

New Strategies for Improving Sensitivity and Resolution in  
Solid-State NMR; Applications to Catalytic Nanoscale Materials,  
Biomolecules and Fossil Fuels

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We will demonstrate the applications of several advanced techniques in solid-state nuclear magnetic resonance spectroscopy to the structural studies of systems comprising small interacting molecules. These latest capabilities were made possible by combining fast MAS (at  $\geq 40$  kHz) with several multiple RF pulse sequences for two-dimensional correlation measurements.

Examples of the studied materials include mesoporous silica nanoparticles (MSN) functionalized with various types of organic groups, where solid-state NMR allows definitive characterization of the structure and absolute/relative concentration of moieties inside the mesopores, their spatial distribution and orientation with respect to the surface, as well as dynamic behavior. The reaction products and intermediates, and catalysts' stability under the reaction conditions can also be studied. In particular, the basic understanding of the dynamics of molecules on the solid-liquid interface, provided by solid-state NMR characterization and theory, served as a predictive tool in the design of a new catalyst for the esterification reaction. In other studies, homo- and heteronuclear correlation solid-state NMR methods provided valuable insights into the arrangement of surfactants in MSN materials. The capabilities of these techniques will be also demonstrated on a naturally abundant tripeptide, a metal-free corrole, and a series of coals.