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Unifying Concepts in Catalysis

UniCat Colloquium

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Structure, Disorder and Function of Solid Materials –an NMR Crystallographic Approach

Solid-state chemists are accustomed to use structure-property relations for tuning the properties of materials. Elucidating the structure of materials is thus a cornerstone for material science and solid-state chemistry. To do so, becomes problematic, if dynamic or static disorder is an inherent feature of the targeted systems, as it is the case for many material classes ranging from layered compounds over porous materials up to supramolecular self-assembly. This lecture will give an overview of how to use and develop NMR crystallographic strategies to elucidate structural and dynamic properties for such systems. In addition, we will show that disorder can be an essential element governing the materials function. NMR crystallography combines scattering experiments with computational chemistry and solid-state NMR spectroscopy (ssNMR) to overcome the loss of information coming along with the disorder.

While scattering provides topologic information, ssNMR allows to access local and intermediate length scales by determining connectivities, distances and orientation correlations based on various homo- and heteronuclear correlation experiments. We demonstrate this approach for two classes – supramolecular polymer additives and hostguest interactions within porous metal-organic frameworks (MOFs). The complex interplay between the molecular structure and the hierarchical self-assembly of the supramolecular additives to nanoparticles with disorder on the mesoscale is addressed and the influence of the particles on the properties of the additive polymer mixtures is elucidated. In the case of MOFs we will show, how disorder of guests and the framework interact with the ability to provide favourable confined environments for guest molecules within the framework. Our studies demonstrate, that for flexible systems, gate-opening effects might be influenced and triggered by this interplay, which provides a new route to control the uptake of guest molecules.

Wednesday, December 05, 2018 at 5:15 PM

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Building C, Lecture Hall **C 264**

Prof. Dr. Risse (FUB)
Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!