

SYNTHESIS OF TITANIA-BEZYLIDENOIMINO HYBRID QUANTUM WELL SOLAR CELL

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ABSTRACT

Solar energy is the biggest advantage over the conventional power generation systems that the sunlight can be directly converted into electricity without any emission of greenhouse gases. In last few years photovoltaic industries have emerged with an annual growth of 40%. Solar cells are renewable pollution free source of electrical energy which can easily replace traditional fossil fuels. Solar power, potentially the most fruitful source of renewable energy. Priorily silicon based solar cell were widely used but according to demand of the community and industries various photovoltaic cells based on inorganic, organic material, multi junctions, hybrid heterojunction combination with quantum wells are widely used now a days.

Keywords: Hybrid Solar Cells, Titania, 2-Bezylidenoimino-6-Substitued Benzothiazoles

I INTRODUCTION

Solar energy is the most promising source of renewable energy. It has the fascinating advantage over the conventional power generation systems that the sunlight can be directly converted into power with the help of solar cells. This type of electrical energy production methods is cost effective, no toxic by products generation, in other words strategy follows sustainable environment.

Priorily the large work has been done on silicon based solar cells, but due to high cost and limitations of conversion efficiencies now a days different type of solar cells like multi junction solar cells, inorganic-organic hybrid cells are widely used for improved efficiency⁽¹⁻¹⁴⁾. Organic quantum well solar cells (OQWSC's) are kind of green energy source show great potential application due to low production costs, mechanical flexibility devices by using simple techniques with low environmental impact. Rapid development of this technology has led to growing interest in OSCs in academic and industrial laboratories. The combination of organic skeleton into inorganic base enomoursly increase the efficiency of photovoltaic cell⁽¹⁵⁻²¹⁾.

Looking the need of photovoltaic cells and benefits of hybrid quantum well (Inorganic/Organic) solar cells here we present an UV responsive inorganic-organic hybrid solar cell based on Titania/2-benzylidenoimino-6-substitued benzothiazole (TiO₂/2-BNZA) heterojunction. In this solar cell, TiO₂ is an ultraviolet light absorber and electronic conductor, 2- benzylidenoimino -6-substitued benzothiazole is a hole conductor, the light-to-electrical conversion is realized by the cooperation for these two components.

II EXPERIMENTAL

Reagent-grade chemicals were used without further purification. The substrates and solvents were used as received. All the melting points are taken in open capillary and uncorrected. The purity of synthesized compounds was checked by Thin Layer Chromatography studies. I.R. spectra were measured on FT-IR Perkin-Elmer (spectrum RX1) spectrophotometer ($\bar{\nu}$ in cm^{-1}) using KBr disc. ^1H NMR were recorded in CDCl_3 and DMSO with Tetramethylsilane (T.M.S.) as the internal standard at 300 MHz on a Bruker DRX-300 spectrophotometer. The chemical shifts are reported as parts per million (ppm). The organic solar cells presented here were prepared by thin-film based technologies. The films in this work have been prepared mainly by spin-coating. The spin-coating method is probably the easiest and fastest for thin film preparation^[22-24] This procedure is typically used to apply thin films on flat substrates. A typical process involves depositing a small puddle of a solution of the desired compound or a mixture of compounds onto the center of a substrate and then spinning the substrate at high speed, generally under controlled atmosphere. Centripetal acceleration will cause the solution to spread to, and eventually off the edge of the substrate, leaving a thin film of the desired compound or mixture on the surface. One of the most important factors in spin-coating is its repeatability.

In the present study, TiO_2 layer and 2- benzylidenoimino - 6-substituted benzothiazoles bulk have been deposited by spin-coating, when used as the main photoactive layer in photovoltaic devices.

