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Solid-State and *in situ* NMR Spectroscopy in Materials Science

Natalia Fulik, Felicitas Kolbe, Silvia Paasch, Julia Pallmann, Tobias Pietsch, Marcus Rauche, Jana Richter, and Eike Brunner*
Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Saxony, GERMANY
eike.brunner@tu-dresden.de, https://tu-dresden.de/mn/chemie/anc/anc1

Solid-state NMR spectroscopy delivers structural information based on the exploitation of short-range interactions. It does not require a long-range (crystalline) order. Based on continuous methodical progresses, it has meanwhile found numerous applications for the characterization of various materials as it will be demonstrated in this contribution for selected examples.

Based on strongly distance-dependent interactions such as the magnetic dipole-dipole interaction, solid-state NMR spectroscopy allows not only bulk materials characterization, but also the selective characterization of interfaces. This is exploited by our group, e.g., to study biominerals[1,2] and other hybrid materials such as metal-organic frameworks (MOFs).[3]

In situ studies of host-guest interactions are particularly powerful to characterize surfaces, e.g., in porous materials such as MOFs. Adsorption/desorption isotherms can be followed by observing the signals of the adsorbed gases. NMR-derived parameters can then be correlated with volumetric adsorption/desorption isotherms. Gases like ^{129}Xe, $^{13}CO_2$, and $^{13}CH_4$ were already used for our investigations. ^{129}Xe NMR spectroscopy for example allows studying adsorption-induced structural transitions since it provides characteristic, structure-sensitive parameters like the chemical shift, the chemical shift anisotropy, signal intensities, and relaxation times.[4,5]

Finally, we are using a combination of solid- and liquid-state NMR spectroscopy for reaction monitoring in ionic liquids.[6]

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