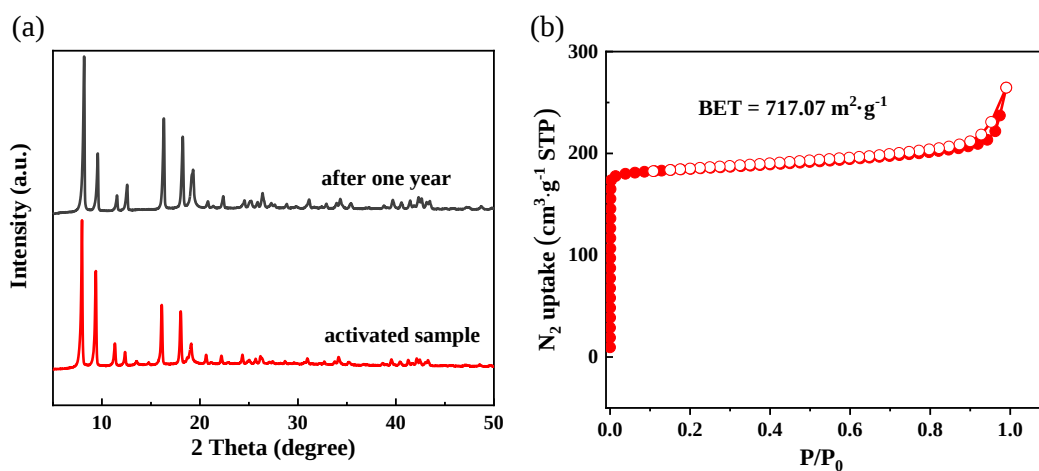


Figure S1. PXRD patterns of $Ni(ADC)(TED)_{0.5}$ (a) and N_2 adsorption and desorption isotherms at 77K (b).

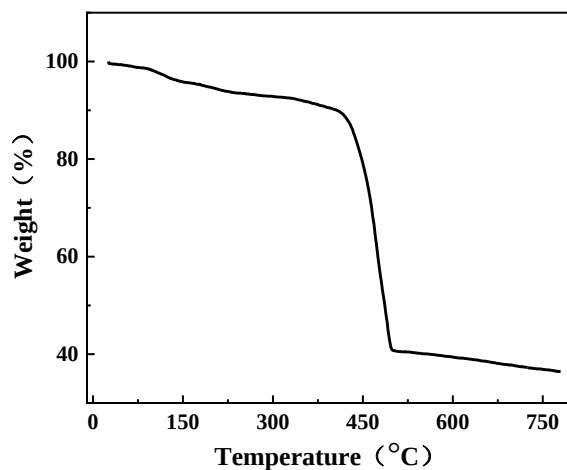


Figure S2. TGA curves of $Ni(ADC)(TED)_{0.5}$.

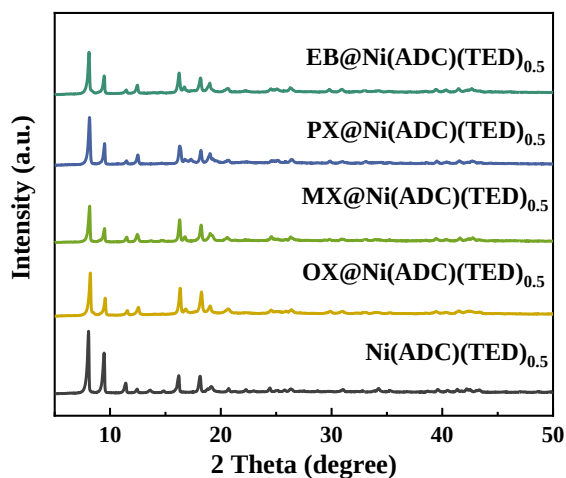


Figure S3. PXRD patterns of the sample and C8 aromatic-included materials.

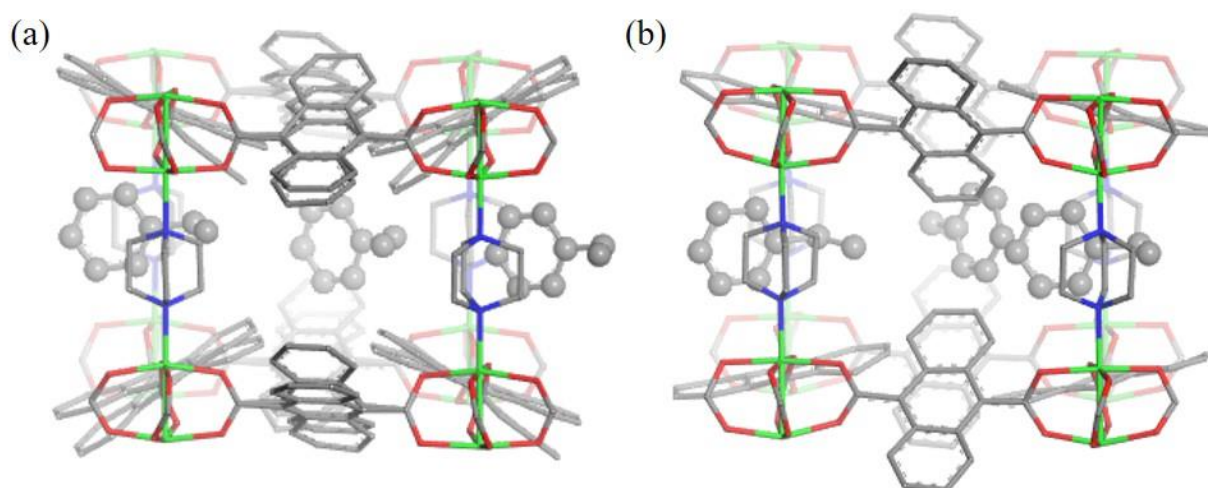


Figure S4. The structure of EB-included for Phase_1 (a) and Phase_2 (b).

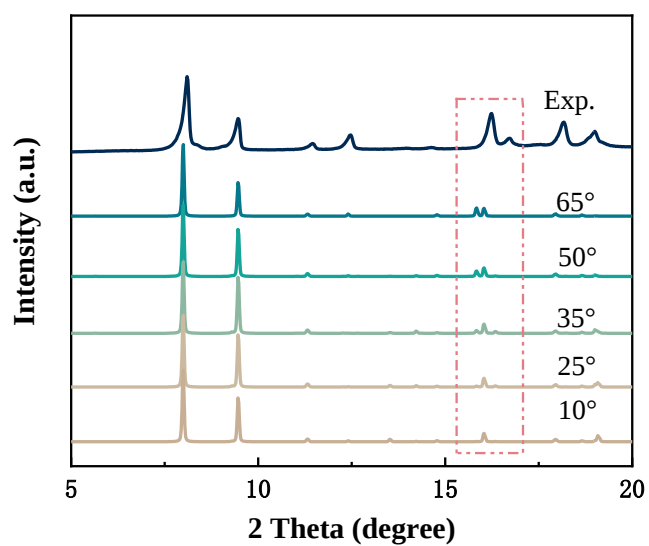


Figure S5. PXRD patterns of simulated the framework with different configurations of anthracene rings.

