

Gas adsorption in Cu-BTC Metal-Organic Frameworks

Juan M. Castillo^{1,2}, Thijs J. H. Vlugt¹, Sofia Calero²

¹Delft University of Technology, Process & Energy Laboratory,
Leeghwaterstraat 44, 2628CA Delft, The Netherlands

²Department of Physical, Chemical, and Natural Systems. University Pablo de Olavide.
Ctra. Utrera km. 1. 41013 Seville, Spain

Molecular simulations were performed to study the adsorption behavior of water, nitrogen, oxygen, and hydrocarbons in the metal-organic framework Cu-BTC. This is one of the better-known materials of this type that is stable upon water adsorption/desorption. The charge of the framework atoms was fitted to reproduce the available experimental water adsorption isotherm. This new set of interaction parameters was used to calculate Henry coefficients as well as the energies, entropies, and enthalpies for the different adsorption sites. Four main adsorption sites for this structure have been identified: site I close to the copper atoms, site I' in the bigger cavities, site II located in the small octahedral cages, and site III at the windows of the four open faces of the octahedral cage. Our simulations show that water has a surprisingly large affinity for the metal center in Cu-BTC. For nitrogen, oxygen, methane, ethane and propane, we identify the octahedral cages (sites II and III) and the big cages (site I') as the preferred positions for adsorption, while site I, near the copper atoms, remains empty over the entire range of pressures analyzed due to its reduced accessibility. This particular behavior could be further exploited for the separation of water from other nonpolar molecules.