Diffusion of host molecules inside mesostructured and hierarchical porous materials by NMR Relaxometry	
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Project :

The synthesis of nanostructured hybrid oxide materials using the so-called, 'surfactant templating' route has attracted a great deal of attention over the past decade. Such materials constitute an ideal playground to material engineers aiming at producing porous objects of controlled size, shape and orientation inside the silica backbone. In particular these materials have potential application in catalysis. The knowledge on the molecular motion of host molecules such as water within different mesostructured materials is primeval to develop new catalysts

This project aims at developing news methodologies in NMR relaxometry and NMR diffusometry for studying fluids embedded in mesostructured and hierarchical porous materials such as silica, titania, zirconia, with the final goal of optimizing the materials properties. NMR (Nuclear Magnetic Resonance) is indeed known for being particularly well suited to this field because, in addition of being non-invasive and relatively fast, it allows the characterization of molecules dynamics, including when the latter are embedded in complex solid materials. "Relaxometry" techniques, which consist in measuring spin relaxation times as a function of the measurement frequency (or equivalently of the static magnetic field B0), are especially used for this kind of studies [1]: they allow the determination in situ of fluid mobility, which is correlated to the materials geometry (pore size and type of structure) and to their surface properties (relaxivity, wettability). The relationship between molecules dynamics and NMR spin relaxation is well known and well established in the case of fast motions (and at relatively high magnetic field). But the characterization of slow motions, such as the ones of embedded molecules in mesoporous media, must be done by using NMR relaxation times measured at low (or very low) magnetic field, and still need appropriate models developments for their analysis. This point will thus constitute a part of the PhD work. NMR relaxometry techniques are also planned to be complemented by self-diffusion measurements (Pulse-field Gradients methods, at high magnetic field) in order to obtain a complete picture of the embedded molecules dynamics [2].

The project is going to benefit from the long-standing collaboration and the complementarity of both partners [3]: on the one hand, specialists from the porous materials field and on the other hand, specialists in NMR spin relaxation methodologies. During the PhD project, the candidate will investigate many aspects in order to evaluate their effect on the embedded fluid mobility: structure of the porous medium (pore size and organization, i.e. simple vs. double porosity or hierarchized porosity), chemical composition (silica, titania, zirconoa), type of fluid (water vs. other solvents). He/she will also have to prepare the porous matrixes and characterize them in detail by SAXS, nitrogen adsorption-desorption analysis, infrared and so on.

References :

[1] E.Steiner, S.Bouguet-Bonnet, A.Robert, D.Canet. Concepts Magn. Reson. (2012) 40A(2), 80-89

[2] M.Yemloul, E.Steiner, A.Robert, S.Bouguet-Bonnet, F.Allix, B.Jamart-Grégoire, D. Canet. J. Phys. Chem. B (2011) 115, 2511-2517

[3] E.Steiner, S.Bouguet-Bonnet, J.-L. Blin, D.Canet. J. Phys. Chem. A (2011) 115, 9941-9946