

Molecular simulation study of the competitive adsorption of H₂O and CO₂ in zeolite 13X

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Pure component isotherms

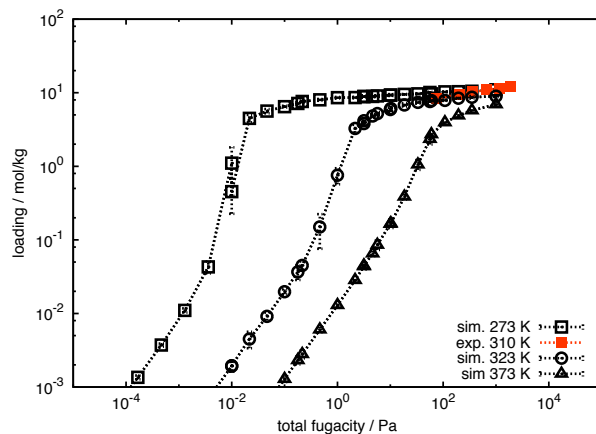


Figure 1: Comparison of the H₂O isotherms obtained from our GCMC simulations and the experimental isotherm at 310 K measured by Ferreira et al.¹

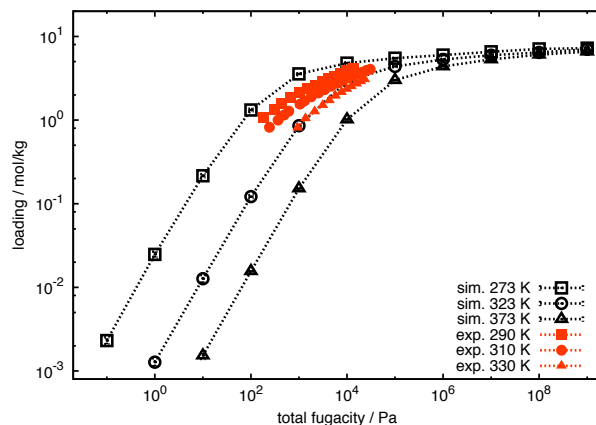


Figure 2: Comparison of the CO₂ isotherms obtained from our GCMC simulations and the experimental isotherms at 290 K, 310 K and 330 K measured by Ferreira et al.¹

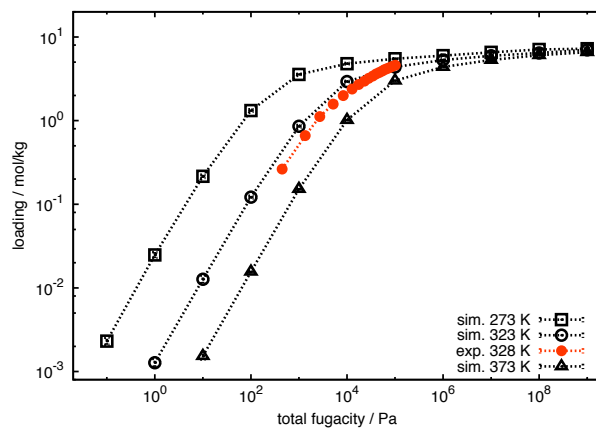


Figure 3: Comparison of the CO₂ isotherms obtained from our GCMC simulations and the experimental isotherm at 328 K measured by Bae et al.²

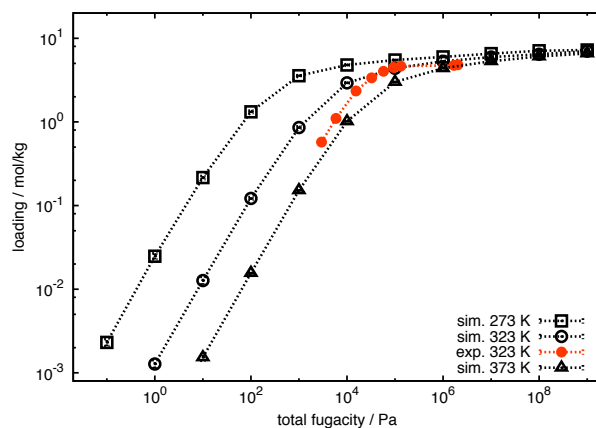


Figure 4: Comparison of the CO₂ isotherms obtained from our GCMC simulations and the experimental isotherm at 323 K measured by Ko et al.³

