

Strategy of improving photovoltage and efficiency of FeS₂ based heterojunction solar cell through absorber, buffer and window layers optimization with SCAPS-1D software

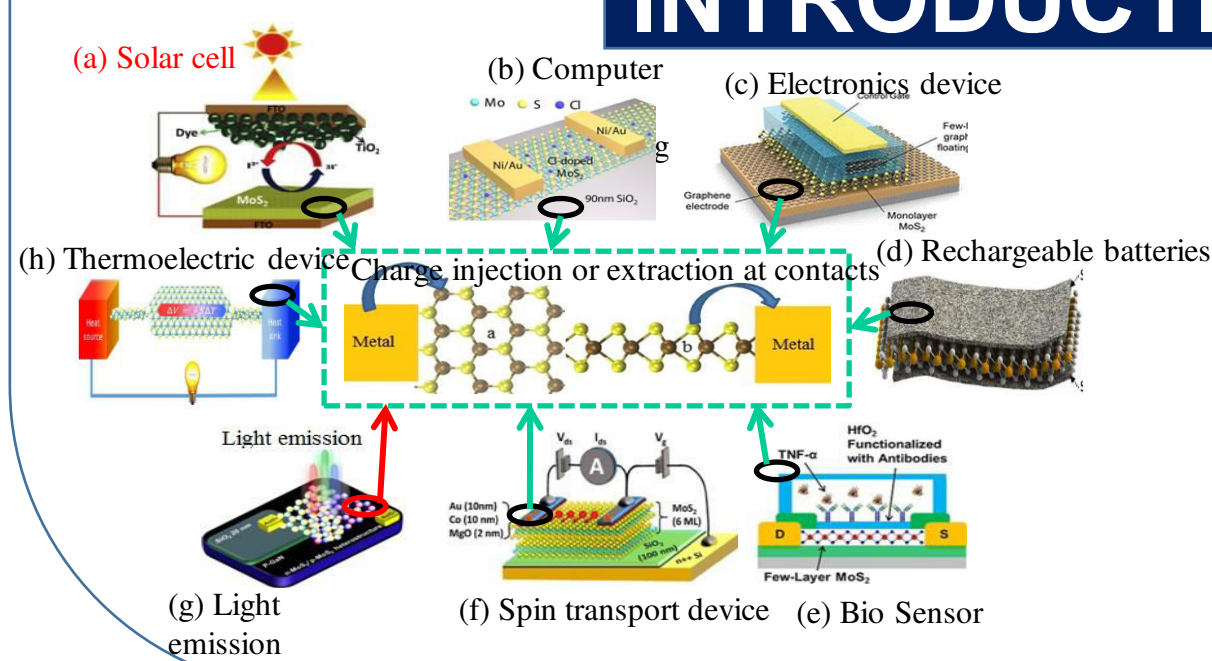
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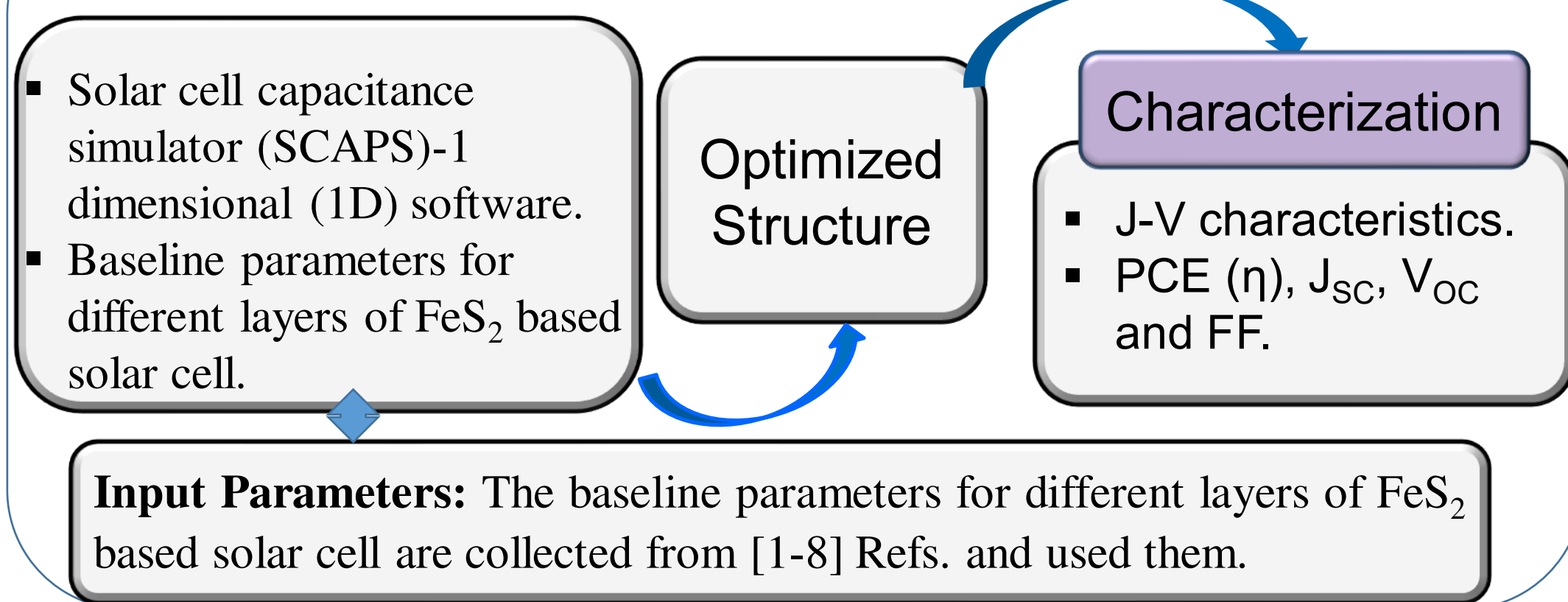
ABSTRACT: In this work, we proposed glass/FTO/ZnO:Al/CdS/FeS₂/MoS₂ solar cell architecture where MoS₂ layer is used to make heterojunction FeS₂(n)/MoS₂(p) along with buffer layer CdS. The photovoltage and the efficiency of iron pyrite (FeS₂) based solar cell have been improved through the component layers optimization. The CdS and MoS₂ layers were studied as electron transporting (ET) and hole transporting (HT) materials for fabricating and improving low-cost, durable and efficient solar cell. The thickness of the absorber layer FeS₂ and HTM-MoS₂ layers gave distinct photovoltaic properties to designing the proposed solar cell device. The results show that MoS₂ layer could considerably improve open circuit voltage and short circuit current density hence power conversion efficiency. Importantly, the absorber and buffer layers thickness affect the cell's parameters and efficiency were extensively simulated. For a optimizing of FeS₂, MoS₂, CdS and ZnO:Al layers with a thickness of 1.40, 0.80, 0.10 and 0.20 μm heterojunction solar cell showed, $\eta=36.60\%$, $J_{SC}=50.20 \text{ mA/cm}^2$, $V_{OC}=0.842 \text{ V}$ and $FF=86.56\%$ without any defect, series and shunt resistances. However, the efficiency is reduced with increasing of series resistance and the operating temperature. This study shows that large thickness of FeS₂ and MoS₂ layers with low band gap favor the formation of solar cell and model equations can be used to predict high efficient solar cell which may lead the way to direction for laboratory experiment.

