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Confinement effects on natural gas within carbon nanotubes[1]
ALEXSANDRO KIRCH, TERESA LANNA, NAIYER RAZMARA, JULIO MENEGHINI, CAETANO MIRANDA, Universidade de So Paulo — The current membrane technology for gas separation displays a low flow rate and/or low selectivity. Improvements in the separation technologies are desirable for natural gas usage as a fuel supply under carbon restrains. Advances in the membrane functionality may be favored by the development of nanotechnology. Notably with the emergence of the nanostructured carbon-based materials could lead to significant phase separation devices due to their fast mass flow and regular pore size. However, the separation process depends on fine-tuned properties of the pore structure which nowadays could be benefited by atomistic level research studies using molecular dynamics simulations (MD). In particular, the understanding of the fluids basic properties in confined geometries and interfaces plays a central role in the separation process optimization. In this work, we investigated the structure and transport of natural gas within carbon nanotubes in the light of fully atomistic MD simulations. Firstly, molecular models of natural gas are explored and confinement and interface effects on gas selectivity were analyzed with decreasing nanotube diameter. Finally, we could evaluate the underlying molecular mechanisms which could lead to the phase separation and influencing nanoflows.

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