Scientific Achievement

Screening amorphous polymeric adsorbents with a large collection of adsorbates is challenging due to adsorption-induced structural changes. Performing this screening for polymers of intrinsic microporosity produced a new database of over 240,000 structures and correlations that can expedite predictions within the amorphous polymer design space.

Significance and Impact

Accurate and efficient predictions of adsorbate-induced restructuring, separation performance, and adsorption as a function of system diversity are essential for developing polymeric adsorbents for industrial applications, e.g. chemical separations.

Research Details

15 PIMs and 24 adsorbates were used to simulate 345 adsorption, swelling, FFV dilation, and surface area expansion isotherms

- The correlations developed are accurate for moderate swelling ($V/V_0 < 1.15$) and are based on routinely characterized system features
- Binary selectivity analysis revealed that chemical modifications evaluated resulted in better separation over PIM-1 for all 345 gas mixtures