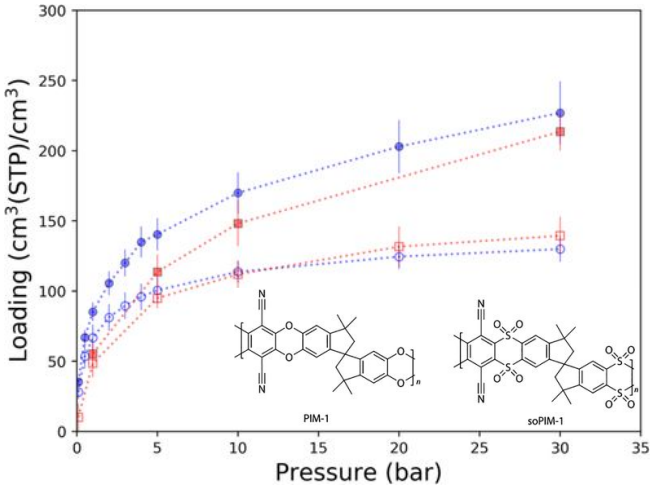
Sulfonyl PIM-1: A Diverse Separation Membrane with Dilation Resistance



The adsorption isotherms for CO_2 in soPIM-1 in blue, and in PIM-1 in red. soPIM-1 is shown to have increased CO_2 uptake with less induced swelling compared to PIM-1, which enables adsorption processes to be operated at lower gas pressures.

Scientific Achievement

The gas phase adsorption properties of a microporous polymer modified with sulfone groups, soPIM-1, were studied with a combined Monte Carlo and molecular dynamics technique. The sulfone-modified polymer was shown to have twice the stiffness of the parent compound, PIM-1, and a greater affinity for CO_2.

Significance and Impact

Identifying adsorbent materials through computational studies is important for the development of sustainable and environmentally conscious technology. Tailoring the chemistry of known polymers with simulations is an efficient strategy for designing promising new materials.

Research Details

GCMC and GCMC/MD simulations were used to describe the adsorption of a diverse set of gasses and adsorbate-induced dynamics on soPIM-1.

- The addition of sulfone groups to PIM structures can improve separation performance in combustion related processes: the heats of adsorption for CO_2, N_2, acetone, and acetaldehyde increased while the values for hydrocarbons was unchanged.

D. M. Anstine, N. F. Mendez, and **C. M. Colina**, "Sulfonyl PIM-1: A diverse separation membrane with dilation resistance," *AIChE J.* **67**, 3, e17006 (2020).

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Work was performed at University of Florida.

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