Scientific Achievement

9 types of hyper-cross-linked polymers (HCPs), a microporous material, were computationally studied and analyzed for their ability to adsorb 24 distinct molecules and for separations of the 276 binary mixtures possible from the unary set, presenting the most diverse set of adsorption data for molecules adsorbing in HCPs available to date.

Significance and Impact

HPCs are typically studied experimentally; this work takes initial steps towards developing computationally efficient models that can rapidly predict molecular adsorption in HCPs without performing extensive molecular simulations.

Research Details

A family of ST-VBC-DVB HCPs were investigated, where 4 materials have 0% divinylbenzene (DVB) but various degrees of cross-linking (25, 50, 75, and 100%), and another 5 materials have 100% cross-linking but different percentages of DVB (10, 20, 30, 40, 50%).