2.1 Synthesis of 2 –benzylidenoimino- 6-substituted benzothiazoles

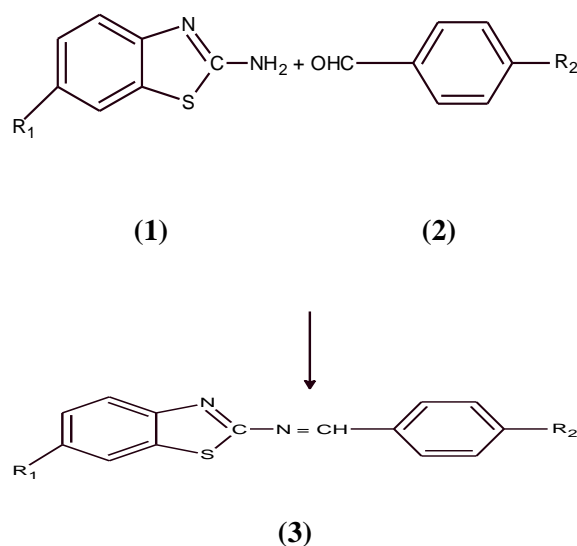
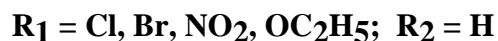


Figure 1

In the present investigation substituted 2- amino benzothiazoles were synthesised by thiocyanogenation of substituted anilines^[25]. To a solution of 2-amino-6-substituted benzothiazole (0.01 mol) (2) in 25 ml of freshly distilled ethanol, 0.01 mol of aromatic aldehyde (3) was added at room temperature, and the reaction mixture was thoroughly mixed to confirm

homogeneity of reaction mixture. The reaction mixture was refluxed on a heating mantle for 4 hours. After cooling residual solvent was evaporated under reduced pressure, during evaporation a solid mass 2-benzylidenoimino-6-substituted benzothiazole derivatives (3) were obtained. Products were recrystallized from ethanol/hexane mixture to give pure (3). (Figure 1)



In the present investigation synthesized 2-benzylidenoimino-6-substituted benzothiazoles were:

- 3a. 2-(benzylidenoimino)-6-chlorobenzothiazole
- 3b. 2-(benzylidenoimino)-6-bromobenzothiazole
- 3c. 2-(benzylidenoimino)-6-nitrobenzothiazole
- 3d. 2-(benzylidenoimino)-6-ethoxybenzothiazole

2.2 Structure elucidation

The structure of synthesized compounds were confirmed by their analytical data, Infrared spectral data and ^1H NMR data.

- 3a** $R_1 = \text{Cl}$, $R_2 = \text{H}$, M.F. $\text{C}_{14}\text{H}_9\text{N}_2\text{SCl}$, M.P. 161 °C, Elemental Analysis C=61.05%, H=0.03%, N=10.27%, IR (KBr) ν_{max} in cm^{-1} 859(C-Cl), 1349(C-S), 1597(C=N), 1447, 1535 (ArC=C), ^1H NMR (300MHz, CDCl_3): δ (4.02(s, 1H,=CHPh), 7.10- 7.632 (m, 8H,ArH),
- 3b** $R_1 = \text{Br}$, $R_2 = \text{H}$, M.F. $\text{C}_{14}\text{H}_9\text{N}_2\text{SBr}$, M.P. 190 °C, Elemental Analysis C=52.99%, H=0.02%, N=8.83%, IR(KBr) ν_{max} in cm^{-1} 809 (C-Br), 1376 (C-S), 1598 (C=N), 1460, 1531 (ArC=C), ^1H NMR (300MHz, CDCl_3): δ 4.0 (s, 1H, =CHPh), 7.02-7.52 (m, 8H, ArH),
- 3c** $R_1 = \text{NO}_2$, $R_2 = \text{H}$, M.F. $\text{C}_{14}\text{H}_9\text{N}_3\text{SO}_2$, M.P. 262 °C, Elemental Analysis C=59.36%, H=0.03%, N=14.84%, IR (KBr) ν_{max} in cm^{-1} 1380, 1510 ($-\text{NO}_2$), 1597 (C=N), 1346 (C-S), 1436, 1490, 1539 (ArC=C), ^1H NMR (300MHz, CDCl_3): δ 5.6 (s, 1H, =CHPh), 7.02-7.90 (m, 8H, ArH),
- 3d** $R_1 = \text{OC}_2\text{H}_5$, $R_2 = \text{H}$, M.F. $\text{C}_{16}\text{H}_{14}\text{N}_2\text{SO}$, M.P. 120 °C, Elemental Analysis C=68.08%, H=0.04%, N=9.92%, IR(KBr) ν_{max} in cm^{-1} 1058 (C-O-Csym.), 1209 (C-O-Casym.), 1457, 1545 (ArC=C), 1596 (C=N), 2974 (C-Hstr.), ^1H NMR (300MHz, CDCl_3): δ 1.45 (t, 3H, CH_3), 4.0 (q, 2H, OCH_2), 5.4 (s, 1H, =CHPh), 7.25-7.55 (ArH)

