Predicting adsorption selectivity of ethane and ethylene in carbon slit pores: a comparison between Monte Carlo simulations and direct numerical integration

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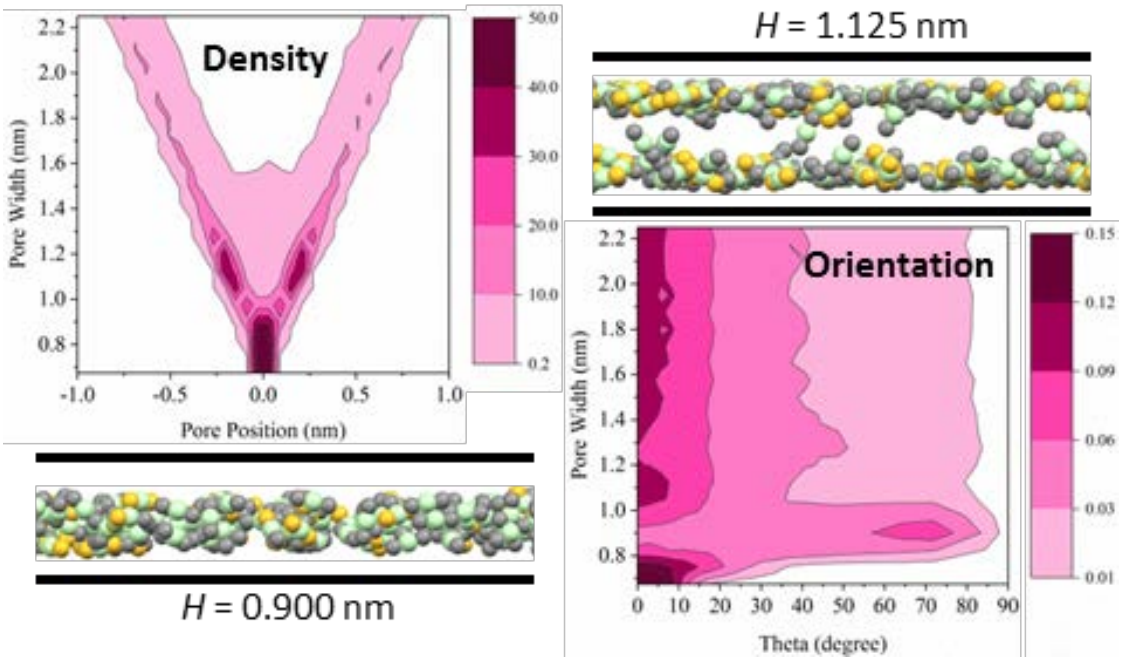
Understanding the behaviour of fluids in confinement is essential to predict adsorption selectivity and develop adsorbents that can address challenging separations, such as ethane/ethylene mixtures [1]. In this work we show that adsorption selectivity for an ethane/ethylene mixture can be predicted from direct numerical integration of the solid-fluid interaction potential because fluid-fluid interactions are negligible when compared to solid-fluid interactions, and adsorption sites are indistinguishable in pure component and mixture simulations. We present a comprehensive analysis of the density and orientation distributions in the pores as a function of pore size and pressure, providing tools that can be used for the design of 2D materials for the selective adsorption of gases.



Reference

[1] W. Liang, Y. Wu, H. Xiao, J. Xiao, Y. Li, Z. Li, Ethane-selective carbon composites CPDA@A-ACs with high uptake and its enhanced ethane/ethylene adsorption selectivity, AIChE J. (2018).

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