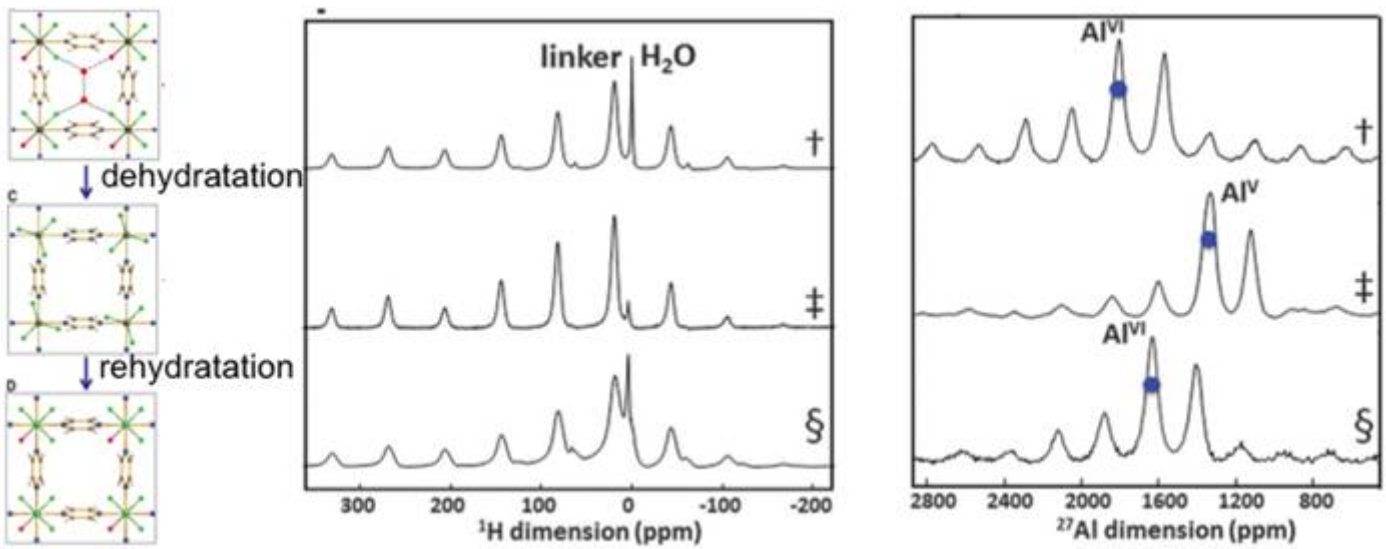
INTERACTIONS@MIM

Solid state NMR and DFT calculations

We develop solid-state NMR measurement methodologies, ranging from sample preparation to adaptation or development of new NMR sequences, with a marked originality on fluorinated / protonated solids. The application of these methods makes it possible to respond unambiguously to structural issues for a number of compounds, such as the location of adsorption sites in fluorinated MOFs, the dynamics of fluoride ions in inorganic solids, the structure of polymeric Nafion based compounds, or polyoligosiloxysilanes. A particular interest is also focused on the characterization of pharmaceutical formulations, in academic or industrial collaborations.



