

# Book of Abstracts



Escola de Engenharia da Universidade do Minho

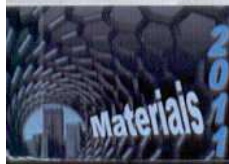
## VI International Materials Symposium

### MATERIAIS 2011

XV Meeting of SPM – Sociedade Portuguesa de Materiais

18-20 Abril 2011

Guimarães, Portugal



## THE INFLUENCE OF ION DOPING PROFILE IN THE FUNCTIONING OF POLYMER LIGHT EMISSION DIODES: A COMPUTER SIMULATION STUDY

A. Pereira<sup>1,2</sup>, J.P. Martins<sup>1,2</sup>, H.M.C. Barbosa<sup>1</sup>, H.M.G. Correia<sup>1</sup>, L. Marques<sup>1,2</sup>, M.M.D. Ramos<sup>1,2</sup>

<sup>1</sup>Centre of Physics, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal, [jpmphysics@gmail.com](mailto:jpmphysics@gmail.com)

<sup>2</sup>Department of Physics, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal

One of the strategies to enhance efficiency of Polymer Light Emission Diodes (PLEDs) is to dope the conjugated polymer with ionic species (organic or inorganic). Although it is proven by experiments that this kind of doping can enhance PLEDs efficiency, it is not clear how the spatial distribution of the ionic species within the polymer layer can affect all the electronic process underlying the PLEDs functioning, and consequently their performance.

In this study, we use computer simulations, combining quantum molecular dynamics simulations at molecular scale with Monte Carlo simulation at device scale, to understand the influence of ion doping profile in PLED functioning, with the polymer active layer of *poly*(p-phenylene vinylene) (PPV). We use five different ion doping profiles, ranging from a random ion distribution throughout the polymer layer to localized ion distribution near the electrodes.

In the results obtained by us it is clear that by changing the ion doping profile there are changes in the electrical and optical properties of doped PLEDs, which affects their efficiency.

**Acknowledgement:** This work is part of the project CONC-REEQ/443/EEI/2005 funded by the Portuguese Foundation of Science and Technology (FCT). A.P. and H.M.G.C. are also indebted to FCT for financial support under PhD grant No. SFRH/BD/62536/2009 and Post-Doctoral grant No. SFRH/BPD/64554/2009, respectively.

**Keywords:** Modelling; PLEDs; Doping.