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Isostructural synthesis of breathing 2D MOFs: Implications for guest selectivity

David M. Jenkins

Department of Chemistry, University of Tennessee, Knoxville, TN 37996 USA

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Since breathing metal-organic frameworks (MOFs) can switch between open and closed configurations, these crystalline materials have been proposed as next-generation materials for complex gas or liquid separations. In the gas phase, guest-selective pore opening and pore closing has been observed in stepwise adsorption isotherms. Because MOFs pore sizes and properties can be tuned through shrewd design of organic linkers, in principle a wide variation in selectivity can be achieved if isostructural systems can be developed.

Our research group has developed a novel method for breathing in anisotropic 2D MOFs. Instead of the entire framework moving through a screw-like motion, which is typical in 3D MOFs, a subunit of the linker (aryl rings) rotates independently to block the pore. This rotational motion is advantageous since the core framework remains stable. Since the framework is permanent, the principles of isostructural design can be applied to prepare MOFs in a variety of sizes. Therefore, both the size of the pore and the breathing subunit can be designed independently to maximize selectivity.

Our 2D MOFs are based on a two-pillared design where metal chains represent the pillars. Two ditopic ligands bind to the metals in a *syn* conformation forming a tubular pore and the width and height of the pore is controlled by the size of the linker. The rotation of the aryl rings is monitored by single crystal X-ray diffraction, PXRD or solid state NMR. Finally, direct comparisons between size of the pore and gas uptake can be measured for this breathing system.

Keywords: MOFs; separations; breathing; 2D