Solid state NMR characterization of materials – combined experimental and ab-initio investigations

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Multinuclear solid-state NMR is an efficient and non perturbing approach to study complex materials, including interactions and interfaces between components, using for instance dipolar 2D correlation spectroscopies. The recent introduction of periodic first principles calculations of NMR parameters (GIPAW method) combined with structural DFT modeling provides additional local and accurate information on these systems at the nanoscale, supporting the interpretation of experimental data.

This approach will be illustrated with a large variety of examples including hybrid materials like small organic molecules adsorbed on an amorphous silica surface[1] or peptide-functionalized Metal Organic Frameworks,[2] preceramic polymers as precursors of functional nitride-based ceramics,[3] fossil samples[4] and glasses for bone regeneration.[5]

In addition, a few results will be presented on the possibility to study the influence of nuclear motion induced by temperature on NMR parameters, using an experimental and theoretical coupled approach.[6]

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