The MARGIN project

MAgnetic **R**esonance studies of **G**as diffusion **I**n **N**anoporous materials: influence of gas-wall interactions

In modern nanoporous materials, gas diffusivity correlates with their efficiency for gas separation and storage or for catalysis. It also correlates with their relevance for investigations of helium superfluid phases and phase transitions with perturbing solid impurities, or confining boundaries since these systems essentially behave as low-density gases of quasi-particles at very low temperatures.
More generally, gas and liquid diffusion measurement techniques are widely used for the characterization of porous media. Nuclear magnetic resonance (NMR) provides a wealth of non-invasive methods for measuring fluid transport in various kinds of porous systems. Gas diffusion NMR is a mandatory tool to address specific problems, such as finding mean free paths in aerogels and characterizing pore sizes and structure.

A precise understanding of all physical processes involved during diffusion measurements is essential to correctly interpret NMR diffusion results obtained in porous media. Gas diffusion in porous media near room temperature is frequently described by diffusion models which take into account the possible presence of adsorbed layers and the spatial structure of pores.
However, usual phenomenological models of gas diffusion fail to account for observations made with strongly adsorbed gases or at low temperatures, because the influence of the attractive wall potential on molecular gas dynamics is overlooked in standard diffusion models. Preliminary results obtained for ^{3}He gas diffusion in an ordered aerogel by the MRS Lab at 4.2 K revealed a significant deviation from the expected behavior, attributed to the increased effect of the aerogel adsorption potential on ^{3}He gas diffusion at low temperatures. This effect of the adsorption potential is believed to manifest itself in an increase of the gas density and in changes of atomic trajectories near the walls in the gas phase.

Theoretical background and experimental data are lacking for gases in porous systems at low temperatures or low gas densities. The MARGIN project is designed to address both issues.

The MARGIN project aims at discriminating between confinement and wall adsorption effects through **NMR investigations of gas diffusion** in several **well-characterized model porous media** over a **wide range of temperatures and gas densities** for which different adsorption regimes are expected, from no adsorption to multilayer adsorption through Henry's, Langmuir's and BET's regimes.

- **Experimentally, ^{3}He will be mainly used as a probe gas** and apparent diffusion will be measured in porous systems such as ordered aerogels, nanopowders, etc., at low temperatures in MRS Lab (Kazan) and at high temperatures in LKB (Paris) using hyperpolarisation methods with laser optical pumping for high sensitivity.
- **Complementary xenon gas diffusion experiments** above 170 K are planned in the same porous media to probe diffusion of atoms with stronger adsorption potentials than for ^{3}He.
- **Numerical simulations of diffusion and nuclear spin dynamics** will be also intensely used to reliably interpret experimental results and draw strong conclusions.

MARGIN aims at demonstrating that NMR could become one of the accepted characterization tools for gas diffusion, instead of being limited to assessing diffusion and relaxation in liquids, inside porous media.

Besides the achievement of its main objectives, namely the detailed characterization of gas diffusion mechanisms in porous media, the MARGIN project is expected to yield data and results which might be relevant for different open questions in fundamental physics.
One of them is related to recently revisited theories of motion-induced magnetic relaxation and frequency shifts in fluids, beyond the standard Redfield approach. On this topic, the planned NMR measurements in samples with near-planar confinement might provide a benchmark for these theories, which have been triggered by new generations of EDM search experiments.