Electronic Supplementary Information (ESI) for:

Effects of De-Fluorination on Hydrophobicity and on CO₂ and CH₄ Adsorption Under High Humidity in MeMOFs, Methylated Analogues of FMOFs

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Contents

S1.	Geometry optimization of methyl functionalized MOFs	S3
S2.	Lennard-Jones (L-J) parameters	S 6
S3.	Excess and absolute adsorption	S 8
S4.	CO_2 uptake and Q_{st} comparison of this work with previously reported data	S9
S5.	Adsorption isotherms and isosteric heats of adsorption at different temperature	S10
S6.	Energy contribution as per GCMC	S15
S7.	Pure component adsorption isotherm fitting	S20
S8.	Calculation of isosteric heats of adsorption at infinite dilution (Q_{st0})	S46
S9.	Calculation of Henry's constants from the slope of the isotherms	S47
S10.	Adsorption selectivity of CO ₂ and CH ₄ over water in FMOF-1c	S50
S11.	Henry's constant and adsorption selectivity of CO ₂ and CH ₄ over water in MeMOF-1c using CBAC and EQeq charge methods	S50
S12.	Convergence analysis of water	S51



S1. Geometry optimization of methyl functionalized MOFs

Figure S1. Forcite geometry optimization: (a) cell lengths and (b) cell angles of MeMOF-1c.



Figure S2. Forcite geometry optimization: (a) density and (b) energy of MeMOF-1c.



Figure S3. Forcite geometry optimization: (a) density and (b) energy of MeMOF-1a.



Figure S4. Forcite geometry optimization: (a) density and (b) energy of MeMOF-1b.

	Energy (kcal/mol)					
	Initial structure	Final structure				
Total energy	4074.407	1599.900				
Valence energy	4220.009	1779.329				
Bond energy	1732.861	0.866				
Angular energy	2402.447	1772.859				
Torsion energy	80.081	5.074				
Inversion energy	4.620	0.530				
Non-bonding energy	-145.602	-179.429				
Van der Waals force	-143.678	-177.233				
Long range correction*	-1.924	-2.196				
Coulomb energy	0.000	0.000				

Table S1. Energy comparison of MeMOF-1c before and after Forcite geometry optimization.

* In our work, we have used UFF (Universal force field) for MOF structures' optimization. During those optimizations, we considered only the van der Waals forces. So, the "long-range correction" term here originates from van der Waals interactions, as a correction factor thereof. As such, the total non-bonding energy is the sum of the van der Waals force and the long-range correction term. To date, many researchers have used this method to efficiently generate feasible crystal structures (e.g., J. Park et al. *Chem. Mater.* 2022, **35**, 9-16; S. Srivastava et al. *Internat. J. H. Energ.* 2022, **47**, 15820-15831; G. Avci et al. *J. Phys. Chem. C* 2019, **123**, 28255-28265; Z. Deng et al. *Chem. Mater.* 2024, **36**, 9806-9821; D. A. Gomez-Gualdron *Chem. Mater.* 2014, **26**, 5632–5639; O. K. Farha et al. *Nat. Chem.* 2010, **2**, 944–948; O. V. Gutov et al. *Chem. Europ. J.* 2014, **20**, 12389–12393).

Structures	$D_i(\mathbf{A})$	$D_f(\mathbf{A})$	$D_{if}(\mathbf{A})$
FMOF-1c	6.731	6.086	6.731
MeMOF-1c	6.700	5.925	6.696
MeMOF-1a	6.447	6.024	6.443
MeMOF-1b	6.213	5.757	6.213

Table S2. Pore sizes of the studied MOFs.*

* D_i is the largest overall diameter; D_f is the restricting pore diameter; D_{if} is the largest diameter along a viable path through the structure.

S2. Lennard-Jones (L-J) parameters

Table S3. Lennard-Jones parameters for the framework.

