Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information

Effect of air humidity on the removal of carbon tetrachloride from air using Cu-BTC Metal-Organic Framework

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Table 1S: Computed surface area of Cu-BTC using different types of molecules. The surface area is given in m^2/g.

Hydrogen	Oxygen	Nitrogen	Argon	CCl_4	Experimental [1]
2563.92	2513.30	2344.28	2296.84	1432.47	1958

Table 2S: Lennard-Jones parameters and partial charges used for Cu-BTC. The Lennard-Jones parameters were taken from the DREIDING generic force field [2], except copper that was taken from the UFF force field [3]. The atomic charges for Cu-BTC were taken from reference [4].

Cu-BTC			
Atoms	Charge [e^-]	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

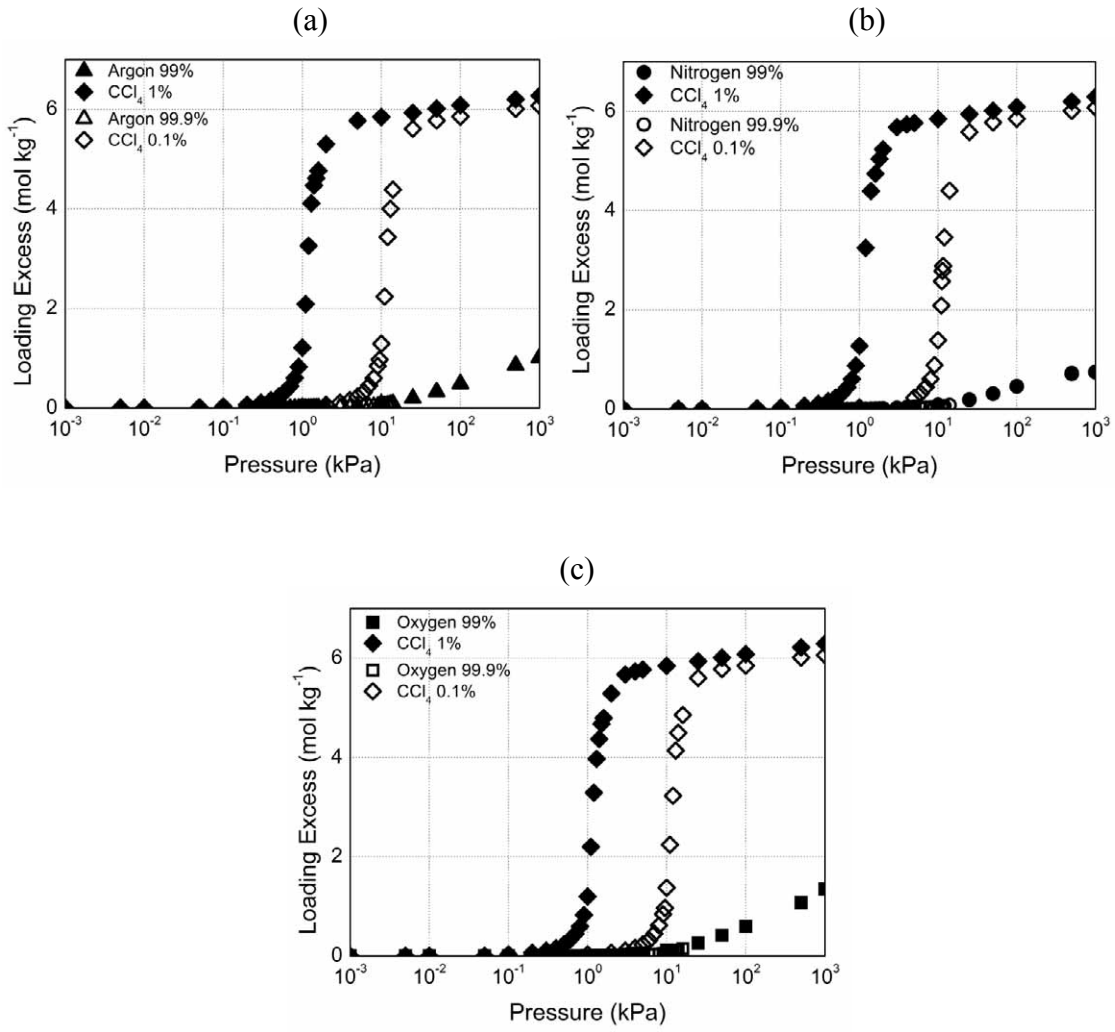

Figure 1S: Adsorption isotherms of (a) Ar/CCl_4, (b) N_2/CCl_4, and (c) O_2/CCl_4 binary mixtures in Cu-BTC. The adsorption isotherms of argon (triangles), nitrogen (circles), oxygen (squares), and carbon tetrachloride (rhombs) were computed at 298 K and at bulk partial fugacity ratio of 99:1 (full symbols) and 99.9:0.1 (empty symbols). Computed error bars are within the symbol size.

