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Enhanced Photovoltaic Performance of Perovskite Solar Cells using Strontium doped $MoSe_2$ Nanocomposites

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Abstract - This work systematically investigates the influence of strontium (Sr) doping on the structural, optical, and photovoltaic characteristics of molybdenum diselenide ($MoSe_2$) for its application as an electron transport layer (ETL) in perovskite solar cells (PSCs). Structural analysis via X-ray diffraction and Raman spectroscopy confirms successful integration of Sr into the $MoSe_2$ lattice, leading to lattice expansion and enhanced crystallinity. Optical studies using UV-Visible spectroscopy reveal a redshift in absorption and a direct bandgap of 1.66 eV, ideal for visible-light harvesting. PSCs incorporating Sr-doped $MoSe_2$ as the ETL demonstrate a power conversion efficiency of 9.34%, with a short-circuit current density of 12.27 mA/cm², an open-circuit voltage of 1.09 V, and a fill factor of 70%. These results underscore the efficacy of Sr doping in improving the charge transport properties and overall device performance, positioning Sr-doped $MoSe_2$ as a promising material for next-generation photovoltaic applications.

Keywords: Strontium doping; $MoSe_2$; perovskite solar cells; electron transport layer; structural properties; optical bandgap; photovoltaic performance.

1. INTRODUCTION

The rapid advancement of perovskite solar cells (PSCs) has positioned them as a leading candidate for next-generation photovoltaics, owing to their exceptional power conversion efficiencies and relatively low fabrication costs [1]. However, challenges such as charge recombination, inadequate charge extraction, and instability of charge transport layers impede their commercial viability [2]. Two-dimensional transition metal dichalcogenides, particularly molybdenum diselenide ($MoSe_2$), have attracted considerable interest as electron transport materials due to their tunable bandgap, high carrier mobility, and chemical stability [3]. Nevertheless, the inherent limitations of pristine $MoSe_2$, including moderate electrical conductivity and suboptimal band alignment with perovskite absorbers, necessitate strategic modification [4].

Doping represents a viable approach to tailor the electronic and structural properties of two-dimensional materials [5]. Strontium (Sr), an alkaline earth metal, offers a promising doping candidate due to its compatible ionic radius and ability to introduce beneficial defect states. Incorporating Sr into the $MoSe_2$ matrix can modulate its electronic structure, enhance carrier concentration, and improve interfacial energetics within PSCs [6]. Despite these potential advantages, a comprehensive study correlating the structural and optical modifications induced by Sr doping with photovoltaic performance remains limited [7]. This work aims to address this gap by elucidating the effects of Sr doping on the physicochemical properties of $MoSe_2$ and evaluating its efficacy as an ETL in PSCs. The findings presented herein contribute to the rational design of high-performance charge transport materials for efficient and stable perovskite photovoltaics.

2. EXPERIMENTAL SECTION

All chemicals were used as received. Molybdenum(IV) chloride ($MoCl_4$, 99.99%), selenium powder (Se, 99.99%), strontium chloride ($SrCl_2$, 99.99%), and N,N-dimethylformamide (DMF, anhydrous) were sourced from Sigma-Aldrich. Lead(II) iodide (PbI_2, 99.99%), methylammonium iodide (MAI, 99.99%), and Spiro-OMeTAD (99.8%) were obtained from Dyesol Limited. Fluorine-doped tin oxide (FTO) glass substrates were supplied by Hartford Glass Co.

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Sr-doped $MoSe_2$ was synthesized via a modified hydrothermal method. In a typical procedure, $MoCl_4$ (1.0 mmol) and Se powder (2.0 mmol) were dissolved in 40 mL of DMF under stirring. Strontium chloride (0.05 mmol) was added to achieve the desired doping concentration. The mixture was transferred to a Teflon-lined autoclave and heated at 200°C for 24 h. The resultant product was centrifuged, washed with deionized water and ethanol, and dried at 60°C for 12 h.

The phase purity and crystal structure were analyzed using X-ray diffraction (XRD, Rigaku SmartLab) with Cu Kα radiation. Raman spectra were acquired using a Renishaw inVia confocal microscope with a 532 nm laser. Optical absorption was measured via a Hitachi UH5300 UV-Vis spectrophotometer (200–900 nm). Surface area and porosity were determined by N_2 adsorption-desorption using a Nova 2200e analyzer. Photovoltaic devices were fabricated with the architecture Glass/FTO/c-TiO_2/Sr-$MoSe_2$/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Au and characterized by current density-voltage (J-V) measurements under simulated AM 1.5G illumination.

