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Fabrication and Characterization of CH3NH3PbBr3-based Planar Heterojunction Photovoltaic Devices

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Abstract: Hybrid halide perovskites, represented by the formula CH3NH3PbX3 (where X = F, Cl, Br, or I), offer a promising avenue for optoelectronic device development. This study presents the fabrication of a perovskite heterojunction device using a cost-effective spin casting process, with the design FTO/PEDOT: PSS/CH3NH3PbBr3/PC61BM/Au. The device's electrical characterization, utilizing current-voltage and impedance measurements, demonstrates low leakage current attributed to the blocking effect of the PEDOT: PSS and PC61BM layers. An energy level diagram elucidates the device's photocurrent generation process, highlighting the roles of the electron transport layer (ETL) and hole transport layer (HTL). In both low and bright light conditions, the device exhibits distinct ideality factors. The study employs various spectroscopic and microscopic techniques to characterize thin films of methylammonium lead bromide, revealing optical properties and surface morphology. Through analysis of photoluminescence and I-V characteristics, the study explores carrier dynamics and device performance, presenting insights into material stability and charge transport mechanisms. The research aims to advance CH3NH3PbBr3-based technologies, particularly in high-performance photodetectors and solar cells.

Keywords: Hybrid halide perovskites, heterojunction device, photovoltaic, charge transport, perovskite solar cells, optoelectronics.

Introduction

Solar cell technology is rapidly evolving to harness sunlight as a renewable energy source to meet the growing global demand for electricity. Among the materials showing promise for solar cell applications are hybrid halide perovskites, known for their exceptional properties. Despite their potential, challenges such as sensitivity to environmental factors like humidity and temperature, as well as issues with material degradation and hysteresis, have hindered the commercialization of perovskite devices. Nonetheless, recent advancements in organo-metal tri-halide perovskites have propelled them to the forefront of solar cell research due to their high efficiency. Notably, in 2018, the most efficient perovskite solar cell achieved an efficiency of 23.3%. Combining perovskites with silicon technology has emerged as a leading strategy, with the aim of achieving efficiencies as high as 30% in the near future [1-4].

Among the various perovskite compositions, chromium bromide perovskites stand out for their larger voltage potential and higher band gap, making them attractive candidates for next-generation solar cells. In particular, CH3NH3PbBr3 has garnered attention for its stability and comparable power conversion efficiency within the photovoltaic community. Planar heterojunction devices, characterized by either mesoporous or planar structures, have gained prominence due to their minimal hysteresis in current-voltage characteristics and lower processing temperature requirements [5].

This study focuses on the fabrication and characterization of a planar heterojunction device comprising FTO/PEDOT: PSS/CH3NH3PbBr3/PC61BM/Au, with perovskite serving as the active layer, PEDOT: PSS as the hole transport material, PC61BM as the electron transport material, and aluminum as the top electrode [6-8]. The device fabrication involves a one-step spin-coating process, and the results demonstrate the potential of Raman spectroscopy in detecting compositional and structural changes at a microscopic level, complementing photoluminescence investigations.

Through a series of spectroscopic, microscopic, and electrical characterization techniques, this research aims to elucidate the optical properties, charge transport mechanisms, and device performance of CH3NH3PbBr3-based heterojunction devices [9]. By addressing key challenges and advancing our understanding of perovskite-based technologies, this study contributes to the ongoing development of high-performance photodetectors and solar cells [10].

Experimental Method

The synthesis of methylammonium bromide (MABr, CH3NH3Br) involved combining methylamine (30 ml, 33 wt% in absolute ethanol) and hydrobromic acid (24 ml, 48 wt% in water) at 0°C for 2 hours in an ice bath with magnetic stirring [11]. The resulting white crystalline solid was obtained by evaporating the solution at 60°C for 45 minutes after stirring, followed by three washes with diethyl ether and vacuum oven drying at

60°C overnight [12].To create CH3NH3PbBr3, MABr and PbBr2 were mixed in a 3:1 molar ratio in 2 ml of DMF and stirred at room temperature [13].

