Multinuclear NMR studies of soft and hard porous materials

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Many natural or man-made materials, including rocks, clays, biological tissues, cellulose derivatives, cements, ceramics or catalysts, can be considered as porous media. Because of their heterogeneous structure and composition, all these soft or hard porous materials interact in a complex manner with moisture, or with imbibed liquids such as water and/or oil phases. Ultimately, this complexity has a significant impact on the final product performance in applications that range from soft matter science, food, packaging and pharmaceutical industry, or chemical engineering and petroleum industry.

NMR offers a number of significant advantages over all other available experimental techniques that can be used to characterize fluid-bearing porous media: it does not require optical transparency, it is quantitative, chemically-selective, multi-nuclear, spatially-resolved (MRI), flow-sensitive, able to probe molecular dynamics, non-invasive and applicable under *operando* conditions.

In this talk, the distinct capabilities of ¹H, ²H and ¹³C NMR/MRI static and MAS spectroscopy and time-domain techniques in selectively investigating spatial and dynamical heterogeneities in soft or hard porous materials will be demonstrated. Selected examples will include the study of water-polymer interactions in wood [1] or cellulose nanocomposites [2,3], as well as new method developments for spatially-resolving multi-site diffusional exchange inside heterogeneous catalyst beds [4]. It will also be shown that when NMR parameters are modelled by molecular dynamics simulations, atomistic-level resolution can be achieved that provides unprecedented insight from NMR data [5].

References:

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