Research proposal

1.Title of the project

Self-assembled organic nanofibers for photovoltaic applications

2.Applicant

Yaroslav V. Aulin

3.FOM research group

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4.Institutioon

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5.Abstract

The project aims fundamental research on the photovoltaic applications of self assembled organic nanofibers. The ability of small organic molecules to form nanostructures will be investigated in order to enhance the efficiency of photovoltaic cells. The morphology of the polymer-nanostructures blends will be analyzed by means of X-Ray diffraction, atomic force microscopy and near field optical microscopy. Photophysical properties will be studied using various spectroscopic methods including time resolved photoluminecence spectroscopy and pump-probe techniques. Finally, efficient devices based on the optimized composite materials will be fabricated.

6.Duration of the project

4 years, starting from September 2010

7.Personnel

Prof M.A. Loi (Associate professor/Leader of the research group)
Y.V. Aulin (Applicant/PhD student)
J. Harkema (Technician)
F. van der Horst (Technician)

8.Cost estimates

8.1 Personnel positions

One ‘Onderzoeker in opleiding’ position for four years

8.2 Running budget

15,000€/year

8.3 Equipment

No equipment is requested

8.4 Other support

8.5 Budget summary of the funding requested

The expenses are summarized in the table:

	2010	2011	2012	2013	2014	Total
PhD students	1	1	1	1	1	
Postdocs	-	-	-	-	-	
Technicians	-	-	-	-	-	
Guests	-	-	-	-	-	
Personnel cost	13,000€	38,000€	43,000€	46,000€	32,000€	172,000€
Running Budget	7,500€	15,000€	15,000€	15,000€	7,500€	75,000€
Equipment	-	-	-	-	-	-
Total	20,500€	53,000€	58,000€	61,000€	39,500€	232,000€

9 Research program

9.1 Introduction

Nowadays organic solar cells based on a bilayer structure or a bulk heterojunction of donor and acceptor materials have several times lower efficiency compared to their inorganic counterparts (maximal efficiencies of 7% and 30% respectively [1]). Their poor performance originates mainly from short exciton diffusion length and low charge carrier mobilities. However, organic photovoltaic cells can be processed from solution, which enables possibility of cheap mass production such as roll to roll and ink jet printing.

Low dimensional nanostructures of organic materials can enhance the photovoltaic performances. They can be designed to have high crystallinity, which will facilitate directional exciton diffusion and charge transport. On the other hand they still can be processed from solution for low cost fabrication.

One dimensional nanomaterials, for instance nanotubes and nanofibers are currently attracting special attention due to 2D confinement, 1D transport of excitons and charges, and the potential to be used as functional components in miniaturized optoelectronic devices in the future. Some prospective applications of organic 1D materials, like OLEDs, field-effect transistors, chemical sensors, optical waveguides, and optically- pumped lasers have been already shown [2,3]. We propose to utilize the properties of 1D organic materials in order to improve the efficiency of organic solar cells.

Self assembled nanofibers of small organic molecules exhibit high charge carrier mobility and exciton delocalization along the nanofiber, moreover there is an opportunity

of tuning their optoelectronic properties, such as absorption spectrum and the efficiency of the exciton dissociation process at the interface by modifying the lateral size of the nanofiber [4].

9.2.Research questions

In our research project we will investigate the performance of organic solar cells based on the hole conducting polymer (poly 3-hexyl thiophene) P3HT and the electron conducting self-assembled molecular nanofibers of perylene diimide derivatives.

P3HT was well studied as a material for polymer-fullerenes bulk heterojunction solar cells [5]. Thus the performances of the P3HT-nanofiber solar cells would be easily evaluated.

The choice of the material for organic nanofibers is dictated by the high values of electron conductivity of perylene, and the ability to tune the properties of the perylene nanostructures by modifying the side-chains of the molecules [2].

In contrast to disordered organic materials such as polymers, excitons and charges are delocalized along the nanofibers. Ordered supramolecular structure arises from the stacking of π-conjugated molecules due to π-π interactions [6]. This relatively strong interaction results in mixing of the molecular orbitals of the neighboring molecules, leading to the delocalization, which is favorable in solar cells.

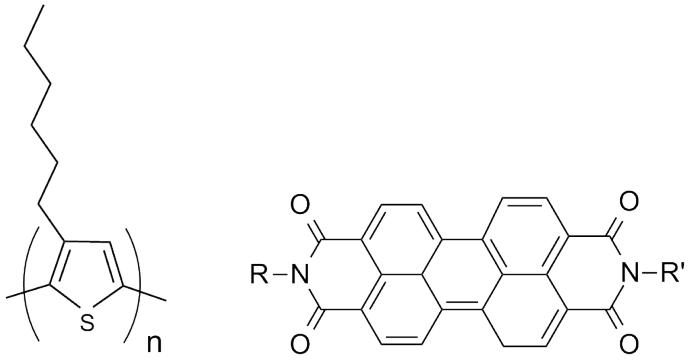


Figure 1. Molecular structures of (poly 3-hexyl thiophene) P3HT, and of perylene diimide (PDI) modified by side chains R and R'.

