Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The effect of GME topology on the multicomponent adsorption in ZIFs

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Supporting Information

Table 1: atom atom interaction parameters

ZIF atoms			adsorbate atoms			
atom	$\sigma(A)$	$\varepsilon/k_B(K)$	atom	$\sigma(A)$	$\varepsilon/k_B(K)$	q(e)
Carbon	3.43	40.27	Carbon CO_2 [a]	2.76	28.13	0.576
Oxygen	3.12	21.75	Oxygen CO_2 [a]	3.03	80.51	-0.288
Hydrogen	2.57	14.14	Nitrogen N_2 [b]	3.31	36.00	-0.482 $(0.964)^{com}$
Nitrogen	3.26	22.72	Oxygen O_2 [c]	3.01	49.05	-0.123 $(0.246)^{com}$
Zinc	2.46	53.4	CH_4	3.73	148.00	
Cl	3.52	99.23	$O(H_2O)$ [d]	3.15	76.58	-0.834 $(0.417)^{H}$
Br	3.73	126.31				

[a] C-O distance (A) :1.18; [b] N-N distance (A) :1.1; [c] O-O distance (A) :1.21;
[d] O-H distance (A) :0.9572, H-O-H angle 104.52^o; ^{com} center of mass charge;
^{H} hydrogen atom charge;

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Table 2: Atomic charges (e) on $Im-Zn-nIm$ fragments for ZIFs 68-78

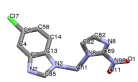
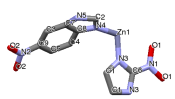
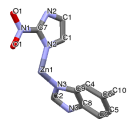
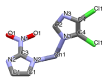
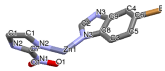
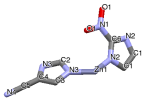
ZIF68		ZIF69		ZIF70		ZIF78	
							
C1	0.225591	Zn1	0.7317525	C1	0.605978456	C1	-0.0106
C2	0.350384	O11	-0.478251	C2	0.001007456	C2	0.128964
C3	0.179233	N2	-0.1558705	C3	0.013118456	C3	0.001442
C4	0.174222	N8	-0.3714605	C4	-0.056530044	C4	-0.219686
C6	-0.1565715	N98	0.731731	H1	0.111105956	C5	-0.121936
C8	-0.143245	C6	0.061975	H2	0.046464456	C6	0.043451
H1	-0.015756	C4	-0.074958	H3	0.073645456	C7	-0.015263
H4	0.013269625	C3	0.092504	N1	0.497581456	C8	0.258017
H6	0.0190095	C13	0.092504	N2	-0.604204044	C9	-0.021719
H8	0.128247	C89	0.350589	N3	-0.201820044	H1	0.1944375
N1	-0.284354	C14	-0.17425	O1	-0.336702544	H2	0.050911
N2	-0.3847325	C58	-0.078663	Zn1	0.863852789	H3	-0.010385
N5	0.588478	C85	0.032752			H4	0.083533
O1	-0.513472	C82	0.0008315			H5	0.152612
Zn1	0.78809075	H86	0.0677			N1	0.549019
		H10	0.08801225			N2	0.637037
		H17	0.100886			N3	-0.1615285
		H15	0.02653			N4	-0.335407
		H5	0.025733			N5	-0.142997
		Cl7	-0.153309			O1	-0.469039
						O2	-0.417138
						Zn1	0.690143

Table 3: Atomic charges (e) on $Im-Zn-nIm$ fragments for ZIFs 79-82

ZIF79		ZIF80		ZIF81		ZIF82	
							
C1	0.032906518	C1	0.006586474	Br1	-0.05360366	C1	0.025438825
C10	-0.060596982	C2	-0.112881026	C1	-0.00844216	C2	0.040290825
C2	0.022409018	C3	0.398487974	C2	0.08614634	C3	-0.086898175
C3	-0.022760982	C4	0.032632474	C3	-0.15867266	C4	0.019024825
C4	-0.294764982	Cl1	-0.104059276	C4	-0.18855966	C5	0.346642825
C5	-0.262450982	H1	0.160282974	C5	-0.09332866	C6	0.330535825
C6	0.142721018	H2	0.074763974	C6	0.03654734	H1	0.122317325
C7	0.246174018	N1	0.428308974	C7	0.33524434	H2	0.092760825
C8	-0.040575982	N2	-0.390102026	C8	0.09322034	H3	0.053276825
C9	0.144435018	N3	-0.051962026	C9	0.14520034	N1	0.549978825
H1	0.100044018	O1	-0.396090026	H1	0.07414009	N2	-0.369172675
H10	0.033027185	Zn1	0.696742974	H2	0.12699134	N3	-0.128532175
H2	0.075918018			H3	0.05665434	N4	-0.498546175
H3	0.009615018			H4	0.12364134	O1	-0.413424675
H4	0.037820018			H5	0.11818534	Zn1	0.679680325
H5	0.164021018			N1	0.72366234		
N1	0.525830018			N2	-0.38018566		
N2	-0.315941482			N3	-0.23377816		
N3	-0.119002982			O1	-0.48827466		
O1	-0.423880482			Zn1	0.72175234		
Zn1	0.664874018						

