

2012 Spring Meeting

**May 14 – 18
Strasbourg, France**

PROGRAMME

CONFERENCE SYMPOSIA

MATERIALS FOR ENERGY

- A Advanced Silicon Materials Research for Electronic and Photovoltaic Applications III
- B Thin Film Chalcogenide Photovoltaic Materials
- C Solid State Ionics: Mass and Charge Transport across and along Interfaces of Functional Materials
- D Unconventional Thermoelectrics: from new materials to energy conversion devices
- E Actinide compounds and properties
- F Solid proton conductors (In honor of Prof. G. Alberti)

BIO / ORGANIC / POLYMERIC MATERIALS

- G Functional Biomaterials
- H Organic and Hybrid Materials for Flexible Electronics: Properties and Applications
- I Biological applications for organic electronic devices
- J DNA Directed Programmable Self-assembly of Nanoparticles into Meta Materials for energy and other applications
- K Surface modifications of carbon-related materials II

MATERIALS FOR ELECTRONIC / PHOTONIC / PLASMONIC

- L Novel Functional Materials and Nanostructures for innovative non-volatile memory devices
- M More than Moore: Novel materials approaches for functionalized Silicon based Microelectronics
- N Control of light at the nanoscale: materials, techniques and applications
- O Applied Nanoplasmonics: Nanoplasmonic Functional Materials and Devices

ADVANCED MATERIALS AND NANO MATERIALS

- P Advanced Hybrid Materials II: design and applications
- Q Novel materials and fabrication methods for new emerging devices
- R Science and technology of nanotubes, graphene and 2D layered materials
- S Novel materials for heterogeneous catalysis
- T Physics and Applications of Novel gain materials based on Nitrogen and Bismuth Containing III-V Compounds
- U Carbon- or Nitrogen-Containing Nanostructured Thin Films

METHODS AND ANALYSIS

- V Laser materials processing for micro and nano applications
 - W Current Trends in Optical and X-Ray Metrology of Advanced Materials for Nanoscale Devices III
 - X Quantitative Microscopy of Energy Materials
 - Y Advanced materials and characterization techniques for solar cells
-

- 14:00 **Thienopyrrolidone-containing Donor/Acceptor alternating copolymers as new electron-donating materials**
Authors : Chiara Ottone(a), Philippe Berrouard(b) , Guy Louarn(c), David Gendron (b), Malgorzata Zagorska (d), Patrice Rannou (a), Ahmed Najari (b), Said Sadki(a), Mario Leclerc(b), Adam Pron(a)
Affiliations : (a) INAC/SPRAM (UMR 5819, CEA-CNRS-Univ. J. Fourier-Grenoble 1) Laboratoire d'Electronique Moléculaire Organique et Hybride, CEA Grenoble, 17 Rue des Martyrs, 38054 Grenoble, France (b) Department of Chemistry, Université Laval Quebec City, QC, G1V 0A6 (Canada) (c) Institut des Matériaux Jean Rouxel (IMN), CNRS-Université de Nantes, BP 32229, 2, rue de la Houssinière, Nantes 44322, France (d) Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00664 Warszawa, Poland
Resume : Pi-conjugated polymers have attracted significant research interests during the past three decades owing to their tuneable by design (electro)chemical, electronic and optical properties. This remarkable and rare combination of features paves the way toward new generations of (opto)electronics devices such as organic FETs, LEDs, Laser & Solar Cells. Designing efficient materials for boosting solar cell's external power conversion efficiency (EPCE) beyond state-of-the-art values exceeding 8.0% require, among other important issues, a strict and full control of their redox properties. Key material parameters are HOMO/LUMO levels and the band gap. Cyclic voltammetry (CV) & UV-Vis spectroscopic studies performed on the three synthesized D/A alternated copolymers showed band gaps inferior to 2.0 eV together with easily varied HOMO and LUMO levels in the -5.62 eV to -5.08 eV and -3.53 eV to -3.13 eV respective ranges as a result of our (macro)molecular engineering approaches. UV-vis-NIR spectroelectrochemical studies confirmed CV results, enabling moreover more accurate determinations of their HOMO levels. In addition, Raman spectroelectrochemistry was used for an in depth probing of the redox stability of these new semiconducting materials incorporating an electron-accepting thienopyrrolidone sub-unit. A preliminary and encouraging EPCE value of 1.6% has been obtained for non-optimized D/A bulk-heterojunction solar cells based on D/A alternated copolymer/PC61BM's active layers. 11 30
- ✚ add to my program → (close full abstract)
- 14:00 **Multiscale modeling of the influence of phase separation in the functioning of organic photovoltaic devices**
Authors : Helena M. G. Correia, Marta M. D. Ramos, Luis Marques, Hélder M. C. Barbosa
Affiliations : Centre of Physics and Department of Physics, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal
Resume : Controlling and understanding the influence of the morphology of the active layer made of polymer/low weight molecules blend in organic solar cells (OSC) is, in our days, seen as one of the key issues to increase its efficiency. Most of the research in this area, is made at experimental level focusing not only on the influence of the molecular structure of the materials used, but also on the deposition conditions that changes the nanomorphology and thus the OSC performance. On the other hand, the few theoretical studies published in the literature that concern the influence of the active layer morphology in OSC functioning, simulate a blend morphology far from what is expected from experimental data. In this communication, we present a study of the influence of polymer/low-weight molecule morphology in OSC functioning, using a multiscale model based on quantum molecular dynamic calculations to obtain the molecular properties of the organic materials and a mesoscopic model that considers not only the main physical processes that are behind OSC functioning, but also simulates different possible polymer/low-weight molecule phase separation. Our results shed some light on how the different polymer/low-weight molecule blend morphologies affects exciton diffusion/dissociation and charge transport/collection processes in OSC performance. 11 31
- ✚ add to my program → (close full abstract)
- 14:00 **ZnCoO as hole extraction layer in polymer solar cells**
Authors : Torsten Otto, Hans Schmidt, Holger Spahr, Tim Bülow, Torsten Rabe, Sami Hamwi, Wolfgang Kowalsky
Affiliations : Institut für Hochfrequenztechnik Technische Universität Braunschweig Schleinitzstr. 22 38106 Braunschweig Germany 11 32
Resume : Polymer solar cells are normally based on liquid polymer solutions applied by spin coating or printing technology. The contact layers at the anode and cathode of those solar cells should feature high transparency and