Working principle of the proposed solar cell is depicted in Fig. 2. and is similar to that one of the bulk heterojunction solar cell. Upon a photon absorption by the active layer an exciton is formed either on the strand of P3HT polymer or in the organic nanofiber.

Upon the exciton dissociation, the charges are transported to the electrodes. Compared to disordered systems, perylene nanofibers can substantially improve the charge extraction due to the high charge mobility and directional transport [7].

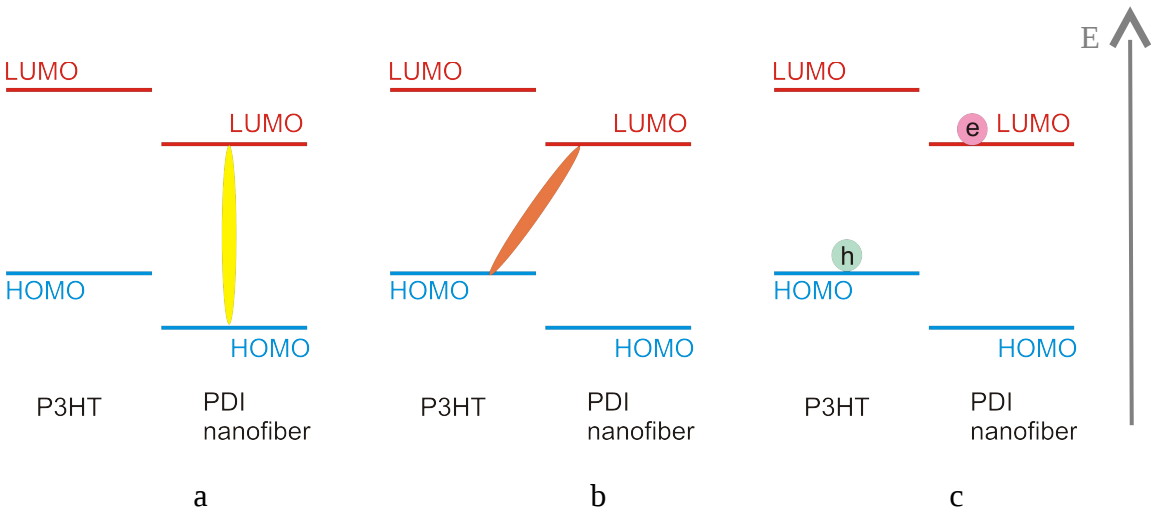
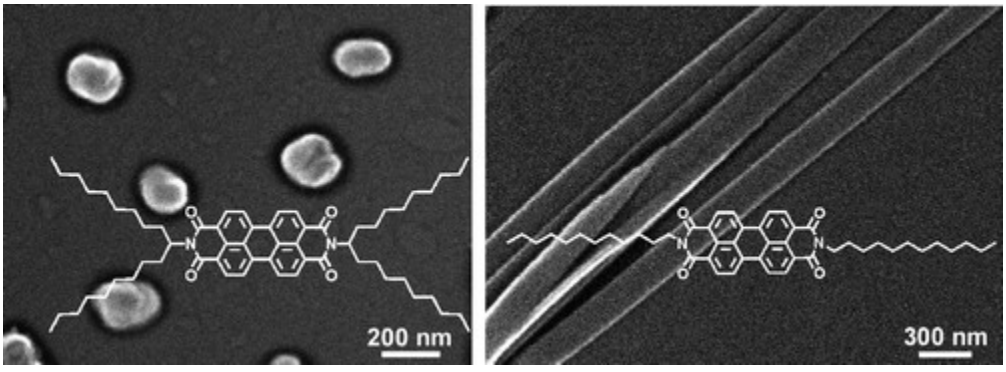


Figure 2. Working principle of the P3HT polymer – self-assembled perylene nanofiber solar cell: a) absorption of the sunlight and the exciton creation either on nanofiber or P3HT polymer strand, b) charge transfer exciton and charge separation at the nanofiber – polymer interface, c) charge carrier transport to the electrodes: the electrons are transported by the nanofibers and the holes by the polymer.

The morphology of the P3HT-perylene blends will play crucial role in the solar cell performance. The requirements to the morphology are dictated by the goal to improve the exciton dissociation efficiency and the charge percolation path. Structures perpendicular to the plane of the device are favorable.

