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The photovoltaic effect in a heterojunction of molybdenyl phthalocyanine and perylene dye

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Abstract

Results of research on the photovoltaic effect in the ITO/*N*,*N*′-dimethyl-3,4,9,10-perylenbis(dicarboximide) (MePTCDI)/molybdenyl phthalocyanine (MoOPc)/Au system are presented. The effect results from photogeneration of charge carriers in the MePTCDI/MoOPc heterojunction. Interface states constituting trapping and recombination centers have been used to interpret the relationship between the open-circuit voltage and the intensity of light.

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1. Introduction

Organic heterojunctions formed from phthalocyanine and perylene dye have been the subject of intensive investigations due to their likely application in thin-film photovoltaic cells [1–5]. A great number of phthalocyanines and perylene dyes enable one to obtain many various heterojunctions, in which phthalocyanine is a p-type semiconductor and the perylene dye – an n-type material. The range of strong optical absorption of these two types of materials is shifted towards each other and, as a result of this shift, a heterojunction formed from them absorbs light from a wide range of wavelength. Particularly strong light absorption (400–900 nm) is obtained with titanyl phthalocyanine (TiOPc) and perylene dye such as *N*,*N*′-dimethyl-3,4,9,10-perylenbis(dicarboximide) (MePTCDI) [6,7]. The same advantage can be expected from systems with vanadyl phthalocyanine (VOPc) [8] or molybdenyl phthalocyanine (MoOPc) [9], since, just as TiOPc, they exhibit absorption expanding up to 900 nm. However, as far as the author is aware, the photovoltaic properties of systems containing these phthalocyanines have been not considered yet.

In this work, results of research on the photovoltaic effect in a system with a heterojunction formed from MoOPc and MePTCDI are presented, in which indium tin oxide (ITO) and gold (Au) were applied as electrodes. Fig. 1 shows the chemical structure of molecules of the used organic compounds and a scheme of the investigated system, hereafter referred to as ITO/MePTCDI/MoOPc/Au.

2. Experimental details

The procedure of preparing the ITO/MePTCDI/MoOPc/Au system has been as follows. A glass substrate half-covered by indium tin oxide (ITO, thickness 35 nm, 100 Ω/square, AWAT) was placed in vacuum of 2×10^{-4} Pa (Auto 306 Turbo, Edwards) after several ultrasonic baths in acetone, methanol and isopropanol and drying in a stream of hot air. With application of proper shadow masks, consecutive layers of MePTCDI (thickness 50 nm), MoOPc (thickness 85 nm) and Au (thickness

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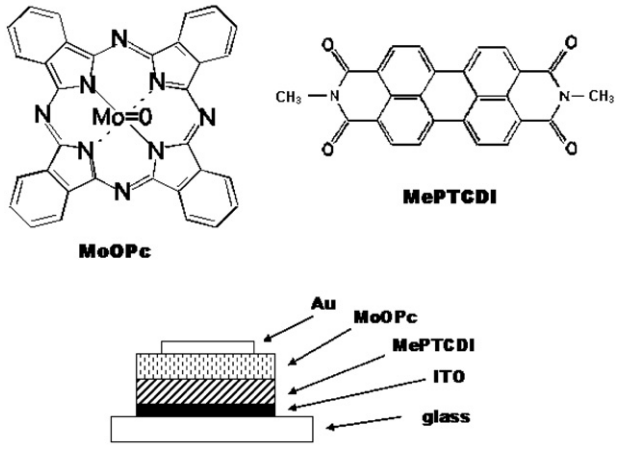

Fig. 1. Chemical structure of the molecules and a scheme the device.

