

Scientific report: Photovoltaics at the nanoscale

Summary

This conference brought together scientists and engineers to exchange and discuss the latest ideas and trends in nanoscale photovoltaics, with the focus on specific research themes in the following fields of organic photovoltaics (OPV): (1) Next generation OPV materials and devices, (2) Advanced characterization from α to Ω , (3) Charge transfer mechanisms and efficiency and (4) Challenges in controlled synthesis of conjugated polymers.

Organisation: The conference was a joint organisation of the INTERREG-project ORGANEXT (Chair: Prof. dr. J. Manca), the European Science Foundation (Chair: Prof. dr. B. Cleuren) and the Belgian Polymer Group (Chair : Prof. dr. D. Vanderzande). A link to the conference website can be found [here](#).

Young scientists training: Additionally, the full program included a one-day school with tutorials, given by Prof. dr. R. A. J. Janssen and Prof. dr. M. Esposito. The content of the tutorials (hand-outs) were available to the participants. A video recording was made of both tutorials and are made available to a wider audience by the internet. Active participation of young researchers was further encouraged by a poster session and programmed group discussions. In order to stimulate a good quality of posters, a poster contest was organised. Only young researchers were allowed to participate. A total of 43 posters participated, and each poster was judged on the criteria layout, content and presentation. Laureats were Dan Credgington from Imperial College London and Bert Conings from IMO Hasselt University.

Conference format: The different themes were programmed as thematic workshops. A thematic day consists of a keynote lecture followed by lectures given by renowned top scientists in the field of that specific theme. All the speakers are selectively invited by the organizers. Every thematic day is finalized with a panel discussion amongst the participants and the speakers.

Numbers: In total there were 172 unique registrations. The attendency numbers per day are:

	24/10	25/10	26/10	27/10	28/10
Theme	Tutorials	Materials	Characterisation	CT & efficiency	Polymers
Registrations	117	143	142	129	114

Scientific content and future outlook

Monday 24/10: Tutorial courses

The first day was devoted to the training of young scientists (graduate students, PhD-students and beginning post-doctoral researchers). Two tutorial courses were scheduled, one on stochastic thermodynamics and a second on novel nanomaterials. The lecturers were asked to give a clear exposition of the material focusing also on a thorough introduction for those unfamiliar with the field. The first tutorial was given by dr. Massimiliano Esposito. He presented a solid introduction to the field of stochastic thermodynamics, which is the adequate tool to study (thermodynamical) energy conversion at a small scale. The second tutorial was programmed in the afternoon session, and was given by prof. dr. R.A.J. Janssen. He gave an overview of the field of organic and polymer solar cells and discussed a.o. phenomena such as photophysics, charge transport, nanoscale morphology and device architecture. Existing loss mechanisms were identified and some hints were given on how to improve material design.

As an extra service to those that could not be present during this day, both lectures were recorded and posted on the internet (youtube). They can be accessed using the following links:

- Tutorial 1: Introduction to stochastic thermodynamics: application to thermo- and photo-electricity in small devices (prof. dr. M. Esposito)
The movie of tutorial 1: [part I](#) and [part II](#).
- Tutorial 2: Novel nanomaterials and concepts for photovoltaic energy conversion (prof. dr. R.A.J. Janssen)
The movie of tutorial 2: [part I](#), [part II](#) and [part III](#).

Tuesday 25/10: Next generation OPV materials and devices

After the official opening of the conference by the rector of the UHasselt, Luc De Schep- per, a keynote lecture has been given by Jef Poortmans from IMEC. He gave a solid overview about where the photovoltaics market and technologies are nowadays. He also discussed technology and material challenges and trends for the future. After this interest- ing contribution, lectures were given by Kees Hummelen (Groningen University), Guy Van Assche (Vrije Universiteit Brussel), Barry Rand (IMEC), Martin Helgesen (Risø, Techni- cal University of Denmark), Moritz Riede (Technische Universitt Dresden) and Paul Blom (Holst Centre). All these speakers are well-established scientists in the field of (organic) photovoltaics focused on material and device physics/chemistry. The two main questions addressed during the panel discussion were: (1) Will fullerenes continue to be the ultimate acceptor material? and (2) Wet processing versus dry processing - who will win?. The short answers are that for the moment fullerenes are still the best and most used acceptor material and there is no real alternative now. However, on the long term it is not excluded that other materials will take over the role that fullerenes are playing now in the world of organic photovoltaics. The competition between wet and dry processing will go on.

