Applications Of Graphene in Perovskite Solar Cells

Chi Zhang *

Department of Physics, Huazhong University of Science and Technology, Wuhan, China

* Corresponding Author Email: u202210173@hust. edu. cn

Abstract. Solar energy is a clean energy source with abundant reserves. Solar cells, which can convert solar energy into electricity, have become a research hotspot. Perovskite solar cell is a type of solar cell that is environmental-friendly and high security. It exhibits high theoretical output potential. People pay much attention to improve the efficiency of perovskite solar cells. As a result, it has garnered significant attention and investment in recent years. Doping nanomaterials with excellent performance are an effective means for modifying perovskite solar cells. Graphene, as a nanomaterial, can enhance the stability and photovoltaic efficiency of perovskite solar cell systems. Therefore, using graphene to modify perovskite solar cells has become a current research hotspot. In this work, the structure, properties, and application of graphene materials in perovskite solar cells are discussed. Perovskite solar cells modified by passivating perovskite solar cells with graphene is highlighted. In addition, graphene oxide combined with TiO_2 is discussed as a way to improve the performance of solar cells. This work helps to inspire new ideas for the modification of perovskite solar cells.

Keywords: Graphene; perovskite solar cells; graphene oxide.

1. Introduction

With the increasing attention to environmental issues, the utilization of renewable energy has become particularly important. There exist various types of renewable energy sources, including solar power, hydroelectric power, wind power, hydrogen energy, and so on. Among the different kinds of renewable energy, solar energy stands out among renewable sources as it is clean, abundant, and environmental-friendly. Additionally, photovoltaic technology directly converts sunlight into electricity, making it an efficient method for energy utilizing. This approach exhibits numerous advantages. As a result, it has garnered significant attention and investment in recent years.

The perovskite solar cells (PSCs) are comparable to traditional solar cells. At present, solar cells based on Si single crystals occupy most of the market for many reasons including excellent stability of the silicon and the complete production technology. PSCs have developed rapidly in recent years. The energy conversion capacity of Si solar cell has reached 26%. This is close to the ultimate efficiency (~29.4%) [1]. PSCs still face numerous challenges. Therefore, it takes scientists a lot of work to overcome these issues. In fact, it is thought that using graphene materials as interfacial elements in PSCs is a potential strategy. Graphene can function as effective layers for electron transport in PSCs. This lowers recombination losses and enhances charge collection overall. Graphene oxide (GO) can be used as hole transport layers in PSCs [2]. These substances encourage charge carrier transit towards the electrode and enable effective hole extraction from the perovskite layer. This lowers charge recombination and improves device performance overall. Graphene is a perfect option to be added to PSCs for improvement of light absorption due to its strong electrical conductivity and exceptionally low optical reflection. Higher power conversion efficiencies can be achieved by improving light absorption and trapping with graphene. Graphene-based materials possess unique characteristics, including ambipolar charge mobilities, significant specific surface area, and exceptional thermal conductivity, rendering them well-suited for augmenting both the stability and photovoltaic efficiency of PSCs. Consequently, one of the main areas of current research and development for perovskite solar cell optimization is the introduction of graphene to the cell.

In this study, two applications of graphene batteries in perovskite batteries are reviewed. One notable application in the realm of PSCs involves utilizing graphene for passivation, with a primary focus on assessing its impact on power conversion efficiency (PCE). Extensive investigations have

been conducted to examine how these graphene-based materials influence the nanostructures of both the electron transport layer (ETL) and hole transport layer (HTL), as well as the alterations they induce in the perovskite layer [2]. Another application is to oxidize graphene to make graphene oxide and prepare titanium dioxide-graphene oxide nanofiber (TiO_2/GO NF) composites by using electrospinning method [3].

2. Passivation of Graphene in PSCs

To address the issue of interfacial charge carrier recombination in PSCs, the application of graphene for surface modification has demonstrated significant potential and effectiveness [4]. Graphene, with its exceptional electrical, mechanical, and optical properties, offers a range of advantages for reducing interfacial recombination and improving PSC performance. This approach allows for voltage control without compromising the short-circuit current (J_{sc}) and fill factor (FF) of the PSCs. Graphene serves as a passivation layer, improving the electrical properties of PSCs and enhancing their overall performance. Specifically, the incorporation of functionalized graphene has demonstrated significant enhancement in the extraction of holes, thereby resulting in a substantial improvement in the open-circuit voltage (V_{oc}) of PSCs [5].

