

NMR Crystallography of Disordered Solids

Disorder is a common cause of diversity of solids, which is present in almost any material and often determines its specific properties. The structure of crystalline solids is usually obtained from diffraction experiments that typically require a highly ordered sample and are inherently limited in the characterisation of disordered systems. An alternative experimental technique for atomic-level characterisation of solids is solid-state NMR spectroscopy (SS-NMR), which does not require a long-range order and is suitable for characterisation of disordered samples. We will study the structure and dynamics of disordered solids by a combination of SS-NMR experiments and advanced quantum-chemical calculations. The newly developed methods will be applied to a wide variety of disordered systems, such as solid hydrates of biomolecules or materials with potential applications in nanodevices. Particular emphasis will be given to investigation of intermolecular interactions in molecular solids responsible for the structure, structural transformations and dynamics of molecules.