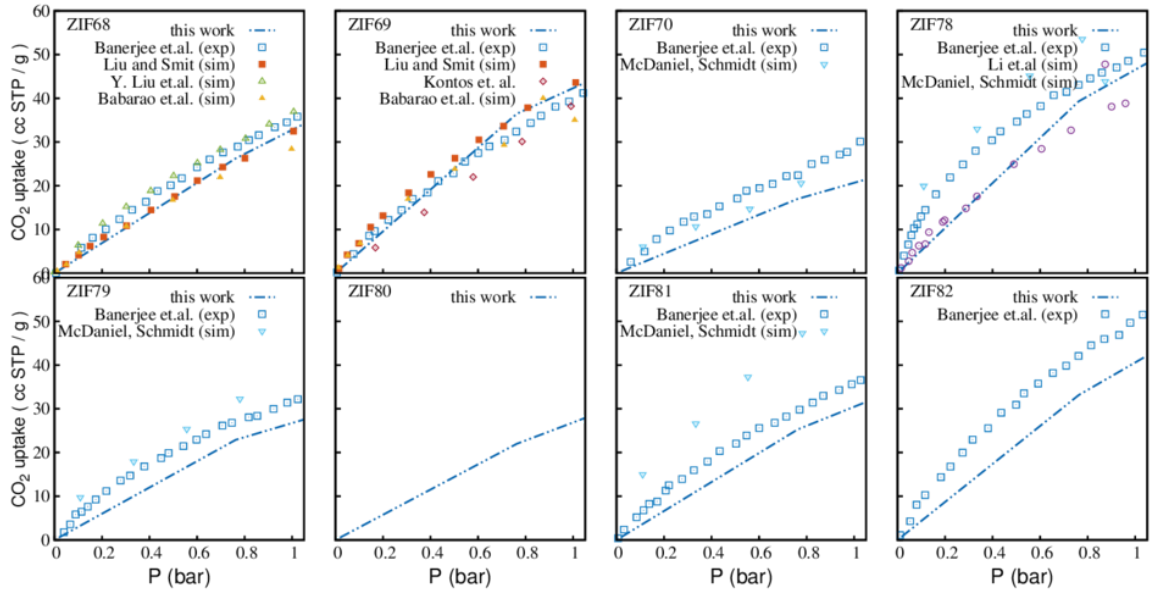


Figure 1: CO_2 adsorption isotherms computed at 298K in this work, compared with a set of experimental and simulated isotherms provided in the literature. The citing articles are included in the reference list of the manuscript