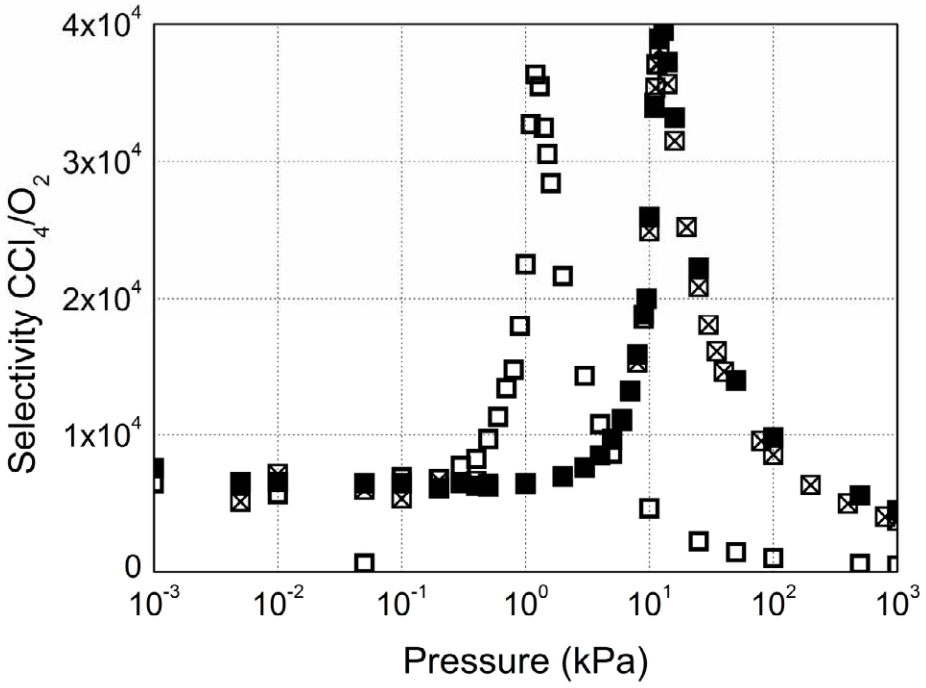

Figure 2S: Adsorption selectivity of carbon tetrachloride over oxygen obtained from the computed adsorption isotherms of O_2/CCl_4 mixtures at a bulk partial fugacity ratio of 99:1 (empty symbols), 99.9:0.1 (full symbols), and 20.979:0.1 (crossed symbols)