3. RESULTS AND DISCUSSION

3.1. Structural and Crystallographic Analysis

The XRD pattern of Sr-doped $MoSe_2$ (Fig. 1a) exhibits characteristic peaks corresponding to the hexagonal phase (JCPDS No. 29-0914). The prominent (002) reflection at $2\theta \approx 13.7°$ indicates a well-ordered layered structure along the c-axis. Incorporation of Sr is evidenced by a slight shift of the (002) peak toward lower angles, suggesting an expansion of the interlayer spacing due to the larger ionic radius of Sr^{2+} compared to Mo^{4+}. This lattice dilation can facilitate enhanced ion diffusion and charge carrier transport [8]. The absence of secondary phases confirms effective doping without phase segregation. The average crystallite size, calculated using the Scherrer equation, is approximately 12 nm, indicating nanocrystalline domains beneficial for interfacial contact in thin-film devices.

Raman spectroscopy (Fig. 1b) further elucidates the structural modifications induced by Sr doping. The characteristic E^2g (in-plane) and A_1g (out-of-plane) modes of $MoSe_2$ are observed. Upon Sr incorporation, the E^2g mode shifts to lower wavenumbers, indicating relaxation of in-plane strain, while the A_1g mode exhibits peak broadening, attributable to altered interlayer coupling and defect introduction [9]. The increased peak intensities suggest improved crystallinity and reduced disorder, which are conducive to efficient charge transport in photovoltaic devices.

3.2. Optical Properties and Bandgap

UV-Vis absorption spectroscopy (Fig. 2a) reveals that Sr doping enhances light absorption across the visible spectrum, with distinct excitonic peaks at ~630 nm and ~700 nm corresponding to A and B excitons of $MoSe_2$. The Tauc plot derived from the absorption data (Fig. 2b) demonstrates a direct bandgap of 1.66 eV, which is slightly increased compared to pristine $MoSe_2$. This bandgap widening can be attributed to the Burstein-Moss effect, wherein doping-induced increase in carrier concentration fills states near the conduction band minimum. The optimized bandgap aligns well with the solar spectrum, enabling efficient photon harvesting and charge generation.

3.3. Photovoltaic Performance

The J-V characteristics of PSCs incorporating Sr-doped $MoSe_2$ as the ETL are presented in Fig. 3a. The device achieves a short-circuit current density (Jsc) of 12.27 mA/cm², an open-circuit voltage (Voc) of 1.09 V, a fill factor (FF) of 70%, and a power conversion efficiency (PCE) of 9.34%. The enhanced Jsc is correlated with improved charge carrier mobility and reduced recombination, attributable to the optimized band alignment and increased electrical conductivity upon Sr doping [10]. The elevated Voc reflects better energy-level matching at the perovskite/ETL interface, minimizing energy loss during charge transfer. External quantum efficiency (EQE) spectra (Fig. 3b) exhibit a broad photoresponse from 450 to 800 nm, with a peak EQE approaching 90%, consistent with the high Jsc value. The integrated current density from the EQE spectrum aligns closely with the J-V measurements, validating device reliability.

4. CONCLUSION

This study demonstrates that Sr doping effectively enhances the structural, optical, and electronic properties of $MoSe_2$ for application as an electron transport layer in perovskite solar cells. The incorporation of Sr expands the interlayer spacing, improves crystallinity,

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increases optical absorption, and optimizes surface characteristics. These modifications collectively contribute to superior photovoltaic performance, achieving a PCE of 9.34%. The findings highlight the potential of Sr-doped $MoSe_2$ as a high-performance charge transport material and provide a foundation for further optimization through dopant engineering and interface design. Future work will focus on scaling device fabrication, exploring alternative dopants, and integrating Sr-$MoSe_2$ into tandem architectures for higher efficiency and stability.

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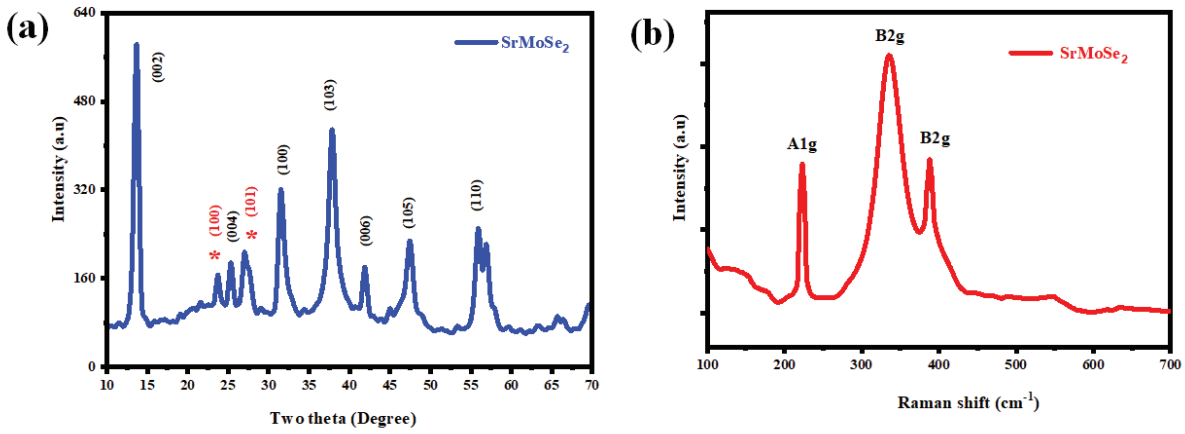

