

Séminaire LIONS



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Solid-state NMR characterization of organic-inorganic interfaces in silica-based hybrid materials: Combined experimental and ab-initio investigations

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A certain number of innovating silica applications are related to its surface properties, and more precisely to the interaction of the latter with organic and/or biological matter. High resolution solid state NMR appears to be a very powerful tool to investigate these hybrid materials since it allows to probe silica surfaces, adsorbed/encapsulated molecules but also interactions between both components. Experiments can be combined with first principles calculations : an amorphous hydroxylated silica surface has been modelled using a periodic *ab initio* approach [1] with the aim to better characterize the reactive sites of films, nanoparticules or mesopores. In a second time, it is possible to compare various modes of adsorption of the studied molecules and determine the most stable configurations. Moreover, NMR parameters can be calculated on these models using also a periodic *ab initio* approach [2] providing additional local and accurate information of these interfaces at the nanoscale, supporting the interpretation of experimental data.

This approach will be illustrated with different examples including the adsorption of small organic molecules (such as glycine [2], ibuprofene and alendronate) and bigger ones (such as a phospholipid [3]) on amorphous silica surfaces. In addition, preliminary results on silica nanoparticles covalently linked by the means of imidazolium-containing ligands will be presented.

[1] F. Tielens, C. Gervais, J.-F. Lambert, F. Mauri, D. Costa *Chem. Mater.* **20** (2008) 3336

[2] C. Bonhomme, C. Gervais, F. Babonneau, C. Coelho, F. Pourpoint, T. Azaïs, S. E. Ashbrook, J. M. Griffin, J. R. Yates, F. Mauri, C. J. Pickard *Chem. Rev.* **112** (2012) 5733

[3] N. Folliet, C. Gervais, D. Costa, G. Laurent, F. Babonneau, L. Stievano, J.-F. Lambert, F. Tielens *J. Phys. Chem. C* **117** (2013) 4104

[4] N. Folliet, C. Roiland, S. Bégu, A. Aubert, T. Mineva, A. Goursot, K. Selvaraj, L. Duma, F. Tielens, F. Mauri, G. Laurent, C. Bonhomme, C. Gervais, F. Babonneau, T. Azaïs *J. Am. Chem. Soc.* **133** (2011) 16815