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AN ATOMISTIC INSIGHT ON CO_2 PLASTICIZATION RESISTANCE OF THERMALLY REARRANGED 6FDA-bisAPAF

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Abstract

An emerging class of thermally rearranged (TR) polymer has been of great interest for its extraordinary transport properties. More importantly, harnessing the full potential of TR polymer as gas separation membrane for CO_2/CH_4 separation is through its ability to resist plasticization at high pressures. Accordingly, we report here on the effect of CO_2-induced plasticization on polyimide precursor (6FDA-bis-APAF: 4,4-hexafluoro isopropylidene- diphthalic anhydride – 2,2'-bis(3-amino-4-hydroxyphenyl) -hexafluoropropane) and on the resulting thermally rearranged polybenzoxazole (TR-PBO) polymer membranes as investigated through the radial distribution function and accessible free volume analyses. Using molecular simulation techniques, structural properties such as d-spacing, glass transition temperature, fractional free volume, etc. were estimated in agreement with wide range of experimental observations, which are published within the last decade. Results showed that, TR polymer displayed restricted % FFV increase up to 40 bar due to its limited chain mobility as indicated by the dihedral distribution, and sorption sites on its backbone with lower affinity to CO_2 as shown by the RDF analyses. Additionally, analysis of free volume elements suggests that the ability of TR polymers to maintain their interconnected microstructure and resistance to CO_2-induced plasticization at high pressures leads also to higher diffusion and hence permeation performances and as a result, make them promising materials in gas separation applications.

Keywords: Molecular simulation, Polyimide, Thermally Rearranged (TR) polymers, Sorption, Plasticization, Membrane-based gas separation