Poster Presentation

MS48.P01

Multiscale structure-properties analysis of photoactive nanocomposite materials

E. Bendeif[1], K. Hsieh[1], D. Schaniel[1], A. Gansmuller[1], S. Pillet[1], T. Woike[2]

[1]CRM2-IJB Université de Lorraine, Vandœuvre les Nancy, France, [2]Institut für Strukturphysik, TU Dresden, Dresden, Germany

In the last decades, the confinement of various types of functional material in mesoporous silica matrices has been used to design hybrid organic-inorganic nanocomposites with unique and fascinating properties. Such nanocomposites have attracted considerable interest owing to their potential applications in various domains [1-2], while reports with precise structural information of such molecular nanomaterials are still rather scarce and quite disparate. However, in order to be able to derive a structure-functionality relationship of such hybrid complexes, a detailed description of the structural organisation of the guest species and of their immediate surrounding is absolutely mandatory. We show in this contribution that detailed structural information can be obtained by using an appropriate multiscale approach combining various experimental techniques such as X-ray total scattering coupled to atomic pair distribution function (PDF) and solid-state NMR spectroscopy. This multiscale approach does provide more extensive and accurate structural information [3]. The PDF approach has allowed the identification of the nature of the incorporated species and their arrangement as well as the distinction of the various existing phases: isolated molecules and nanoparticles. The multi-nuclei Solid State NMR investigation has provided information on both the amorphous host and the molecular guest and adds a dynamic dimension to the classical static structural characterisation. We also discuss the influence of the structural changes on the physical properties of the investigated materials

[1] *C. Sanchez, B. Lebeau, F. Chaput, and J.-P. Boilot, Adv. Mater., 2003, 15, 1969–1994,* ***[2]*** *P. Durand, S. Pillet, E.-E. Bendeif, et al., J. Mater. Chem. C, 2013, 1, 1933–1942.,* ***[3]*** *K.-Y. Hsieh, E.-E. Bendeif, A. Guansmuller, et al., RSC. Advances., 2013, 3, 26132-26141*

Keywords: Nanocrystallography, Pair distribution function (PDF), Photoactive materials