Condensed Matter and Nanophysics — Internship offer 2014-2015

Modeling of Organic Solar Cells: focus on the Cell Morphology

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Summary:

Over the past few decades, organic solar cells have given rise to intensive research, since they are flexible, lightweight, and can be produced at low price. However, if much effort has been devoted to experimental studies, only few theoretical models have been developed. Among the various architectures of organic solar cells, the bulk heterojunction is one of the most common: the active layer of the cell is composed of a blend of the donor and acceptor materials allowing an efficient generation of free charges [1].

Numerical approaches seem to be valuable tools in order to better understand the various mechanisms taking place within cells, or to optimize their performances. A 2D model has been developed in our group [2-3], based on the accepted hypothesis of free charge generation mechanisms, and leading to the electrical characteristics of the cell (charge carrier densities, I-V curves, transient responses, performance, . . .).

The morphology of a bulk heterojunction is quite complex as it originates from the phase separation process taking place between the donor and acceptor materials. Consequently, one important hypothesis in the 2D model is the choice of the simulated morphology. The electrical characteristics of cells have been shown to be sensitive to the sizes of the donor and acceptor domains, even when the donor / acceptor ratio is fixed [2]. It is commonly accepted that a periodic structure with typical sizes for the donor and acceptor domains allows to reproduce the behavior associated with the morphology of a real bulk heterojunction [4]. Nevertheless, this particular assumption has never been verified: it is the purpose of this internship project.

The applicant must show good scientific computing skills as well as good programming skills.

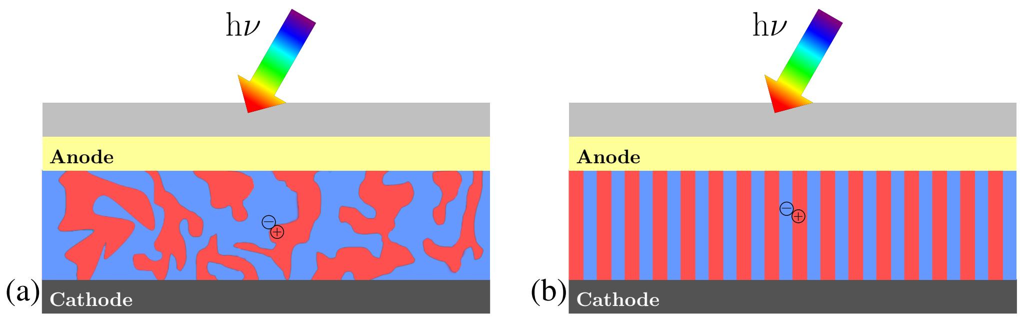

Figure 1: *Morphology of a real bulk heterojunction solar cell (a) versus a modeled cell (b).*

References:

[1] C. Deibel and V. Dyakonov, *Rep. Prog. Phys.* 73, 096401 (2010)

[2] A. Raba, A.-S. Cordan and Y. Leroy, *J. Nanosci. Nanotechnol.*, 13(7), 5164 (2013)

[3] A. Raba, Y. Leroy and A.-S. Cordan, *J. Appl. Phys.*, 115, 054508 (2014)

[4] H. R. Kodali and B. Ganapathysubramanian, *Modelling Simul. Mater. Sci. Eng.*, 20, 035015 (2012)