Confined Ionic Liquids (IL) in carbon-based materials for CO_2/CH_4 separation: insights from computer simulations.

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Abstract
Among the several suggested approaches to design tailored sorbents for CO_2 capture and separation, the incorporation of ionic liquids (IL) within the micropores of solid porous materials is recently considered as an alternative method to control the CO_2 thermodynamic sorption selectivity [1]. The major drawback of IL in carbon capture applications arises from their high viscosity, which further increases upon CO_2 capture. This issue can be overcome by designing composite materials, where the IL cations and anions impregnate the pores of a solid porous support. In this context, the present study aims to shed some light upon the role of the IL concentration in model hybrid composite materials, consisted of ethyl-methyl-imidazolium ($Emim^+$)-(BF_4^-) IL and a prototype model of three-dimensional carbon nanotube networks, on the separation of CO_2 / CH_4 fluid mixtures [2]. A combination of force-field based Grand Canonical Monte Carlo (GCMC) and MD simulations was employed for this reason. The results obtained reveals that the adsorption selectivity increases with the increase of the IL concentration for the whole investigated pressure range and it becomes higher as the pressure increases. Moreover, it was found that tuning of the ionic liquid concentration is very crucial in determining the mechanisms of the translational dynamics of the confined molecules at different time scales.

References

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Figures

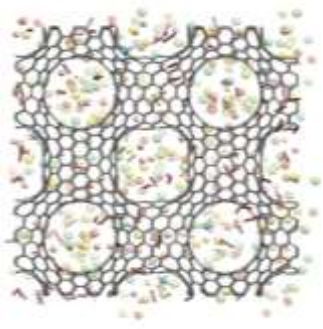

Figure 1: Snapshot of the IL-loaded carbon-based composite material taken from molecular simulations.

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