There is great belief that both processing methods can exist next to each other, probably contributing to different future applications.

Wednesday 26/10: Characterisation from α to Ω

This day was attributed to the characterization of organic photovoltaics starting with the materials and devices going to the lifetime and stability of such devices. The keynote lecture has been given by Alberto Salleo from Stanford University. He addressed studies at different lengthscales of the used materials, going from the device scale to the nanoscale order with different techniques. Afterwards, lectures have been given by Aram Amasian (KAUST), Eric Hoke (Stanford University), Paolo Samori (Université Strasbourg), Carsten Deibel (University of Würzburg), Ronald Österbacka (Åbo Akademi University), Jean-Luc Gardette (Université Blaise Pascal) and Hans-Joachim Egelhaaf (Konarka Technologies). The main question that was addressed during the panel discussion was 'Is the well-known P3HT system a good model system?'. From the discussion it appeared that people have to be careful to use the workhorse polymer P3HT as a model system. The quest for a good model system is still running, although some people suggested that it will be very difficult to find one model system, because the active materials used in the applications can be very different, raising different properties and characteristics. Discussion about degradation mechanisms and lifetime of the devices has put forward that degradation can occur in many different ways at different places in the device: active material, contacts, interfaces, . . . The lifetime of working devices also depends tremendously on the environment where they are placed. For some regions, the temperature can be the main degrading factor, while in other regions it will be more the weather conditions like rain, hail, that will determine the lifetime.

Thursday 27/10: Charge Transfer mechanisms and efficiency

The central theme of fourth day was on charge transfer mechanisms and efficiency of organic solar cells. The keynote lecture on was given by Prof. James Durrant (Imperial College London) who discussed several factors (such as film microstructure, molecular structure and crystallinity) that influence the kinetics and yields of charge separation and recombination in organic solar cells. Each of the subsequent lectures focused on a more specific topic related to the central theme. The speakers were: J. Cornil (University of Mons, Theoretical simulations of electronic processes governing the operation of organic solar cells); A. Bakulin (Cambridge university, Importance of driving energy and delocalized states for charge separation in organic semiconductors); K. Tvingstedt (Linköping University, Charge transfer excitons probed by steady state electro- and photoluminescence spectroscopy); P. Würfel (Karlsruhe University, How solar cells work); T. Kirchartz (Imperial College London, Influence of disorder on subgap absorption and emission spectra in polymer: fullerene solar cells); J. Nelson (Imperial College London, Experimental and modelling studies of the competition between charge transfer and other excited states in polymer: fullerene blend films); K. Vandewal (Linköping University, Charge-transfer absorption and emission in organic donor/acceptor solar cells). The day was closed by the panel discussion, during which the following questions were addressed: Which efficiency

can be expected? Can OPV beat CIGS, CdT or Si? Are CTC beneficial or detrimental for solar cells? Will CT absorption and emission be detectable in all good donor:acceptor blends? Is such ground state material interaction needed for a good organic solar cell? Effect of excess energy lost in converting polymer excitons to free charge carriers. Does this energy aid in charge separation? How to measure this excess energy?

