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Photovoltaic effect in bulk heterojunction system with glass forming indandione derivative DMABI-6Ph

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Abstract

The aim of the work is to evaluate possible use of 2-[[4-(bis(2-trityloxyethyl)amino)phenyl]methylene]indane-1,3-dione (DMABI-6Ph) as light absorbing material for solar cells. DMABI-6Ph is a perspective material due to its good photoelectrical, thermal and chemical properties. The main advantage of DMABI-6Ph is its ability to form amorphous films by wet-casting methods thus allowing using the compound in organic solar cells made from solution. For now most popular materials for solution processable solar cells are polymer P3HT and fullerene derivative PCBM, but lot of investigations are in the field of new low molecular weight materials to replace the polymer. Photoelectrical measurements were made to determine molecule ionization and electron affinity levels of DMABI-6Ph. Difference of 2.06 eV between DMABI-6Ph ionization level and PCBM affinity level was obtained. Accordingly open circuit voltage of system DMABI-6Ph:PCBM was measured up to 0.78 V. The best power conversation efficiency was 0.11 % for the DMABI-6Ph:PCBM mass fraction 2:1. Limiting factor for high efficiency could be low charge carrier mobility which can be increase by additional DMABI-6Ph modification.

Keywords: indandione group; bulk heterojunction; energy levels; power conversion efficiency; glass forming structure

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1. Introduction

Renewable energy is becoming more and more popular [1, 2]. Significant part of it is solar energy and photovoltaic cells, especially silicon solar panels [3]. However, new kind of solar panels are necessary which could be integrated into buildings, windows and other objects. Such solar panel should be semi-transparent and flexible [4]. Organic solar panels could be one of the solutions. These panels could also ensure low environmental impact due to easy and cheap manufacturing process [5–7]. Investigations must be done to find new materials to improve efficiency and lifetime of organic solar cells. Regarding to production technique of organic solar cells evaporation in vacuum is expensive and complicated. More promising is solution processed solar cells [8, 9]. This method allows using less expensive roll to roll method for solar cell production. Nowadays most popular materials for solution processable solar cells are polymer poly(3-hexylthiophene) (P3HT) and fullerene derivative [6,6]-phenyl C61-butyric acid methylester (PCBM) made as bulk heterojunction system with reported efficiencies 3–6 % [10–14]. Replacement of the polymer by low molecular weight materials could offer lower production costs, better repeatability of synthesis and easy recycling [15].

Dimetilaminobenzylidene-1,3-indandione (DMABI) is a perspective material due to its good photoelectrical, thermal and chemical properties [16]. However, the only way how to produce pure thin film from these molecules is thermal evaporation in vacuum. Recently our research has shown the possibility to overcome this issue by attaching bulky trityloxyethyl groups to the molecule [17, 18]. These groups assist amorphous thin film formation from solution. The aim of this work is to evaluate possible use of 2-[[4-(bis(2-trityloxyethyl)amino)phenyl] methylene]indane-1,3-dione (DMABI-6Ph) as organic material for solar cells. DMABI-6Ph with added two trityloxyethyl groups allows forming glass structure by wet-casting. Photoelectrical measurements were made to determine molecule ionization and electron affinity levels of DMABI-6Ph. The photovoltaic characteristics as power conversion efficiency and fill factor of bulk heterojunction solar cell containing PCBM and DMABI-6Ph made by spin-coating method were measured and the dependencies of these parameters on DMABI-6Ph concentration in system were investigated.

2. Description of experimental research

2.1. Materials

Well known electron acceptor and transporter fullerene derivative [6,6]-phenyl C61-butyric acid methylester (PCBM) (Sigma Aldrich 684457) and newly synthesized indandione derivative DMABI-6Ph (see Fig. 1) were used to make a bulk heterojunction layer in solar cell. Attached tri-phenyl groups in the indandione derivative ensure amorphous state formation in active layer from organic solvents. There were made measurements also with poly(3-hexylthiophene-2,5-diyl) (P3HT) (Sigma Aldrich 445703) to ensure correct energy level comparison.