Atom type	σ (Å)	$\epsilon/k_B(\mathbf{K})$	Force field
Ν	3.26	34.60	UFF^1
С	3.43	52.40	UFF^1
F	3.09	25.20	UFF^1
Н	2.57	22.14	UFF^1
Ag	2.81	18.12	UFF^1
Zn	4.05	27.68	DREIDING ²

Table S4. Framework charges.^{3–6}

Atom type	Charges, q (e)*
Agı	$0.390,^3 0.509^6$
Ag ₂	$0.350,^3 0.342^6$
N_1	-0.384, ³ -0.253 ⁶
N_2	-0.347, ³ -0.098 ⁶
C_1	$0.345,^3 0.099^6$
C2_(CF3)	$0.510,^4 0.5232^5$
F	$-0.170,^4 -0.1744^5$
C2_(CH3)	-0.0489, ⁵ -0.155 ⁶
Н	$0.0163,^{5}0.010^{6}$

* One important factor in calculating gas adsorption in MOFs is the consideration of electrostatic interactions with the framework. To consider the electrostatic interactions, we must assign charges on the framework atoms. In this work, we used the CBAC method for CH₃ in MeMOF-1c. For FMOF-1c, we first used charges from a previous simulation,³ where CF₃ charges were taken from Dalvi et al.⁴ We then used CBAC charges⁵ for CF₃ for simulating CO₂ adsorption isotherms in FMOF-1c and compared the data (Figure S5) with our former simulation³ to make our study consistent. Further, we used EQ_{eq} charges⁶ for MeMOF-1c to study the influence of point charges on CO₂ adsorption for MeMOF-1c (Figure 3b of the main article).

Adsorbate	Atom type	σ (Å)	ϵ/k_B (K)	q (e)	Force field
Carbon dioxide	O_CO ₂	3.05	79.0	-0.35	TraPPE ⁷
	C_{CO_2}	2.80	27.0	0.70	TraPPE ⁷
Methane	CH4	3.73	148	0.0	TraPPE ⁸
	O_H ₂ O	3.15	78.0	_	TIP4P ⁹
Water	H_H ₂ O	_	_	0.52	TIP4P ⁹
	M_H_2O	_	_	-1.04	TIP4P ⁹

Table S5. Lennard-Jones parameters and partial charges for the adsorbates used in this work.

S3. Excess and absolute adsorption

Excess adsorption amount is obtained from experimental measurements, whereas absolute uptake is calculated from simulations. The excess (n^{ex}) and absolute (n^{abs}) uptake are related to each other as per the following equation,¹⁰

$$n^{ex} = n^{abs} - V^g \rho^g \tag{1}$$

Where V^g is the pore volume of the MOF and ρ^g is the molar density of the bulk gas phase. Generally, RASPA2 software calculate the absolute adsorption first.¹¹ During simulation we specify the pore volume of the MOF as void fraction (probed with helium), and ρ^g is calculated by the Peng-Robinson equation of state. After obtaining all the parameters, RASPA2 determine the excess adsorption amount using equation (1).

S4. CO₂ uptake and Q_{st} comparison of this work with previously reported data



Figure S5. Comparison of CO₂ uptake with previous data at 298 K in FMOF-1c.^{3-5,12}



Figure S6. Comparison of isosteric heat of adsorption of CO₂ with previous data³ at 298 K in FMOF-1c.

S5. Adsorption isotherms and isosteric heats of adsorption at different temperature predicted from GCMC



Figure S7. Comparison of CO₂ and CH₄ adsorption isotherms in FMOF-1c and MeMOF-1c at 288 K.



Figure S8. Comparison of CO₂ and CH₄ adsorption isotherms in FMOF-1c and MeMOF-1c at 308 K.



Figure S9. Comparison of CO₂ and CH₄ adsorption isotherms in MeMOF-1a and MeMOF-1b at 298 K.



Figure S10. Isosteric heats of adsorption of CO₂ and CH₄ in FMOF-1c at different loading at different temperature.



Figure S11. Isosteric heats of adsorption of CO₂ and CH₄ in FMOF-1c at different pressure at different temperature.



Figure S12. Isosteric heats of adsorption of CO₂ and CH₄ in MeMOF-1c at different loading at different temperature.



Figure S13. Isosteric heats of adsorption of CO₂ and CH₄ in MeMOF-1c at different pressure at different temperature.



Figure S14. Simulated isosteric heats of adsorption of CO₂ and CH₄ in MOFs: (a) as a function of uptake and (b) as a function of pressure at 298 K.



Figure S15. Contribution of -CH₃ group on increased percentage of adsorption amount and on isosteric heats at infinite dilution.



Figure S16. Henry's constant (*K*_H) of CO₂ and CH₄ in MeMOF-1a and MeMOF-1b at 298 K.

S6. Energy contribution as per GCMC



Figure S17. The breakdown of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in FMOF-1c at 288 K.



