

What solid-state NMR can do to characterize metal-organic frameworks?

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Metal-organic frameworks (MOFs) are a novel type of materials with many current and potential applications in gas capture/storage/separation, catalysis, sensing and drug delivery. Structural characterization of MOFs is crucial, since an understanding of the relationship between the macroscopic properties of these industrially relevant materials and their molecular-level structures allows for development of new applications and improvements in their current performance. Solid-state NMR spectroscopy is an important characterization technique, which provides information truly complementary to that obtained from X-ray diffraction. In this talk, we will present our recent solid-state NMR work on (1) resolving crystallographically inequivalent and/or chemically very similar sites in unit cells; (2) refining the local metal geometry; (3) monitoring the dynamic behavior of gas species (*e.g.* CO₂, H₂, CH₄ *etc.*) adsorbed in MOF frameworks and identifying the binding sites.