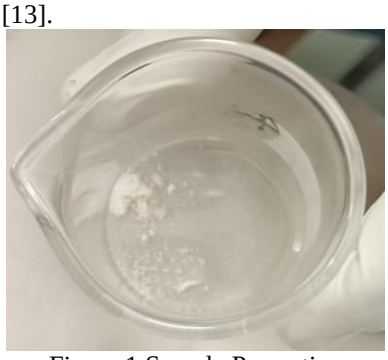

Figure 1 Sample Prepration

The fabrication of the heterojunction device (FTO/PEDOT: PSS/CH3NH3PbBr3/PC61BM/Au) commenced with thorough rinsing of the glass substrate with FTO coating using an ultrasonic bath sonicator [14]. Subsequently, the cleaned FTO was spin-coated with a PEDOT:PSS polymer hole transport layer (HTL) and left at room temperature. A perovskite active layer (CH3NH3PbBr3) was then deposited over the PEDOT: PSS layer and heated to 110°C for 2 minutes. Following this, an electron transport layer (ETL) consisting of PC61BM was deposited on top of the perovskite layer, and the device was left at room temperature in a glove compartment for four hours for preparation. Finally, the top electrode of the finished device was deposited via thermal evaporation of Au [15].

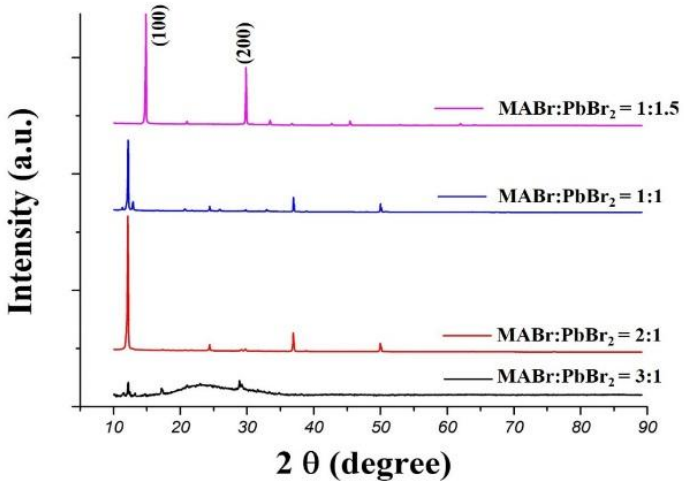

Figure 2 XRD of CH3NH3PbBr3 in different concentration ratio

Characterization of thin films of methylammonium lead bromide (CH3NH3PbBr3) involved X-ray diffractionmeter of Analytical Technologies [16]. The optical absorption spectra of the perovskite thin films were measured using a UV-VISLabtronics and using COXEM for SEM. Photoluminescence spectrometry was utilized to retrieve PL parameters. The I-V characteristics of the photovoltaic device under illumination were tested using a manual probe station (LA-100 DC, Semiprobe USA) and a Keithley source meter 2612 [18]. Electrochemical impedance spectroscopy (EIS) was conducted using an electrochemical workstation (Autolab PGSTAT30), and the eisanalyser program was employed for data analysis [19-22].

Results and Discussion

The study focuses on the fabrication of a transparent device using a thin film of CH3NH3PbBr3 nanoparticles, which cover nearly the entire surface area without visible agglomerations or pinholes [23]. The thin film allows the device to become transparent to visible light, and the UV-Vis absorption spectra reveal three distinct peaks at 300 nm, 430 nm, and 615 nm [24]. The material's degradation causes the first peak (300 nm) to appear. Absorption begins at approximately 650 nm in the red portion of the visible spectrum and reaches saturation at about 400 nm in the violet portion. The absorption of the material in the spectra region can be attributed to the temperature of MABr during synthesis, which occurs just below the energy gap [25].

$$\alpha_E = A\left(E - E_g\right)^{\frac{1}{2}}$$

The lead bromide-based perovskite layer is placed on top of the glass/FTO substrate, sandwiched between the p-type hole transport layer PEDOT: PSS and the n-type electron transport layer PC61BM. The top electrode, made of aluminum, serves as the cathode and collects the electrons. Surface morphology analysis using FESEM images shows the highly resolved vibrational modes of spin-coated MAPbBr3 onto glass-slide. Raman spectra show two distinct peaks within the 190–1410 cm−1 area, with two distinct peaks at 550 and 1105 cm−1 and two less intense peaks at 670 and 1190 cm−1. The spectrum is red-shifted, reaching its peak at 559 nm and pointing towards the blue end of the spectrum [26].