Recently, profound research on self -assembled organic nanostructures has been done for the derivatives of oligophenylenes, phthalocyanines, porphyrins and perylenes. It has been shown that organic nanofibers with uniform widths could be formed under certain conditions. Fig.3 represents nanoparticles and nanofibers of perylene diimide derivatives.



a b

Figure 3. Effect of side-chain substitutions on the morphology of self-assembly of perylene diimide molecules on example of two derivatives modified with different side-chains: a) *N*,*N*‘-di(dodecyl)-perylene-3,4,9,10-tetracarboxylic diimide (DD-PTCDI) and b) *N*,*N*‘-di(nonyldecyl)-perylene-3,4,9,10-tetracarboxylic diimide (ND-PTCDI) [8]

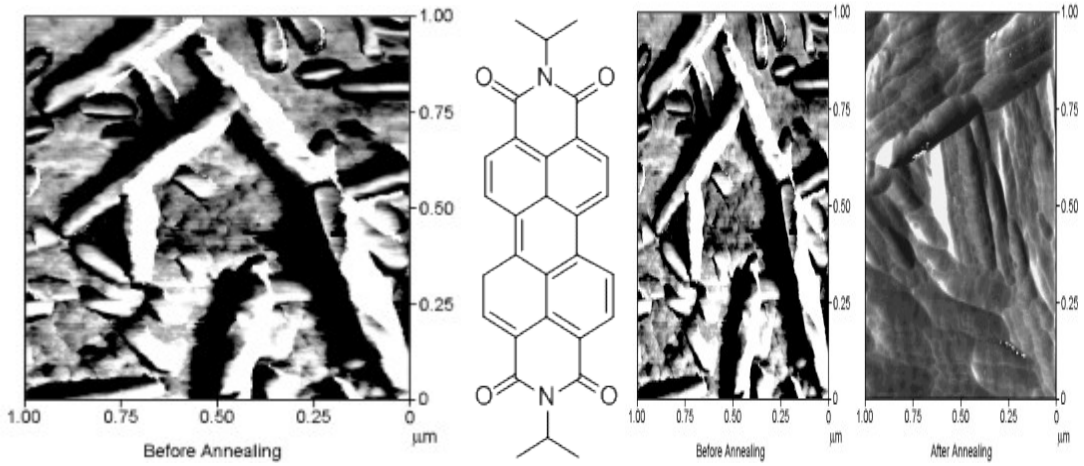


Figure 4. AFM images of the layers formed from the blend of perylene diimide derivative EP-PTC (3,4:9,10-perylene bis(tetracarboxyl diimide)) with P3HT for different processing conditions [9].

Experiments on the P3HT -EP-PTC (3,4:9,10-perylene bis(tetracarboxyl diimide)) blends showed that the morphology of spin-cast layers could be controlled significantly by varying the processing conditions. In Fig. 4 the examples of different morphologies of the blends are provided.

Still, the control of the organic nanofibers orientation remains a challenge. Several experimental techniques have been elaborated to achieve directional growth of nanofibers including vertical spincoating, external electric field application and vapor deposition technique [10,11].

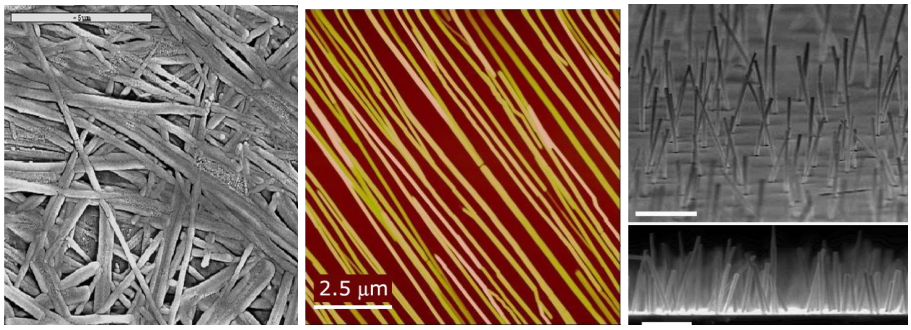


Figure 5. Self assembled molecular nanofibers and control of their orientation: a) SEM image of randomly oriented fibers of 1,3-diphenyl-2-pyrazoline [2] [2], b) AFM image of the organic nanofibers of para-sexiphenyl molecules grown by hot wall epitaxy technique and oriented in the plane of the substrates [10], c) vertical organic nanowire array of 1,5-diaminoanthraquinone molecules formed by the physical vapor transport method [11]

. The self assembley of small molecules into nanofibers in blends with polymers and the ability to control nanofiber size and the orientation in the blend has yet to be investigated

9.3 Research methods

The ability of PDI derivatives to form nanofibers in the blends with P3HT polymer will be studied. Samples will be fabricated using various methods with the ultimate goal to obtain nanofibers embedded into the polymer matrix and oriented mostly perpendicular to the surface of the substrate – geometry ideal for the solar cell.