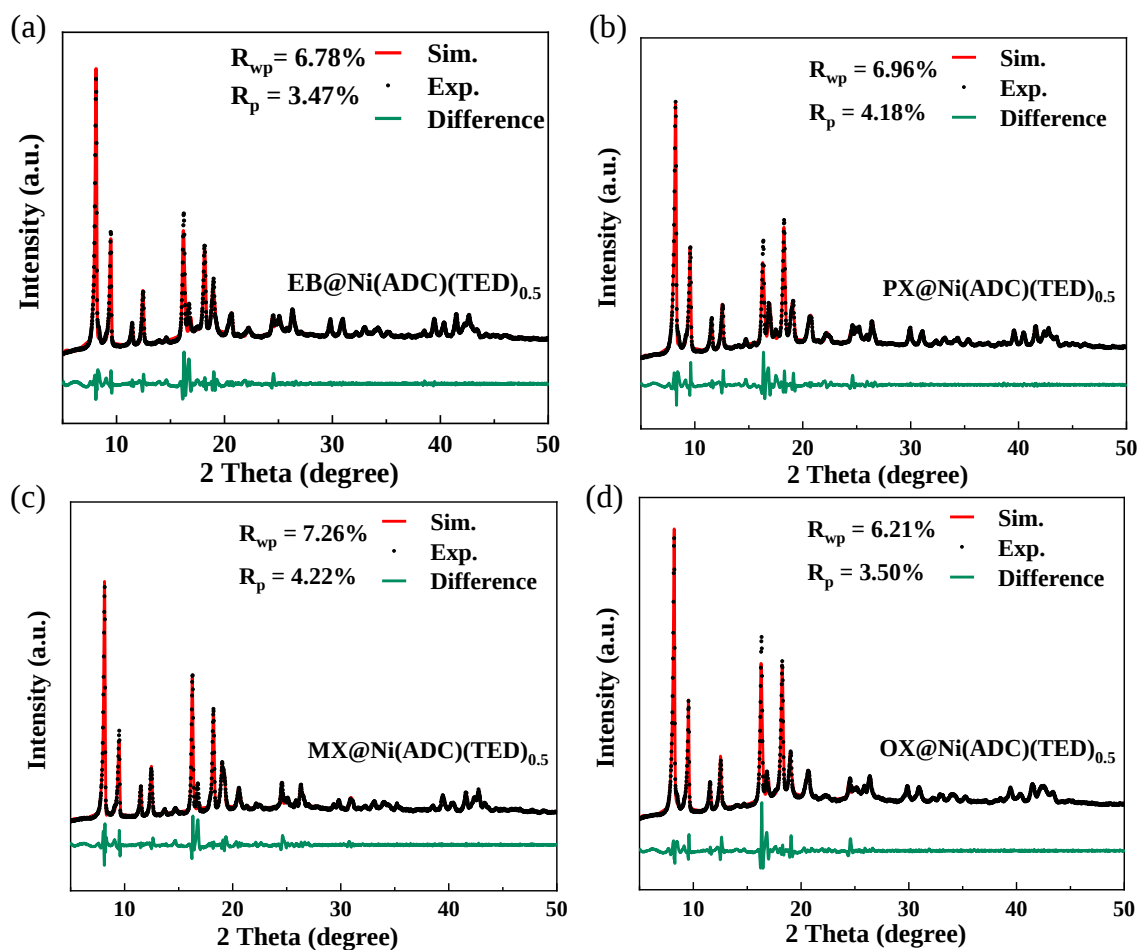


Figure S6. Pawley refinement of MOF structures: (a) EB@ Ni(ADC)(TED)_{0.5}, (b) PX@ Ni(ADC)(TED)_{0.5}, (c) MX@ Ni(ADC)(TED)_{0.5}, (d) OX@ Ni(ADC)(TED)_{0.5}.

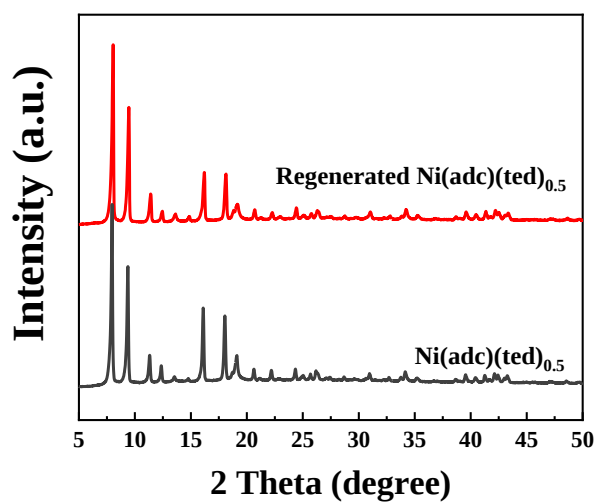


Figure S7. PXRD of Ni(ADC)(TED)_{0.5} and the regenerated sample.