Figure S18. The breakdown of percentage of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in FMOF-1c at 288 K.



Figure S19. The breakdown of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in FMOF-1c at 308 K.



Figure S20. The breakdown of percentage of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in FMOF-1c at 308 K.



Figure S21. The breakdown of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in MeMOF-1c at 288 K.



Figure S22. The breakdown of percentage of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in MeMOF-1c at 288 K.



Figure 23. The breakdown of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in MeMOF-1c at 298 K.



Figure 24. The breakdown of percentage of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in MeMOF-1c at 298 3K.



Figure S25. The breakdown of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in MeMOF-1c at 308 K.



Figure S26. The breakdown of percentage of total potential energy contribution into host-guest and guest-guest contribution for CO₂ and CH₄ adsorption in MeMOF-1c at 308 K.



Figure S27. Adsorption energy of (a) CO₂ and (b) CH₄ in the studied MOFs, predicted from MC.

S7: Pure component adsorption isotherm fitting

Langmuir model is one of the most frequently used models that considers the surface homogeneity and the dominant adsorbate – adsorbent interactions. The equation is as follows:¹³

$$n_L = \frac{a_L b_L P}{1 + b_L P} \tag{2}$$

where n_L is the amount adsorbed in mol/kg; a_L is the maximum adsorption capacity, b_L is the Langmuir isotherm constant also known as affinity constant and P is the pressure in the unit of Pascal.

Langmuir-Freundlich is the combination of Freundlich and Langmuir isotherm models. In 1984, Sips¹⁴ proposed this hybrid model that can characterize the structure heterogeneity and overthrown the constraints of the Freundlich model.¹⁵ The Langmuir-Freundlich equation is:

$$n_{FL} = \frac{a_{LF}b_{LF}P^m}{1+b_{LF}P^m} \tag{3}$$

where n_{LF} and a_{LF} are the adsorbed amount and maximal adsorption capacity, P is the pressure, b_{LF} is affinity constant and m is the system heterogeneity parameter. This parameter is generally larger than unity and, therefore, the greater this parameter is, the more heterogeneous the structure is. At high pressure, it describes the Langmuir isotherm, whereas at low pressure, this isotherm approaches to the Freundlich's model and does not portray the Henry's law characteristics.

We considered the Toth isotherm as it contemplates both the surface incongruity and depicts the Henry's law type performance at low pressure region. The empirical Toth equation¹⁶ is,

$$n_T = \frac{a_T b_T P}{\left[1 + (b_T P)^m\right]^{1/m}} \tag{4}$$

here n_T is the amount adsorbed; a_T is the maximum amount adsorbed, b_T is the Toth isotherm constant and *m* characterize the system heterogeneity.

Residual root-mean square error (RMSE) and chi-square test defined in equations (5) and (6) respectively were used to study the goodness of the fitting of the models.

$$RMSE = \sqrt{\frac{1}{n-2}} \sum_{i=1}^{n} (q_{im} - q_{is})^2$$
(5)

$$\chi^{2} = \sum_{i=1}^{n} \frac{(q_{im} - q_{is})^{2}}{q_{im}}$$
(6)

Here q_{is} is the consideration from the simulation isotherms, q_{im} is the prediction from the isotherm models and *n* in the number of considerations in the simulations. The lower value of RMSE and χ^2 demonstrates the better fitting of the models to the simulated data.



Figure S28. Langmuir, Langmuir-Freundlich, and Toth fitting curves of CO₂ and CH₄ in FMOF-1c at 288 K.



Figure S29. Langmuir, Langmuir-Freundlich, and Toth fitting curves of CO₂ and CH₄ in FMOF-1c at 298 K.



Figure S30. Langmuir, Langmuir-Freundlich, and Toth fitting curves of CO₂ and CH₄ in FMOF-1c at 308 K.



Figure S31. Langmuir curve fit for the adsorption of CO₂ in FMOF-1c at 288 K.



Figure S32. Langmuir curve fit for the adsorption of CH₄ in FMOF-1c at 288 K.



Figure S33. Langmuir curve fit for the adsorption of CO₂ in FMOF-1c at 298 K.



Figure S34. Langmuir curve fit for the adsorption of CH₄ in FMOF-1c at 298 K.



Figure S35. Langmuir curve fit for the adsorption of CO₂ in FMOF-1c at 308 K.



Figure S36. Langmuir curve fit for the adsorption of CH₄ in FMOF-1c at 308 K.

