Revealing structural design and defect engineering of Metal-Organic Frameworks and their applications by employing X-ray absorption spectroscopy

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Abstract

Metal-organic frameworks (MOFs) are novel crystalline porous materials, which combine the rigid, well-defined structures of crystalline inorganic networks and the flexibility and versatility of organic-based moieties as a synergistic unit. The tremendous diversity of precursor components reveals broad perspectives for systematic, bottom-up designs and fine tunings of MOFs framework structures, characteristic features, and chemical properties. Rational design of chemical functionalities and engineering of structural defects within MOF structures provide the mechanistic understanding of controlled phase formation and crystal morphology. Moreover, they also exhibit emerging functional properties, which can be further applied for selective catalysts, and sensing materials. X-ray absorption spectroscopy (XAS) is one of the crucial characterization techniques to examine the detailed structural engineering and the presence of catalytic active sites in MOF structures, especially at the metal clusters. In details, X-ray absorption near-edge structure (XANES) confirms the existing of highly reactive $Ru^{II,II}$ centers in Ru-based HKUST-1 analogue MOF. X-ray absorption fine structure (EXAFS) is used to monitor the mechanistic crystalline-phase formation of Zr-based MOFs synthesized by controlled secondary building approach at mild conditions and reveals the presence of both Cr and Fe at the same metal nodes within the mixed-metal MOFs. In additions, EXAFS analysis provides the strong evidence to identify the different local defect concentration within Zr-based MOF, of which plays a crucial role as catalytic active sites for monosaccharide sugar conversion to lactic acid.

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