Using modeling tools is essential when conducting experiments to examine how different elements like the ETL, HTL, absorber layer doping concentration, and interface defect density impact the performance of PSCs. The SCAPS-1D modeling tool is widely utilized for this purpose [6]. SCAPS-1D is a simulation software tailored for in-depth analysis of solar cells, leveraging principles from the Poisson equation and semiconductor equations for electrons and holes. Researchers utilize it to conduct detailed simulations, probing the influence of device design and material properties on solar cell performance. With SCAPS-1D, they can explore and optimize various parameters affecting the efficiency and characteristics of PSCs [5]. This tool empowers researchers to investigate the impact of different factors such as ETLs, HTLs, absorber layer doping concentration, and interface defect density on solar cell performance. By employing SCAPS-1D, researchers gain valuable insights into the underlying physics and mechanisms governing PSCs. Furthermore, SCAPS-1D facilitates the design and optimization of device architectures, material selection, and process parameters to enhance PSC performance and efficiency. It enables comprehensive evaluations of diverse factors influencing solar cell efficiency and behavior, aiding researchers in advancing the development and understanding of perovskite solar cell technology.

By utilizing SCAPS-1D, researchers and engineers can study and optimize different aspects of solar cell design, such as layer thicknesses, material properties, composition, and architecture, to enhance the performance and efficiency of the devices. The software provides valuable insights into the relationship between the electrical characteristics of devices, enabling informed decision-making in solar cell research and development.

The experiment is structured into two control groups: one utilizing graphene-passivated PSCs, and the other employing graphene-free PCS. Experimental data is observed and recorded under identical light conditions. J-V curves are plotted for both groups, and PCE, FF, J_{sc}, and V_{oc} values of PCS in both groups are measured and computed [5]. By comparing the PCE, FF, Jsc, and Voc values between the two experimental groups and analyzing the J-V curves, conclusions can be made regarding the mitigation of defect states at the interface through passivation. Specifically, the efficiency of PCS is enhanced through graphene passivation. Passivation of perovskite layers effectively reduces recombination losses and prolongs carrier lifetimes, as opposed to unpassivated perovskite films.

Indeed, the studies conducted by Li et al. and Eli Danladi, both utilizing graphene passivation in PSCs, offer compelling evidence supporting the notion that graphene passivation enhances the efficiency of perovskite cells. Li et al. employed graphene passivation in PSCs fabricated with methylammonium lead triiodide ($MAPbI_{3-x}Cl_3$), while Eli Danladi utilized graphene passivation in PSCs made of methylammonium lead triiodide ($MAPbI_3$) [5,7].

It can be conclusively inferred that graphene passivation significantly enhances the efficiency of PSCs, regardless of minor variations in the perovskite composition.

3. Graphene Oxide Modified TiO_2

In conventional PSCs, titanium dioxide (TiO_2) serves as the electron transport layer (ETL) [4]. TiO_2 is favored for this role due to its affordability, chemical stability, and ease of fabrication. Within PSCs, it serves as a mediator for hole transport. This facilitation promotes effective movement of charge carriers, thereby significantly enhancing the overall functionality and performance of the solar cell [8].

At present, scientists have made many attempts to improve the stability and efficiency of PSC. One of the most effective methods is to introduce metal oxides into the TiO_2 nanoparticles.

Furthermore, one technique for preparing nanofibers is electrospinning. The advantages of preparing nanomaterials using this technology include a high surface area-to-volume ratio, high pliability, the ability to achieve material thickness ranging from a few microns to nanometers, and enhanced adhesion between the photoanode-electrolyte interface and the photoelectrode/electrolyte interface.

During the sunlight capture process in PSCs, the absorption of sunlight by TiO_2 nanoparticles is indeed pivotal. This underscores the significance of TiO_2 nanoparticles in the anode, as they efficiently absorb sunlight. Additionally, TiO_2 nanoparticles play a crucial role in facilitating the migration of charge carriers generated upon photoexcitation of perovskite molecules. The combination of metals, metal oxides, and carbon-based materials with TiO_2 nanoparticles presents a promising approach to enhancing the energy conversion efficiency of PSCs, particularly at the anode. The inclusion of carbon-based materials notably contributes to improving the power conversion efficiency of PSCs [8,9].

And the method used to prepare TiO_2 nanoparticles,is hydrothermal ,which is one of the best way to obtain pure graphene. The method has several advantages such as being environment-friendly, low energy consumption and low cost [10].

However, using TiO_2 as the electron transport layer has several disadvantages. For example, TiO_2 can decompose the light-absorbing material under ultraviolet light, resulting in rapid deterioration of battery performance. The electron mobility of TiO_2 is much lower than that of perovskite materials, and the transport of photoelectrons after injection into the TiO_2 skeleton is not as good as direct migration in perovskite materials. And also, the surface trap of TiO_2 nanostructure can hinder electron injection and destroy the stability of the device. To solve this disadvantage, graphene oxide was combined with TiO_2 to build a better electron transport layer [10].

