Seminar: “From NMR of noncovalent interactions to the local structural features of solids”

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The mechanical and chemical properties of solids depend on their morphology. There are many methods designed to determine the composition of very complex materials. There is a lack of methods suitable to study intermolecular interactions and associated local structural features even into simple noncrystalline solids. Magnetic resonance spectroscopy (NMR) is the method of choice for such applications. The only critical requirement of NMR is the presence in the system of interest of spin-labels that can provide solutions of problems under consideration.

This presentation will cover the following aspects:

(i) What nuclei can serve as most suitable spin-labels?
(ii) How noncovalent interactions affect NMR parameters? [1,2]
(iii) What one can learn about the morphology of surfaces using solid-state NMR? [3-5]
(iv) Time-efficient DFT calculations as a complement to solid-state NMR. [1,6]
(v) Reconstruction of the morphology of noncrystalline organic solids from NMR parameters of spin-labels. [7,8]

References