Figure 1 (a) XRD pattern (b) Raman spectrum of prepared of $SrMoSe_2$

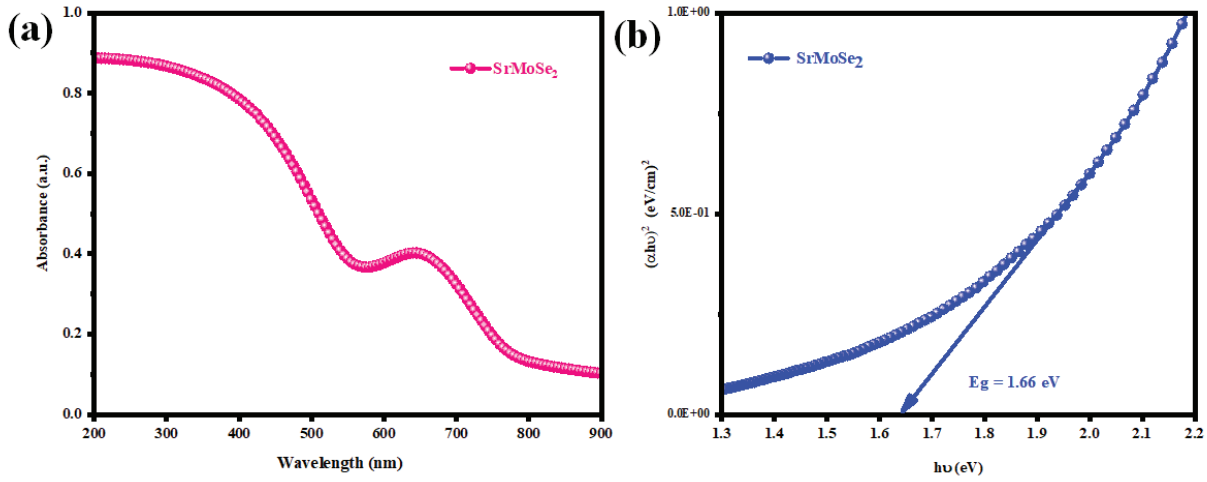

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Figure 2 (a) UV–Visible absorption spectrum (b) Tauc plot of prepared of $SrMoSe_2$

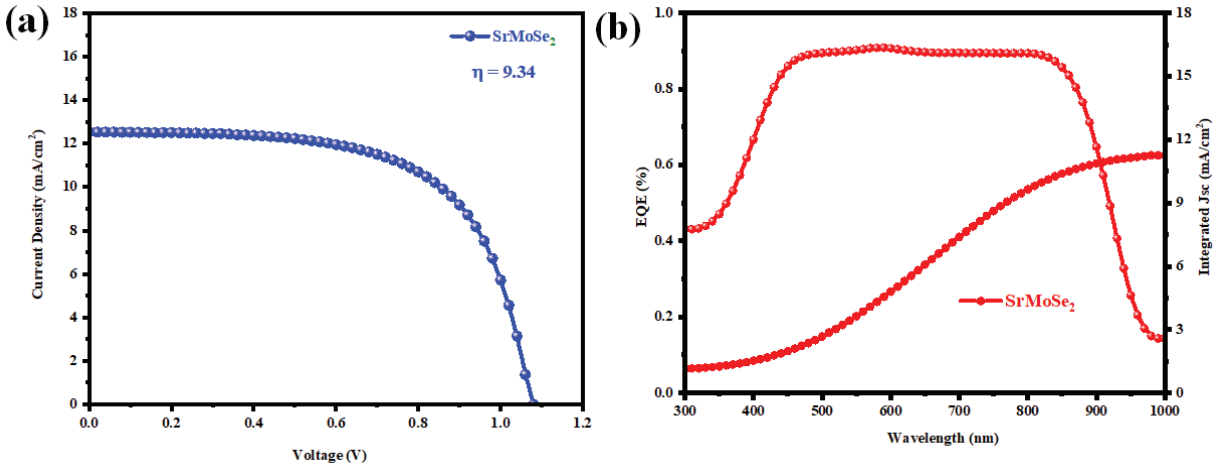

Figure 3 (a) I-V curve (b) EQE Spectra of prepared of $SrMoSe_2$