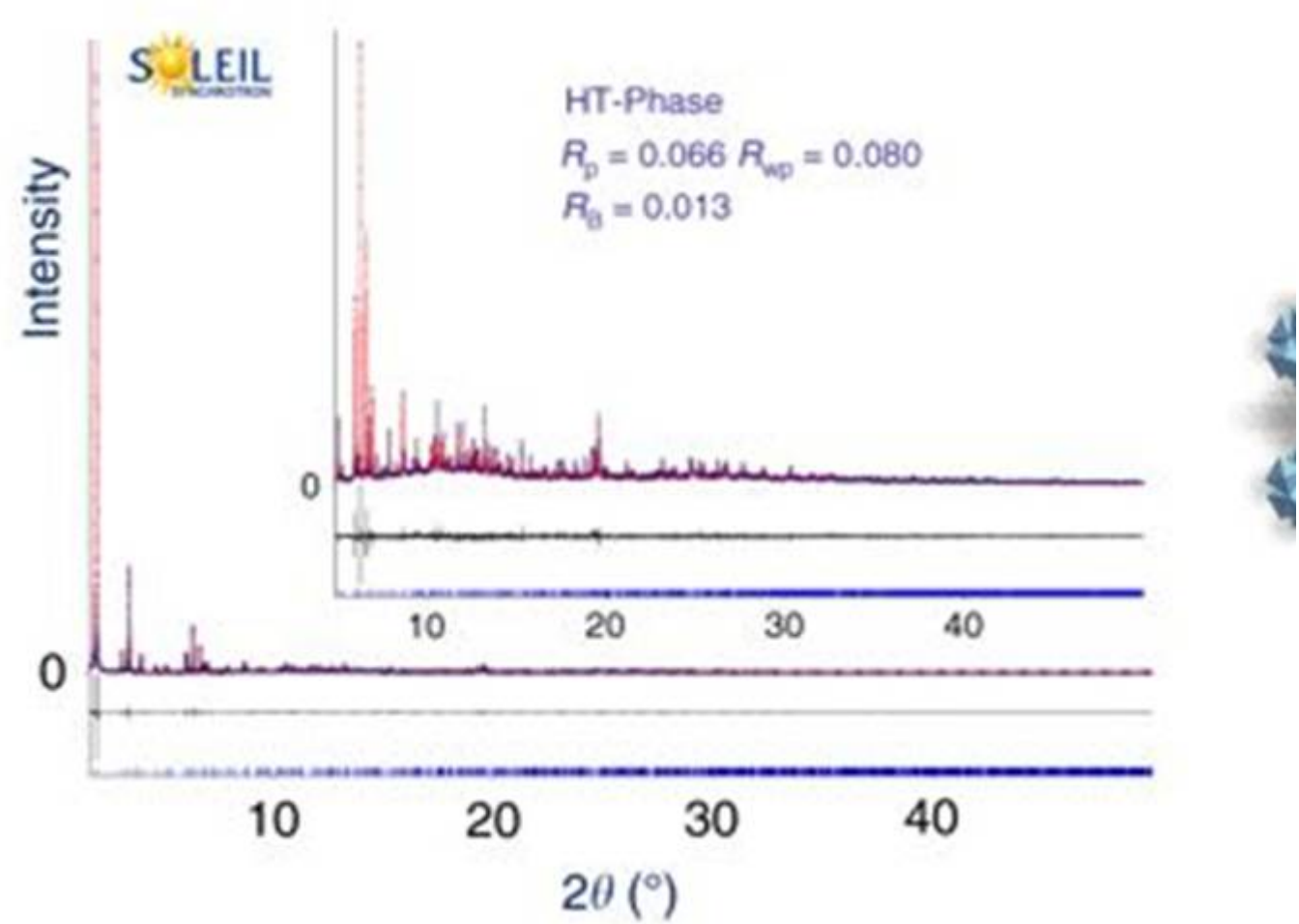
Recent publications

Science, 2017, 356 731 (link)

Nat. Commun. 2018, 1660 (link)

X-ray diffraction

The knowledge of structure / property relationships of powdered solid state materials (e.g. MOFs) is a prerequisite for their rational use. Therefore the *ab initio* structural resolution from powder X-ray diffraction data is clearly needed. We elucidate strutures from conventional and synchrotrons sources (SOLEIL and ESRF). A systematic search for complementary experimental data, such as the pair distribution function (PDF), can be combined with the "load flipping" and / or simulated annealing methods coupled with the use of rigid groups to expand investigation to poorly crystallized materials.



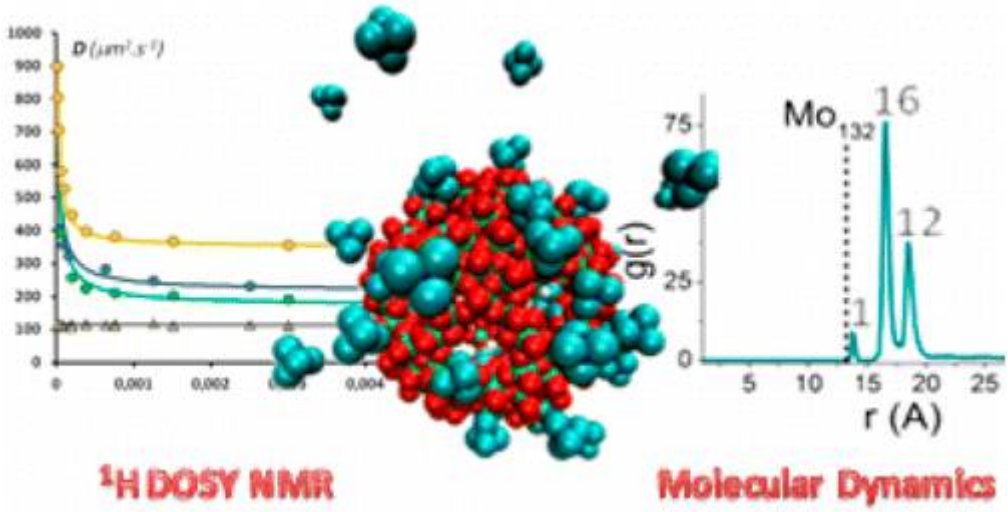
Recent publications

Chem. Commun. 2016, 52, 9063 (link)
Nat. Commun. 2018, 1660 (link)

Liquid NMR and physical-chemistry of solutions

For NMR-related activities, we seek to develop and apply NMR methodologies for the study of crystallogenesis of porous materials and the chemistry of polyoxometalates in solution. Particular attention is given to multinuclear approach and multidimensional techniques like DOSY (Diffusion Ordered SpectroscopY). Such method is used not only

to determine the size of the aggregates and their dynamic properties, but also to study the physicochemical behavior in solution through weak attractive or repulsive interactions by hydrophobic / chaotropic effect.



Recent publications

J. Am. Chem. Soc. 2015, 137, 5845 (link)