Carbon-Based Nanoporous Networks as Media for the Separation of CH4/CO2 Mixtures: A Molecular Dynamics Approach

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Gas adsorption and separation are very important processes for industrial and environmental applications. These processes can lead to an important reduce of the release of harmful gases in the environment. Porous solids acting as adsorbents or membrane fillers are playing key roles in capture, adsorptions, separations and purifications of various chemicals that we encounter in our daily activities, directly or indirectly[1]. There are several families of porous materials that have been synthesized in the last few years[2,3]. They exhibit advanced properties, compared to traditional porous materials such as zeolites or polymeric membranes. Carbon based (CB) materials are promising candidates of this kind.

In present work molecular dynamics simulation techniques have been employed to investigate the adsorption and separation of equimolar binary mixture CH_4/CO_2 at ambient temperature, using recently design 3D-carbon-based nanostructure: a 3D Porous Nanotube Network (PNN)[4]. The calculation performed have shown that CO_2 molecules are preferentially adsorbed over CH_4 ones, yielding a very satisfactory selectivity for carbon dioxide. Mean square displacements of CO_2 and CH_4 molecules have also been calculated predicting higher diffusivities for CH_4 molecules inside the PNN compared to CO_2 ones, but significantly lower than in bulk gas mixture[5].

The results obtained signify that rational design of novel CB nanostructured porous networks might lead to the development of promising candidates for CH_4/CO_2 separation.

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