TITLE: Systematic Study of Defects in Zeolitic Imidazolate Frameworks for Enhanced Adsorption and Diffusion Properties

Summary: Metal-organic frameworks (MOFs) exhibit diverse properties that are often influenced by the presence of defects and associated disorder within their structures. Despite their importance, the identification, characterization, and modification of these defects are still challenging. As a promising subfamily of MOFs with structures similar to inorganic zeolites, zeolitic imidazolate frameworks (ZIFs) present an excellent opportunity to explore the impact of inherent and deliberately created defects on their adsorption properties. A young researcher will undertake a systematic study of defects in ZIFs, focusing on their type, location, amount, and distribution, and evaluating their impact on the adsorption and diffusion of small molecules. The understanding of adsorption mechanisms is crucial for optimizing these materials for efficient adsorption-based molecular separation processes and enhancing their performance in low-temperature heat reallocation systems.

Research techniques used: Advanced solid-state NMR (SSNMR) methods will be employed to obtain structural characterization of ZIFs. To tackle the defects in ZIFs and study host-guest interactions during adsorption, new approaches will be developed, such as the use of NMR-sensitive probe molecules. The young researcher will have the opportunity to work with state-of-the-art equipment, including a 600 MHz spectrometer specifically designed for studying solids and a pulsed-field gradient (PFG) NMR probe for investigating molecular diffusion. These cutting-edge instruments are expected to be installed and ready for use in 2024, providing our young researcher with an exciting opportunity to work with the latest technology in the field of SSNMR.

The reason why the topic is innovative: ZIFs were recently identified as the fourth type of melt-quenched glasses, and the first to have a permanent microporosity accessible to gases without any post-synthetic treatments. This breakthrough has opened up new possibilities for shaping these functional materials into glass monoliths and crystal-glass composites. Glassy ZIFs represent an extreme case of disordered materials, and despite their potential for practical applications, the current understanding of their atomic-level structure and host-guest interactions is extremely limited. SSNMR is one of the few experimental techniques capable of providing important insights into these materials.

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