20 nm) were subsequently evaporated through thermal sublimation (deposition rate 0.5 Å/s). The substrate temperature during deposition of the organic layers was (65 ± 5) °C. Molybdenyl phthalocyanine was provided by Dr A. Kempa and MePTCDI was purchased from Sensient Imaging Techn. Syn Tec Div. Both organic materials were additionally purified by sublimation in a stream of N_2 (train sublimation) [10]. Four samples were produced in one cycle, each of them with 5 mm^2 of active electrode surface. The absorption spectra of MePTCDI and MoOPc were measured with a Perkin Elmer Lambda 10 spectrometer. A Kethley 6517 electrometer with a computer controlling voltage source was used for electric measurements. Reproducibility of experimental results of electric measurements performed on various samples from the same series was around 10%. An Xe (ILC 201) lamp provided with an AMO filter (Oriel) was a source of white light simulating solar light. Spectra of photocurrents were obtained using a CM110 monochromator (CVI) with a constant flux of photons in the whole wavelength range. The system was always illuminated through ITO. All measurements were performed in ambient air at room temperature.

3. Results and discussion

3.1. Current–voltage curves

The sample's current–voltage characteristics while in the dark and under illumination with white light are presented in Fig. 2. Positive voltage ($U > 0$) refers to a higher potential on ITO, e.g. to the +ITO/−Au polarization. The obtained curves exhibit an asymmetry consisting in higher currents flow with the −ITO/+Au polarization. However, the rectification ratio is not very high. As an example, at $U = 0.4$ V it equals 4.5 for the dark curve (inset) and as little as 2.0 under illumination (Fig. 2). Moreover, the observed photovoltaic effect exhibits rather low values of open-circuit voltage, U_{oc} (less than 100 mV under illumination with white light of 20 mW/cm^2) and a fill factor of 0.29. The short-circuit current flows through the junction from MePTCDI to MoOPc, in agreement with the built-in electric field appearing after equalization of the electrodes' Fermi levels. In general, charge carrier transport through a system formed from electrodes and organic layers is limited by structural disorder and potential barriers existing at the electrodes and at organic–organic interfaces. Information about the height of such barriers can be obtained from an analysis of the energy-level diagram of the used materials. A diagram of Fermi levels of electrodes

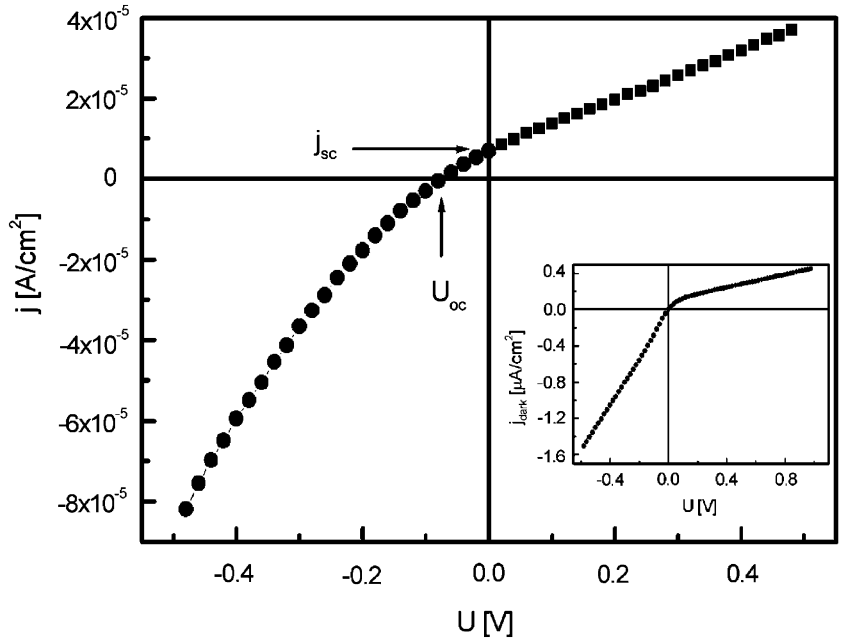

Fig. 2. Current density versus applied voltage: photocurrent under illumination through ITO with white light of 20 mW/cm^2 and current in the dark (inset).