

# Effect of water and coexisting impurities on the adsorption of CO<sub>2</sub> in CuBTC and zeolite 13X

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MOFs and zeolites have been intensely studied for CO<sub>2</sub> adsorption and separation through experimental techniques and computational simulation methods in recent years. However, and in spite of the great importance from their practical implementation, the investigation of the effect of coexisting components or impurities such as water, SO<sub>2</sub> and others, in flue gases was less explored.<sup>1,2</sup> For practical applications, the adsorbents should not only possess a high adsorption capacity for CO<sub>2</sub> and high CO<sub>2</sub> selectivity over other species, but also exhibit good behavior under impurities and water. The main objective is to assess the adsorption potential of MOF CuBTC and zeolite 13X for application in CO<sub>2</sub> adsorption separation from gas mixtures, with the impurities found in real processes, as a further step in finding optimal materials for CO<sub>2</sub> capture and separation. To this purpose, Grand Canonical Monte Carlo (GCMC) simulations are used in order to obtain the main properties related to CO<sub>2</sub> capture on these porous materials<sup>3</sup>.

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