Electronic Supplementary Material (ESI) for CrystEngComm.

Adenine-based bio-MOFs with high water and acid-base stability for ammonia capture

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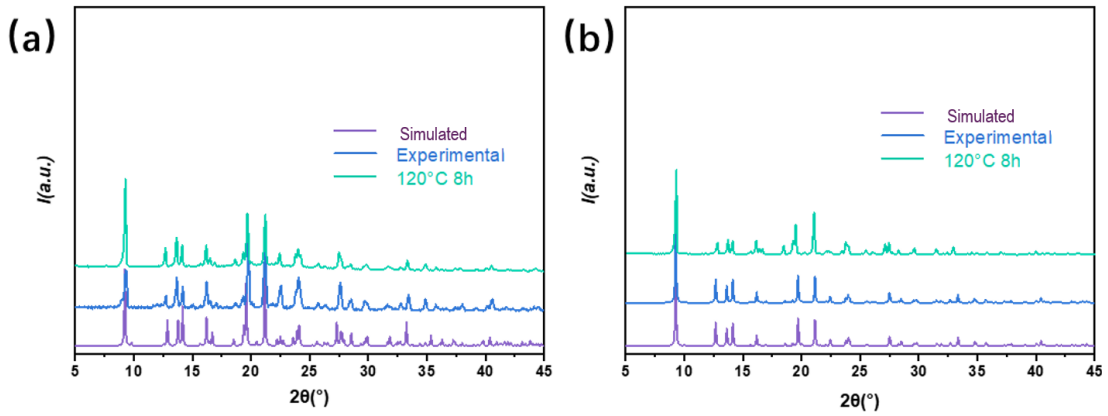

Fig. S1 PXRD patterns of Zn(3-AIN)(AD)•DMF (a) and Zn(3-AIN)(AD)•DMA(b).

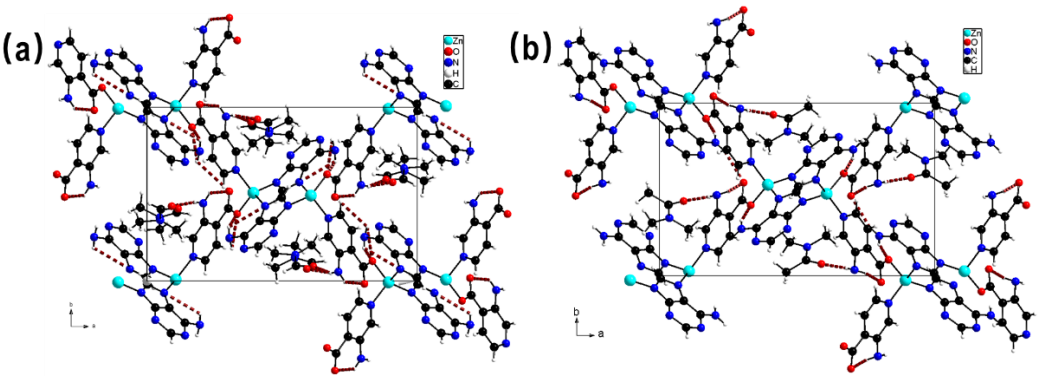

Fig. S2 N-H…O and N-H…N hydrogen bond networks (dash line) for Zn(3-AIN)(AD)•DMF (a) and N-H…O hydrogen bond networks (dash line) for Zn(3-AIN)(AD)•DMA.

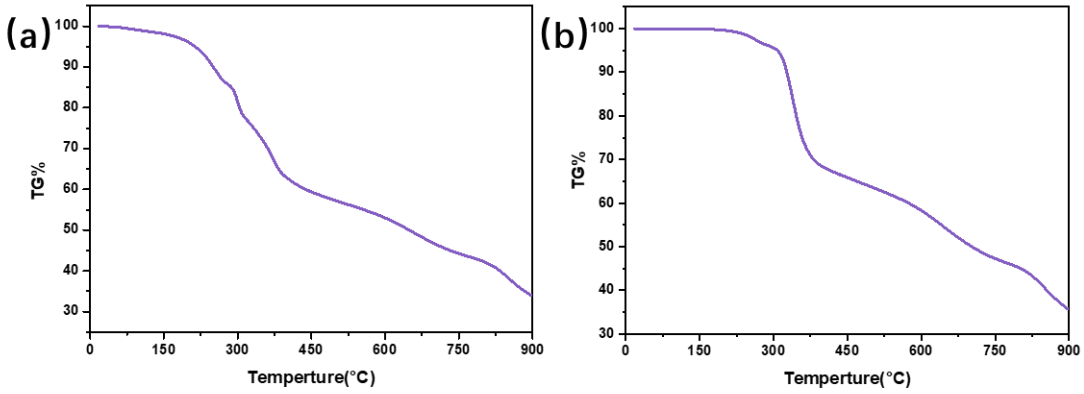

Fig. S3 TG curves of Zn(3-AIN)(AD)•DMF (a) and Zn(3-AIN)(AD)•DMA(b).

