Supporting Information

Polyporous Metal-Coordination Frameworks

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Section 1. Figure for simulated nitrogen uptake

Grand canonical Monte Carlo simulations (Figure SI1) were carried out using the crystallographic data file for CD-MCF.

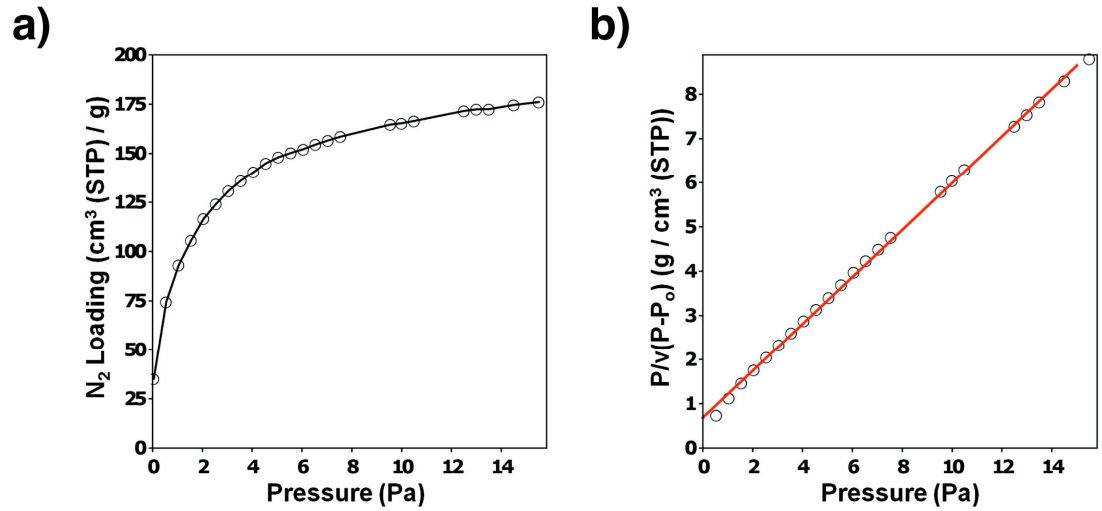

Figure SI1. a) Simulated adsorption N_2 isotherm for CD-MCF at 77 K. (b) BET analysis of the simulated isotherm shows that CD-MCF has an accessible surface area of 820 m^2/g.

Section 2. Computation studies for chiral and gas separation

The complex porosity of CD-MCF led us to investigate the possibility of its use as a material for chromatographic separations. The use of porous materials for stationary phases for chromatographic separations in both the single[1] and bulk crystalline states[2] has been investigated previously. Specifically, microporous materials that have homochiral components[3] are of interest for chiral separation processes. Here, we investigated the ability of CD-MCF to adsorb left-handed enantiomers selectively from racemic mixtures of 1,2-dimethylcyclobutane. Using multicomponent GCMC simulations, following the approach of Clark[4] and others[5] we find (Figure SI2a) that CD-MCF is indeed predicted to be enantioselective for (*SS*)-1,2-dimethylcyclobutane. The long helical void spaces of CD-MCF can also be useful for a different type of separation. As a result of the exceptionally tortuous and narrow nature of the helical cavites of CD-MCF, it is also a potentially useful adsorbent for size-selective separation of gas mixtures where the components are of similar size and shape, e.g., separating Xe and Kr mixtures. Using multicomponent GCMC simulations,[6] we here modeled the selective adsorption of Xe in CD-MCF from an industrially relevant mixture of 80/20 Xe/Kr gas. The simulation (Figure SI2b) shows that CD-MCF is predicted to be selective for Xe gas over Kr at intermediate pressures.

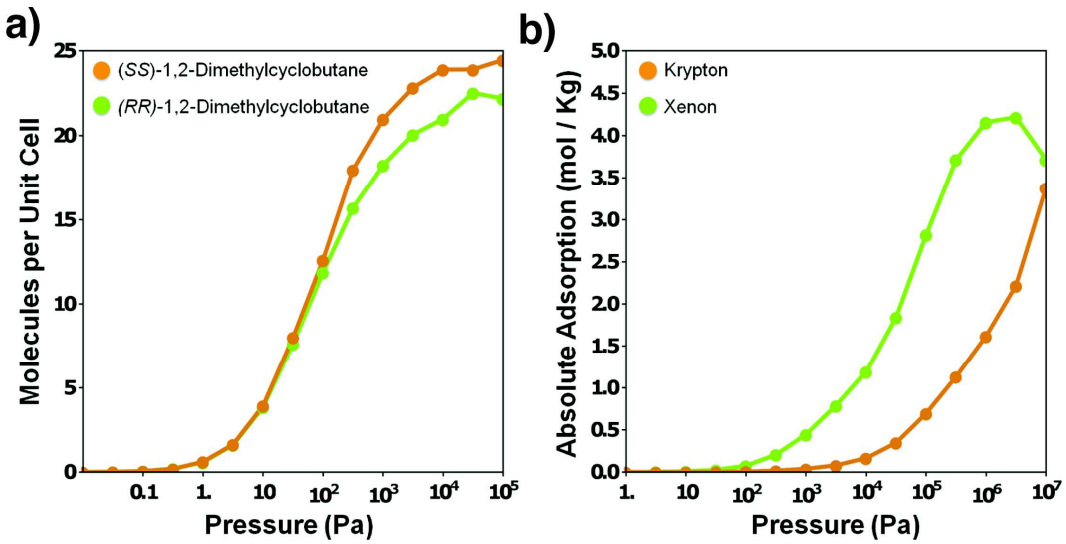

Figure SI2. (a) Simulated adsorption isotherms of the (*RR*) and (*SS*) enantiomers of 1,2-dimethylcyclobutane with CD-MCF. The simulation shows that there is a preference for the adsorption of the (*SS*) enantiomer near atmospheric pressure. (b) Simulated adsorption isotherms of a Xe/Kr mixture within CD-MCF. The simulation shows that CD-MCF has a preference for Xe over Kr at higher pressures.

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