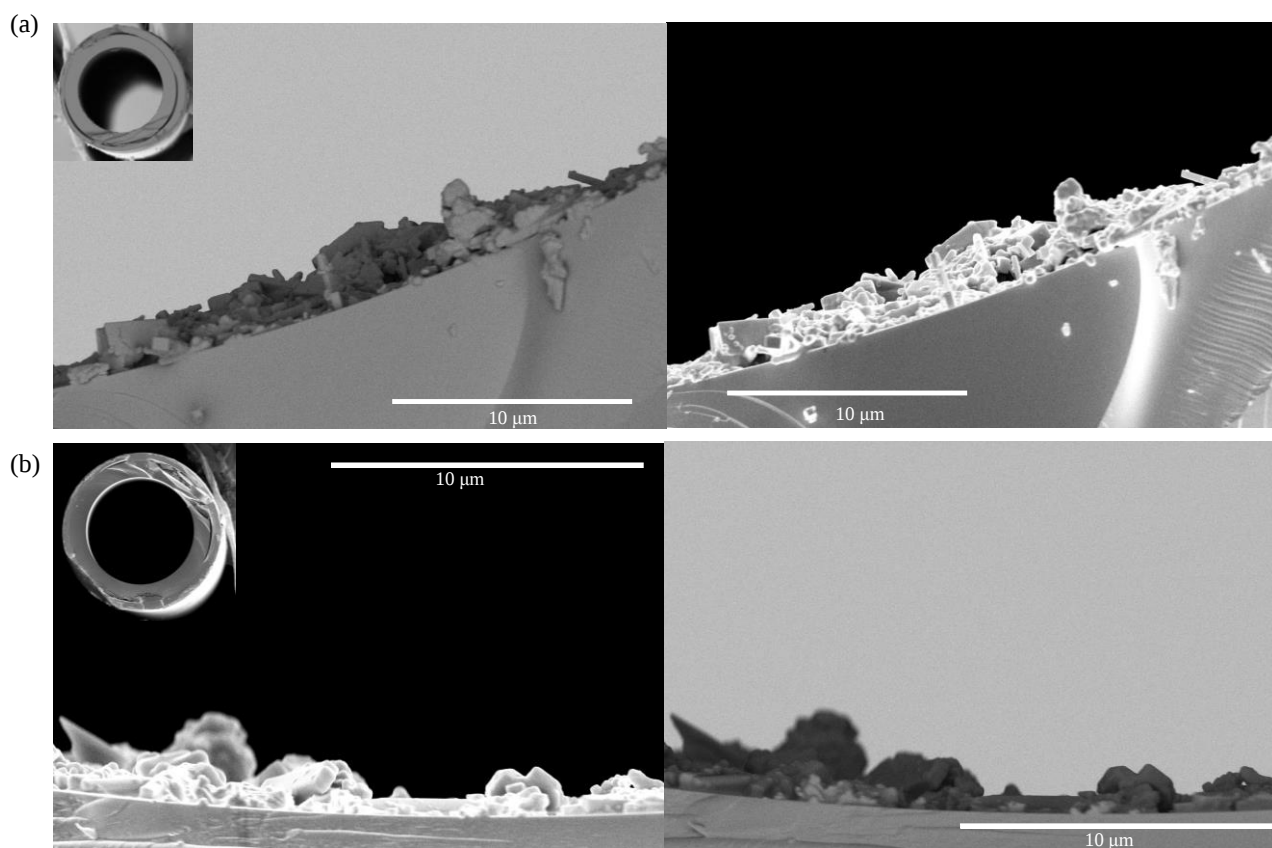


Figure S8. Ni(ADC)(TED)_{0.5} coated capillary column ((a): 2.5 μm thickness; (b): 1.6 μm thickness)

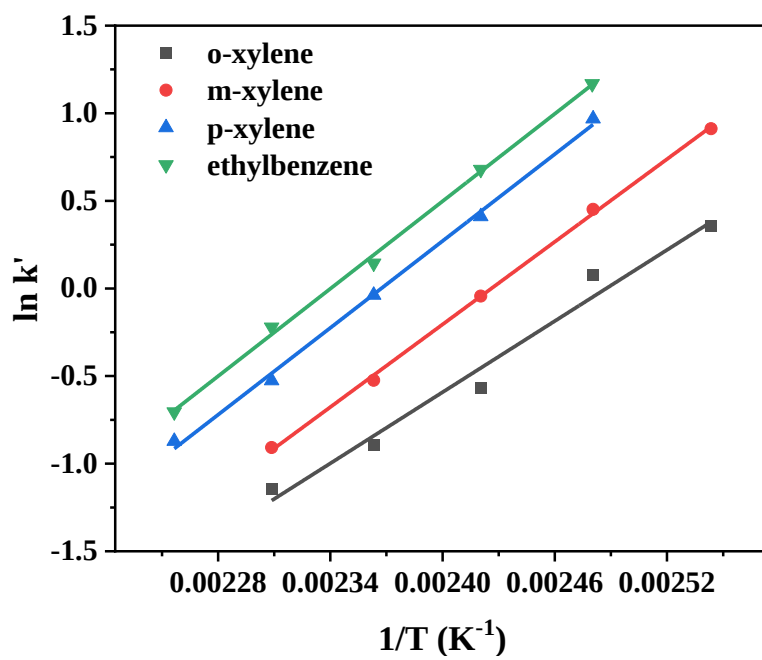


Figure S9. The van't Hoff plots of xylene isomers and ethylbenzene on the Ni(ADC)(TED)_{0.5} GC column.

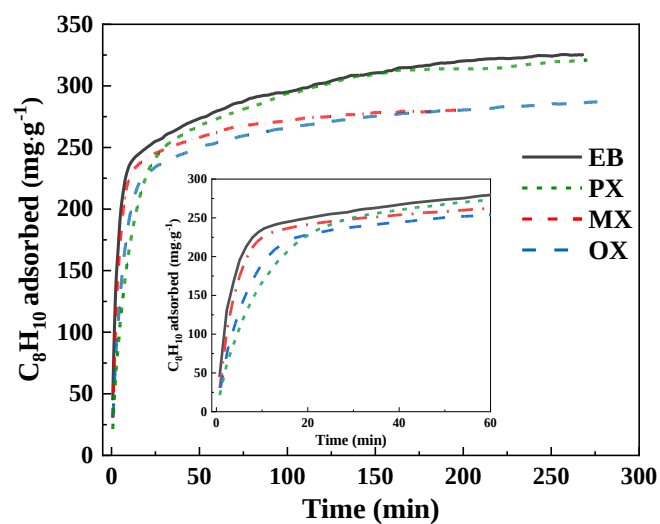


Figure S10. The kinetic adsorption isotherms of the sample.