Т	288 K		298 K		308 K	
CO ₂ /CH ₄	CO ₂	CH4	CO ₂	CH4	CO ₂	CH4
a_L	3.860	2.546	3.912	2.410	3.637	2.353
b_L	1.262×10 ⁻⁶	6.010×10 ⁻⁷	7.870×10 ⁻⁷	5.502×10 ⁻⁷	7.370×10 ⁻⁷	4.513×10 ⁻⁷
RMSE	0.1665	0.0149	0.2823	0.3382	0.8849	0.0055
χ^2	0.0167	0.0008	0.0157	0.0003	0.0089	0.0003

Table S6: Langmuir parameters of FMOF-1c.



Figure S37. Langmuir-Freundlich curve fit for the adsorption of CO₂ in FMOF-1c at 288 K.



Figure S38. Langmuir-Freundlich curve fit for the adsorption of CH₄ in FMOF-1c at 288 K.



Figure S39. Langmuir-Freundlich curve fit for the adsorption of CO₂ in FMOF-1c at 298 K.



Figure S40. Langmuir-Freundlich curve fit for the adsorption of CH₄ in FMOF-1c at 298 K.



Figure S41. Langmuir-Freundlich curve fit for the adsorption of CO₂ in FMOF-1c at 308 K.



Figure S42. Langmuir-Freundlich curve fit for the adsorption of CH₄ in FMOF-1c at 308 K.

Т	288 K		298 K		308 K	
CO ₂ /CH ₄	CO_2	CH4	CO ₂	CH4	CO ₂	CH4
a_{LF}	3.373	2.287	3.198	2.207	3.063	2.122
b_{LF}	1.236×10 ⁻⁹	9.870×10 ⁻⁷	1.537×10 ⁻⁹	1.147×10 ⁻⁷	2.842×10 ⁻⁹	1.230×10 ⁻⁷
т	1.5295	1.1457	1.4905	1.1222	1.4238	1.1062
RMSE	0.0374	0.0054	0.0436	0.0033	0.0336	0.0020
χ^2	0.0022	0.0003	0.0026	0.0002	0.0020	0.0001

 Table S7: Langmuir- Freundlich parameters of FMOF-1c.



Figure S43. Toth curve fit for the adsorption of CO₂ in FMOF-1c at 288 K.



Figure S44. Toth curve fit for the adsorption of CH₄ in FMOF-1c at 288 K.



Figure S45. Toth curve fit for the adsorption of CO₂ in FMOF-1c at 298 K.



Figure S46. Toth curve fit for the adsorption of CH₄ in FMOF-1c at 298 K.



Figure S47. Toth curve fit for the adsorption of CO₂ in FMOF-1c at 308 K.



Figure S48. Toth curve fit for the adsorption of CH₄ in FMOF-1c at 308 K.

Т	288 K		8 K 298 K		308 K	
CO ₂ /CH ₄	CO ₂	CH4	CO ₂	CH4	CO ₂	CH4
a_T	3.193	2.110	2.973	2.030	2.792	1.946
b_T	8.239×10 ⁻⁷	5.904×10 ⁻⁷	6.859×10 ⁻⁷	5.240×10 ⁻⁷	5.849×10 ⁻⁷	4.690×10 ⁻⁷
1/m	0.3804	0.6706	0.3735	0.7012	0.3930	0.7233
RMSE	0.0054	0.0020	0.0022	0.0014	0.0018	0.0008
χ^2	0.0003	0.0001	0.0001	0.00007	0.0001	0.00005

 Table S8. Toth parameters of FMOF-1c.



Figure S49. Langmuir, Langmuir-Freundlich and Toth fitting curves of CO_2 and CH_4 in MeMOF-1c at 288 K.



Figure S50. Langmuir, Langmuir-Freundlich and Toth fitting curves of CO_2 and CH_4 in MeMOF-1c at 298 K.



Figure S51. Langmuir, Langmuir-Freundlich and Toth fitting curves of CO_2 and CH_4 in MeMOF-1c at 308 K.



Figure S52 Langmuir curve fit for the adsorption of CO₂ in MeMOF-1c at 288 K.



Figure S53. Langmuir curve fit for the adsorption of CH₄ in MeMOF-1c at 288 K.



Figure S54. Langmuir curve fit for the adsorption of CO₂ in MeMOF-1c at 298 K.