We propose to study application of the following methods to achieve the desired morphology:

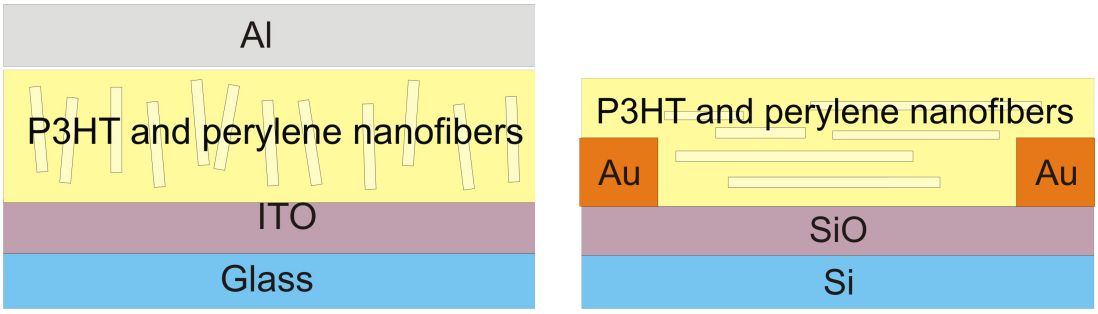
i) processing from the solution (spincoating or doctor blading) with external electrical field applied perpendicular to the substrate in order to orient the nanofibers [12]

ii) processing from the solution onto a precursor layer of perylene diimide derivatives to which nanofibers formed in the solution should attach due to π- π interactions,

iii) vapor deposition teqhniques.

Samples with the nanofibers oriented in the plane of substrate will be also fabricated using vertical spincoating technique [13], or orientation in applied electric field [12].

Research on the samples anisotropy will provide additional information on the mechanisms of charge transport and exciton dissociation in this class of materials. The composites with the nanofibers oriented in the plane of the substrate are attractive materials for polarization sensitive light detection in field effect transistor geometry.



a b

Figure 6. Structure of the solar cell with the nanofibers oriented perpendicular to the substrate surface (a) and of the field effect transistors with the nanofibers oriented in plane of the active layer (b).

Structural analysis of the fabricated films of P3HT –PDI nanofibers will be performed using X-ray techniques, AFM (atomic force microscopy), SNOM (scanning near field optical microscopy [14]). The spatial orientation of the fibers embedded into the polymer will be determined by probing the samples with polarized light [15].

In order to improve solar cell performance following material properties should be optimized: exciton lifetime, diffusion and delocalization lengths, efficiency of the exciton dissociation at the nanofiber-polymer interface, charge-carrier mobilities. In order to shed light on the behavior of the excitons and charges in this class of materials the

problem will be tackled using wide range of experimental techniques. Measurement of the exciton lifetime will help to understand and improve the exciton dissociation process. The efficiency of charge generation by light in the material will be investigated using pump-probe and photoinduced absorption techniques. Charge carrier mobilities will be extracted from the measurement of microwave conductivity [16], the method that allows to eliminate the influence of the electrodes.

Solar cells and field effect transistors with the active layer from the composite materials with optimized structure and optoelectronic properties will be created during the final phase of the project. Device layouts of the proposed solar cell and a transistor are shown in Fig. 6.

9.4 Research plan

September 2010–August 2011	Investigation of an ability to controll the nanostructure of P3HT – perylene diimide derivatives blend and the orientation of organnic nanofibers in the blend by different methods. Study of the films by AFM, far and near field optical microscopy, electron microscopy and X-Ray diffraction techniques
September 2011–August 2012	Specroscopic study of the samples using time resolved spectroscopy, optical pump-probe and transient absorption techniques Study of the charge transport properties of the blends by microwave conductivity
September 2012– August 2013	Fabrication of efficient solar cells and photo-diodes/photo-transistors Optimization of the device performance
September 2013–August 2014	Investigation of possible applications of the other materials in polymer -organic nanofiber solar cells Writing the thesis

9.5 Application perspective in industry, other disciplines or society

In addition to fundamental investigation of the self-assembled organic nanofibers current research project has direct industrial applications in the field of solar energy harvesting. We attempt to improve the efficiency of organic solar cells by introducing self-assembled organic nanostructures into the active layer. The efficiency improvement will lead to commercialization of the technology, and its application in various novel optoelectronic devices.

References

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