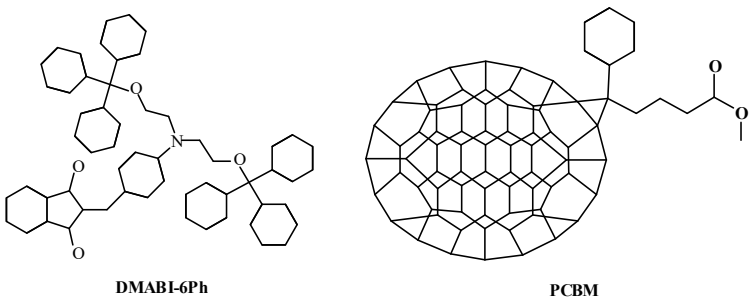

Fig. 1. Structural formulas of the investigated molecules.

2.2. Preparation of samples

Several types of samples were made for various measurements.

Threshold energy of photoconductivity determination was made on sandwich type samples – thin film of material is between two semi-transparent electrodes. Indium tin oxide (ITO) covered glass was used as the substrate. PCBM layer was made by thermal evaporation in vacuum and DMABI-6Ph by spin-coating. For both films the thickness was about 500 nm. Aluminium (Al) layer with thickness of 30 nm was deposited as a top electrode. For ionization energy measurements similar samples were used only without top electrode.

Thin film of studied compounds with the thickness of 30 nm was deposited on a quartz substrate for absorption spectra measurements.

The sandwich type samples with the structure where organic bulk heterojunction layer is between ITO as a bottom electrode covered with PEDOT:PSS and aluminium as a top electrode were made for photovoltaic measurements. ITO coated glass was used as a substrate. It was covered by PEDOT:PSS using spin-coating technique. The parameters of spin-coating were 2500 rpm for 80 seconds. After coating the PEDOT:PSS layer was dried at 160 °C for 30 minutes. The solution of organic compounds was made using chlorobenzene and chloroform as solvents with proportion 2:1, respectively. Five solutions were made dissolving DMABI-6Ph and PCBM in different mass ratios between 1:1 and 6:1, respectively. The thickness of all samples was about 60 nm. It was obtained from 10 mg/ml solution at the spin-coating parameters 500 rpm for 40 sec. After active layer coating the samples were dried at 70 °C for 10 minutes followed by temperature increase to 120 °C and treated additional 15 minutes. Al was used as the top electrode and was deposited at pressure of $6 \cdot 10^{-6}$ mBar using thermal evaporation in vacuum in an evaporation system EDWARD AUTO 306. The thickness of the top electrode was 80 nm. The area of each photovoltaic pixel was defined by Al and ITO electrode overlapping area and was 10 mm^2.

2.3. Experimental methods

Optical microscope Nikon ECLIPSE L150 was used to make optical images of thin films. Calibrated spectrometer Ocean Optics HR4000 was used to measure absorption spectra of thin films.

Ionization energy of materials was determined on a self-made experimental system. Energetiq LDLS EQ-99 light source attached to monochromator was used to provide light with spectral width of 2 nm for sample illumination. The distance between electrode and sample was ~20 mm and the voltage 20 V was applied between them. Measurements were made in vacuum at pressure $1 \cdot 10^{-5}$ mBar. For electric measurements an electrometer Keithley 617 with an incorporated DC voltage supply was used. From the film emitted electron current was measured as a dependence on illuminated light wavelength. Photoelectron emission quantum yield (PEQY) dependence on photon energy was calculated. Photoconductivity measurements were performed at the same experimental setup. In this case there was no distance between electrode and sample. Sandwich type samples were used for these measurements. Photoconductivity measurement process and calculations of threshold values of compounds were made by procedure described elsewhere [19].

The current-voltage characteristics for photovoltaic measurements were obtained by computer controlled Keithley 6517 which was used as voltage source and electrometer. As a light source a solar simulator ScienceTech SS150 was used providing an irradiance of 100 mW/cm^2 with AM 1.5 filter. All photovoltaic measurements were carried out in ambient conditions without encapsulation of the samples.

3. Results and discussion

Thin film of DMABI-6Ph was obtained amorphous and it has good quality.

Absorption spectrum of investigated compound covers visible spectral range from 420 nm to 540 nm (see Fig. 2).