Carbon-based materials, including GO, are extensively utilized in the fabrication of photoanodes for solar cells owing to their affordability and notable electrocatalytic prowess. GO offers several advantageous properties that make it suitable for this application. Firstly, GO possesses a high surface area, allowing for increased active sites for light absorption and charge transfer reactions. This property enhances the overall efficiency of the photoanode. Secondly, GO exhibits excellent mechanical strength, which is essential for maintaining the structural integrity of the photoanode during fabrication and operation. This strength helps to prevent deformation or damage to the material. Thirdly, GO has remarkable catalytic action, enabling efficient charge carrier transport and reducing recombination losses. The catalytic activity of GO facilitates the rapid transfer of charges generated by light absorption in the photoanode, thereby increasing the photocurrent and overall device performance. Lastly, the thermal stability of GO is advantageous in the preparation process. GO can withstand high temperatures during fabrication processes such as roasting or annealing without degradation. This thermal stability ensures the integrity and functionality of the composite material during the device fabrication steps. Overall, the combination of high surface area of GO, mechanical strength, catalytic action, and thermal stability makes it an excellent choice for incorporating carbon-

based materials into photoanodes, contributing to enhanced performance and cost-effectiveness in solar cells.

To produce GO using Hummers' method, graphite powder is initially mixed with sulfuric acid in a round-bottomed flask, followed by placement in an ice bath at 0–5°C with continuous stirring for 4 hours. The ice bath is periodically changed every 30 minutes to maintain the desired temperature. Hydrogen peroxide is then added to the solution. For purification, the yellow GO is washed multiple times with a mixture of 10% hydrochloric acid (HCl) and deionized water. This washing step is crucial for removing impurities and enhancing the purity of the GO. Subsequently, the GO suspension is filtered to obtain GO sheets, which are then dried under vacuum conditions at 60°C. This process results in the formation of graphene oxide suitable for various applications. This drying process was repeated daily to ensure that the GO sheets were thoroughly dried and ready for further use or characterization. In order to confirm the complete oxidation of graphite to graphene oxide, infrared spectral analysis was performed. By analyzing the peaks in the infrared spectrum, the graphite can be completely oxidized to graphene oxide [9,10].

The synthesis of GO-TiO_2 NFs (nanofibers) was conducted using a manual electrospinning system. Among various precipitation methods, electrospinning has garnered significant interest due to its capability to produce nanoparticles with high aspect ratios and porosity. Additionally, the electrospinning method offers advantages such as shorter fabrication times, easy regulation of nanomaterials, and eco-friendliness, making it particularly suitable for applications in biomedical engineering.

The electrospinning system consists of two electrodes that connect the injection pump to a rotating drum covered with aluminum foil at a speed of 450 rpm. Initially, 5 mg of GO was dispersed by ultrasonic treatment in 3 ml of absolute ethanol. In the subsequent stage, the dispersed graphene oxide is combined with a 50 ml volume of a yellow TiO_2-PVP ethanol colloidal solution. This blend is then transferred into an injection pump, connected to a positive electrode. Concurrently, a rotating drum is linked to the negative electrode [9]. The injection pump meticulously dispenses the mixture, while an electric field is established between the positive and negative electrodes. This arrangement enables the electrospinning process, wherein the electric field induces the creation of nanofibers from the solution. As a result, PVP-GO-TiO_2 nanofibers are deposited onto a surface, typically covered aluminum foil, as a substrate. Finally, after the deposition process, the nanofibers are separated from the substrate by applying a sharp force. The separated nanofibers are then subjected to a heat treatment process known as roasting. They are heated to a temperature of 400°C and maintained at this temperature for one hour. During this process, any remaining PVP and other organic species are thermally decomposed and burned off, leaving behind GO-TiO_2 nanofibers. The roasting process further enhances the structural and chemical properties of the nanofibers, resulting in the desired final product [11]. The required amounts of ethanol and ethyl cellulose are used to prepare TiO_2 and GO-TiO_2, and for spuncoating. The thickness of the substrate was regulated through ethanol dilution and spin coating. Subsequently, the prepared samples underwent roasting at 550°C for a duration of 1 hour, followed by cooling to room temperature. The edge conduction band and energy gap mapped at the site by ETM indicate that the energy gap of graphene oxide is reduced or decreased, which leads to the transfer of photoexcited electrons from the ETM layer and TiO_2 to graphene oxide. Therefore, PVSC based on GO/TiO_2 nanocomposites should have better collection and charge transfer performance, which can improve the efficiency of PSC.

4. Conclusion

In this study, it was found that PSCs can be optimized by using graphene. The optimization methods discussed in this experiment are divided into two kinds. To passivate PSCs by graphene was discussed firstly.It is shown that the PSC efficiency of graphene passivation is improved. The second way is to oxidize graphene and then use electrostatic spinning technology combined with TiO_2 to make TiO_2/GO. For this method, PCS can easily collect charge, and improve the efficiency of PCS.

Through the analysis of experimental data, it can be clearly known that TiO_2/GO has better collection and charge transfer performance, which can help to improve efficiency of PSCs. Therefore, using graphene to modify PSCs is an effective way to promote their application in the future.

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