Friday 28/10: Challenges in controlled synthesis of conjugated polymers

The last day of the conference was devoted toward synthetic methods for polymer semi-conducting materials. The morning session started with a key-note lecture by Prof. Mats Anderson of Chalmers University of Technology discussing his recent work on 'Design and synthesis of conjugated polymers for solar cells', highlighting the most recent developments in the field. Next, three contributing presentations then focused on different approaches to control the polymerization process. The first by Prof. Guy Koeckelberghs (KULeuven) explored different approaches toward block copolymers: 'The controlled polymerization of poly(thiophene)s and derivatives: toward all-conjugated block-copolymers'. Dr. Noémie Hergué (University of Mons) discussed other approaches to the 'Molecular design and controlled synthesis of block copolymers based on poly(3-hexylthiophene)'. Finally the most recent efforts on 'Living p-quinodimethane polymerization for the synthesis of well-defined PPV materials: Progress and challenges' was presented by Prof. Thomas Junkers (University of Hasselt). These contributing oral presentations were intended as a preparation toward the afternoon workshop which was entirely devoted to the PhD-students and young post-docs present in the audience. This group of about 30 people was divided in three groups of about 10 people with a young post-doc moderator and reporter. The three themes for discussion were presented before lunch and introduced: Theme 1: 'A need for controlled synthesis?'; Theme 2: 'A polymerization reaction as a black box'; Theme 3: 'Phase separation and nano-morphology'. Each group received also the assignment based on introductory questions to prepare in two sessions of an hour and ten minutes a 7-slide powerpoint presentation to express their views and conclusions on the theme to be presented at the last activity the 'Roundup discussion'. An example of the introductory questions for theme 1 is given below. Questions: 'How strong is the necessity for controlled synthesis of conjugated polymers?; Is this necessity proven or demonstrated already? What can be done in this way which cannot be realized by classical homo-polymers and copolymers? What should be understood by 'controlled synthesis', meaning which aspects must be controlled in function of photovoltaic applications ? Is there further need to other approaches toward control on the synthesis?'. The roundup discussion showed a very nice compilation of the lively discussion that occurred in the different groups. Seemingly the goal of the workshop activity to stimulate specifically the young people to discuss the science they are involved in was quite successful and can be used as a model for future workshops. Finally the conference was closed by Prof. Dirk Vanderzande, director of imo-imomec.

Program

Time	Monday 24th October: Tutorial courses
9h00-10h00	<i>Registration and coffee</i>
10h00-12h00	Tutorial 1: Introduction to stochastic thermodynamics: application to thermo- and photo-electricity in small devices (prof. dr. M. Esposito)
12h00-13h30	<i>Lunch</i>
13h30-16h00	Tutorial 2: Novel nanomaterials and concepts for photovoltaic energy conversion (prof. dr. R.A.J. Janssen)
17h30-...	<i>Evening activity</i>

Time	Tuesday 25th October: Next generation OPV materials and devices
8h30-9h30	<i>Registration and coffee</i>
9h30-10h00	Welcome by the rector of UHasselt (prof. dr. L. De Schepper)
10h00-11h00	Opening keynote: Quo vadis, Photovoltaics? (prof. dr. J. Poortmans)
11h00-11h20	<i>Coffee break</i>
11h20-11h55	Lecture: Pathways to a new efficiency regime for organic solar cells (prof. dr. J.C. Hummelen)
11h55-12h30	Lecture: Relations between phase diagram, kinetics of thermal annealing process, and morphological stability in polymer: fullerene blends for bulk heterojunction solar cells (prof. dr. G. Van Assche)
12h30-14h00	<i>Lunch</i>
14h00-14h35	Lecture: An overview of ultrasonic spray coating for large area polymer solar cells and modules (dr. B. Rand)
14h35-15h10	Lecture: Roll to Roll processing, demonstration and advanced materials for polymer solar cells (dr. M. Helgesen)
15h10-15h30	<i>Coffee break</i>
15h30-16h05	Lecture: Vacuum-processed OPV (dr. M. Riede)
16h05-16h40	Lecture: Charge transport and recombination in organic solar cells (prof. dr. P. Blom)
16h40-17h15	Panel discussion
17h15-19h00	Poster session

