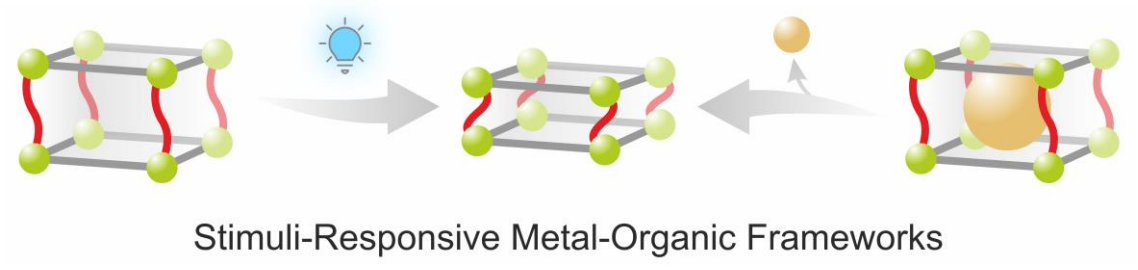
Stimuli-Responsive Metal-Organic Frameworks: Structural Dynamics and Sorption Properties

Stimuli-responsive materials have the remarkable ability to change their properties in response to environmental cues such as temperature, light, or presence of guest molecules. These materials can adapt, self-heal, or transform, positioning them as key players in the development of smart technologies. Among the exciting advancements in this field is the discovery of flexible metal-organic frameworks (MOFs). Unlike traditional materials with rigid structures, flexible MOFs can alter their shape, volume, or porosity in response to external stimuli. Notably, photoresponsive materials represent a significant leap in adaptive technologies, capable of adjusting their properties precisely and reversibly with light. Incorporating photoresponsive elements like azobenzene into flexible MOFs enables the creation of structures that not only adapt their form but also their functional properties under specific light conditions. This versatility allows them to function as *dynamic sponges*, ideal for a variety of applications including gas storage and separation, sensing, water purification, energy applications, and drug delivery.



The proposed research project aims to delve into the structural dynamics of a series of stimuli-responsive materials. Our primary objectives include designing and synthesizing flexible MOFs with novel organic linkers inspired by azobenzene-based dyes. These MOFs are categorized into three main groups: (i) pillar-layered MOFs, (ii) multivariate MOFs (MTV-MOFs) and/or MOF-on-MOF architectures, and (iii) stable MOFs functionalized with photoresponsive ligands. Through this approach, we intend to conduct an in-depth investigation of the materials' stability and structural dynamics. Advanced structural characterization techniques and computational simulations will be utilized to understand the dynamics observed. Furthermore, we will assess the potential applications of selected candidates in challenging areas such as hydrogen isotope separation (H_2/D_2) and controlled drug delivery.