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Keywords: MOF, kinetic assembly, powder structure determination

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Structure and gas adsorption study on metal organic frameworks

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Recent work in the field of hydrogen storage and CO_2 sequestration has been overwhelmingly dominated by the use of a narrow range of materials, specifically high surface area carbons (including carbon nanotubes) zeolites and metal hydrides. Activated carbons have the attraction that they are very cheap, their capacities on a weight % basis are very good due to their very low densities, and the adsorption process is readily reversible under mild conditions. Their shortcomings stem from the fact that the fundamental interactions between carbons and hydrogen are non-bonding in nature (i.e. they involve physisorption) and are therefore rather weak. Metal hydrides, adsorb hydrogen by a chemisorption process that is accompanied by dissociation of the dihydrogen molecules. The interaction is much stronger, but facile reversibility is a problem in many cases and such systems are often prone to irreversible poisoning by oxygen. There is clearly an urgent need to develop new classes of materials that have the potential to provide superior performance for hydrogen storage and CO_2 sequestration. Some of the more recent developments in this area include the use of Metal Organic Frameworks (MOFs). Our strategy is aimed at the development of new materials systems where the host-guest interactions are intermediate between those found in the carbons and the metal hydrides.

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Photo-responsive Pores of Porous Coordination Polymers

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Porous coordination polymers (PCPs) or metal–organic frameworks (MOFs), which are constructed from metal ions and organic ligands, have been extensively investigated to provide the nanometer-sized space that is potentially applicable in separation, heterogeneous catalysis, and gas separation/storage. Recently, we reported porous crystalline materials that can be activated by photostimulation [1] and demonstrated that photochemical modification is a powerful method for the control of physical properties of PCPs or MOFs.

In this report, synthesis and properties of new PCPs containing *trans*-1,2-bis(4-pyridyl)ethene (bpe) as a photoreactive module will be presented. The photoreactive PCPs adsorb gaseous molecules such as carbon dioxide. The bpe molecules quantitatively take place topochemical [2+2] cycloaddition reactions and the PCPs show single-crystal to single-crystal (SCSC) transformations upon UV irradiation (> 300 nm). We will discuss not only the SCSC transformations but also the impact on the photochemical transformations on the sorption properties.

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Pressure-induced magnetic switching in molecular framework materials

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The design and characterization of molecular materials with targeted functionalities, such as magnetism and/or nanoporosity, is part of a major international push aimed at developing systems with technologically important applications (e.g., molecular sensing and storage). As such, the accurate elucidation of their often complex structure-function relationships presents a crucial step in their advancement. For molecular magnetism, these approaches are commonly focused on variations of temperature and/or magnetic field, while comparatively little attention has been given to how these materials behave as a function of pressure. Here, we report magneto-structural investigations of magnetic molecular materials using synchrotron-based structural studies (powder diffraction and pair distribution function) and magnetic susceptibility measurements at high pressures. These studies have revealed a range of interesting phenomena such as orbital reorientations, spin crossover, phase transitions, and extreme compressibility [1].

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The crystal structure of Ziegler-Natta catalyst supports

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