Alternative materials in organic solar cells

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Introduction

Organic solar cells (OSC) are promising devices for harvesting solar energy because:

-they are environmentally less aggressive

-more suitable for fabrication in large scale than inorganic solar cells

Conjugated polymer in organic solar cell

- Alternated single and double bonds allow the electron transfer
- Defects in polymer chains and spatial configuration of polymer chains have negative effects on electron transport.





Photon-Polymer interaction

- The delocalized orbitals with π electrons in the conjugated polymer enable the photon absorption
- Frenkel excitons confines the electronhole pair on the same molecule
- Wannier excitons extend the electron-hole pair between two neighboring molecules



Exciton diffusion and decay

- Photon absorption
- Exciton generation
- Exciton decaying
- Charge carrier separation



Charge transport

The need of acceptor

The acceptor role is:

- To form p-n junction with the donor
- To separate charge carriers
- To lead the carriers to the external electrode to preventing recombination



Energy levels

- Material workfunction W_f
- HOMO and LUMO level
- Band gap E_g
- Fermi level E_f





Monolayer OSC

- The active layer is composed of the organic film, the donor
- The exciton decay takes place at the organic (polymer)-ITO interface
- Poor efficiency between 0,005 and 0,8 %



Bilayer OSC

- The active region is composed of two separate layers, the donor and acceptor
- The exciton decay takes place at the donor-acceptor interface
- The efficiency is better than in monolayer SC between 0,1 and 3 %



Bulk-Heterojunction OSC (BH-OSC)

 The bulk hetero-junction OSC structure forms a large polymer -acceptor interface with a well spread network of electron conducting paths

The efficiency is ~5



Materials in BH-OSC

- The materials are divided based on their function on:
 - Acceptors

[6,6]-phenyl-C₆₁butyric acid methyl ester-**PCBM C60** LUMO=-3,75eV $E_g=2,35eV$ HOMO=-6,1eV [6,6]-phenyl-C₇₀ butyric acid methyl ester-**PCBM C70** LUMO=- $E_g=$ HOMO=-

Polymers

poly(3-hexylthiophene) (**P3HT**) LUMO=-3,52eV $E_g=1,68eV$ HOMO=-5,2eV poly[2-methoxy-5-(2'-ethylhexyloxy)-*p*phenylene vinylene] (**MEH-PPV**) LUMO=-2,7eV $E_g=2,32eV$ HOMO=-5,02eV

MEH-PPV

Materials for electric contac

• Metals for electrical contact Metals with high workfunctions Al $W_f = 4,3eV$ Li $W_f = 2,49eV$ Metals with low workfunctions ITO $W_f = 4,7eV$

Substrates

- -glass or
- -plastic foil

Both covered by a transparent and conductive indium-tin oxide (ITO) layer. $W_f=4,7eV$ $R=20\Omega$





PEDOT:PSS

- is a mixture of two polymers that are applied as a dispersion of gelled particles in water
- minimizes the roughness of the ITO surface
- facilitates the hole transport in to ITO layer



Polymer P3HT

- P3HT is a conjugated polymer
- Absorption range between 300nm and 700nm

Band gap of 1,68 eV



Acceptor PCBM

- PCBM is a fullerene molecule with 61 carbon atoms
- PCBM is a acceptor material
- The attached side group is to increase the solubility



Fabrication of OSC

- Preparation of solution
 - mixing and dilution of materials
 - stirring
- Substrate preparation
 - etching the ITO layer
 - substrate cleaning



Fabrication of OCS



• Evaporation of the back contact

• Device annealing

I-V measurements

0.005

- The I-V measurements are performed in dark and under illumination
- The shape of the I-V curve determinate the solar cell properties





I-V measurements

- Calculation of parameters
 - Maximum power point (P_{max})

$$P_{\max} = I_{\max} * U_{\max}$$



I-λ measurements

I-λ measurements gives the current wavelength dependence – the spectral response SR



I-λ measurements

 From the I-λ data it is possible to calculate the external quantum efficiency (EQE)



New acceptor material Mo₆S₃I₆ nanowires

- Nanowires are fabricated by direct synthesis from elemental materials
- Their physical properties are suitable for implementation in OSC structure because:

-they are soluble in most organic solvents
-their energy levels are suitable for charge transport in OSC

HOMO=-4,78eV LUMO =-3,58eV $E_g=1,2eV$



New organic-inorganic SC structure

Embedded MoSI nanowires in the active layer



I-V measurements

I-V measurements of BH-OSC with embedded MoSI nanowires



I- λ measurements

I-λ measurements of BH-OSC with embedded MoSI nanowires



EQE calculations

EQE calculations for BH-OSC with embedded MoSI nanowires



Ft-IR investigations

Ft-IR spectroscopy investigations of solutions





The efficiency of OSC is the main factor that determinate the ability of converting the light in to electrical power.

By chemical tailoring of the primary materials and improving the OSC structure it is possible to influence on the efficiency of these devices.

Our attempts to affect on the solar cell efficiency by adding a new material in to the structure demonstrates that with a accurate material selection it is possible to influence on some properties.

Thank you for your attention