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Electrical properties of a perovskite solar cell with a novel structure of Cesium lead bromide with MXene and multi-well carbon nanotubes

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Abstract

The electrical characteristics of a perovskite solar cell made of multi-walled carbon nanotubes (MWCNTs), cesium lead bromide (CsPbBr₃QD), and MXene show promise for enhancing photovoltaic performance. Both MXene and MWCNTs enhance charge collection and reduce recombination by serving as electron transport layers (ETLs) and/or hole transport layers (HTLs). With its long carrier diffusion lengths, high absorption coefficient, and advantageous bandgap, CsPbBr₃QD functions as a light absorber and helps achieve a 3.5% power conversion efficiency. The power efficiency achieved surpasses that of CsPbBr₃QD either alone or in conjunction with MXene.

Keywords: CsPbBr₃ QD, MXene, MWCNTs, ETLs, HTLs, and PCEs

1. Introduction

Creation of photovoltaic technology of the future. Due to their remarkable optoelectronic properties, inexpensive manufacturing methods, and rapidly increasing power conversion efficiencies (PCEs), perovskite solar cells (PSCs) have garnered considerable attention [1, 2]. Because they are more resistant to heat and moisture than their hybrid organic-inorganic cousins, all-inorganic perovskites, including cesium lead bromide (CsPbBr₃), have shown great promise for long-term device stability [3, 4]. CsPbBr₃ perovskites are ideal for tandem solar cells, light-emitting devices, and photodetectors because of their broad bandgap (~2.3 eV), excellent photoluminescence quantum yield, and effective charge carrier mobility [5, 6]. Notwithstanding these benefits, problems including inadequate charge transport and recombination losses in the active layer continue to restrict the performance of CsPbBr₃-based solar cells [7]. Researchers have looked into adding sophisticated nanomaterials with specialised electrical characteristics to the perovskite matrix to overcome these difficulties. Perovskite quantum dots can be hybridized with two-dimensional transition metal carbides and nitrides, or MXenes, which provide superior mechanical strength, adjustable surface functionality, and high electrical conductivity [8]. This is a promising approach. MXenes, like Ti₃C₂T_x, may efficiently inhibit interface recombination and enable charge extraction, improving the overall stability and efficiency of the device [9]. In parallel, because of their enormous surface area and one-dimensional conductive pathways, multi-walled carbon nanotubes (MWCNTs) have also shown promise as effective materials for electron or hole transport [10]. The limitations of individual components may be overcome by combining MWCNTs with perovskite and MXene structures to form a ternary nanocomposite with synergistic benefits. Effective charge transport across interfaces, improved charge carrier separation, and decreased series resistance are all possible with the integrated architecture [11]. The purpose of this work is to examine the electrical properties of a new CsPbBr₃-based perovskite solar cell that combines MWCNTs with MXene nanosheets. Through an analysis of this ternary composite's carrier dynamics, impedance response, and current voltage behavior, the study aims to clarify the reasons behind the enhanced performance and offer guidance for the sensible design of stable, high-efficiency perovskite solar cells. If these nanostructured materials are successfully integrated, it might lead to the development of long-lasting and scalable solar systems that can be used in practical settings.

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2. Materials and Methods

2.1 Synthesis of CsPbBr₃ QDs

At room temperature (24 °C), in an ambient environment, the CsPbBr₃ QDs were created [12]. To be more precise, the Cs⁺ precursor was made by dissolving 2.35 g of Aladin's 99% Cs₂CO₃ powder in 4 mL of 99.5% propionic acid, and the Pb²⁺ precursor, 1.835 g of Aladin's 99% PbBr₂ powder, in 10 mL of a mixture of butylamine (99.5%), 2-propanol (99.5%), and propionic acid (1:1:1). Next, 100 µL of the Cs⁺ precursor was quickly added to the combination of 2 propanol (20 mL) and hexane (40 mL), along with the Pb²⁺ precursor (1080 µL), while being aggressively stirred for 5 s. Two centrifugation processes at 1500 and 3000 r/min produced high-quality CsPbBr₃ QDs, which were then dispersed in toluene.