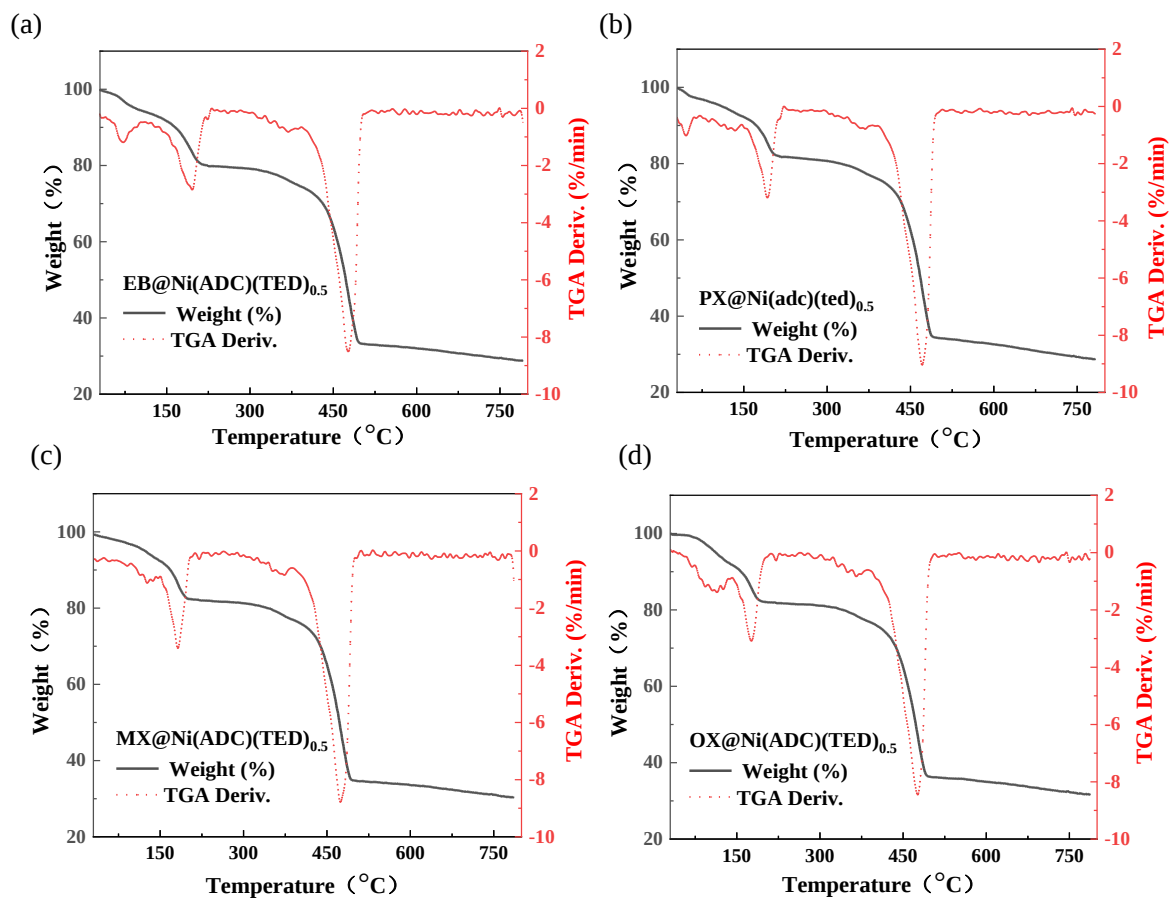


Figure S11. TGA patterns of the C8 aromatic-included sample.

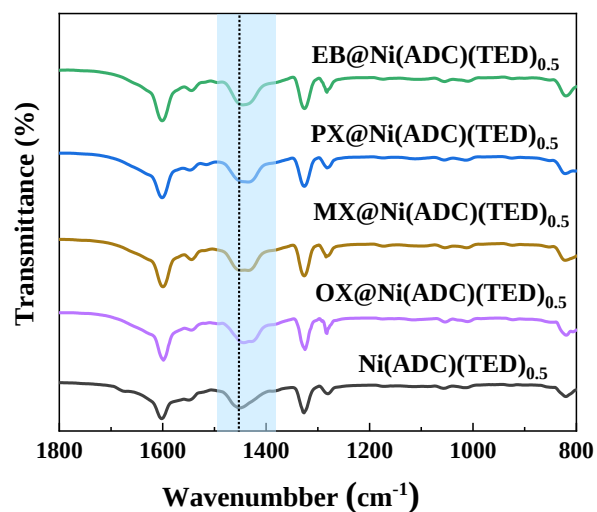


Figure S12. FT-IR patterns of the C8 aromatic-included sample and original one.

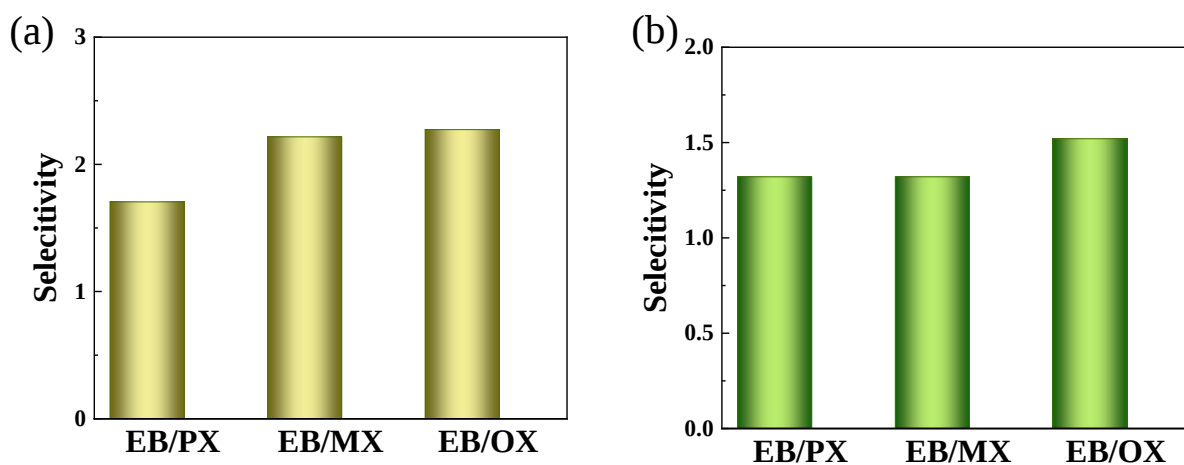


Figure S13. Separation performance of Ni(ADC)(TED)_{0.5} in binary vapor phase experiments (a) and multi-component vapor phase experiments (b).

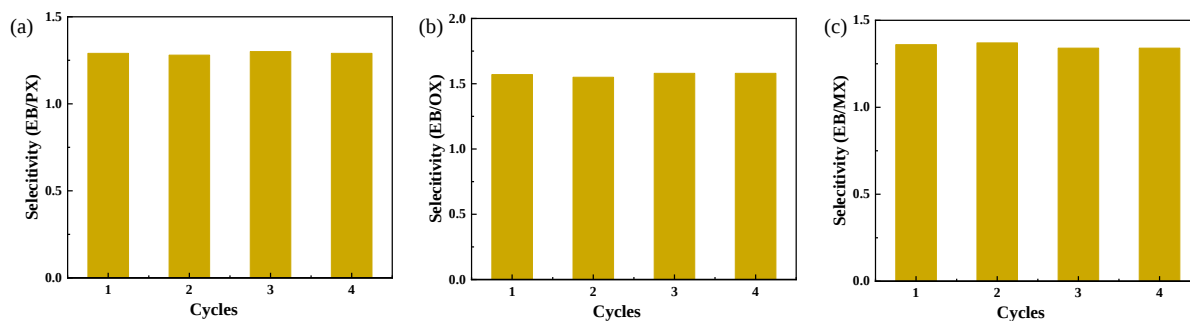


Figure S14. Adsorption cycles for the separation of an equimolar mixture of C8 aromatic isomers (vapor phase).