Isotherms on a linear scale

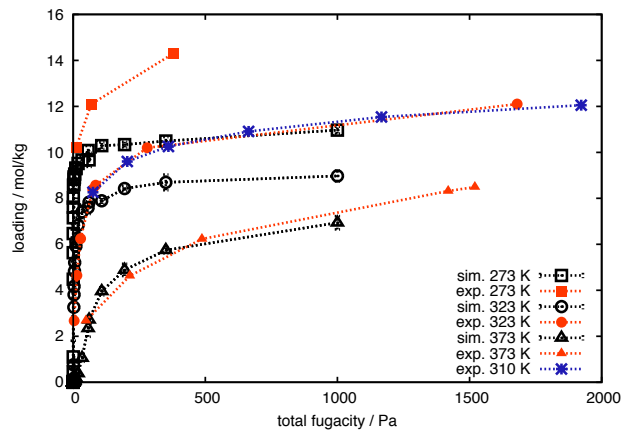


Figure 5: H₂O isotherms on a linear scale and comparison with experimental data. Red data points from Wang et al.,⁴ blue data points from Ferreira et al.¹

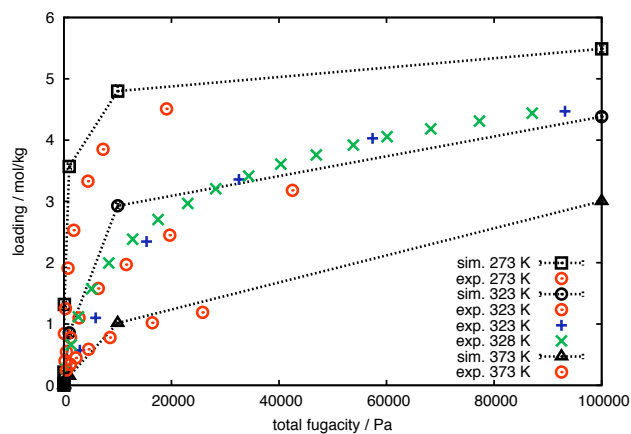


Figure 6: CO₂ isotherms on a linear scale and comparison with experimental data. Red data points from Wang et al.,⁴ blue data points from Ko et al.³ and green from Bae et al.²

Mixture isotherms

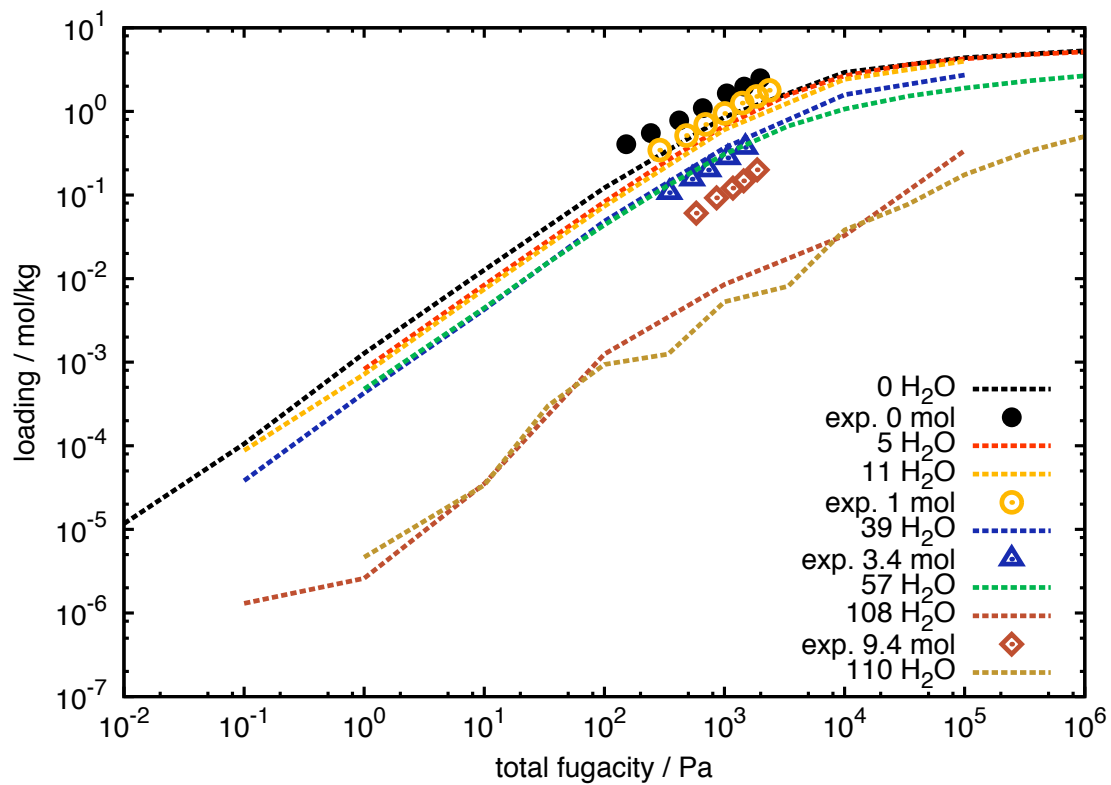


Figure 7: Comparison of the H₂O/CO₂ isotherms obtained from our GCMC simulations and the experimental isotherms at 323 K measured by Wang et al.⁵

References

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