Solid-State NMR Spectroscopy as Tool for Investigation of Surface Modified Silica Particles

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Due to their large effective surface, functionalized mesoporous silica particles are successfully used in various fields of chemistry and materials science. A wide variety of synthesis techniques can be used to accomplish surface functionalization through various organic groups, metal complexes, or even enzymes.

In this process, the investigation of such functionalized particles by various spectroscopic methods is clearly of particular importance since they facilitate precise information about the structural environment of the components or composites on a microscopic level. They enable statements about the quality of the particle, particle coating and the reproducibility of the used syntheses. Furthermore, the understanding of microscopic properties can provide indications of the desired macroscopic properties such as catalytic activity or magnetic cooperativity.

Supplemented by analysis techniques such as X-ray diffraction, vibrational spectroscopy and N₂ sorption analysis, the focus of this contribution is the use of modern high-resolution solid-state NMR, as a non-destructive, element-selective, and inherently quantitative technique of structural analysis. Examples discussed in this presentation include (a) orthogonally functionalized mesoporous hybrid silica particles for catalytic applications,[1] and (b) lanthanide doped upconverting nanoparticles, which are covered with a mesoporous silica shell and functionalized with the photosensitizer silicone phthalocyanine for use as a theragnostic agent.

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