Modelling and Performance Analysis of Physical and Electrical Properties of $BaZrS_3$ Chalcogenide Perovskite Solar Cells

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Abstract: **This study explores the application and utility of $BaZrS_3$-based perovskite solar cells (PSCs) for thin-film photovoltaic applications. The proposed device exhibited stable current up to 1.1 eV and maintained over 65% quantum efficiency across a broad spectrum. The Mott-Schottky analysis indicated a bandgap of approximately 1.7 eV. Nyquist and Bode plots confirmed robust impedance behaviour. The device displayed V_{oc} =1.33 V, J_{sc} = 16.56 mA/cm^2, FF = 83.97%, and Efficiency = 18.58%. $BaZrS_3$'s exceptional optical and electrical properties, coupled with environmental stability, position it as a promising material for advanced PSCs.**

Keywords: Mott Schottky, Capacitance, Conductance, $BaZrS_3$, SCAPS-1D

I. INTRODUCTION

Perovskite solar cells (PSCs) have rapidly advanced since their introduction as visible light sensitizers for photovoltaics in 2009, when they achieved a 3.8% efficiency. Laboratory-scale single-junction PSCs now reach efficiencies of 31.63%, and tandem perovskite/silicon PVs have surpassed 32%, highlighting their potential for high efficiency, stability, endurance, and cost-effective manufacturing [1]. Chalcogenide perovskites, like $CaTiS_3$, $BaZrS_3$, $CaZrSe_3$, and $CaHfSe_3$, offer significant advantages for solar cells, including favourable band gaps for efficient solar energy conversion and better optical absorption attributions. These materials address critical issues found in halide perovskites, including moisture-induced instability and the presence of harmful lead, making them more sustainable and environmentally friendly [2]. $BaZrS_3$, specifically, stands out due to its robustness against pressure, oxidation, and moisture, and an exceptionally high absorption coefficient. Additionally, it offers high carrier mobility and stability under various environmental conditions, thus solidifying it as an extremely suitable material for thin-film photovoltaic implementations [3]. In this study, SCAPS -1D was utilized for the numerical modelling of the device under illumination using the AM1.5 spectra at a temperature of 300K and an incident power density of 1000 W/m^2.

II. DEVICE SCHEMATICS

Figure 1 shows the device schematics of the proposed structure. It consists of $BaZrS_3$ deployed as the absorber layer with TiO_2 and Cu_2O as the electron transport material (ETM) and hole transport material (HTM) respectively. Metals with work functions of 3.9 eV (Ti) and 5.3 eV (Au) serve as the front and back metal contacts respectively.

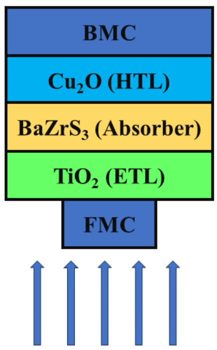

Fig 1: Layered Structure of the Proposed Device

III. RESULTS AND DISCUSSION

Figure 2 represents the I-V curve of the proposed device structure with an inset curve showing the trend of the quantum efficiency (QE) and energy of the photons as a variable dependent on the wavelength of the incident light beams. It is observed that the device maintains a steady current till a voltage of 1.1 eV, after which the current density begins to fall rapidly. This is due to the increased probability of recombination rates at higher voltages. The QE curve represents the ratio of collected electron-hole pairs to incident photons on the device. As observed, the device maintains more than 65% QE for a significant range of the spectrum.

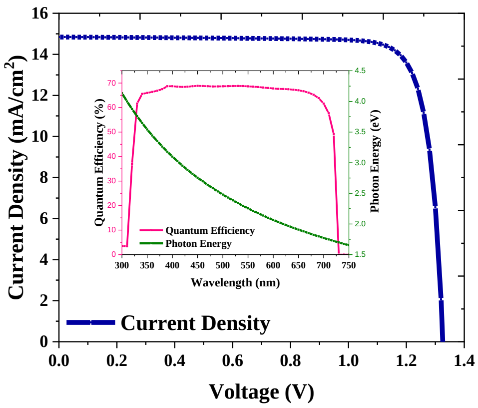

Fig 2: I-V Curve of the device and trend of Quantum Efficiency (QE) and Photon Energy as a function of the wavelength

Figure 3 provides the Mott Schottky Curve while simultaneously presenting the impact of the voltage on the conductance and capacitance of the device. The Mott Schottky curve has an intercept of approximately 1.7 eV which is equivalent to the bandgap of the absorber layer. Furthermore, the slope of the Mott Schottky curves also corresponds to the shallow donor density of the absorber layer (~10^{18} cm^{-3}). The capacitance increases with applied voltage due to the narrowing of the depletion region and increased charge storage capacity. Simultaneously, conductance increases due to enhanced carrier injection and reduced potential barriers, leading to higher current flow through the cell.

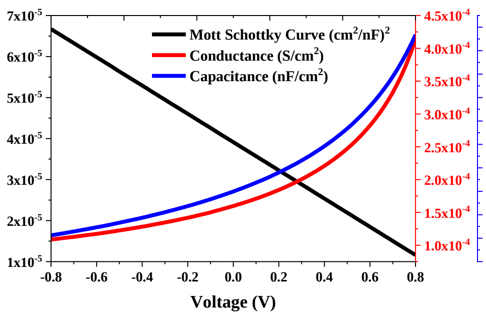

Fig 3: Mott Schottky Curve and Effect of Applied Voltage on Capacitance and Conductance

Figures 4 and 5 illustrate the Nyquist and Bode Plots for the proposed device structure. The arc within the Nyquist plot shows the response of the absorber bulk material. The almost circular shape is owed to the formation of an RC pair in the device. The Bode plot provides the change in the total impedance of the device as a function of the frequency. At high frequencies, the impedance is often dominated by the series resistance, while at low frequencies, it includes contributions from both the series and parallel resistances.

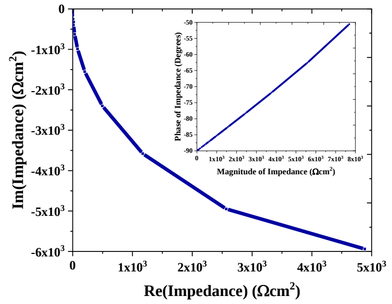

Fig 4: Nyquist Curve for the Proposed Device Structure

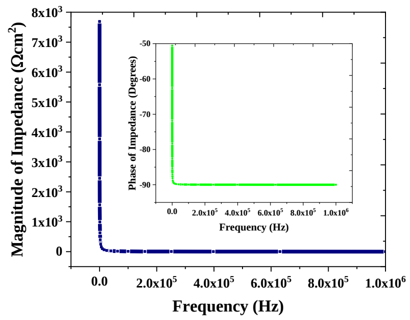

Fig 5: Bode Plot for the Proposed Device Structure

Table 1: Comparative Analysis of Proposed and Previously Reported Work

Sr. No.	Efficiency (%)	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	Reference
1	7.33	12.90	1.06	53.30	[3]
2	18.58	16.56	1.33	83.97	This Work

IV. CONCLUSION

This study demonstrates the potential of BaZrS3-based perovskite solar cells (PSCs) for thin-film photovoltaics. Numerical modelling using SCAPS-1D under standard illumination showed a stable current up to 1.1 eV, with high quantum efficiency (over 65%) across a broad spectrum. The Mott-Schottky plot revealed a bandgap of approximately 1.7 eV. Nyquist and Bode plots confirmed the robust impedance response of the absorber material. This work helps establish a more robust framework for the commercialisation and operationalisation of chalcogenide perovskite solar cells.

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