Christian Bonhomme, J Material Sci Eng 2016, 5:8 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.049

NMR crystallography: When nuclear magnetic resonance and diffraction meet

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This presentation will expose an overview and the latest methodological developments in NMR Crystallography. Such a concept appeared recently in the solid state NMR community following the pioneering work of Pickard and Mauri and their implementation of the GIPAW method. Such a method allows the calculations of NMR parameters from first principles (at the DFT level) under periodic boundary conditions. Such calculations lead to full NMR tensorial parameters for all interactions (chemical shift, quadrupolar, J coupling, Knight shift) and for all nuclei described in the asymmetric unit of the crystal. GIAPW has been also extended to amorphous and disordered derivatives. The complementarity of diffraction techniques (X-rays and neutrons) and solid state NMR will be presented in the frame of NMR Crystallography. The goal of this approach is to propose new perspectives for the refinement of structures. The following questions will be raised: are NMR parameters sufficient for a full description of a crystal structure? Are a limited number of chemical environment representative of glassy architecture? A large panel of examples will illustrate the NMR Crystallography concept: inorganic structures, organic/inorganic hybrids, disordered materials such as biocompatible glasses doped with various cations. Applications of GIPAW will be presented as well in the frame of EPR and other spectroscopies.

Biography

Christian Bonhomme has completed his PhD from Pierre et Marie Curie University (UPMC) in Paris, France. Currently, he is full Professor at UPMC. He has been Invited Professor at the Department of Physics, Warwick University, UK. He is the leader of the SMiLES group at the Laboratoire de Chimie de la Matière Condensée de Paris. He has published more than 105 papers in reputed journals and has given 50 invited conferences in the fields of NMR, NMR Crystallography and Materials Science.

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