Molecular simulation study of the competitive adsorption of H_2O and CO_2 in zeolite 13X

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Pure component isotherms

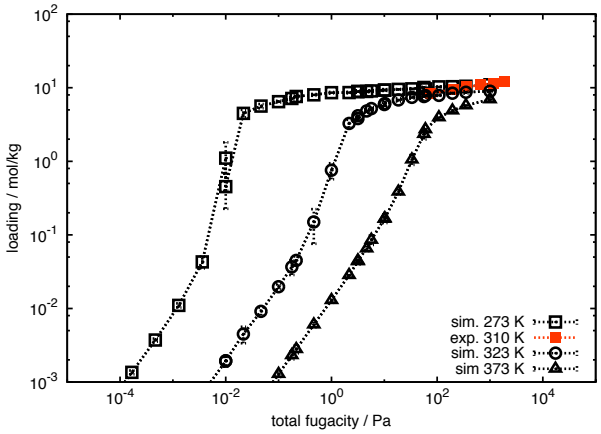

Figure 1: Comparison of the H_2O isotherms obtained from our GCMC simulations and the experimental isotherm at 310 K measured by Ferreira et al.[1]

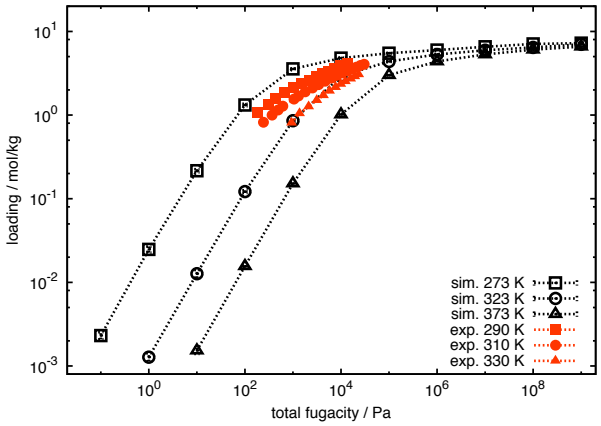

Figure 2: Comparison of the CO_2 isotherms obtained from our GCMC simulations and the experimental isotherms at 290 K, 310 K and 330 K measured by Ferreira et al.[1]

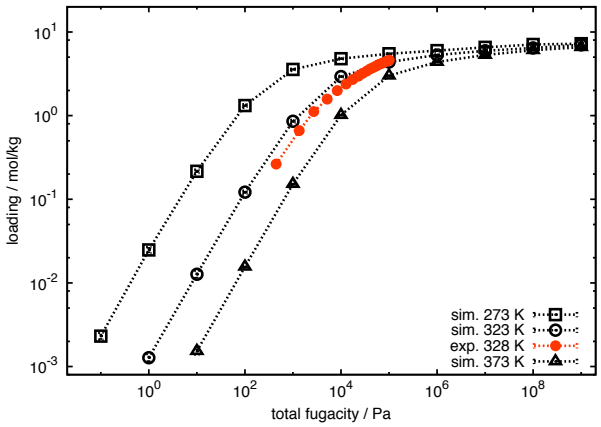

Figure 3: Comparison of the CO_2 isotherms obtained from our GCMC simulations and the experimental isotherm at 328 K measured by Bae et al.[2]

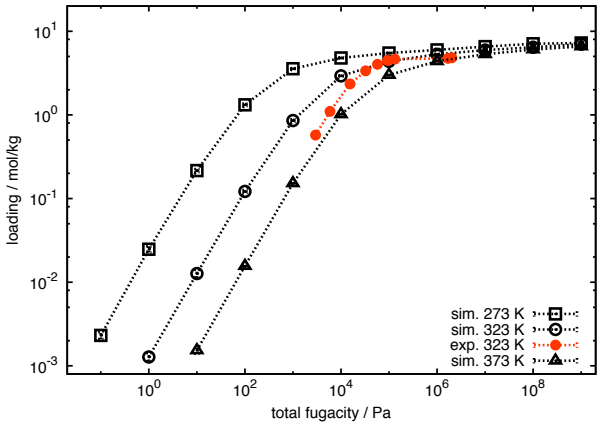

Figure 4: Comparison of the CO_2 isotherms obtained from our GCMC simulations and the experimental isotherm at 323 K measured by Ko et al.[3]

Isotherms on a linear scale

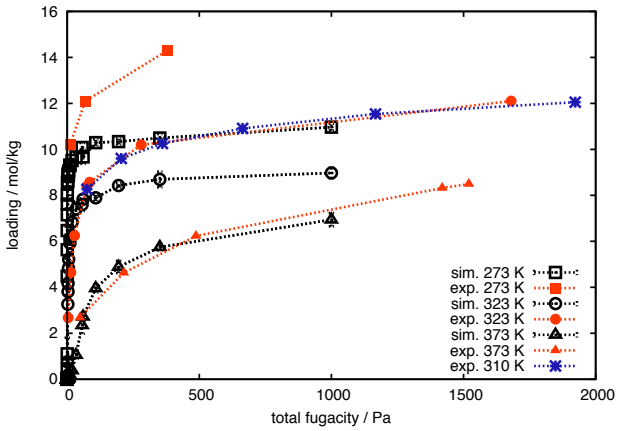

Figure 5: H_2O isotherms on a linear scale and comparison with experimental data. Red data points from Wang et al.,[4] blue data points from Ferreira et al.[1]

