Supplementary Material (ESI) for Chemical Communications

On the performance of Cu-BTC Metal Organic Framework for Carbon Tetrachloride Gas Removal

Sofía Calero,*[a] Ana Martín-Carlvo,[a] Said Hamad[a] , and Elena García-Pérez[a]

[a]*Department of Physical, Chemical, and Natural Systems, University Pablo de Olavide, Seville, Spain. Fax+34 95434 9814; Tel: +34 95497 7594; E-mail: scalero@upo.es*

Supporting Information

Table 1. Point charges and Lennard-Jones parameters used in this work

Cu-BTC			
Atoms	Charge [e^-]	Lennard-Jones parameters	
		ε/k_B [K]	σ [Å]
Cu	1.0	2.518	3.114
O_b	-0.6	48.19	3.03
C_a	0.7	47.86	3.47
C_b	0.0	47.86	3.47
C_c	-0.15	47.86	3.47
H	0.15	7.65	2.85
Adsorbed Molecules			
Atoms	Charge [e^-]	Lennard-Jones parameters	
		ε/k_B [K]	σ [Å]
O (O_2)	-0.112	53.023	3.045
Dummy (O_2)	0.224	-	-
N (N_2)	-0.405	38.298	3.306
Dummy (N_2)	0.810	-	-
Ar	-	124.070	3.380
CCl_4	-	519.730	5.140

Figure 1S compares our computed adsorption values of carbon tetrachloride with experimental adsorption previously reported in several materials[1]. As shown in the figure, the amount of carbon tetrachloride that we obtain at saturation on Cu-BTC is higher than the obtained for other materials such as activated carbon BPL, hydrophobic zeolite Y and silicalite-1 and only comparable with the obtained for MCM-41. However, we can indicate two main reasons to prioritize Cu-BTC over MCM-41. The first reason is that saturation on Cu-BTC is reached at lower pressures than on MCM-41. The second reason is that Cu-BTC is stable upon hydration /dehydration[2], whereas MCM-41 collapses upon rehydration at room temperature, and also when it is left in air for three months[3].

