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Photovoltaic effect in single-layer organic solar cell devices fabricated with two new imidazolin-5-one molecules

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ABSTRACT

Organic solar cells were fabricated with two new imidazolin-5-one molecules as active layers. The use of imidazolin-5-ones, derivatives of a biomolecule chromophore, for photovoltaic applications is particularly attractive due to its biodegradable nature and tunable properties. Single-layer devices with two analogues of imidazolin-5-ones were prepared and characterized. Devices fabricated with one of the molecules as the active layer showed a maximum J_{sc} of 0.52 μA cm^{-2} and V_{oc} of 0.68 V at an incident power of 20.32 mW cm^{-2}, while the other set of devices showed a maximum J_{sc} of 0.63 μA cm^{-2} and V_{oc} of 0.57 V at the same incident power.

1. Introduction

Organic solar cells (OSCs) have undergone a rapid growth in the past 20 years ever since the development of a two-layer organic photovoltaic cell by Tang in 1985 [1]. Availability of inexpensive and varied raw materials accompanied by an easy fabrication procedure and the ability to tune molecular properties has made organic photovoltaic an attractive proposition [2–4]. However, OSCs still suffer from problems such as low efficiency, poor reliability and instability. Hence the quest for a material, which will solve these problems, is still an area of active research today [5,6].

Imidazolin-5-one is the main chromophore, which is responsible for the high fluorescence property of green fluorescent proteins (GFPs) [7,8]. In the protein the chromophore, 4-(*p*-hydroxybenzylidene) imidazolin-5-one, is attached to the peptide backbone through 1 and 2 positions of the ring [9]. It is formed via a post-translational internal cyclization of the Ser^{65}-Ty^{66}-Gly^{67} tripeptide followed by 1,2-dehydrogenation of tyrosine [10]. The substituents attached to imidazolin-5-one ring can be varied to modulate the optical and electrical properties of the molecule that can thus be engineered for absorption in a desired frequency range [11]. This ability to tune imidazolin-5-ones provides the designer with flexibility to alter the molecular properties as per his/her desire. In addition, the molecules score over most other known materials for solar cell application in terms of their biodegradable nature, thus making them environment and user friendly.

In this paper, characteristics of the two set of devices using a single layer of imidazolin-5-one molecules as the active layer have been discussed. The devices showed photovoltaic effect when exposed to light and the current density–voltage (*J*–*V*) relations of the same have been studied.

2. Materials

In our work, we have investigated two molecules as potential candidates for solar cell applications. The chemical structure of these two molecules is depicted in Fig. 1(a) and their energy band diagram is given in Fig. 1(b).

The two molecules are

Molecule A: (4Z)-4-(4-methoxybenzylidene)-2-((E)-4-methoxystyryl)-1-phenyl-1,4-dihydro-5H-imidazolin-5-one.
Molecule B: (4Z)-4-(4-*N*,*N*-dimethylaminobenzylidene) -1-methyl-2-phenyl-5H-imidazolin-5-one.

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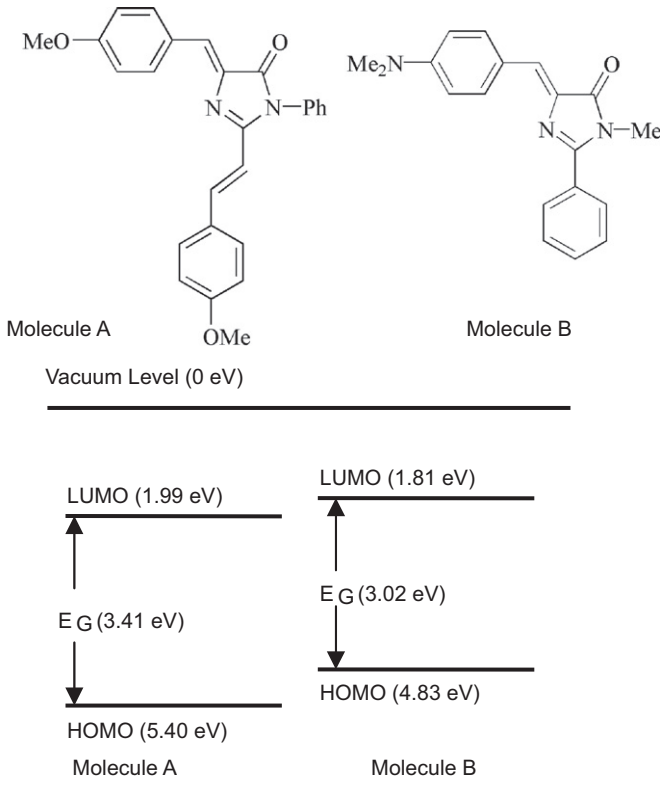

Fig. 1. (a) Molecular structures of the two new imidazolin-5-one molecules synthesized based on the chromophore of green fluorescent protein; (b) energy level band diagram of the molecules denoting the HOMO–LUMO levels and the energy gap drawn with respect to the vacuum level.

