Leipzig Spin Resonance Colloquium

June 2nd, 2021 – 16:00 Leipzig time – on Zoom

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Investigating Disorder in Solids using NMR Spectroscopy, Isotopic Enrichment and First-Principles Calculations

NMR spectroscopy provides an element-specific, sensitive probe of the local environment, enabling detailed information to be extracted. However, in the solid state the vast majority of this information remains unexploited, owing to the challenges associated with obtaining high-resolution spectra with good sensivity and the ease with which these can be interpreted. Recent advances enabling accurate and efficient calculation of NMR parameters in periodic systems have revolutionized the application of such approaches in solid-state NMR spectroscopy, particularly among experimentalists. Improvements in sensitivity can be obtained in a number of ways, but for nuclei with low natural abundance isotopic enrichment is a key approach. However, the high cost of enriched reagents often means that new cost-effective and atom-efficient synthetic approaches are required.

Many of the interesting physical and chemical properties of materials result from a deviation of the periodic and translational symmetry characteristic of the solid state, i.e., compositional, positional or temporal disorder. Although diffraction produces an average structural picture in these cases, the sensitivity of NMR to the atomic-scale environment provides a potentially powerful tool for studying disordered materials, and the combination of experiment with first-principles calculations offers a particularly attractive approach. In this talk I will give a brief overview of solid-state NMR spectroscopy, and the approaches used to improve resolution, sensitivity and the extraction of chemical information. I will illustrate this with examples for our work on O NMR spectroscopy of microporous materials (where isotopic enrichment is vital to overcome to 0.037% natural abundance), and show how we have combined calculation and experiment to investigate disorder in phosphate frameworks and ceramic materials proposed for the encapsulation of radioactive waste.

June 2nd, 2021 - 16:00 CEST (Berlin) - 22:00 CST (Peking) - 07:00 PST (San Francisco) - 10:00 EST (New York)

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