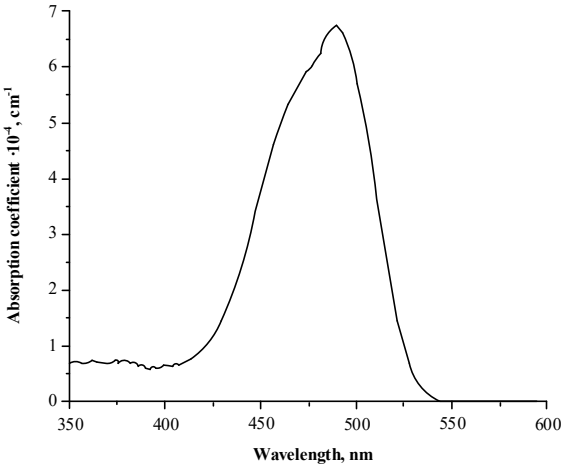

Fig. 2. Absorption spectrum of DMABI-6Ph.

It is necessary to determine energetic levels of organic compound to design good solar cell [20, 21]. Important processes are charge carrier photogeneration and separation. In those processes a molecule ionization energy I_f gives information about hole transport level and electron affinity level E_{Af} gives information about electron transport level. To make comparison, we obtained energetic levels not only for DMABI-6Ph, but also for commercially available compounds PCBM and P3HT.

In Fig. 3(a) obtaining of molecule ionization energy in thin film I_f for compound DMABI-6Ph can be seen. A rapid growth of PEQY was obtained in ultraviolet region around 6 eV and here can be seen that growth of PEQY at power of 2/5 is linear. Molecule ionization energy value can be obtained in a point of intersection with X axis.

In Fig. 3(b) a determination of threshold energy of photoconductivity value E_{Th} can be seen for compound DMABI-6Ph. Here the values of β(hν) were raised to the power of 2/5 [19]. This method can be used as there was observed anti-correlation between absorption curve and quantum efficiency of photoconductivity β(hν). It shows that photogeneration process is in volume of sample. In opposite case it would be in the interface between organic film and electrode. From E_{th} we can obtain difference between hole transport levels and electron transport levels. These energy levels were obtained also for compounds PCBM and P3HT.

Energy levels of investigated compounds DMABI-6Ph, PCBM and P3HT can be seen in Fig. 4. Energy diagram shows that DMABI-6Ph has better energy level position as P3HT. Combining PCBM with compound DMABI-6Ph the difference between electron affinity levels is only 0.06 eV compared to 0.44 eV for P3HT:PCBM system.

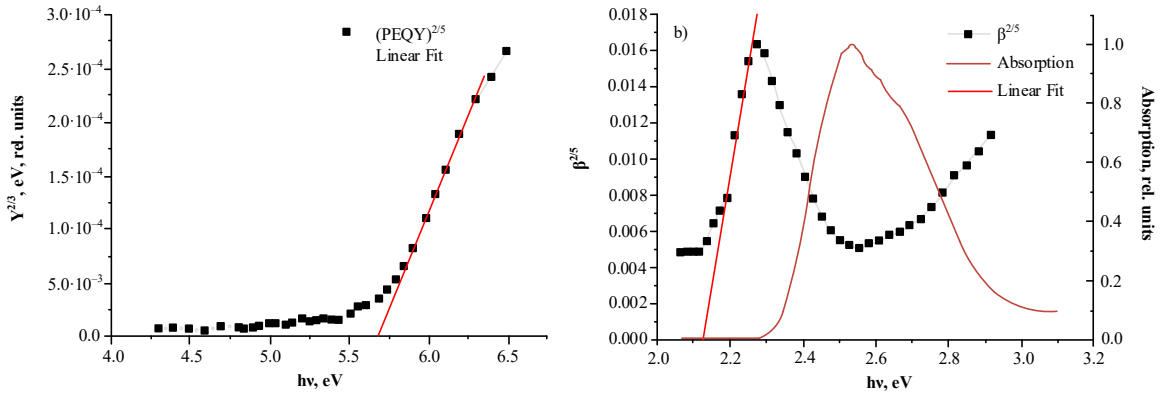

Fig. 3. Determination of: (a) molecule ionization energy in thin film I_f; (b) threshold energy of photoconductivity value E_{Th} for compound DMABI-6Ph.