The intensity of the photoluminescence (PL) spectrum at the interface between the perovskite and PC61BM/PEDOT: PSS films, as well as the lifespan of free charge carriers in the active layer (perovskite), are directly correlated [27]. The lifespan of an exciton (charge carrier) is being extended by the greater intensity of the PL spectrum. Improving perovskite's performance is mostly dependent on temperature, and the stability of the material is a major concern due to the lead content, which causes it to decay rapidly when exposed to air [28].

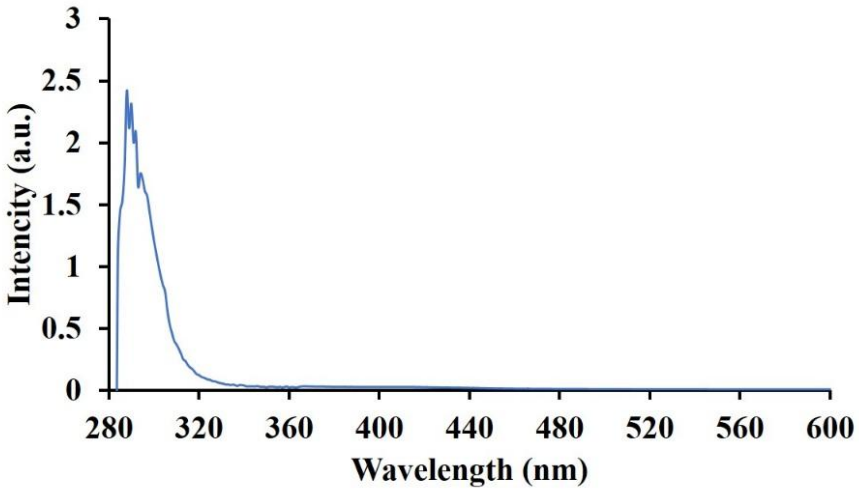

Figure 2 Absorption of perovskite sample

The planar heterojunction device was tested using I-V measurements in both dark and light environments. The device showed a nearly nonexistent leakage current, indicating typical diode behavior. The energy band diagram under forward applied voltage showed that the positive and negative terminals of the semiconductor are connected to FTO and Al, respectively. Under reverse bias conditions, PC61BM and PEDOT: PSS successfully block carriers, improving the dark I-V characteristics and reducing leakage current. The device's photocurrent is generated when charge carriers, including free electrons and holes, make their way to the Al and FTO electrodes via the associated charge transport layers. As an ETL (HTL), PCBM(PEDOTS:PSS) effectively removes photo generated holes from the perovskite layer at the interface between the two materials, reducing the likelihood of recombination and enhancing the device's photocurrent. The ideality factor (n) and reverse saturation current (Is) were calculated using the Mott Gurney Law,

$$J = \frac{9}{8}\mu_n \varepsilon_0 \varepsilon_r \frac{V^2}{L^3}$$

With the estimated value of (Is) in darkness being 1.604×10-5 A and 1.79 in illumination. The device's dark I-V characteristics were also examined using the Mott Gurney Law. The impedance spectra (IS) were examined between 100 Hz and 1 MHz, and simulation results were used to evaluate the impedance parameters.

$$\tau_n = R_P \times C_P$$

The series resistance (R1) and shunt resistance (R2) were analyzed to simulate the effects of defective capacitance. A dark I-V curve and high R2 indicate less leakage current, possibly due to charge injection blockage by HTL and ETL under reverse bias conditions [29].

Conclusions

Thin films made of the CH3NH3PbBr3 perovskite material have had their optical light response and transport characteristics investigated. You can use these nanoparticles as an active layer material in a heterojunction device after they were chemically produced. According to spectrophotometric measurements, the

optical band gap (Eg) is around 2.3 eV. At room temperature, the device's I-V curve shows a very little leakage current. We have obtained the device's ideality factor and reverse saturation current from the semi-logarithmic I-V curve. The SCLC model was used to determine the carrier mobility, which was determined to be 1.6×10-3cm2v-1s-1. By examining the IS results, we were able to obtain the device's intrinsic circuit parameters. We anticipate that our research will contribute to the advancement of CH3NH3PbBr3 based technologies, particularly high-performance photodetectors and solar cells.

Acknowledgement

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Conflict of Interest Statement

The authors conducted ethical and transparent research, demonstrating the importance of ethical practices in scientific research.

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