Time	Wednesday 26th October: Characterisation from α to Ω
8h30-9h00	<i>Registration and coffee</i>
9h00-10h00	Keynote: Characterization of organic semiconductors for photovoltaics: do we understand the role of structure? (prof. dr. A. Salleo)
10h00-10h35	Lecture: Organic solar cells: molecular design and low-cost solution processing (dr. A. Amassian)
10h35-10h55	<i>Coffee break</i>
10h55-11h30	Lecture: Molecular packing in bulk heterojunction solar cells (Eric Hoke)
11h30-12h05	Lecture: Supramolecular electronics: towards multifunctional systems and devices (prof. dr. P. Samori)
12h05-13h30	<i>Lunch and group picture</i>
13h30-14h05	Lecture: Nongeminate recombination in polymer-fullerene solar cells (dr. C. Deibel)
14h05-14h40	Lecture: Effect of spontaneous charge transfer and dipole formation on charge transport in polymer OPVs (prof. dr. R. Österbacka)
14h40-15h00	<i>Coffee break</i>
15h00-15h35	Lecture: Photodegradation of organic materials used as active layers and encapsulation of OPV (prof. dr. J.-L. Gardette)
15h35-16h10	Lecture: OPV Stability – From cells to modules (dr. H.-J. Egelhaaf)
16h10-16h45	Panel discussion
16h45-19h30	Lab visit (optional) or <i>leisure time</i>
19h30-...	<i>Conference dinner</i>

Time	Thursday 27th October: CT mechanisms & efficiency
8h30-9h00	<i>Registration and coffee</i>
9h00-10h00	Keynote: Factors influencing charge separation and recombination in polymer/fullerene solar cells (prof. dr. J. Durrant)
10h00-10h35	Lecture: Theoretical simulations of electronic processes governing the operation of organic solar cells (prof. dr. J. Cornil)
10h35-10h55	<i>Coffee break</i>
10h55-11h30	Lecture: Importance of driving energy and delocalized states for charge separation in organic semiconductors (dr. A. Bakulin)
11h30-12h05	Lecture: Charge transfer excitons probed by steady state electro- and photoluminescence spectroscopy (dr. K. Tvingstedt)
12h05-13h30	<i>Lunch</i>
13h30-14h05	Lecture: How solar cells work (prof. dr. P. Würfel)
14h05-14h40	Lecture: Influence of disorder on subgap absorption and emission spectra in polymer: fullerene solar cells (dr. T. Kirchartz)
14h40-15h00	<i>Coffee break</i>
15h00-15h35	Lecture: Experimental and modelling studies of the competition between charge transfer and other excited states in polymer: fullerene blend films (prof. dr. J. Nelson)
15h35-16h10	Lecture: Charge-transfer absorption and emission in organic donor/acceptor solar cells (dr. K. Vandewal)
16h10-16h45	Panel discussion

Time	Friday 28th October: Challenges in controlled synthesis of conjugated polymers
8h30-9h00	<i>Registration and coffee</i>
9h00-10h00	Keynote: Design and synthesis of conjugated polymers for solar cells (prof. dr. M. Andersson)
10h00-10h35	Lecture: Controlled polymerization of poly(thiophene)s and derivatives: towards all-conjugated block-copolymers (prof. dr. G. Koeckelberghs)
10h35-10h55	<i>Coffee break</i>
10h55-11h30	Lecture: Molecular design and controlled synthesis of block copolymers based on poly(3hexylthiophene) (dr. N. Hergué)
11h30-12h05	Lecture: Living p-Quinodimethane polymerization for the synthesis of well-defined PPV materials: progress and challenges (prof. dr. T. Junkers)
12h05-13h30	<i>Lunch</i>
13h30-14h40	Theme workshop discussion on challenges of controlled synthesis - Session I
14h40-15h00	<i>Coffee break</i>
15h00-16h10	Theme workshop discussion on challenges of controlled synthesis - Session II
16h10-16h45	Roundup discussion
16h45-17h00	Closing remarks