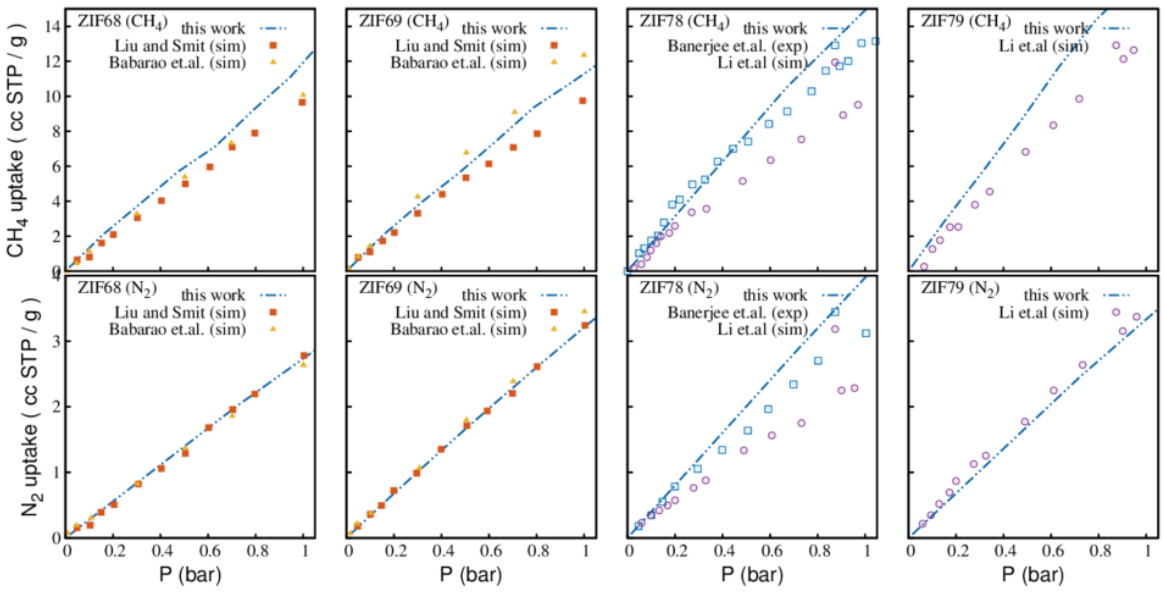


Figure 2: CH_4 and N_2 adsorption isotherms computed at 298K in this work, for ZIF68, ZIF69, ZIF78 and ZIF79, compared with a set of experimental and simulated isotherms provided in the literature.The citing articles are included in the reference list of the manuscript

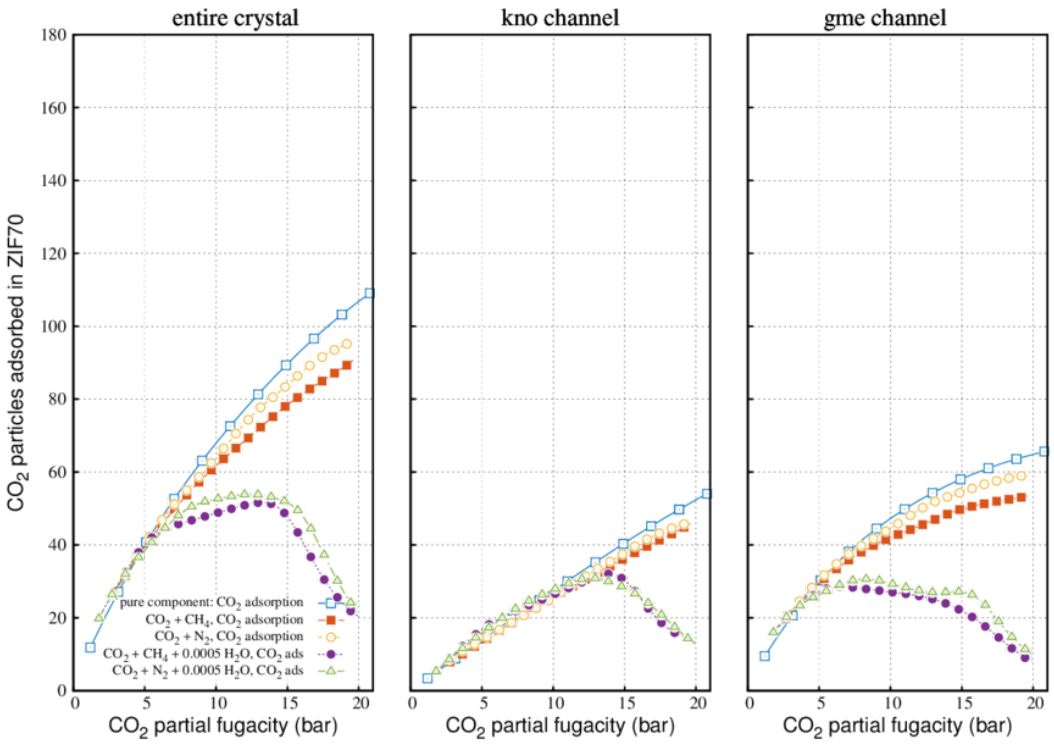


Figure 3: CO_2 adsorption in the unit cell, the *kno* and *gme* channels of ZIF70, for single and multicomponent systems.

