Molecular simulation study of the competitive adsorption of H$_2$O and CO$_2$ in zeolite 13X

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Pure component isotherms

Figure 1: Comparison of the H$_2$O isotherms obtained from our GCMC simulations and the experimental isotherm at 310 K measured by Ferreira et al.$^1$

Figure 2: Comparison of the CO$_2$ isotherms obtained from our GCMC simulations and the experimental isotherms at 290 K, 310 K and 330 K measured by Ferreira et al.$^1$
Figure 3: Comparison of the CO$_2$ isotherms obtained from our GCMC simulations and the experimental isotherm at 328 K measured by Bae et al.$^2$

Figure 4: Comparison of the CO$_2$ isotherms obtained from our GCMC simulations and the experimental isotherm at 323 K measured by Ko et al.$^3$
Isotherms on a linear scale

Figure 5: H$_2$O isotherms on a linear scale and comparison with experimental data. Red data points from Wang et al.,$^4$ blue data points from Ferreira et al.$^1$

Figure 6: CO$_2$ isotherms on a linear scale and comparison with experimental data. Red data points from Wang et al.,$^4$ blue data points from Ko et al.$^3$ and green from Bae et al.$^2$
Mixture isotherms

Figure 7: Comparison of the H$_2$O/CO$_2$ isotherms obtained from our GCMC simulations and the experimental isotherms at 323 K measured by Wang et al.$^5$


References