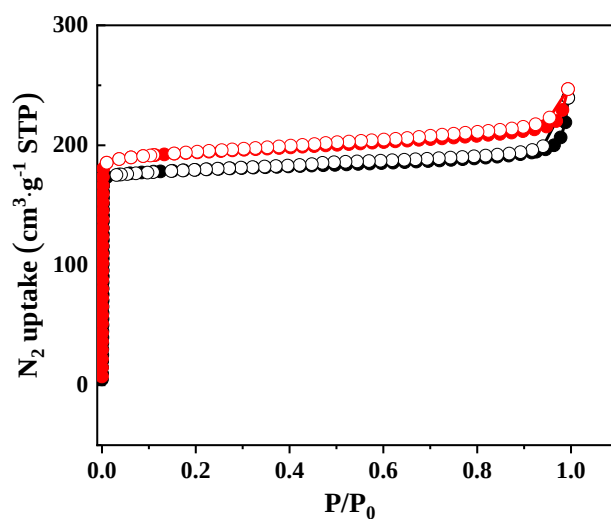


Figure S15. N₂ adsorption and desorption isotherms at 77K (red: the activated sample; black: the regenerated sample).

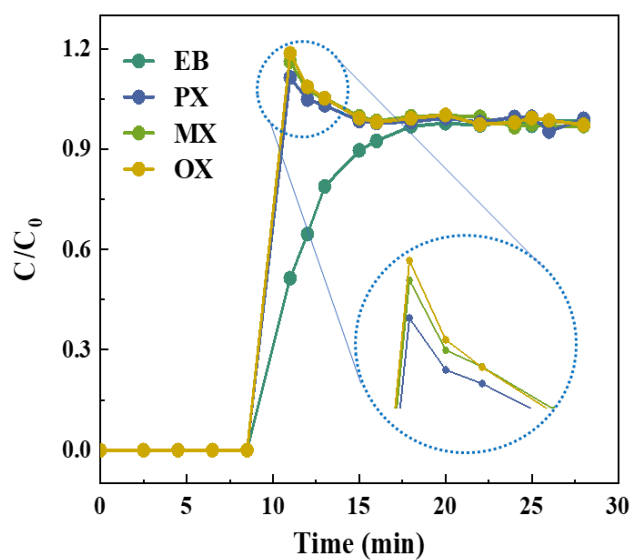


Figure S16. Multicomponent liquid phase breakthrough measurements for an equimolar mixture of C8 aromatics of Ni(ADC)(TED)_{0.5}.

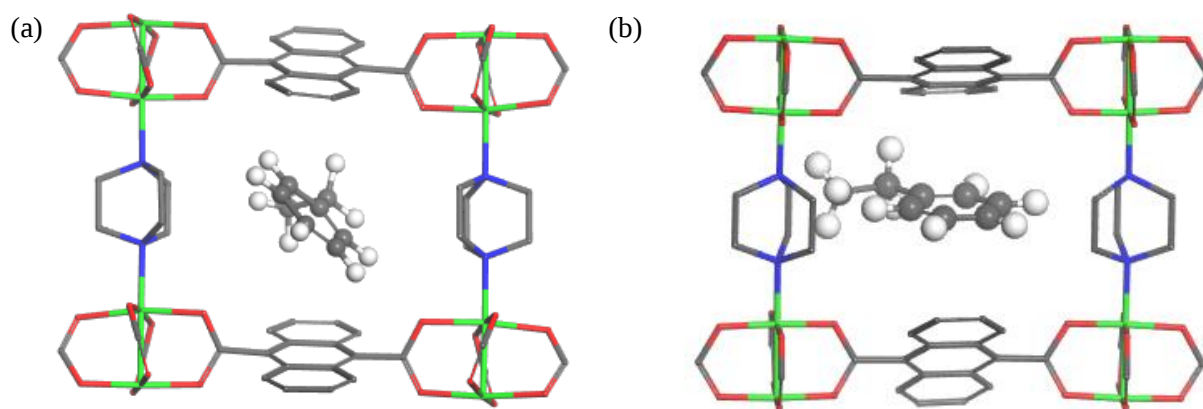


Figure S17. The adsorption configurations of the edge-to-face (a) and face-to-face configurations (b) by taking EB@ Ni(ADC)(TED)_{0.5} as an example.

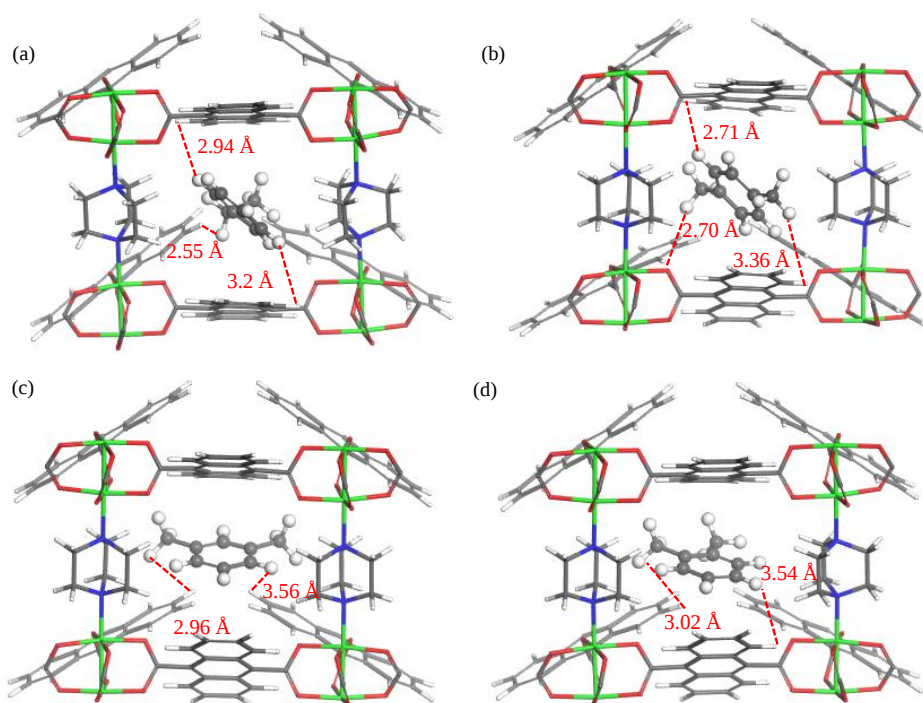


Figure S18. Optimized configurations of EB (a), PX (b), MX (c), OX (d) on the framework.

