Recent advances in solid-state NMR studies of zeolite catalysts

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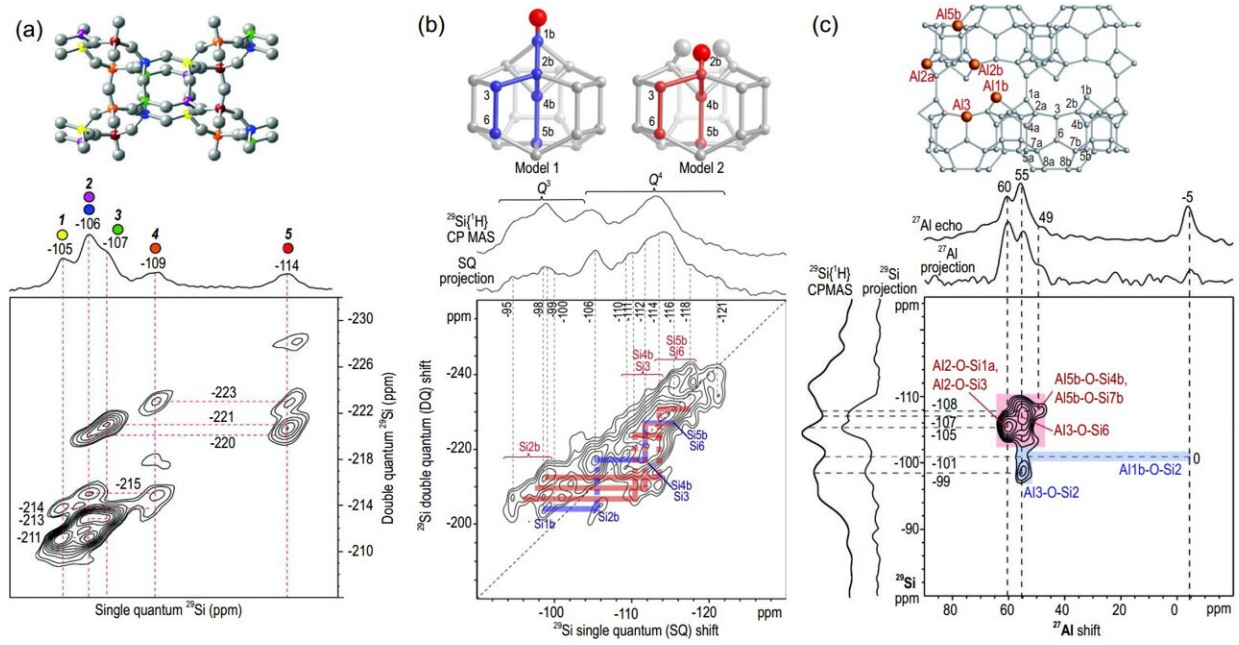

(a) 2D refocused INADEQUATE (J-mediated) 29Si{29Si} DQ NMR spectrum of as-synthesized zeolite ITW. (b) DNP-enhanced 2D 29Si{29Si} J-mediated correlation spectrum of calcined Si-SSZ-70. (c) Schematic diagram of the framework structure of Al-SSZ-70 (orange color indicates the T sites that are occupied by Al heteroatoms), and 2D 27Al{29Si} J-HMQC NMR spectrum of calcined Al-SSZ-70. Credit: Science China Press

Zeolites are important inorganic crystalline microporous materials with a broad range of application in the areas of catalysis, ion exchange, and

adsorption/separations. Due to their unique pore structure, high thermal stability and tunable acid-base property, zeolites are one kind of the most important heterogeneous catalysts used in petrochemical industry and fine chemical industry.

The design of efficient zeolites with improved properties depends on the understanding of the structure–activity relationship, which requires the fundamental characterization of the zeolites. Solid-state NMR (ssNMR) spectroscopy is a well-established tool in the study of zeolites and relevant catalytic reactions because of its advantage in providing atomic-level insights into molecular structure and dynamic behavior.

In a new review published in *National Science Review*, scientists at the State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics in Wuhan, China, summarize the recent advances in ssNMR of zeolite catalysts, mainly including the new applications of ssNMR to investigate zeolite framework structure, catalytically active sites, intermolecular interactions and catalytic reaction mechanisms. The authors also discuss the current limitations and the future prospects of ssNMR technique for its application in zeolite catalysts.

The authors indicate that, combined with advanced instrumentation and experimental techniques, ssNMR has demonstrated to be a powerful analytic tool in zeolites characterization. The direct detection of framework structure and acid sites is enabled by using various 1D and 2D ssNMR methods. The obtained knowledge has made it possible for zeolite scientists to optimize zeolites with improved catalytic performance in many important reactions such as methanol conversion, cracking of hydrocarbons and oligomerization of alkenes.

Meanwhile, 1D and 2D correlation spectroscopy allows ssNMR to probe the internuclear spatial proximities, which are associated with host-guest and guest-guest interactions in zeolites. The characterization of various

interactions allows scientists to gain better understandings in zeolite synthesis, adsorption/desorption and catalytic reactions.

Moreover, the utilization of ssNMR for the observation and identification of critical active intermediates in zeolite-catalyzed reactions has become a key approach for the elucidation of reaction mechanism. The knowledge on the reaction mechanism and the involved intermediates has been applied to the synthesis of new zeolites capable of controlling reaction pathway in a complex reaction such as methanol conversion.

More information: Weiyu Wang et al, Recent advances in solid-state NMR of zeolite catalysts, *National Science Review* (2022). DOI: 10.1093/nsr/nwac155

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