2.2 Synthesis of Ti₃C₂TX nanosheets

The improved least intensive layer delamination (MILD) technique was used to create MXene (Ti₃C₂TX) nanosheets [13]. To put it briefly, 40 mL of HCl (9 mol/L) was mixed with 2 g of lithium fluoride (LiF, 99.9%, Aladdin) and 2 g of Ti₃AlC₂ powders (Forsman Scientific Co., Ltd.) while being stirred for 24 hours at room temperature. Following etching, accordion-like multilayer MXenes powders were repeatedly cleaned with deionized water until the pH reached >6.

Following centrifugation, 1 g of black sediment was mixed with 280 mL of DI water and 20 mL of dimethyl sulfoxide solution (DMSO, 99.5%) to create an intercalation solution, which was stirred for 24 hours. After three rounds of washing with deionized water to get rid of any remaining DMSO, the resultant multiple layered MXenes were subjected to sonication for 300 minutes in DI water while under argon gas. Following a 15-minute centrifugation at 8000 rpm, the Ti₃C₂TX nano-sheets were ultimately produced by an overnight vacuum drying procedure at 60 °C.

2.3 Compound manufacturing CsPbBr₃ QD /MXene

Using ethanol as the solvent, CsPbBr₃ crystals and an MXene-based substance were combined to create the composite at a concentration of 0.05 mg/mL. To guarantee uniform dispersion, the mixture was agitated with a magnetic stirrer at ambient temperature (about 25°C). For a suitable amount of time (usually 30 to 60 minutes), the stirring operation was continued in order to promote even dispersion of MXene particles inside the CsPbBr₃ matrix. It is anticipated that this process would improve the components' physical or chemical interactions and the final composite's qualities for possible use in electrical or optoelectronic devices [14]. As in Show Fig 1.1.

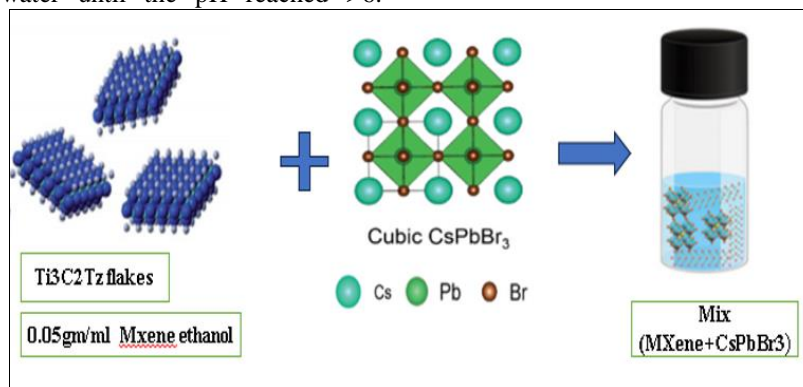


Fig (1.1): Compound manufacturing CsPbBr₃/MXene

2.4 Synthesis of a compound from mixing CsPbBr₃ QD /MXene and MWCNTs

Using ethanol as an organic solvent, 0.01 grams of carbon nanotubes (MWCNTs) and 1 gram of CsPbBr₃/MXene were combined to create a nanocomposite. To guarantee even dispersion and encourage efficient interaction between the nanomaterials, the mixture was sonicated for 30 minutes. This

process produces a well-integrated nanocomposite by promoting improved surface contact and uniform component distribution. Because of the elements' synergistic effects, it is anticipated that the addition of CNTs to the CsPbBr₃/MXene matrix will enhance the final material's electrical and physical characteristics. As shown in the numbered Fig. (1.2)