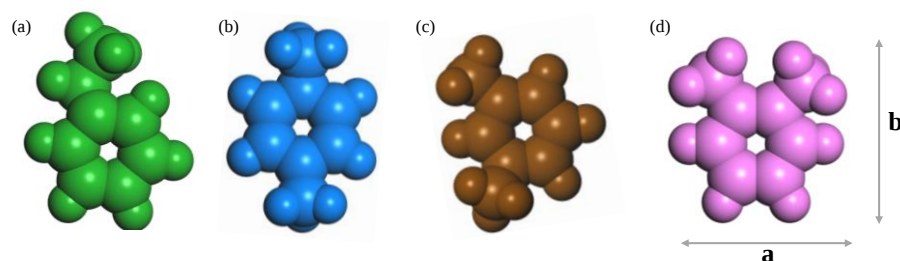


Figure S19. Molecular shapes of C8 aromatic isomers ((a) green: EB; (b) blue: PX; (c) brown: MX; (d) pink: OX).

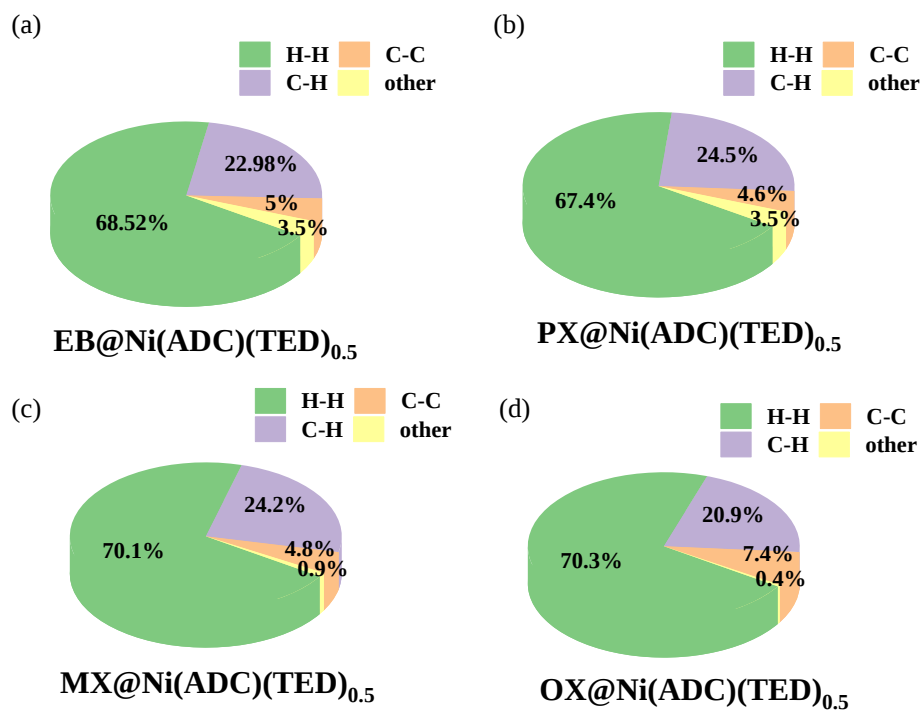


Figure S20. Relative contribution to the Hirshfeld surface area for various molecular contacts in guest-included Ni(ADC)(TED)_{0.5}.

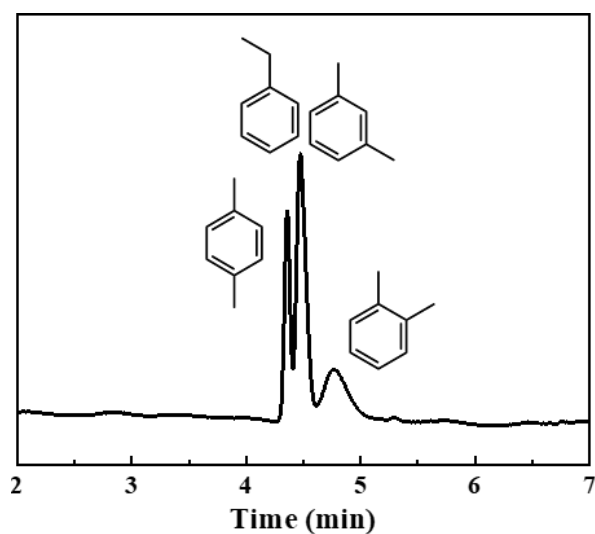


Figure S21. GC chromatograms on the Ni(BDC)(TED)_{0.5} capillary column for the separation of C8 aromatic isomers

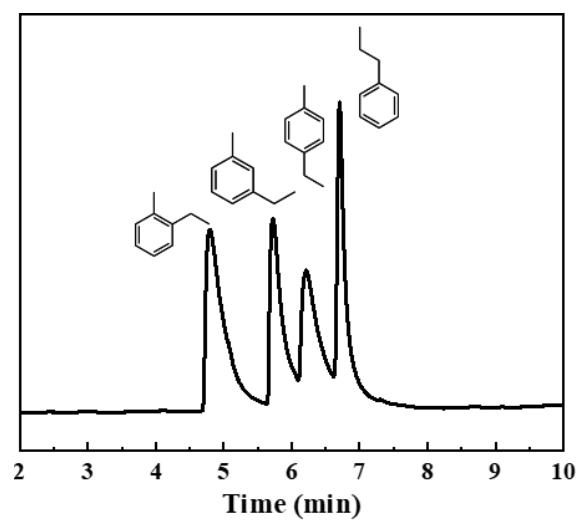


Figure S22. GC chromatograms on the Ni(ADC)(TED)_{0.5} capillary column for the separation of ethyltoluene isomers and n-propylbenzene.

3. Supplementary Tables

Table S1. Crystallographic and refinement information for Phase_1.

Identification code	Phase_1
Empirical formula	C ₃₈ H ₂₈ N ₂ Ni ₂ O ₈
Formula weight	758.03
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	I222
a/Å	13.770(3)
b/Å	16.220(3)
c/Å	18.220(4)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	4069.4(14)
Z	8
ρ_{calc} g/cm ³	1.451
F(000)	684.0
2 Θ range for data collection/°	0.118 to 2.072
Index ranges	-19 ≤ h ≤ 19, -22 ≤ k ≤ 21, -25 ≤ l ≤ 25
Reflections collected	90373
Independent reflections	6198 [R_{int} = 0.3369, R_{sigma} = 0.1230]
Data/restraints/parameters	6198/920/141
Goodness-of-fit on F ²	1.328
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.1590, wR_2 = 0.3742
Final R indexes [all data]	R_1 = 0.1801, wR_2 = 0.3858

Table S2. Crystallographic and refinement information for Phase_2.