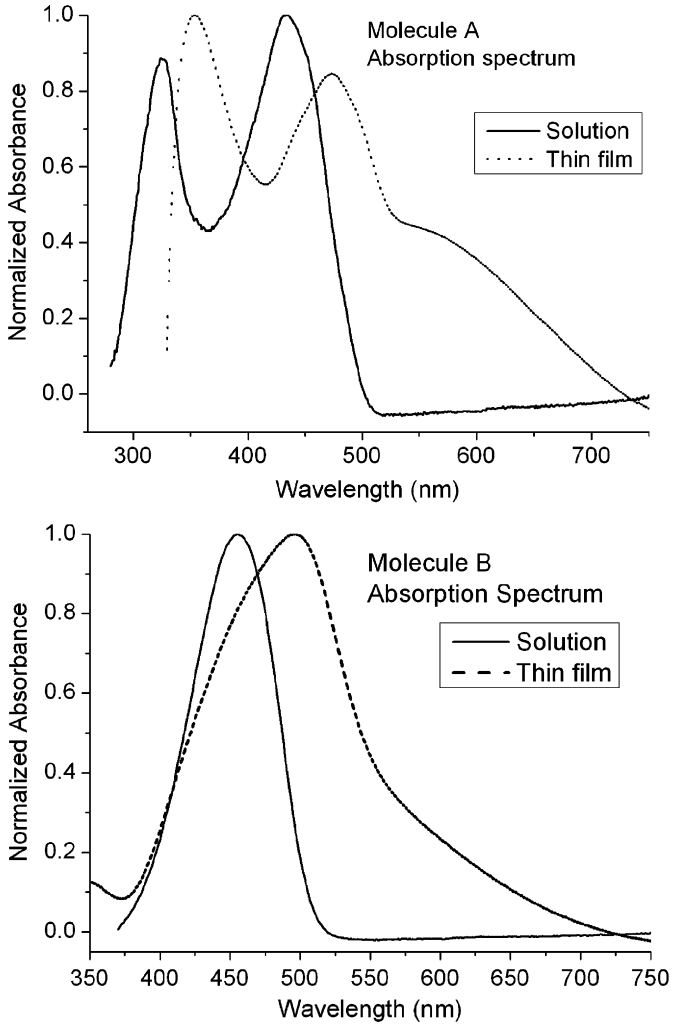

Fig. 2. Absorption spectra of the two imidazolin-5-one molecules (Molecules A and B) in solution and thin film form. The broadening and red shift of absorption spectrum in thin film form compared to the solution form can be observed.

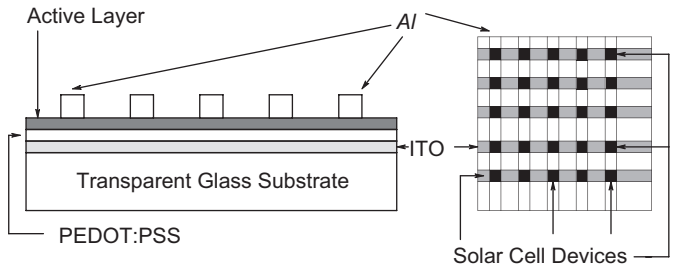

Fig. 3. Schematic cross-section and top view of the fabricated device structure. Devices are formed at the intersection of the horizontal anode and vertical cathode lines. Active layer denotes the imidazolin-5-one molecule layer, which can be a single layer of Molecule A or B.

Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels were estimated using the Gaussian 98 programme [12], which makes use of the time-dependent density function theoretical calculations (TDDFT B3LYP) [13]. Cyclic voltametry (CV) [14] was also performed on the molecules in dichloromethane solution and HOMO level energy was found to be in good agreement with the theoretical values.

The absorption spectra (absorbance) of the materials in solution and thin film form are shown in Fig. 2. All the absorption peaks lie in the blue region.

The solutions were prepared by dissolving the compounds in chloroform. The thin films were prepared by heating powders of the compound in a metal boat kept inside a high vacuum (4×10^{-6} mbar pressure) chamber. The vapours of the compound were depositing on a glass substrate kept above the boat.

It can be observed from all the figures that the absorption spectrum in thin film form is broader as compared to that in solution form. Also the absorption peak for thin film is red shifted in comparison to the solution peak. These observations can be explained by taking into account the intermolecular interactions in thin film form, where the molecules are on an average closer with a wider spread in their spacing [15].

3. Experimental

The structure of the fabricated devices consisted of the following layers (Fig. 3):

Indium tin oxide (ITO)/poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS)/imidazolin-5-one (Molecule A or B)/aluminium.

ITO-coated glass substrates were first patterned using photolithography to obtain ITO strips of 3 mm width. The patterned substrates were RCA cleaned and dried to remove any moisture content. These substrates were further exposed to UV-ozone gas for 15 min to improve the ITO work function. PEDOT:PSS solution (Baytron) was filtered and then spin-coated onto these substrates at 1000 rpm for 60 s and dried at 120 °C for 1 h. The thickness of PEDOT:PSS layer was measured to be 120 nm using Alpha Stepper