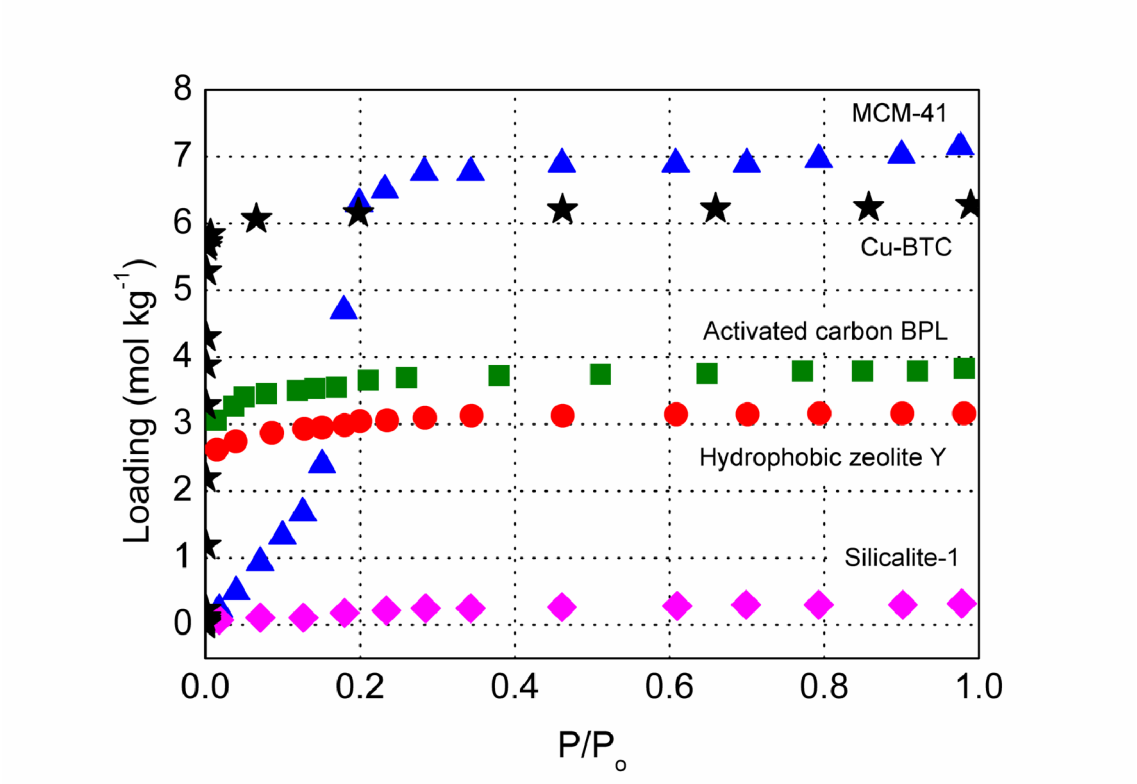

Figure 1S: Adsorption isotherms of carbon tetrachloride over several adsorbents.

We have performed additional simulations to check the effect with water as competing molecule. Simulations were performed in what we think could be one of the worst of the scenarios, i.e. 100% relative air humidity (4% of water at room conditions). The obtained results show preferential adsorption of carbon tetrachloride over water (Figure 2S) and demonstrate that carbon tetrachloride selectivity over N2, O2, and Ar increases even more with ambient humidity. It is also interesting to note that recent experimental and simulation studies have also reported an enhancement of selectivity of CO2 with water content in this structure[4].

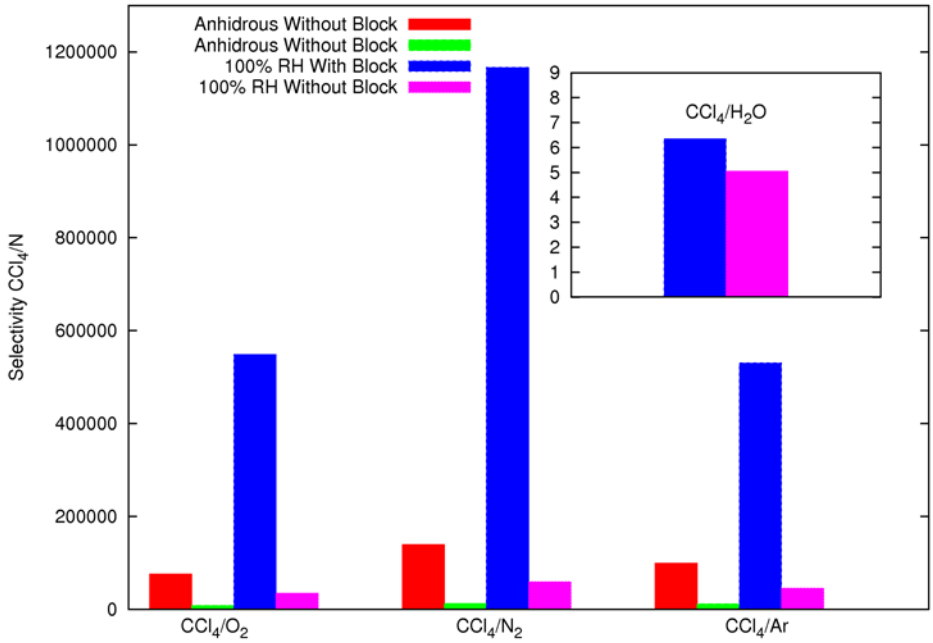

Figure 2S: Adsorption selectivity of carbon tetrachloride over the main components of the air in anhydrous conditions and for air relative humidity 100%. Comparison between the values obtained for the blocked and for the non-blocked structures.

1. X. S. Zhao, Q. Ma and G. Q. M. Lu, *Energy & Fuels*, 1998, **12**, 1051-1054.
2. J. M. Castillo, T. J. H. Vlugt and S. Calero, *Journal of Physical Chemistry C*, 2008, **112**, 15934-15939.
3. X. S. Zhao, F. Audsley and G. Q. Lu, *Journal of Physical Chemistry B*, 1998, **102**, 4143-4146.
4. A. O. Yazaydin, A. I. Benin, S. A. Faheem, P. Jakubczak, J. J. Low, R. R. Willis and R. Q. Snurr, *Chem. Mat.*, 2009, **21**, 1425–1430.