*Specialized i*NANO lecture
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Title: Chemistry by diffraction: unveiling bonding from the wealth of experiments
Time: Thursday 23 February 2010, at 15.15
Location: 1531-113 Aud-D1, Department of Mathematical Sciences

Abstract: In this lecture I will show how a combination of methods, primarily based on diffraction techniques, can uncover the chemistry and bonding in the solid state. The studied substances, light hydrides and metal-organic frameworks (MOFs), are prospective hydrogen storage materials. First we observe their transformations at different pressure-temperature conditions, exploring the behaviour and bonding preferences of different structural units. Analysis of polymorphism points to the crystal chemistry and the building principles, responsible not only for the structure but also for properties. The latter can also be explored by diffraction, since most intermediates and decomposition products are crystalline. Hydrogen absorption/desorption, thermal decomposition, trapped reaction intermediates are studied *in-situ* under operating conditions. The obtained knowledge suggests the ways to the rational synthesis of new materials and modification of their stability by chemical substitution.

Interesting findings in the chemistry of these systems, obtained from the state-of-the-art synchrotron diffraction experiments, will be presented. Fast *in-situ* experiments allow to visualize chemical processes, while the high-quality powder and single-crystal diffraction – to look on the underlying chemical interactions. The findings prove to be rather unexpected: the seemingly simple metal borohydrides, $M(BH_4)_n$, reveal a strikingly diversified chemistry. Numerous practical applications of the diffraction techniques to study highly reactive compounds and MOFs, recommendations and examples will be given.