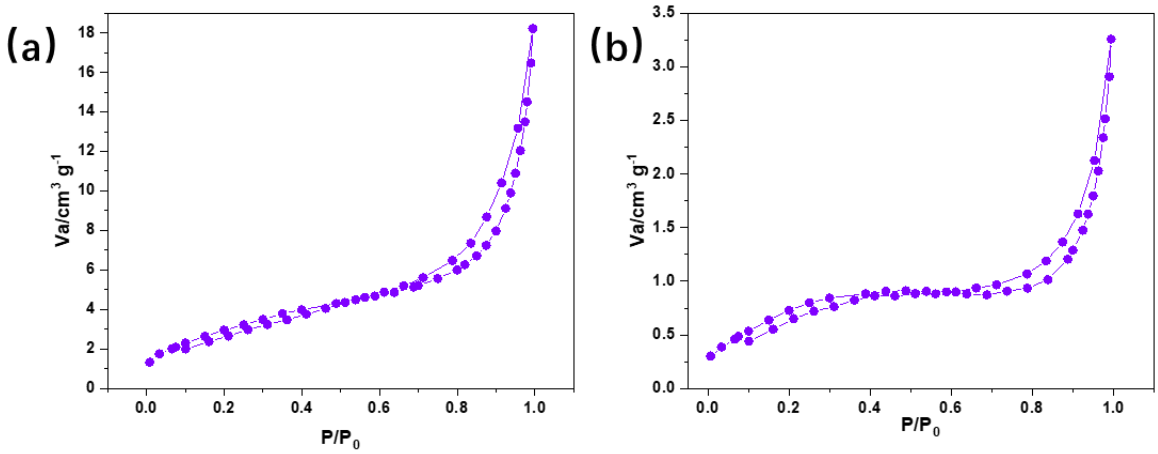

Fig. S4 N2 adsorption isotherms of Zn(3-AIN)(AD)•DMA (a) and Zn(3-AIN)(AD)•DMF(b)

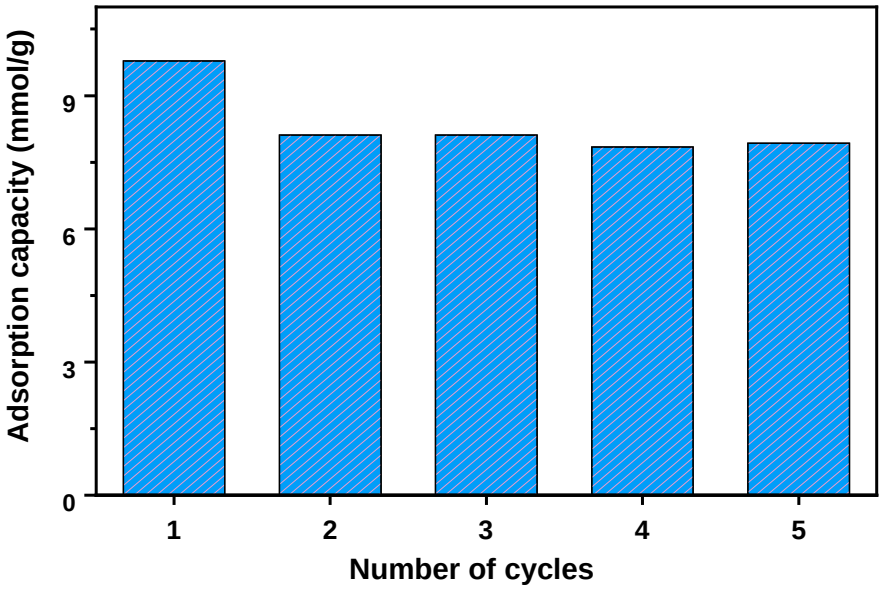

Fig. S5 Comparison of NH3 uptake of Zn(3-AIN)(AD)•DMA in the five adsorption cycles.

Table S1 Crystal data and structure refinement for (3-AIN)(AD)•DMA) and Zn(3-AIN)(AD)•DMF