Identification code	Phase_2
Empirical formula	C ₃₈ H ₂₈ N ₂ Ni ₂ O ₈
Formula weight	758.03
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	<i>Pca</i> 2 ₁
a/Å	21.220(4)
b/Å	10.730(2)
c/Å	18.190(4)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	4141.7(14)
Z	4
ρ_{calc} g/cm ³	2.121
2 Θ range for data collection/°	0.134 to 2.052
Index ranges	-25 $\leq$ h $\leq$ 27, -14 $\leq$ k $\leq$ 13, -25 $\leq$ l $\leq$ 23
Reflections collected	71469
Independent reflections	10318 [R_{int} = 0.2575, R_{sigma} = 0.1777]
Data/restraints/parameters	10318/945/172
Goodness-of-fit on F ²	1.085
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.1391, wR_2 = 0.3241
Final R indexes [all data]	R_1 = 0.1645, wR_2 = 0.3447

Table S3. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Phase_1.

Atom	x	y	z	U(eq)
Ni1	5000	5000	5698(2)	16.7(9)
Ni2	0	10000	5703(2)	13.4(8)
O19	4122(5)	5925(5)	4435(4)	11.3(15)
C15	3833(9)	6180(8)	4996(6)	33(3)
O17	1119(5)	9224(5)	4358(4)	12.6(14)
O20	3881(7)	5694(6)	5534(5)	22.8(18)
O18	778(7)	8963(6)	5562(5)	24.5(19)
C16	1257(6)	8922(5)	4962(4)	9.5(17)
C5D	8120(13)	4061(9)	6808(7)	58(3)
C6D	8369(13)	4389(7)	7488(9)	58(3)
C1D	8320(14)	3900(10)	8113(7)	58(3)
C2D	8021(13)	3083(9)	8059(7)	58(3)
C3D	7772(12)	2756(7)	7380(9)	58(3)
C4D	7822(13)	3245(10)	6754(7)	58(3)
C1A	2937(10)	8877(9)	5878(7)	21.7(15)
C2A	3771(11)	8861(10)	6273(8)	34(2)
C3A	4375(12)	8178(9)	6300(9)	34(2)
C4A	4113(11)	7470(10)	5935(9)	21.7(15)
C14A	3274(10)	7486(8)	5497(8)	14.3(12)
C5A	1942(12)	6048(10)	4320(9)	21.7(15)
C6A	1040(13)	5974(11)	4025(12)	34(2)
C7A	466(13)	6681(10)	3959(11)	34(2)
C8A	756(12)	7387(10)	4292(10)	21.7(15)
C11A	1623(11)	7451(9)	4674(9)	14.3(12)
C9A	1895(11)	8187(9)	5006(10)	19.2(16)
C13A	2651(10)	8171(8)	5491(8)	14.3(12)
C10A	3086(11)	6815(9)	5052(9)	19.2(16)
C12A	2217(11)	6756(10)	4701(9)	14.3(12)
C5B	1902(14)	5954(12)	4519(7)	21.7(15)
C6B	965(15)	5822(14)	4290(9)	34(2)
C7B	315(15)	6494(12)	4276(9)	34(2)
C8B	621(14)	7271(12)	4487(8)	21.7(15)
C11B	1581(13)	7409(11)	4725(7)	14.3(12)
C1B	3123(13)	9138(11)	5387(7)	21.7(15)
C2B	4067(14)	9240(13)	5615(9)	34(2)
C3B	4701(15)	8561(11)	5620(9)	34(2)
C4B	4435(12)	7773(11)	5414(7)	21.7(15)
C14B	3464(11)	7667(9)	5179(7)	14.3(12)
C10B	3176(13)	6875(11)	4966(7)	19.2(16)
C12B	2231(13)	6738(12)	4740(7)	14.3(12)
C9B	1881(12)	8195(12)	4942(5)	19.2(16)
C13B	2825(11)	8344(9)	5173(6)	14.3(12)
N1C	5000	5000	6805(7)	25(3)
C3C	5337(16)	4189(9)	7049(9)	31(2)
N2C	5000	5000	8175(6)	17(2)

C4C	5325(16)	4184(9)	7915(9)	31(2)
C5C	5657(15)	5645(12)	7050(9)	31(2)
C6C	5687(14)	5608(12)	7905(9)	31(2)
C7C	4004(10)	5155(15)	7048(9)	31(2)
C8C	4020(10)	5125(15)	7908(9)	31(2)

Table S4. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Phase_2 squeeze.

Atom	x	y	z	U(eq)
Ni2	2476.7(12)	-490.1(18)	4932.5(15)	6.9(3)
O20B	6577(4)	245(5)	6288(3)	14.1(9)
O20C	2373(4)	1340(6)	5126(3)	13.7(13)
C15B	3667(4)	-316(6)	5686(3)	5.3(13)
O16C	2345(4)	7699(5)	6252(4)	13.9(9)
O19B	6583(4)	823(5)	5156(3)	14.1(9)
O17B	3406(4)	-755(5)	6261(3)	14.5(9)
C15C	2494(5)	7130(6)	5678(4)	9.1(13)
O16B	3366(4)	-189(5)	5081(3)	14.5(9)
O17C	2571(4)	7614(6)	5060(3)	13.9(9)
C18B	6315(4)	559(6)	5715(3)	4.4(13)
C18C	2505(5)	1796(7)	5716(4)	15.0(16)
O19C	2665(4)	1191(6)	6241(4)	15.2(13)
C8B	4212(5)	1316(6)	6683(4)	21.2(9)
C7B	4482(4)	2202(6)	7130(4)	24.8(9)
C6B	5117(4)	2470(7)	7097(4)	24.8(9)
C5B	5512(5)	1733(7)	6693(4)	21.2(9)
C14B	5247(4)	953(7)	6152(4)	21.0(9)
C4B	5778(5)	-1316(7)	4754(4)	21.2(9)
C3B	5538(4)	-2126(8)	4252(4)	24.8(9)
C2B	4887(4)	-2300(8)	4196(5)	24.8(9)
C1B	4520(5)	-1756(7)	4728(4)	21.2(9)
C11B	4724(4)	-757(7)	5171(4)	21.0(9)
C9B	4348(4)	-112(6)	5654(4)	10.8(10)
C13B	4605(4)	661(7)	6181(4)	21.0(9)
C10B	5632(4)	338(6)	5667(4)	10.8(10)
C12B	5389(4)	-566(7)	5207(4)	21.0(9)
N1A	2508(3)	-549(5)	3877(4)	11.7(9)
C5A	3026(5)	-1272(9)	3581(5)	38.5(11)
N2A	2458(3)	-604(5)	2476(4)	11.7(9)
C8A	2978(5)	-1341(9)	2731(5)	38.5(11)
C3A	1939(5)	-1024(10)	3599(5)	38.5(11)
C6A	1913(5)	-1178(9)	2760(5)	38.5(11)
C4A	2536(6)	688(9)	3566(6)	38.5(11)
C7A	2574(6)	630(9)	2725(6)	38.5(11)
C1C	1431(4)	3144(9)	6054(4)	35.2(11)
C2C	901(6)	3820(10)	6179(4)	63.1(18)
C3C	905(6)	5103(10)	6136(5)	63.1(18)
C4C	1397(4)	5734(9)	5839(6)	35.2(11)
C14C	1977(4)	5109(6)	5755(4)	13.7(7)

