

Physics Seminar

Friday, 20th January 2012 at 11h00
(coffee at 10h45)

Campus Belval

Room F011

Talk by **Dr. Alain Lafond**

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X-rays Crystallographic Investigations of Photovoltaic Chalcogenide Compounds

First, results issued from crystal structure investigations of Cu-poor Ga-rich compounds in the $\text{Cu}_2\text{Se-In}_2\text{Se}_3\text{-Ga}_2\text{Se}_3$ system will be discussed. This study highlights the high flexibility of the crystal structure of CIGSe compounds towards the In/Ga substitution and the presence of Cu-vacancies in a large amount. This structure flexibility is very likely one of the key points for the success met by CIGSe as photovoltaic material.

Second, I will introduce preliminary results on the crystal chemistry of $\text{Cu}_2\text{ZnSnS}_4$ and its derivatives (CZTS). It is well known that the higher solar cell performances are acquired with Cu-poor Zn-rich CZTS absorbers. So far, no structure determination of the non-stoichiometric compounds is reported in the literature. We want to address the question of the stability domains of single phases in the vicinity of the $\text{Cu}_2\text{ZnSnS}_4$ composition as well as the real distribution of the cations onto the different crystallographic sites. Because a lot of secondary phases such as ZnS and Cu_2SnS_3 can be formed during the synthesis, it is of importance to investigate the actual homogeneity of the samples. The use of the Wavelength Dispersion Spectrometry technique and the Rietveld analysis of powder diffraction patterns can address this issue in the case of high temperature synthesized powders. Our first results demonstrate the existence of a well-defined phase with a composition close to $\text{Cu}_{1.7}\text{Zn}_{1.18}\text{Sn}_{0.99}\text{S}_4$ for which a single crystal structure refinement has been successfully carried out.

Next Physics Seminars to be precised later