2.3 Photocurrent measurement

After the photovoltaic samples were prepared, their current-voltage (J - V) characteristics were measured under dark and white-light illumination. By recording the J - V curves of illuminated solar cell, it is possible to determine the maximum power output, and thus the power conversion efficiency. Most of the photovoltaic parameters can be directly derived from the J - V characteristics, like short circuit current (J_{sc}), open circuit voltage (J_{oc}), calculated fill factor (FF), and power conversion efficiency. J_{sc} is the current, which flows with zero internal resistance (at $V = 0$, when no bias voltage is applied). U_{oc} is the voltage in the open-circuit conditions, i.e. when no current flows through the cell. The power

conversion efficiency of the device (η) can be calculated from the defined parameters. is the ratio of the generated power to the incident optical power (P_0). In the end, (η) is the most important parameter of any given solar cell. Hence, (η) can be expressed as following expression⁽²²⁻²⁴⁾:

$$\eta = \frac{P_{\max}}{P_0} = \frac{FF \cdot J_{sc} \cdot U_{oc}}{P_0}$$

FF is the maximum power that can be withdrawn from the device (P_{\max}) and theoretical power:

$$FF = \frac{P_{\max}}{J_{sc} \cdot U_{oc}} = \frac{J_{\max} \cdot U_{\max}}{J_{sc} \cdot U_{oc}}$$

FF is directly related to the series and shunt resistance of the solar cell. Higher FF is desirable and corresponds to a more "square-like" shape of the J - V curve. Following Figure shows the schematic diagram of J - V curves of an ideal photovoltaic device both in the dark and in a white-light illumination. In the dark, the solar cell photocurrent passing through the cell until the voltage is high enough or in other words the cell behaves like a diode. When the solar cell is illuminated, the J - V curve shifts downwards by the amount of photocurrent generated. The power (P) produced by the cell can be calculated along the J - V sweep by the equation $P = JU$. The power is zero at the J_{sc} and U_{oc} points, and the maximum power (P_{\max}) between the two points (shaded square in Figure 2).

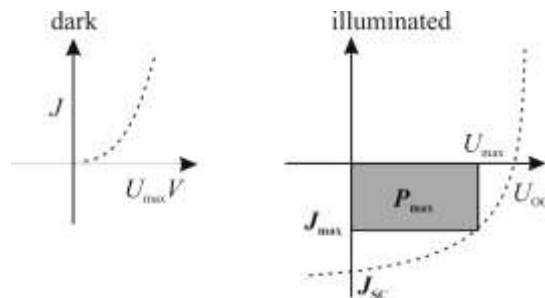


Fig. 2 Current-voltage (J - V) characteristics of an ideal solar cell both in the dark (left) and under illumination (right).

In this work, the J - V curves were recorded in the dark and under ANI 1.5 sunlight illumination. All the measurements were carried out in an open air at room temperature.

III RESULTS AND DISCUSSION

The synthesis of heterocyclic compounds and fabricating on inorganic base Titania open the new pathway for enhanced efficiency of photovoltaic cells. Doping quantum wells of other inorganic materials in hybrid solar cell may enhance the photovoltaic performance of the cell.

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