Figure S55. Langmuir curve fit for the adsorption of CH₄ in MeMOF-1c at 298 K.



Figure S56. Langmuir curve fit for the adsorption of CO₂ in MeMOF-1c at 308 K.



Figure S57. Langmuir curve fit for the adsorption of CH₄ in MeMOF-1c at 308 K.

Т	288 K		298 K		308 K	
CO ₂ /CH ₄	CO_2	CH ₄	CO_2	CH ₄	CO ₂	CH ₄
a_L	7.474	5.865	7.514	5.7902	7.297	5.660
b_L	4.553×10 ⁻⁶	1.320×10 ⁻⁶	2.734×10 ⁻⁶	1.054×10 ⁻⁶	2.025×10 ⁻⁶	8.244×10 ⁻⁷
RMSE	0.3301	0.1823	0.1076	0.2163	0.0925	0.1000
χ^2	0.0331	0.0101	0.0598	0.0120	0.0514	0.0056

Table S9: Langmuir parameters of MeMOF-1c.



Figure S58. Langmuir-Freundlich curve fit for the adsorption of CO₂ in MeMOF-1c at 288 K.



Figure S59. Langmuir-Freundlich curve fit for the adsorption of CH₄ in MeMOF-1c at 288 K.



Figure S60. Langmuir-Freundlich curve fit for the adsorption of CO₂ in MeMOF-1c at 298 K.



Figure S61. Langmuir-Freundlich curve fit for the adsorption of CH₄ in MeMOF-1c at 298 K.



Figure S62. Langmuir-Freundlich curve fit for the adsorption of CO₂ in MeMOF-1c at 308 K.



Figure S63. Langmuir-Freundlich curve fit for the adsorption of CH₄ in MeMOF-1c at 308 K.

Т	288 K		298 K		308 K	
CO ₂ /CH ₄	CO_2	CH4	CO ₂	CH4	CO ₂	CH4
a_{FL}	7.156	5.435	6.956	5.254	6.675	5.135
b_{FL}	3.593×10 ⁻⁸	1.280×10 ⁻⁷	3.365×10 ⁻⁸	7.350×10 ⁻⁸	2.688×10 ⁻⁸	1.006×10 ⁻⁷
т	1.385	1.188	1.3589	1.313	1.349	1.169
RMSE	0.1453	0.0474	0.1074	0.0700	0.1326	0.0235
χ^2	0.0086	0.0028	0.0063	0.0041	0.0078	0.0014

 Table S10: Langmuir-Freundlich parameters of MeMOF-1c.



Figure S64. Toth curve fit for the adsorption of CO₂ in MeMOF-1c at 288 K.



Figure S65. Toth curve fit for the adsorption of CH₄ in MeMOF-1c at 288 K.



Figure S66. Toth curve fit for the adsorption of CO₂ in MeMOF-1c at 298 K.



Figure S67. Toth curve fit for the adsorption of CH₄ in MeMOF-1c at 298 K.



Figure S68. Toth curve fit for the adsorption of CO₂ in MeMOF-1c at 308 K.



Figure S69. Toth curve fit for the adsorption of CH₄ in MeMOF-1c at 308 K.

Т	288 K		299	298 K		3 K
CO ₂ /CH ₄	CO ₂	CH ₄	CO_2	CH ₄	CO_2	CH ₄
a_T	7.032	5.214	6.890	4.965	6.462	4.998
b_T	2.511×10 ⁻⁶	1.119×10 ⁻⁶	2.051×10 ⁻⁶	9.100×10 ⁻⁷	1.464×10 ⁻⁶	7.827×10 ⁻⁷
1/m	0.5552	0.6702	0.6375	0.6164	0.5371	0.7480
RMSE	0.0432	0.0134	0.0382	0.0240	0.0007	0.1126
χ^2	0.0025	0.0008	0.0008	0.0015	0.0121	0.0001

 Table S11. Toth parameters of MeMOF-1c.

S8: Calculation of isosteric heats of adsorption at infinite dilution (Q_{st0})

The isosteric heats of adsorption at infinite dilution for CO₂ and CH₄ were calculated using the pure component adsorption data attained at 288, 298 and 308 K. The simulated isotherms were first fitted to different isotherm models to obtain the best fit. Toth model showed the best fitting. We then generated the pressure (*p*)-loading (*n*) pairs at each temperature and used the Clausius-Clapeyron equation¹⁷ (equation 7) to estimate the Q_{st0} values.

$$\Delta Q_{st0}(n) = R. \ln\left(\frac{P_2}{P_1}\right) \frac{T_1 T_2}{(T_2 - T_1)}$$
(7)

Where, R is the ideal gas constant, P is the pressure and T is the temperature.