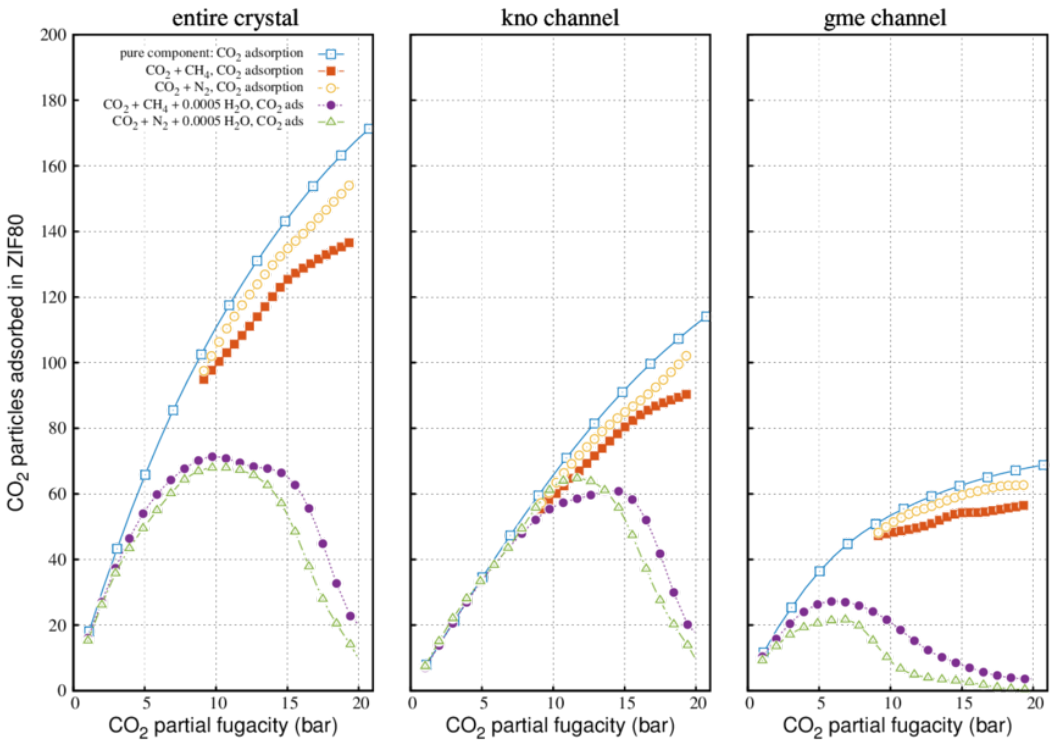


Figure 4: CO_2 adsorption in the unit cell, the *kno* and *gme* channels of ZIF80, for single and multicomponent systems.

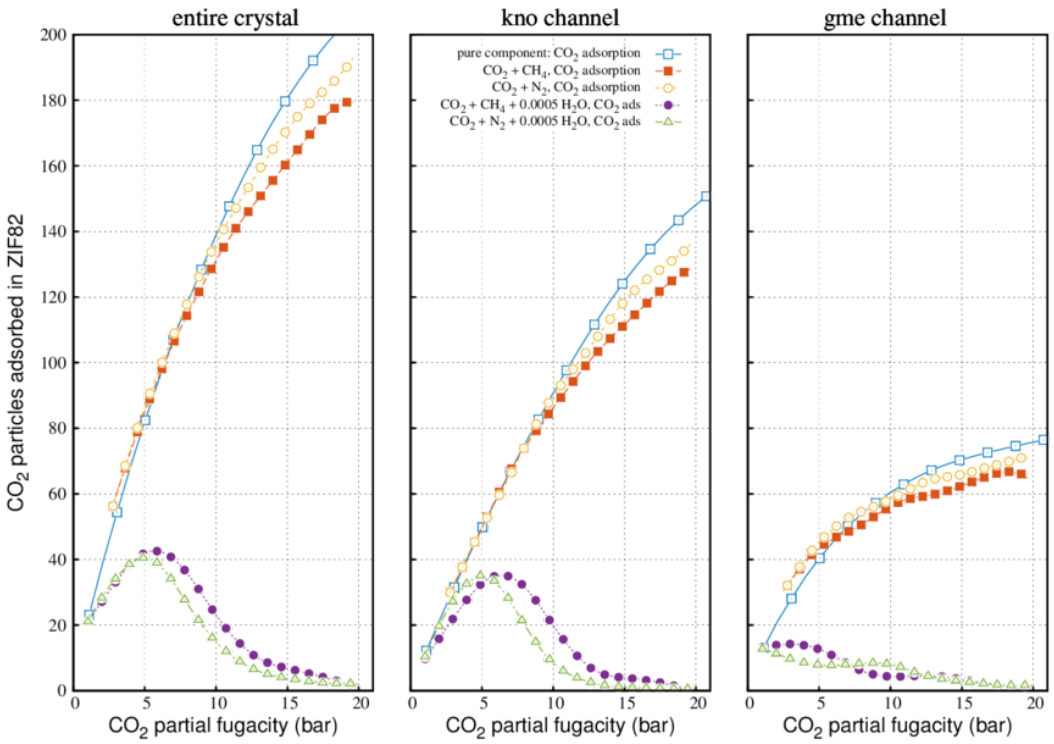


Figure 5: CO_2 adsorption in the unit cell, the *kno* and *gme* channels of ZIF82, for single and multicomponent systems.