Condensed Matter and Nanophysics — Internship projects

Physical modeling of organic solar cells: a Monte Carlo approach

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Collaborations:	Experimental group in MaCEPV team Experimental groups in the RhinSolar Consortium (a German-Swiss-French Interreg Network, http://www.rhinsolar.eu/)

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. But 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.

Numerical approaches seem to be valuable tools in order to better understand the various mechanisms taking place within the cell, or to optimize their performance. A 2D model has already been developed in our group, 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, performance).

The purpose of this training course is to develop a complementary Monte-Carlo approach which could provide relevant information on the charge carrier mobilities, very useful for the existing model. Indeed, since the mobilities are key parameters of the model, it is essential to know their dependence to the electric field, charge densities and temperature.

The required work will proceed in several stages, of which a first phase of bibliographic search to find the already existing models. Then the best approach will be chosen and analyzed, with rewriting and adaptation to the considered system.
All the simulated results will be compared with experimental results of the experimental group in MaCEPV team of our laboratory, and also of German teams (RhinSolar).

References:

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