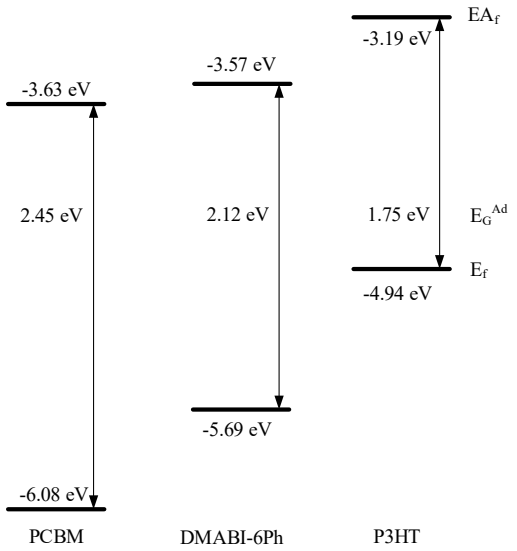

Fig. 4. Energy levels of investigated compounds. Upper levels correspond to the electron affinity level in thin film E_{Af}. The lower levels correspond to the molecule ionization energy level in thin film I_f. The values given between the levels correspond to the values of threshold energy of photoconductivity E_{Th}.

It means that electron could be easier transferred to PCBM due to small difference between electron affinity values.

Molecule ionization energy is lower for DMABI-6Ph molecule compared to P3HT. Consequently it should give higher open circuit voltage [22, 23]. In case of system P3HT:PCBM difference between donor ionization and acceptor affinity levels was 1.31 eV. Open circuit voltage for such system is average 0.60 V [24–27]. In our system DMABI-6Ph:PCBM difference between donor ionization and acceptor affinity levels was 2.06 eV, accordingly we could expect higher open circuit voltage for the system DMABI-6Ph:PCBM.

Photovoltaic measurements were made for samples with different DMABI-6Ph mass fraction in system to investigate photovoltaic parameters change on DMABI-6Ph mass fraction changes.

Obtained short circuit current I_{sc} and open circuit voltage U_{oc} values are shown in Fig. 5(a). I_{sc} values were around 0.50 mA/cm^2. Comparing to P3HT:PCBM system, obtained current values and efficiency of our system is lower. It could be due to low charge carrier generation or poor charge carrier extraction from the active layer. It can be observed that I_{sc} values decrease rapidly as mass friction of DMABI-6Ph increases significantly. Two explanations could be given. First is increase of the distance between interface and second is decrease of charge carrier mobility. Open-circuit voltage values for system DMABI-6Ph:PCBM slightly change on concentration and is between 0.70 V to 0.78 V (see Fig. 5(a)). These values are higher than for well-known system P3HT:PCBM containing polymer as it was predicted.

Power conversion efficiency and fill factor change on DMABI-6Ph mass friction can be seen in Fig. 5(b). Best value of power conversion efficiency was obtained for sample with mass fraction 0.67 of DMABI-6Ph and reached 0.11 %. If samples with different mass fractions of DMABI-6Ph in system are compared, it is observed that best values of power conversion efficiency can be reached if mass fraction of DMABI-6Ph in system is between 0.60 and 0.75. It is more than one order of magnitude less in comparison to P3HT:PCBM. The reason is low fill factor and short circuit current. The fill factor values were not dependent on mass fraction of DMABI-6Ph in system and were about 0.26. Average fill factor values for polymer solar cells P3HT:PCBM are about 0.50 [28–30].