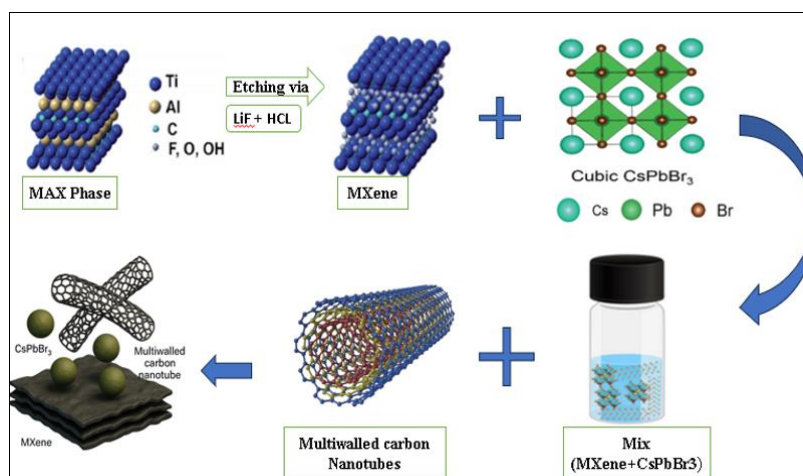


Fig (1.2): Mixing CsPbBr₃ QD /MXene and MWCNTs

2.5 Thin film preparation of ZrO₂/Graphene Nanocomposite (HEL): ZrO₂/G NC was made by mixing 0.25 g of G and 20 g of ZrO₂ in 60 ml of distilled water, ultrasonically agitating the mixture for 4 hours, and then placing the suspension in a 100 ml Teflon-lined stainless-steel autoclave. The autoclave was then maintained for ten hours at a precise temperature of 140°C. The black product was repeatedly washed with distilled water after it had cooled to room temperature. ZrO₂/G was then separated.

2.6 Thin film preparation of TiO₂/G (ETL)

Using the doctor blade approach, a paste made of TiO₂/G nanoparticles was created and evenly distributed across an FTO substrate to produce uniform films with nanostructures. Remarkably, 0.02 g of graphene was combined with 1 g of TiO₂ in 4 ml of ethanol, followed by 50 ml of deionized water. The mixture was then cooked using a hydrothermal process for 72 hours at 160°C in an autoclave device. The autoclave was allowed to cool to room temperature once the reaction was finished.

To create the nanocomposite TiO₂/G powder, the resultant precipitate was filtered, repeatedly cleaned with distilled water and ethanol, and then dried at 40°C for an entire night. 0.5g of TiO₂/G nanocomposite was combined with 4ml of ethanol to make the TiO₂/G paste. A magnetic stirrer was then used to mix the solution with 0.25g of ethyl cellulose and 0.1 ml of citric acid for 36 hours at room temperature. TiO₂/G film is made using the doctor blade approach, which involves dripping a droplet of solution onto the sample and letting it cure at room temperature. Following drying, these as-fabricated TiO₂/G films ETL are annealed at 450°C to increase adhesion between the film and FTO.

2.7 Counter Electrode Preparation

The TEV method is used to produce the counter electrode

(CE). With a CE film surface area of 2cm², copper is deposited on a high-density zirconium/copper oxide (ZrO₂/G HTL) layer by placing the strips 9 cm from a tungsten vessel into which copper oxide is evaporated under a pressure of 10-5 Torr.

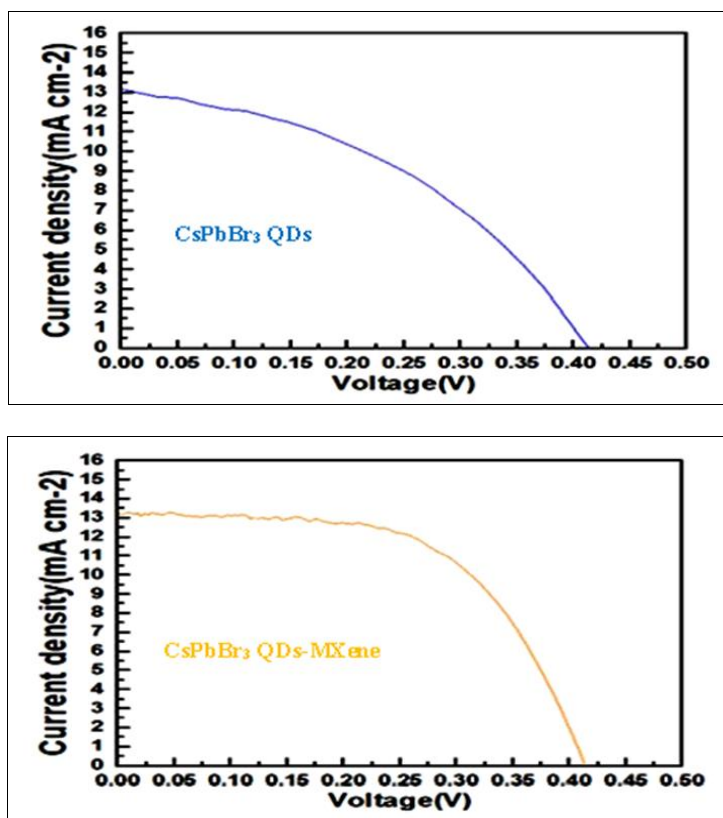
3 Results and Discussion

3.1 (I-V) Characteristics of Solar Cell

For solar cells, measuring the current-voltage under illumination circumstances is crucial since it allows one to ascertain the cell's characteristics and, consequently, its efficiency. The short-circuit current value (J_{sc}) was set at ($R \rightarrow \text{Zero}$, so that $V=0$), and the open-circuit voltage (V_{oc}) was set at ($I = 0$) (as with an infinite load resistance). The power output value is obtained by multiplying the open circuit voltage by the short circuit current ($P_{Out} = V_{oc} \cdot J_{sc}$)

