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► **To cite this version:**

Raphael Clerc. Physics of Organic Diode Operation: Application to Solar Cell and Photodiodes.. 223rd Electro Chemical Society Meeting MA2013-01 May 12 - 16, 2013 Toronto, Ontario, Canada, May 2013, Toronto, Canada. hal-00917104

HAL Id: hal-00917104

<https://hal.science/hal-00917104>

Submitted on 11 Dec 2013

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Physics of Organic Diode Operation : Application to Solar Cell and Photodiodes.

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Introduction: the development of photosensitive organic materials has attracted tremendous attention during recent years [1-5]. Indeed, as these materials are mostly composed of polymers, they can essentially be deposited by low cost solution-based processes, such as spin coating, dip coating, or inkjet printing [1][3]. The earliest and potentially most significant applications of these materials are photovoltaic cells [1-5] and, to a lesser extent, organic photodetectors [6-7]. These organic devices have shown great potential to become flexible, printable, low-cost and light-weight products. Moreover, these organic materials can be deposited on large surfaces, which is usually not possible using more conventional crystalline semiconductors.

Similarly, a considerable effort has been dedicated to the analysis and modelling of the operation, performances and limitations of these devices. The aim of this paper is twofold: first, the state of the art and main trends of the understanding, modelling and simulation of such devices, focusing on the Bulk HeteroJunction (BHJ) polymer based devices, will be reviewed. In a second part, recent finding, combining experiments and modelling (numerical as well as analytical) will also be presented.

Drift Diffusion models based on the virtual semiconductor approach:

First attempts to model BHJ OPV have given birth to the extensively used “virtual semiconductor” or “effective media approach” [8]. Similar approach has already been implemented in commercial 2D simulation software. It relies on the following assumptions: 1/ Acceptor and donor materials are supposed to be perfectly mixed, in order to dissociate efficiently and homogeneously the excitons 2/ As a consequence, the full blend is considered as a homogenized effective semiconductor, featuring the HOMO of the donor and the LUMO of the acceptor. 3/ transport of free carriers is described in the framework of the drift and diffusion model, well known in organic electronics. It includes non geminate Langevin recombinations [9] and, if needed, trap assisted recombinations [10], as in inorganic semiconductor.

Advanced models taking into account the detail morphology of bulk heterojunction: In the meantime, alternative approaches have also been investigated to improve the “effective media” approach.

The main alternative relies on the hopping theory [11], which, in principle, should describe more accurately transport in disordered semiconductors. Such an approach has been extensively used in organic electronics for instance to predict the field and temperature dependencies of bulk mobility used in drift diffusion model. Full OPV devices have also been simulated in the framework of the

hopping model, employing the Monte Carlo technique. This approach has the great advantage to be able to account easily for the fine morphology of the intermixed blend of donor and acceptor semiconductors. Indeed, in these works, a so called Ising model is first used to generate a series of blend morphologies with varying scales of phase separation. The transport of charges created by exciton dissociation at each interfaces is then computed according to hopping equations. Moreover, the impact of phase separation on OPV blend can also be investigated in the framework of a pure Drift Diffusion model. The group of Prof. Alam at Purdue university [12] for instance was able to calculate the structure of the phase separation versus process parameters (annealing temperature and duration) and then to compute the 3D transport of electron and hole using the drift and diffusion approaches. Such an approach constitutes an attractive alternative to more time consuming hopping simulations, without using the effective media approximation

Open questions: Despite significant recent progresses in the characterisation and modelling of BHJ devices, several issues are still under deep investigations. First of all, the capability of these models to reproduce experimental data (dark and illuminated currents, External quantum efficiency ...) has to be confirmed by a careful analysis. Moreover, the accurate understanding of the impact and nature of recombination mechanisms is still under discussion. More specifically, the nature, localisation and characterisation of traps versus materials and architecture are of particular interest. Similarly, the impact of the morphology on performances has also to be deeper investigated.

Recent insights on these issues, combining the results of electric and optical measurements, as well as analytical modelling, will be discussed in this talk.

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