C5C	3638(4)	5713(9)	5360(6)	35.2(11)
C6C	4182(6)	5047(10)	5306(7)	63.1(18)
C7C	4188(6)	3746(10)	5352(7)	63.1(18)
C8C	3624(4)	3181(9)	5431(5)	35.2(11)
C11C	3079(4)	3810(6)	5582(4)	13.7(7)
C9C	2519(4)	3181(6)	5648(5)	10.0(10)
C13C	1978(4)	3815(6)	5879(4)	13.7(7)
C10C	2540(4)	5768(6)	5672(5)	10.0(10)
C12C	3074(4)	5108(6)	5474(4)	13.7(7)
NiI	2501.1(12)	-631.4(18)	6330.9(14)	6.9(3)

Table S5. The pore size of the Ni(ADC)(TED)_{0.5} and the guest-included sample.

MOFs	Pore size*
Ni(ADC)(TED) _{0.5}	0.569
EB@Ni(ADC)(TED) _{0.5}	0.510
PX@Ni(ADC)(TED) _{0.5}	0.519
MX@Ni(ADC)(TED) _{0.5}	0.519
OX@Ni(ADC)(TED) _{0.5}	0.514

*Calculated by Zeo++⁴

Table S6. Selectivity of C8 aromatic isomers for the Ni(ADC)(TED)_{0.5} packed column.

	EB	PX	MX	OX
EB	-	1.13	1.36	4.77
PX	0.88	-	1.21	1.47
MX	0.73	0.83	-	1.22
OX	0.60	0.68	0.82	-

Table S7. Values of ΔH and ΔS for structural isomers of xylene isomers and ethylbenzene on the Ni(ADC)(TED)_{0.5} GC column.

Analytes	o-xylene	m-xylene	p-xylene	Ethylbenzene
ΔH (kJ·mol ⁻¹)	-56.27	-65.36	-68.68	-69.16
ΔS (J·mol ⁻¹ ·K ⁻¹)	-132.70	-151.31	-155.33	-154.52

Table S8. The weight loss temperature of the guest molecules in the framework.

Aromatics	Temperature(°C)
EB	196.34
PX	192.71
MX	182.10
OX	176.59

Table S9. The binding energy of C8 aromatic isomers on the framework by the edge-to-face configuration and face-to-face configuration, respectively.

Adsorption configuration	Adsorbate molecule	Binding Energy (kJ·mol ⁻¹)
Edge-to Face configuration	EB	-90.70
	PX	-85.32
	MX	-81.14
	OX	-71.80
Face-to Face configuration	EB	-82.85
	PX	-84.80
	MX	-74.70
	OX	-69.14

Table S10 Molecular sizes of C8 aromatic isomers.

Aromatics	a (Å)	b (Å)
EB	6.7	9.6
PX	6.6	9.2
MX	7.3	8.9
OX	7.5	7.6

Table S11. The sum of the minimum distances of various guest-host contracts in guest-included sample.

Aromatics	The minimum distances (Å)			
	H···H	H···C	C···H	C···C
ethylbenzene	2.00	2.67	2.9	3.6
p-xylene	2.27	2.7	2.8	3.6
m-xylene	2.43	2.95	2.8	3.4
o-xylene	2.37	3.2	2.8	3.5

Table S12. Selectivity of ethyltoluene isomers and n-propylbenzene for the Ni(ADC)(TED)_{0.5} packed column.

	N-PB	P-ET	M-ET	O-ET
N-PB	-	1.10	1.22	6.37
P-ET	0.91	-	1.11	1.40
M-ET	0.82	0.90	-	1.26
O-ET	0.65	0.72	0.80	-

Table S13. Column resolution for ethyltoluene isomers and n-propylbenzene on the Ni(ADC)(TED)_{0.5} packed column.

Rs	R _{P-ET/M-ET}	R _{M-ET/O-ET}	R _{N-PB/M-ET}
Ni(ADC)(TED) _{0.5} column	1.32	0.79	0.85

Table S14. Comparison of separation of C8 aromatic isomers on the Ni(ADC)(TED)_{0.5} and the reported columns.

Materials	Elution order	References
co-pillar[4+1]arene	MX < OX < PX < EB	5
MOF-5	EB < MX $\approx$ PX < OX	6
Zr-BTB-C ₁₄	EB < MX < OX < PX	7
UiO-66	PX < MX < EB < OX	8
MIL-47	EB < PX $\approx$ MX < OX	9
CD-MOF ^a	PX < MX < EB < OX	10
MIL-101	PX < MX < EB < OX	11
MIL-53(Fe) ^a	EB < PX < MX < OX	12
MIL-53(Al) ^a	EB < PX = MX < OX	13
Untwisted Zr-BTB-FA	EB < MX < OX < PX	14
VF-WAXMS	EB < PX < MX < OX	14
HP-5MS	EB < PX = MX < OX	14
Ni(ADC)(TED) _{0.5}	OX < MX < PX < EB	This work

a: liquid chromatographic separation

Table S15. Summary of separation selectivity of C8 aromatics in various materials.

Materials	Separation selectivity			References
	EB/PX	EB/MX	EB/OX	
Zn ₂ (aip) ₂ (bpy)	0.33	2	2	15
Zn ₂ (aip) ₂ (bpe)	0.312	0.526	0.769	15
Co ₂ (dobdc)	3.21	2.05	1.21	16
MIL-53(Al)	0.32	0.26	0.092	22
MIL-101(Cr)	NG	1.1	0.714	17
MOF-5	0.51	0.427	0.241	6
H/ZSM-5	0.148	NG	NG	18
Li/ZSM-5	0.251	NG	NG	18
Na/ZSM-5	0.498	NG	NG	18
K/ZSM-5	0.908	NG	NG	18
UiO-66	1.03	NG	1.77	19
MIL-125(Ti)-NH ₂	0.625	NG	NG	20
Cu(CDC)	0.2	NG	NG	21
MIL-47	0.55	0.71	0.72	22
SqI-1-Co-NCS	0.14	0.26	0.017	23
[Ce(HTCPB)]	0.42	NG	NG	24
AZO-cage	0.15	1.11	1.83	25
[Zn(o-phen)(2,6-NDC)·DMF]	1.5	0.017	0.09	26
Ni(ADC)(TED) _{0.5}	1.86	2.68	3.75	This work

Note: NG refers to not mentioned.

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