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ABSTRACTS' BOOKLET



SPOF, Sociedade Portuguesa para a Investigação e Desenvolvimento em Óptica e Fotónica
contact@spidof.pt
Rua 1º de Maio, 2, 2º, 4730-734 Vila Verde
Portugal

Room 3:Fri. 18:00 to 19:30 pm

18:00 pm: **Morphology in thin polymer blend films for solution-processed solar cells using advanced spectroscopic tools** (*Invited Paper*), Ellen Moons, Ana Sofia Anselmo, Andrzej Dzwilewski, Krister Svensson, Karlstad Univ. (Sweden); Jakub Rysz, Andrzej Budkowski, Jagiellonian Univ. (Poland); Andrzej Bernasik, AGH Univ. of Science and Technology (Poland); Jan van Stam, Karlstad Univ. (Sweden) [8001-89]
Polymer-based photovoltaics opens the way to inexpensive, thin, and lightweight solutions for renewable and mobile power supply. The energy conversion efficiency of these solution-processed solar cells is closely linked to the distribution of donor and acceptor molecules in the film, i.e. the morphology. Morphological control is indispensable for the development of high-performance polymer photovoltaics. In this talk I present our current understanding of the formation of lateral and vertical compositional gradients in spin-coated polymer:fullerene films, based on complementary results from Atomic Force Microscopy, Near-Edge X-ray Absorption Fine Structure spectroscopy (NEXAFS), and Dynamic Secondary Ion Mass Spectrometry (dSIMS).

18:30 pm: **Multi-scale modelling of polymer-based optoelectronic devices** (*Invited Paper*), Marta M. D. Ramos, Helena M. G. Correia, Helder M. C. Barbosa, Univ. do Minho (Portugal) [8001-109]
The optimization of polymer-based optoelectronic devices such as light-emitting diodes (LEDs), photodetectors and photovoltaic cells requires the understanding how molecular properties and the spatial arrangement of the conjugated strands affect the electronic processes underlying the functioning of these

devices. Since some of the important features are determined largely by the individual molecular strands and other features depend strongly on the nanostructure, a multi-scale modelling of materials and device properties is needed. In this work we discuss the atomistic and nanoscale modelling of charge injection, transport, trapping and recombination in LEDs, as well as exciton formation and migration in photodetectors.

→ 19:00 pm: **Computational study of the presence of defects in semiconducting polymers on exciton formation**, Helena Correia, Helder Barbosa, Marta Ramos, Univ. of Minho (Portugal) [8001-179]
Although semiconducting polymers are very attractive to be used in optoelectronic devices due to their molecular properties, they are not pristine semiconductors. After deposition it is possible to find out several structural and chemical defects that strongly influence exciton dynamics, since they create deep energetic sites where excitons can be trapped leading to their quenching or reducing exciton diffusion length. By using a self-consistent quantum molecular dynamics method we performed a computational study to understand the influence of well-known polymer defects on excitons dynamics. Our results show that these defects influences mainly intramolecular exciton localization and exciton energy.

19:15 pm: **The influence of generated charges on the functioning of polymer photodiodes: a computer simulation study**, André Pereira, Helder M. Barbosa, Helena M. Correia, Marta M. Ramos, Univ. of Minho (Portugal) [8001-27]
The use of semiconducting polymers in solar cells and photodetectors is very attractive because of their low cost, lightweight and flexibility. When a photon is absorbed by the polymer it generates a quasi-particle known as exciton, which can dissociate leading to the formation of a pair of charges of opposite sign. However it is not clear from the experiments how the electric field of the generated charges can affect the exciton dissociation efficiency in these devices. To understand this effect we performed computer simulations of a polymer photodiode using a developed multi-scale model.