The supervisory board of the Kestcells Project announces the Seminar AMU-01:

"*Ab-Initio Modeling and Simulation of materials for solar cells*"

Dates: 6th of September, 2013.
Place: AMU, Domaine Universitaire de Saint Jérôme Case 231 - 13397, Marseille, France

Program

Time	Subject	Speaker
10:30 – 12:00	Ab-initio methods in condensed matter physics	Laurent RAYMOND
14:00 – 15:30	Electronic excitations in CZTS from first-principles	Silvana BOTTI

Summary

Ab-initio methods in condensed matter physics

Laurent RAYMOND

Nowadays, Ab-initio calculations are widely used, in a lot of fields. Most of the time, according to who is speaking, a precise method is associated to this term, but this association is very context dependent, and changes along the time. To point a method, or a class of methods, one has to use a less common name possibly designing a program. In this short review, we will start from a very general form of the problem to be solved in condensed matter. The chain of approximations and the principal results that make the computation feasible will be reviewed. We will try this way to give more meaning to the different abbreviations hidden in the Ab-initio designation (DFT, TDTDF, LDA, LSDA, GW, (L)APW, (FP)LO, ...).

Electronic excitations in CZTS from first-principles

Silvana BOTTI

$Cu(In,Ga)(Se,S)_2$ (CIGS) thin-film solar cells have emerged as a technology that can challenge the current hegemony of silicon solar panels. The family of kesterites $Cu_2ZnSe(S,Se)_4$ exhibits very similar electronic properties. For the past years we have witnessed a growing interest in kesterites for their potential application in photovoltaics. However, there is still a strong need for fundamental knowledge on the electronic properties and defect physics of this family of semiconductor. From the theoretical perspective,

the study of electronic properties of kesterites is particularly hard since standard density functional theory yields often results in quantitative and qualitative disagreement with experiments. By presenting some examples of calculations, I will analyse which theoretical approaches are reliable to calculate band structures, defect levels and absorption spectra including excitonic effects, and I will discuss the physical insight that they allow to gain on electronic excitations in new materials for photovoltaics.