MULTISCALE MODELLING OF THE INFLUENCE OF PHASE SEPARATION IN THE FUNCTIONING OF ORGANIC PHOTOVOLTAIC DEVICES



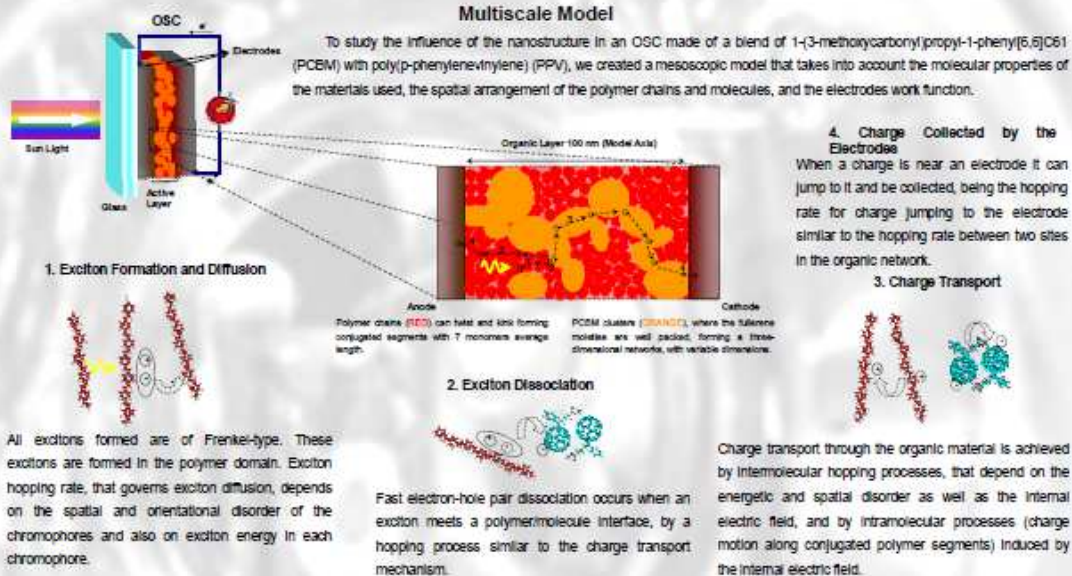
Helena M. G. Correia, Marta M. D. Ramos*, Luís Marques and Hélder M. C. Barbosa

 Centre and Department of Physics, University of Minho, Campus de Gualtar, 4710 – 057 Braga, Portugal

Abstract

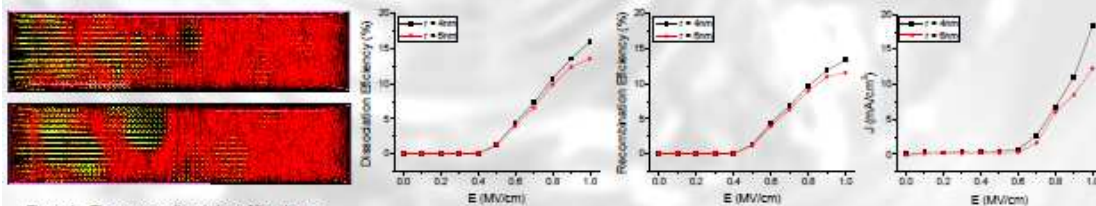
Controlling and understanding the influence of the active layer morphology in polymer/low weight molecules blend organic solar cells (OSC) is, actually, seen as one of the key issues to increase its efficiency. In this communication, we present a study of the influence of polymer/low-weight molecule morphology in OSC functioning, using a multiscale model based on quantum molecular dynamic calculations to obtain the molecular properties of the organic materials and a mesoscopic model that considers not only the main physical processes that are behind OSC functioning, but also simulates different possible polymer/low-weight molecule phase separation. Our results shed some light on how the different polymer/low-weight molecule blend morphologies affects exciton diffusion/dissociation and charge transport/collection processes and their consequences for OSC performance.

Multiscale Model



Results and Conclusions

The active layers studied in this work consist of a mixture of PCBM and PPV in a 1:1 weight ratio and PCBM-rich spherical regions with an average radius, r , of 4 and 6 nm.



The decreasing of phase separation (i.e. increase of rich PCBM domains with small radius) leads to a change on blend morphology by increasing polymer/molecule interface area. As a result, there is an increase of both exciton dissociation efficiency and charge recombination efficiency, the effect being less pronounced for the recombination process.

Since the percolation paths for electron transport are formed more easily when PCBM-rich particles are smaller, the current density increases with the decrease of the radius of the phase-separated PCBM domains.