3.2 Current-Voltage (I-V) calculations for PSC devices

Current-voltage (I-V) measurements were performed to determine the electrical behaviour and efficiency of the solar cell. The current-voltage curves of the solar cell were used to calculate the open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), and fill factor (FF). The cell efficiency (PCE) of each solar cell was determined. Assuming that the conduction band edge of the quantum dots lies between the perovskite conduction edge and the occupied molecular orbital from the top of the carrier transition layer, charge carrier mobility is enhanced, which increases the fill factor value and, consequently, the conversion efficiency of the solar cell. The prepared PSCs have efficiencies of 2.3%, 3.22% and 3.5% for (FTO /TiO₂-G/CsPbBr₃QD /ZrO₂-G/Cu), (FTO /TiO₂-G/CsPbBr₃QD-MXene/ZrO₂-G/Cu) and (FTO /TiO₂-G/CsPbBr₃QD-MXene-MWCNTs/ZrO₂-G/Cu), respectively, as shown in Fig. 3.1 and Table 3.1.



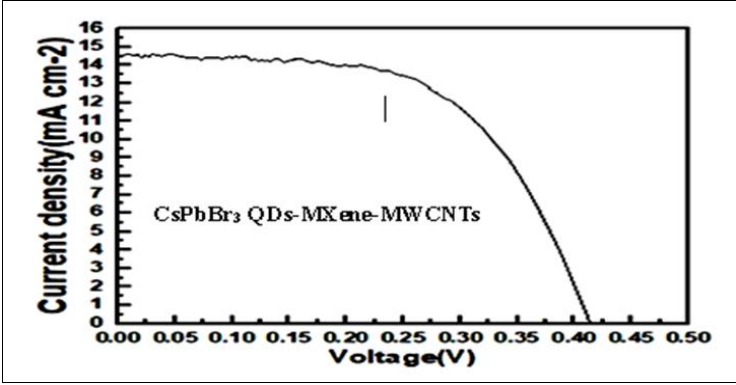


Fig 3.1: I-V measurements of three solar configuration CsPbBr₃ QDs, CsPbBr₃ QDs /MXene and CsPbBr₃ QDs /MXene - MWCNTs

Table 3.1: Photovoltaic Parameters of PSCs for all Configurations.

Solar Cells (Configurations)	Jsc (mA/cm ²)	Voc (V)	FF	PCE (%)
FTO /TiO ₂ -G/CsPbBr ₃ QD /ZrO ₂ -G/Cu	13	0.42	0.42	2.3
FTO \TiO ₂ -G\CsPbBr ₃ QD-MXene\ZrO ₂ -G\Cu	13.1	0.41	0.6	3.22
FTO \TiO ₂ -G\CsPbBr ₃ QD-MXene-MWCNTs \ZrO ₂ -G\Cu	14.5	0.42	0.58	3.5

Cell 3 (CsPbBr₃ QDs + MXene + MWCNTs - 3.5% efficiency) by adding carbon nanotubes (MWCNTs) to the mixture, an additional increase in efficiency was observed, attributed to: Further improvement in electrical conductivity: MWCNTs provide a three-dimensional network that helps accelerate charge movement across the active layer. Increased Effective Surface Area: MWCNTs create additional charge transport pathways, increasing photocurrent collection. Strengthened Active Layer Structure: The composite structure of quantum dots, MXene, and MWCNTs creates a more cohesive and conductive layer. Improved Light Absorption: MWCNTs contribute to broader light absorption and improved charge conversion efficiency.

4.1 Conclusions

The obtained results showed that the effect of adding multi-walled carbon nanotubes (MWCNTs) to the CsPbBr₃ QD-MXene perovskite layer led to an improvement in efficiency by 3.5%, as well as an improvement in electrical conductivity, which became higher compared to the formulations containing MXene, as well as better extraction and transport of charges, and also an improvement in the shape of the perovskite layer.

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