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Molecular Engineering of Intrinsically Microporous Polybenzimidazole for Energy-efficient Gas Separation

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Abstract : Polybenzimidazole (PBI) is a high-performance polymer that exhibits high thermal and chemical stability. However, it suffers from low porosity and low fractional free volume, which hinder its application as separation material. Herein, we demonstrate the molecular engineering of gas separation materials by manipulating a PBI backbone possessing kinked moieties. PBI was selected as it contains NH groups which increase the affinity towards CO_2, increase sorption capacity, and favors CO_2 over other gasses. We have designed and synthesized an intrinsically microporous polybenzimidazole (iPBI) featuring a spirobisindane structure. Introducing a kinked moiety in conjunction with crosslinking enhanced the polymer properties, markedly increasing the gas separation performance. In particular, the BET surface area of PBI increased 30-fold by replacing a flat benzene ring with a kinked structure. iPBI displayed a good CO_2 uptake of 1.4 mmol g^{-1} at 1 bar and 3.6 mmol g^{-1} at 10 bar. Gas sorption uptake and breakthrough experiments were conducted using mixtures of CO_2/CH_4 (50%/50%) and CO_2/N_2 (50%/50%), which revealed the high selectivity of CO_2 over both CH_4 and N_2. The obtained CO_2/N_2 selectivity is attractive for power plant flue gas application requiring CO_2 capturing materials. Energy and process simulations of biogas CO_2 removal demonstrated that up to 70% of the capture energy could be saved when iPBI was used rather than the current amine technology (methyl diethanolamine [MDEA]). Similarly, the combination of iPBI and MDEA in a hybrid system exhibited the highest CO_2 capture yield (99%), resulting in nearly 50% energy saving. The concept of enhancing the porosity of PBI using kinked moieties provides new scope for designing highly porous polybenzimidazoles for various separation processes.

Keywords : polybenzimidazole (PBI), intrinsically microporous polybenzimidazole (iPBI), gas separation, pnergy and process simulations
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