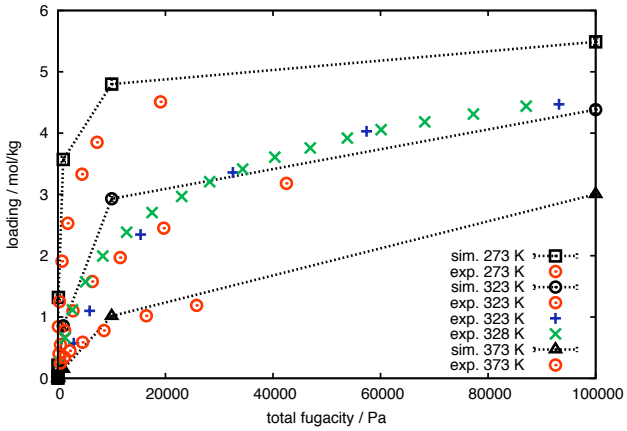

Figure 6: CO_2 isotherms on a linear scale and comparison with experimental data. Red data points from Wang et al.,[4] blue data points from Ko et al.[3] and green from Bae et al.[2]

Mixture isotherms

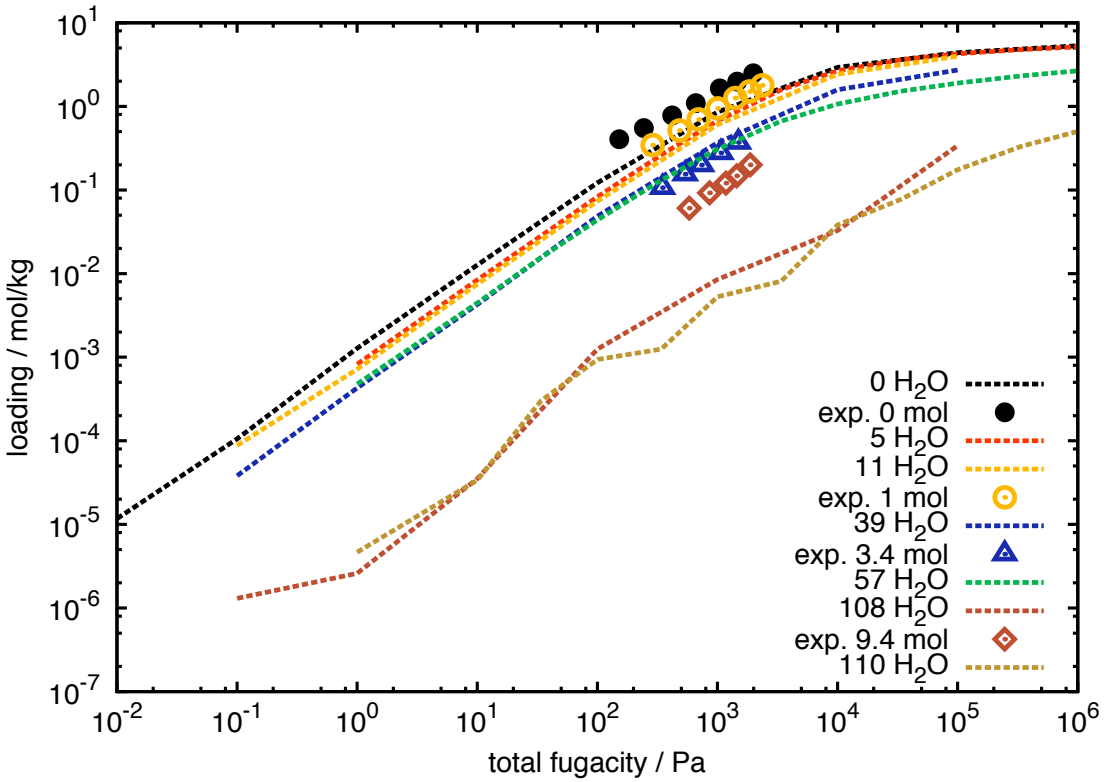

Figure 7: Comparison of the H_2O/CO_2 isotherms obtained from our GCMC simulations and the experimental isotherms at 323 K measured by Wang et al.[5]

References

[1] Ferreira, D.; Magalhães, R.; Taveira, P.; Mendes, A. *Ind. Eng. Chem. Res.* **2011**, *50*, 10201–10210.

[2] Bae, T.-H.; Hudson, M. R.; Mason, J. A.; Queen, W. L.; Dutton, J. J.; Sumida, K.; Micklash, K. J.; Kaye, S. S.; Brown, C. M.; Long, J. R. *Energy Environ. Sci.* **2013**, *6*, 128–138.

[3] Ko, D.; Siriwardane, R.; Biegler, L. T. *Ind. Eng. Chem. Res.* **2003**, *42*, 339–348.

[4] Wang, Y.; LeVan, M. D. *J. Chem. Eng. Data* **2009**, *54*, 2839–2844.

[5] Wang, Y.; LeVan, M. D. *J. Chem. Eng. Data* **2010**, *55*, 3189–3195.