

Supplementary material: Theoretical and experimental investigations of ^{129}Xe NMR chemical shift isotherms in metal-organic frameworks

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Chemical shift values

Table A1 Theoretical values of the chemical shift of ^{129}Xe as a function of pressure (GCMC, model systems). For all theoretical values, 47 ppm have been subtracted.

Pressure [bar]	$\delta_{\text{theo,UiO-66}}$ [ppm]	$\delta_{\text{theo,UiO-67}}$ [ppm]
1	200.86	133.49
2	239.39	159.15
3	243.73	172.41
4	249.37	191.55
5	261.84	202.06
6	252.38	199.22
7	263.64	210.25
8	256.31	223.15
9	262.93	225.41
10	259.18	227.94
11	271.54	230.09
12	276.31	240.09
13	268.01	234.28
14	286.46	239.86
15	284.52	234.68
16	291.81	245.86
17	270.65	248.62

Table A2 Experimental values of the chemical shift of ^{129}Xe as a function of pressure. The first pressure range indicates adsorption, the second one desorption.

UiO-66		UiO-67	
Pressure [bar]	δ_{exp} [ppm]	Pressure [bar]	δ_{exp} [ppm]
2.06	235.96	1.18	153.86
3.05	244.09	1.81	168.34
4.11	249.55	2.39	178.18
5.08	253.16	3.24	189.11
6.08	255.92	4.29	206.24
7.07	258.35	5.33	213.38
8.01	260.40	6.48	219.58
9.12	264.00	7.51	223.72
10.05	266.50	8.63	227.92
11.07	268.70	9.84	231.82
12.01	270.30	10.76	234.48
13.05	271.50	11.82	236.74
14.63	274.50	13.25	239.57
16.23	276.29	13.85	241.50
17.23	276.43	15.07	243.05
		16.01	244.91
		17.26	245.95
15.03	276.05	16.09	245.86
9.52	265.74	14.91	242.79
8.04	263.40	12.92	239.29
6.01	256.79	8.54	227.53
3.99	249.16	4.26	206.20
1.99	235.08	1.07	152.10
1.00	217.06	0.83	138.70
0.73	207.11	0.43	114.53
0.40	190.31		

^{129}Xe NMR spectra

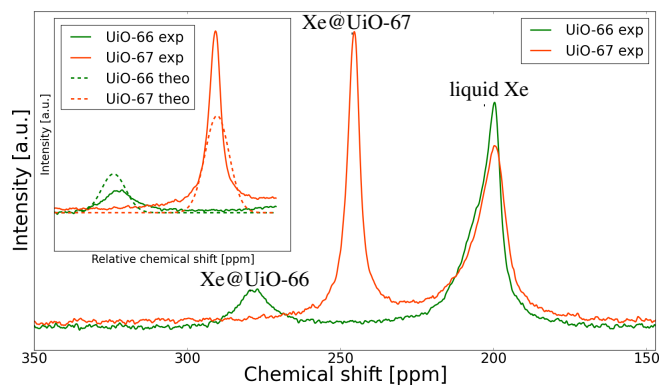


Figure A1 High pressure ($p = 1.73$ MPa) ^{129}Xe NMR spectra of UiO-66 and UiO-67. Comparison of experimental NMR spectrum (exp) with the theoretical prediction using the model systems (theo)¹.

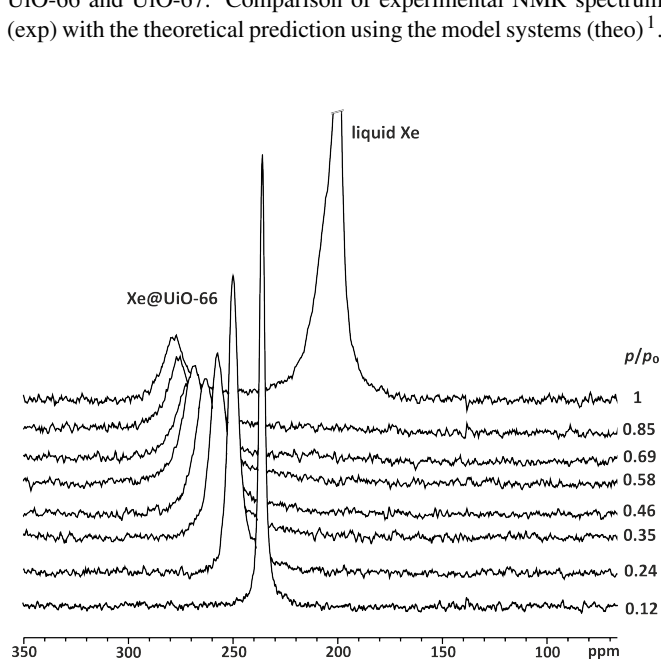


Figure A2 ^{129}Xe NMR spectra of xenon adsorbed on UiO-66 measured for variable pressure at $T = 237$ K.

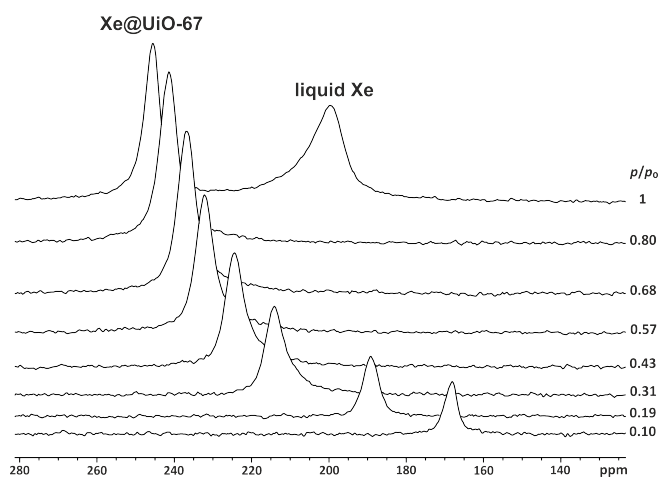


Figure A3 ^{129}Xe NMR spectra of xenon adsorbed on UiO-67 measured for variable pressure at $T = 237$ K.

References

- 1 K. Trepte, J. Schaber, S. Schwalbe, F. Drache, I. Senkowska, S. Kaskel, J. Kortus, E. Brunner and G. Seifert, *Physical Chemistry Chemical Physics*, 2017, **19**, 10020–10027.