S9: Calculation of Henry's constants from the slope of the isotherms

Figure S70. Adsorption range for the calculation of Henry's constant ($K_{\rm H}$) of CO₂ in FMOF-1c.



Figure S71. Adsorption range for the calculation of Henry's constant ($K_{\rm H}$) of CO₂ in MeMOF-1c.



Figure S72. Adsorption range for the calculation of Henry's constant ($K_{\rm H}$) of CH₄ in FMOF-1c.



Figure S73. Adsorption range for the calculation of Henry's constant ($K_{\rm H}$) of CH₄ in MeMOF-1c.

Temperature (K)	Structures	Methods	CO2 (mol/Kg/Pa)	CH4 (mol/Kg/Pa)
288	FMOF-1c	$K_{ m H,\ RASPA}$	2.180 ×10 ⁻⁶	1.450 ×10 ⁻⁶
		$K_{ m H,\ Toth}$	2.631×10 ⁻⁶	1.246 ×10 ⁻⁶
	MeMOF-1c	$K_{ m H,\ RASPA}$	1.870 ×10 ⁻⁵	6.610 ×10 ⁻⁶
		$K_{ m H,\ Toth}$	1.766 ×10 ⁻⁵	5.834 ×10 ⁻⁶
298	FMOF-1c	$K_{ m H,\ RASPA}$	1.810 ×10 ⁻⁶	1.230 ×10 ⁻⁶
		$K_{ m H,\ Toth}$	2.039 ×10 ⁻⁶	1.064 ×10 ⁻⁶
	MeMOF-1c	$K_{ m H,\ RASPA}$	1.560 ×10 ⁻⁵	5.150 ×10 ⁻⁶
		$K_{ m H,\ Toth}$	1.412 ×10 ⁻⁵	4.518 ×10 ⁻⁶
	FMOF-1c	$K_{ m H,\ RASPA}$	1.520 ×10 ⁻⁶	1.060 ×10 ⁻⁶
308		$K_{ m H,\ Toth}$	1.633 ×10 ⁻⁶	9.127 ×10 ⁻⁷
	MeMOF-1c	$K_{ m H,\ RASPA}$	1.010 ×10 ⁻⁵	4.150 ×10 ⁻⁶
		$K_{ m H,\ Toth}$	9.460 ×10 ⁻⁶	3.912 ×10 ⁻⁶

Table S12. $K_{\rm H}$ of CO₂ and CH₄ in FMOF-1c and MeMOF-1c, obtained from RASPA2 and Toth isotherms.





Figure S74. Selectivity of CO₂ and CH₄ over water for FMOF-1c using different methods at 298 K.

S11: Henry's constant and adsorption selectivity of CO₂ and CH₄ over water in MeMOF-1c using CBAC and EQeq charge methods

As water interaction is highly sensitive to the charges of framework atoms, we have used two different charge methods, CBAC⁵ and EQeq⁶, to determine the $K_{\rm H}$ values of CO₂, CH₄ and H₂O in MeMOF-1c. It is apparent that the $K_{\rm H}$ value of H₂O based on the CBAC charge method is higher than that of the value obtained by the EQeq charge method, in MeMOF-1c. This higher $K_{\rm H}$ value of H₂O leads to the lower selectivity for CO₂ and CH₄ over H₂O for CBAC compared to EQeq.

Parameter	Adsorbate/ Selectivity	CBAC	EQeq
$K_{ m H}$	H ₂ O	5.756 ×10 ⁻⁶	1.536 ×10 ⁻⁶
	CO_2	1.560 ×10 ⁻⁵	1.826 ×10 ⁻⁵
	CH ₄	5.150 ×10 ⁻⁶	5.166 ×10 ⁻⁶
Selectivity	CO ₂ /H ₂ O	2.7	11.9
	CH ₄ /H ₂ O	0.9	3.4

Table S13. *K*_H and selectivity in MeMOF-1c at 298 K using CBAC and EQeq charge methods.

S12: Convergence analysis of water



Figure S75. Number of water molecules adsorbed in FMOF-1c at 298 K at a pressure of 4500 Pa.

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