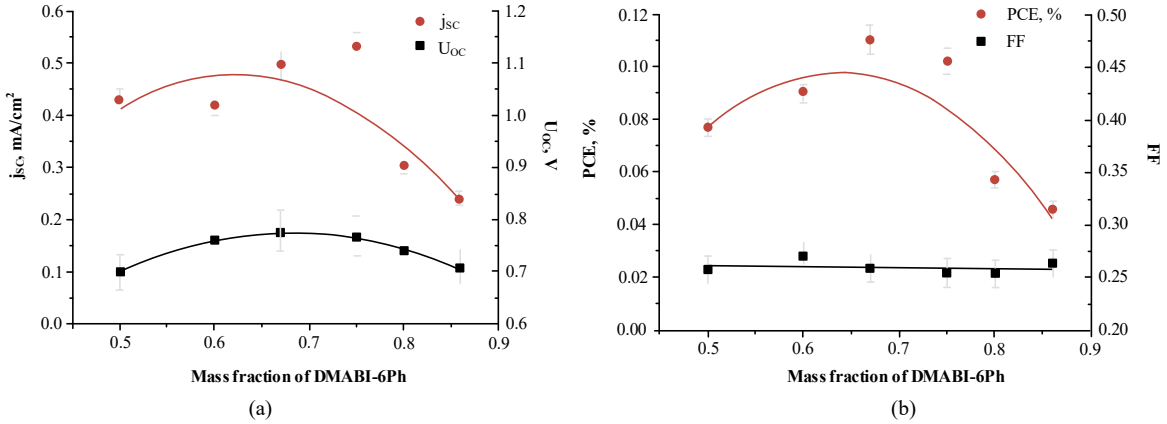

Fig. 5. Solar cell photovoltaic characteristics dependence on mass fraction of DMABI-6Ph in system DMABI-6Ph:PCBM: (a) short circuit current and open circuit voltage; (b) power conversation efficiency and fill factor.

Measurements on spectral dependence of incident photon to charge carrier efficiency (IPCE) were performed (Fig. 6) to explain low I_{sc}. If we assume that one excition is generated at each absorption case and this excition is separated in charge carriers, then IPCE should follow absorption spectrum. But for our samples IPCE spectrum do not correlate with the system absorption spectra. It means that in the spectral regions with low absorption were generated less excitions but proportionally higher amount of charge carriers was collected in comparison to the regions with high absorption where higher number of excitons was generated. Most likely the reason could be charge carrier transport through the active layer. At high density charge carrier generation part of them stay at the PCBM:DMABI-6Ph interfaces and recombines. This effect reduces short circuit current and could be reason of low FF because FF is higher for low absorbing region and lower for high absorbing region.

4. Conclusions

The glass forming indandione derivative DMABI-6Ph is possible to use to convert visible light to electricity as the photoelectrical effect was observed. The relatively high value of open circuit voltage allows assuming that DMABI-6Ph in combination with well-known fullerene derivative PCBM is promising as bulk heterojunction system for organic solar cells, thus, making possible solution processed organic solar cell without use of polymer. Avoiding polymer ease the production and recycling of solar cell.

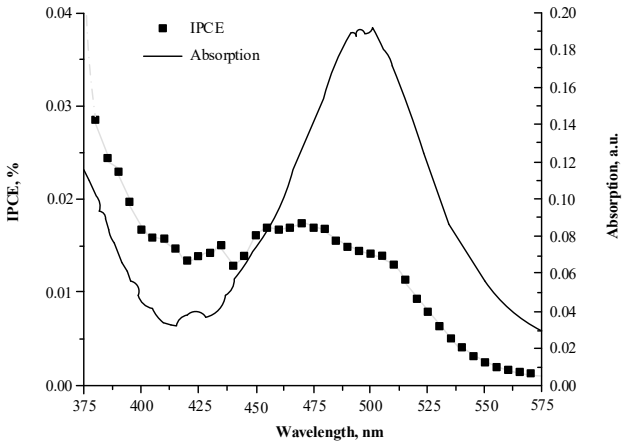

Fig. 6. Anti-correlation between incident photon to charge carrier efficiency (IPCE) and absorption for system DMABI-6Ph:PCBM in case of mass fraction of DMABI-6Ph in system 0.50.

Most likely, charge carriers' mobility is low for DMABI-6Ph. It significantly reduces charge carriers transfer to electrodes. Mobility could be improved by modifying DMABI-6Ph with attached different hole transport groups. Fill factor could be improved in the same way or by adding extra electron and hole transfer layers in the system.

The best power conversion efficiency of system DMABI-6Ph:PCBM was obtained for the mass ratio of DMABI-6Ph in the system of 67 % (DMABI-6Ph:PCBM 2:1). It also has to be taken into consideration that samples were made without encapsulation and photovoltaic measurements were carried into ambient atmosphere. Better results would be expected if all measurements were made in vacuum or inert atmosphere. Solar cell efficiency can be also significantly improved with encapsulation of samples to prevent impact of oxygen and environment [31]. In case of our studies the emphasis was on determination of solar cell characteristics dependence on mass fraction of DMABI-6Ph in system therefore multilayer system was avoided and encapsulation of samples was not done.

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