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# Competitive adsorption of $CO_2$ and $CH_4$ in functionalized amorphous-silica nanopores

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We investigate the mechanisms of competitive adsorption of $CO_2$ and $CH_4$ molecules in silica nanopores characterized by different physico-chemical features. We study the influence of different physical properties (e.g., surface roughness and the geometric arrangement of functional groups) and chemical heterogeneity (e.g., the number of hydroxyl, -OH, and ethoxyl, -$OCH_2$-$CH_3$, groups at the nanopore surface) on the affinity for $CO_2$ and $CH_4$, as well as on the resulting mobility. Notably, hydroxyl (Fig 1a) and ethoxyl (Fig 1b) are among the most common surface groups found on silica substrates that are synthesized from the Tetraethyl orthosilicate (TEOS) precursor. A recent work [1] showed the potential of hydrophilic (high density of -OH groups) and hydrophobic (high density of -$OCH_2$-$CH_3$) membranes for fluid separation. From the results of molecular dynamic (MD) simulations, we extract the most relevant parameters that describe the adsorption of the $CO_2$, $CH_4$, and mixtures of the two. We report the key findings of the atomistic investigation and discuss the relevant surface properties that need to be considered for a faithful upscaled description of the resulting macroscopic flow and of the adsorption of $CO_2$/$CH_4$ in nanoporous silica. In particular, we focus on the differences between the two functionalizations of the surface and their selectivity towards the two gases. The results of the MD simulations enable the rational design of amorphous adsorbents that can be tailored to adsorb the required ratio of $CO_2$ to $CH_4$ molecules. Precisely designed selective adsorbents can find application, for instance, in shifting the equilibrium of the methanation reaction ($CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$), which is gaining attention in synthetic fuel production aiming at mitigating $CO_2$ emission.

## Participation

In-Person

## References

[1] Eva Loccufier et al. “Silica nanofibrous membranes for the separation of heterogeneous azeotropes”. In: Advanced Functional Materials 28.44 (2018), p. 1804138.

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