Identification code	**(3-AIN)(AD)•DMA)**	**Zn(3-AIN)(AD)•DMF**
Empirical formula	$C_{11}H_9N_7O_2Zn•C_4H_9NO$	$(C_{11}H_9N_7O_2Zn)_2•C_3H_7NO$
Formula weight	423.74	746.34
Temperature/K	170.00(10)	293(2)
Crystal system	orthorhombic	orthorhombic
Space group	$Pna2_1$	$Pna2_1$
a/Å	18.0312(5)	17.6657(3)
b/Å	11.2975(5)	11.3205(2)
c/Å	8.6680(3)	8.8645(2)
α/°	90	90
β/°	90	90
γ/°	90	90
Volume/Å^3	1765.74(11)	1772.76(6)
Z	4	2
ρ_{calc}g/cm^3	1.594	1.398
μ/mm^{-1}	2.253	2.139
F(000)	872.0	760.0
Crystal size/mm^3	0.19 × 0.16 × 0.15	0.19 × 0.19 × 0.15
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.238 to 143.058	9.278 to 143.104
Index ranges	$-22 \le h \le 21$, $-13 \le k \le 13$, $-5 \le l \le 10$	$-12 \le h \le 21$, $-13 \le k \le 13$, $-9 \le l \le 10$
Reflections collected	4578	5570
Independent reflections	2338 [R_{int} = 0.0251, R_{sigma} = 0.0317]	2800 [R_{int} = 0.0255, R_{sigma} = 0.0364]
Data/restraints/parameters	2338/1/248	2800/262/282
Goodness-of-fit on F^2	1.121	1.141
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.1110	R_1 = 0.0561, wR_2 = 0.1605
Final R indexes [all data]	R_1 = 0.0393, wR_2 = 0.1132	R_1 = 0.0580, wR_2 = 0.1645
Largest diff. peak/hole / e Å^{-3}	0.64/-0.60	1.03/-0.47
Flack parameter	0.07(6)	-0.02(3)

Table S2. Hydrogen bonds for Zn(3-AIN)(AD)•DMF [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(3)	0.86	2.13	2.97(2)	162.6
N(2)-H(2A)...O(4)	0.86	2.19	3.02(2)	163.0
N(2)-H(2B)...O(2)	0.86	2.11	2.729(9)	128.9
N(6)-H(6A)...O(1)#4	0.86	2.31	3.045(8)	143.5
N(6)-H(6A)...N(7)	0.86	2.77	3.128(7)	107.0
N(6)-H(6B)...O(2)#5	0.86	2.97	3.263(8)	102.3
C(2)-H(2)...O(2)	0.93	3.09	3.474(12)	106.6
C(2)-H(2)...N(3)#4	0.93	2.57	3.421(9)	152.3
C(2)-H(2)...N(9)#4	0.93	2.98	3.429(11)	111.2
C(8)-H(8)...O(1)	0.93	2.39	2.719(8)	100.3
C(9)-H(9)...N(7)#6	0.93	3.03	3.422(8)	106.9
C(10)-H(10)...O(3)	0.93	2.61	3.38(3)	140.5
C(10)-H(10)...O(4)	0.93	2.67	3.44(3)	141.0
C(16)-H(16A)...O(4)#7	0.96	2.94	3.46(4)	115.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,z+1/2 #2 -x+1,-y+1,z+1/2 #3 -x+1/2,y-1/2,z-1/2 #4 -x+1,-y+1,z-1/2 #5 x+1/2,-y+3/2,z #6 x-1/2,-y+1/2,z #7 -x,-y+1,z-1/2

Table S3. Hydrogen bonds for Zn(3-AIN)(AD)•DMA [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2B)...O(3)	0.87	2.19	3.040(8)	165.1
N(6)-H(6A)...O(2)#5	0.86	2.38	3.213(6)	162.7
N(6)-H(6B)...O(1)#4	0.86	2.22	3.041(7)	160.9
C(2)-H(2)...N(3)#4	0.93	2.59	3.449(9)	153.3
C(2)-H(2)...N(9)#4	0.93	2.94	3.378(9)	110.1
C(8)-H(8)...O(1)	0.93	2.39	2.713(7)	100.2
C(9)-H(9)...N(2)#6	0.93	2.78	3.490(9)	134.0
C(9)-H(9)...N(7)#7	0.93	3.03	3.438(7)	108.1
C(10)-H(10)...O(3)	0.93	2.50	3.301(8)	144.3
C(12)-H(12B)...N(1)#3	0.96	2.82	3.493(11)	128.2
C(14)-H(14A)...O(2)#3	0.96	2.70	3.452(13)	135.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y-1/2,z+1/2 #2 -x+1,-y+1,z+1/2 #3 -x+3/2,y+1/2,z-1/2 #4 -x+1,-y+1,z-1/2 #5 x-1/2,-y+1/2,z #6 -x+3/2,y+1/2,z+1/2 #7 x+1/2,-y+3/2,z

Table S4 The calculated atom distance (d) of the hydrogen bond between NH_3 and interaction site in the activied Zn(3-AIN)(AD)•DMA and adsorption energy (E_{ads}).

Adsorption site	Site 1	Site 2	Site 3	Site 4	Site 5	Site 6	Site 7
d (Å)	2.24	2.21	2.29	2.24	2.18	2.24	1.98
E_{ads} (kJ/mol)	-656.1	-508.4	-653.2	-685.9	-581.8	-617.5	-585.6