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Enhancing dye-sensitized solar cell performance by employing an innovative WSe_2:Zn counter electrode for improved electrocatalytic activity

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Abstract

In this research, we introduced a novel counter electrode (CE) for dye-sensitized solar cells (DSSCs) based on crystalline WSe_2 doped with Zn impurities. The crystalline nature of these CEs was confirmed through X-ray diffraction (XRD) analysis. Additionally, we demonstrated that Zn dopants significantly enhances the electrochemical and electrocatalytic properties of the CEs. These improvements were verified using electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and Tafel analysis with iodine-based electrolytes. Collectively, these enhancements resulted in a remarkable 42% increase in DSSC efficiency, improving it from 5.78% to 8.19% under optimized conditions. Notably, this surpassed the performance of platinum-based CEs, which achieved 7.66% efficiency. The proposed CE holds great promise for advancing DSSCs by elevating their efficiency and reducing fabrication costs.

Introduction

In recent years, the photovoltaic (PV) industry has concentrated its efforts on enhancing the efficiency and long-term stability of PV technologies while striving for cost-effective production [1]. This pursuit has led to the evolution of various types of solar cells. Among these, silicon-based solar cells have emerged as dominant players in the PV market due to their high efficiency and extended operational lifespans [2]. However, silicon-based technologies present challenges associated with purification processes, intricate production procedures, and the need for costly infrastructure. These hurdles have hindered their further progress in achieving greater efficiency and sustainability goals [3].

In contrast, a new generation of solar cell technologies, known as third-generation solar cells, including dye-sensitized solar cells (DSSCs) [4,5], perovskite solar cells (PSCs) [6], organic solar cells (OPVs) [7,8], and quantum dot solar cells (QDSCs) [9], have emerged as promising alternatives. Among these, DSSCs have garnered attention as a viable alternative to silicon solar cells due to their use of low-cost raw materials, a straightforward fabrication process, and a wide range of materials [10,11].

Since their initial introduction by O'Regan and Gratzel in 1991, DSSCs have seen significant advancements, with power conversion efficiency (PCE) exceeding 15%. The DSSC industry has been committed to continuous efficiency improvements through material, layer, and architecture engineering. Typically, a DSSC consists of a sandwich-like structure comprising a photoanode, a sensitizing dye, an electrolyte, and a counter electrode (CE). Commercial DSSCs employ materials such as TiO_2, ruthenium (Ru)-based N719 dye sensitizers, iodide/triiodide (I^-/I_3^-) electrolytes, and platinum (Pt) as the CE [[12], [13], [14]]. Notably, advancements in nanostructured photoanode materials, high-efficiency sensitizers, and robust electrolytes have made DSSCs increasingly competitive among PV technologies [[15], [16], [17]]. In DSSC architecture, the CE's primary functions are to collect and facilitate the flow of charges to and from the external circuit into the liquid electrolyte. Traditional Pt-based CEs, while efficient, face limitations due to their rarity, high cost, and dissolution issues, driving ongoing research into alternative CE materials and designs [18,19].

Transition metal dichalcogenides (TMDs) have emerged as promising materials for cutting-edge PV devices, thanks to their exceptional optoelectronic properties, including superior charge carrier mobility and tunable electronic structures. TMDs consist of transition metals bonded to chalcogen atoms (S, Se, and Te), forming triatomic layers held together by weak van der Waals interactions. Their high surface-to-volume ratio, cost-effectiveness, and environmental friendliness make them attractive for PV applications [20,21]. Among TMDs, tungsten diselenide (WSe_2) has gained prominence as a CE material in DSSCs due to its high abundance, d-electron-rich characteristics, polarizability, electrochemical stability, and efficient electrocatalytic activity for I_3^- reduction. However, the full potential of WSe_2-based materials in DSSC applications remains largely untapped, necessitating advanced research.

One approach to enhance DSSC performance is through alloying Pt with other materials or replacing Pt with Pt-free alternatives. Various Pt-free CE materials, including carbon-based materials, transition metal oxides, chalcogenides, alloys, conducting polymers, and composites, have been explored. Within this landscape, this study introduces a novel approach: the doping of WSe_2 with zinc (Zn) atoms to create WSe_2:Zn as a CE material for DSSCs. Different Zn doping levels were achieved using magnetron sputtering, a versatile and controllable technique known for producing high-purity, compact, and uniform films. Up to our best knowledge, this study marks the second reported use of WSe_2:Zn as a CE material for PV applications after Ari et al. who used co-sputtering technique with two different targets to prepare the CE and could achieve efficiencies of 7.41% which was comparable to the golden standard of Pt-based CEs [22]. In our work, we employ the solid-state reaction method to prepare WSe_2:Zn targets which are later used to prepare the CEs using RF sputtering method. We believe, the solid-state reaction method is a capable method to prepare reproducible targets and with versatile properties.

The motivation behind incorporating Zn in WSe_2 is to modify the structural and electronic properties of WSe_2. This approach offers several advantages: tunable electrical property, preserving the crystalline properties of the material, enhanced electrochemical properties, and cost-effectiveness. These properties have the potential to meet the requirements of CE materials in DSSC applications, opening new possibilities for improved photovoltaic performance in the future. In summary, this paper explores the doping of WSe_2 with Zn to create WSe_2:Zn as a novel CE material for DSSCs. This innovative approach offers the potential to tailor the material's properties to meet the demands of CE materials in DSSC applications, thereby advancing the field of photovoltaics.

Section snippets

Target preparation

We employed the solid solid-state reaction method to prepare WSe_2 targets doped with varying ratios of Zn. Initially, 7.65 g nano-powder WSe_2 (≥99.995% Ossila) was combined with different weight ratios of ZnSe (Sigma-Aldrich 99.99%) —specifically, 0, 100, 206, 320 mg —inside a ball milling apparatus, along with 20 mL of pure ethanol. The weight ratio of the composite material to the balls was set at 1:12. The ball milling apparatus began operating at a speed of 550 rpm and was halted after…

Results and discussion

To investigate the crystalline properties and structure of the prepared electrodes, X-ray diffraction (XRD) patterns were obtained. Fig. 1 illustrates the diffraction patterns for WSe_2:Zn0, WSe_2:Zn3, WSe_2:Zn6, and WSe_2:Zn9 samples. The peaks observed at angles 13.49, 31.83, 38.21, 47.23, 56.41, and 69.02° correspond to (002), (100), (103), (105), (008) and (203) crystal planes of hexagonal-phase WSe_2 with spatial symmetry $P6_3/mmc$ These peaks closely match the standard card number 00-038-1388,…

Conclusion

In this study, we proposed a new counter electrode for DSSCs based on the crystalline form of the WSe_2 doped with the Zn dopants. The crystalline structures of the CEs were confirmed by the XRD analysis although we noticed that the introduction of too much Zn content will perturb the crystalline structure while affecting the electrical and optical properties of the material. Furthermore, Zn doping and the nanoflake structures in WSe_2 can significantly enhance the electrochemical and…

CRediT authorship contribution statement

Manal Abdulwahid Abbood: Formal analysis, Conceptualization. **Ebraheem Abdu Musad Saleh:** Writing – review & editing, Supervision. **Abhinav Kumar:** Writing – original draft, Visualization. **Paul Rodrigues:** Project administration, Funding acquisition. **Shavan Askar:** Methodology, Investigation. **Taif Alawsi:** Validation, Investigation. **Ahmed Alawadi:** Formal analysis, Data curation. **Ali Alsalamy:** Validation, Investigation.…

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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