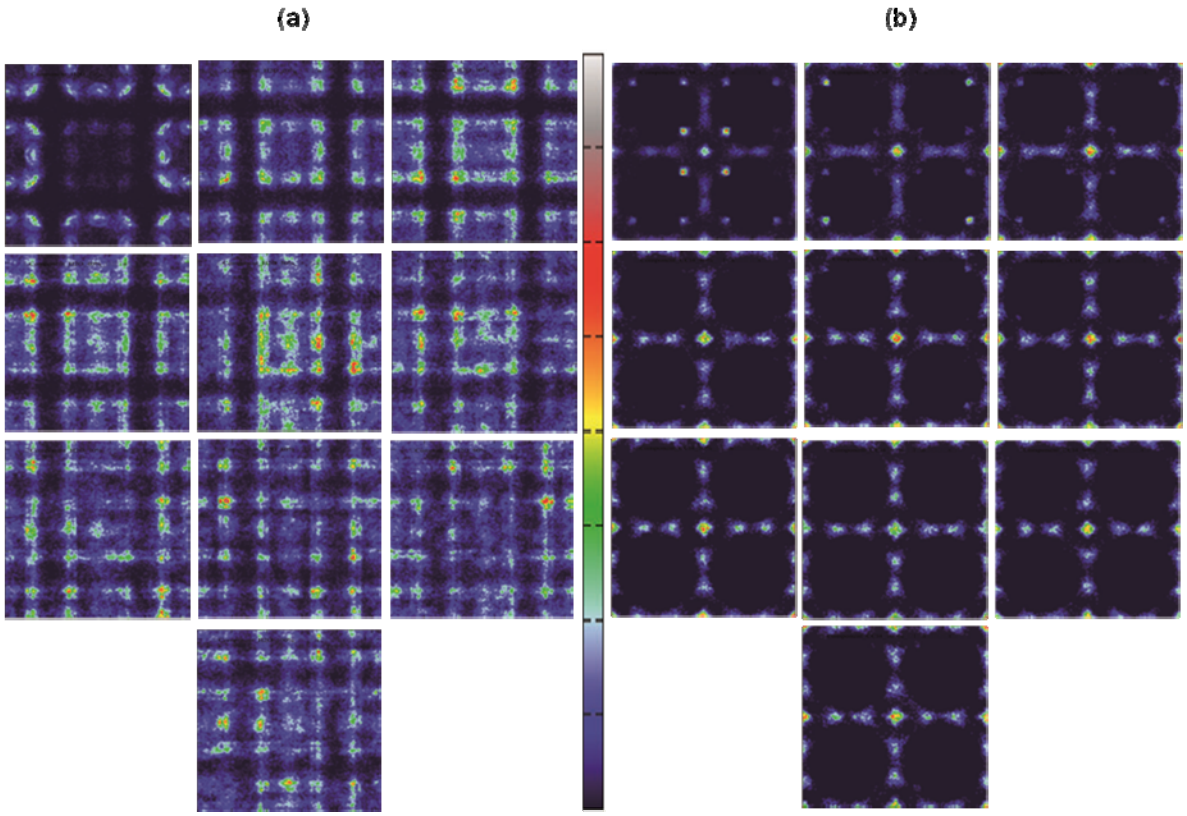

Figure 3S: Average occupation profiles of (a) water and (b) carbon tetrachloride in Cu-BTC. The profiles were obtained from the molecular simulations of five-component mixtures of carbon tetrachloride in air with relative humidity from 10%-30% (top left-top right) to 100% (bottom). The same color gradation (from dark blue to white) is employed in all figures, although the total number of molecules present in the unit cell is different for each calculation.

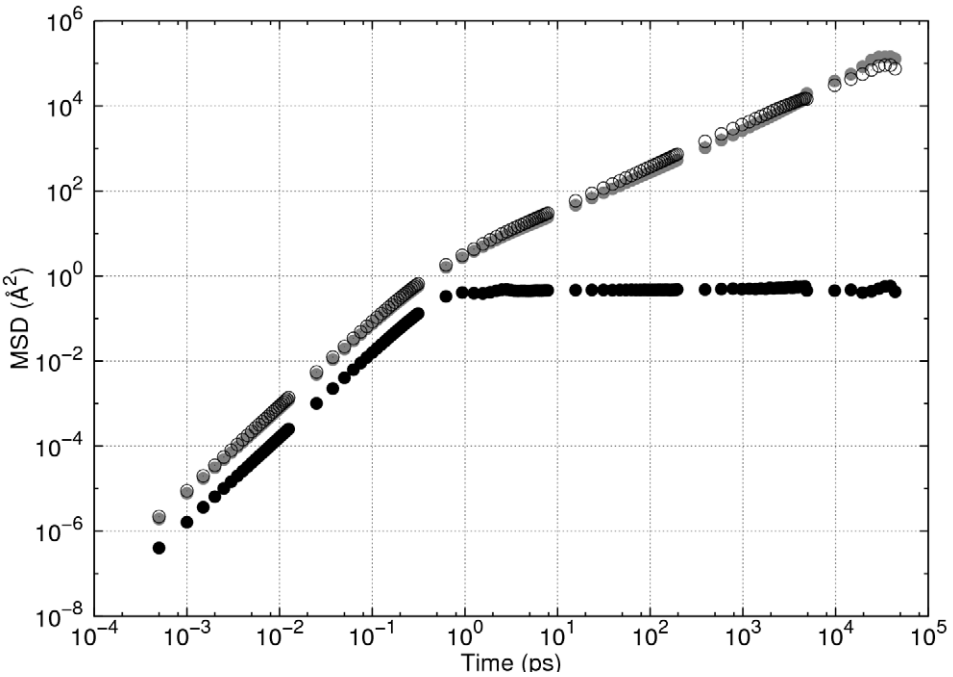

Figure 4S: Representation of the Mean Square Displacement (MSD) of oxygen (gray circles), nitrogen (empty circles), and carbon tetrachloride (black circles) as pure components.

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