INTRODUCTION



- Among 23 existing photovoltaic materials including Si, FeS₂ outstands all of them in terms of the highest availability that may potentially lead to lower costs than Si-solar cells.
- A $\sim 10^5 \text{ cm}^{-1}$ for $h\nu > 1.4 \text{ eV}$, mobility $\sim 360 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and diffusion length (100-1000 nm).
- Nontoxic, robust, earth abundance and biocompatible elements. Indirect $E_g=0.95-1.38 \text{ eV}$ and direct $E_g=1.10-1.19 \text{ eV}$.
- $J_{SC}=30-42 \text{ mA/cm}^2$, $QE \sim 90\%$.
- $V_{OC} < 0.2 \text{ eV}$ and PCE never exceeded 2.8%.

METHODOLOGY



Input Parameters: The baseline parameters for different layers of FeS₂ based solar cell are collected from [1-8] Refs. and used them.

RESULTS AND DISCUSSION

Optimized cell parameters

Layer	Thickness (μm)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF%	Efficiency (η)%
ZnO:Al	0.2-0.25	0.842	50.20	86.56	36.60
CdS	0.1-0.15	0.842	50.20	86.56	36.60
FeS ₂	0.8-0.9	0.842	50.20	86.56	36.60
MoS ₂	0.3-0.4	0.842	50.20	86.56	36.60

Fig.1(a) shows optimized device architecture of the proposed solar cell.

Fig. 1(b) shows the band alignment of the different layers which is essential for carrier transport to the respective electrodes.

Fig. 1(c) shows the band diagram alignment of the different layers which is obtained from SCAPS-1D. In Fig.1(d) it is evident that MoS₂ acts as hole transport and other layers act as electron transport medium

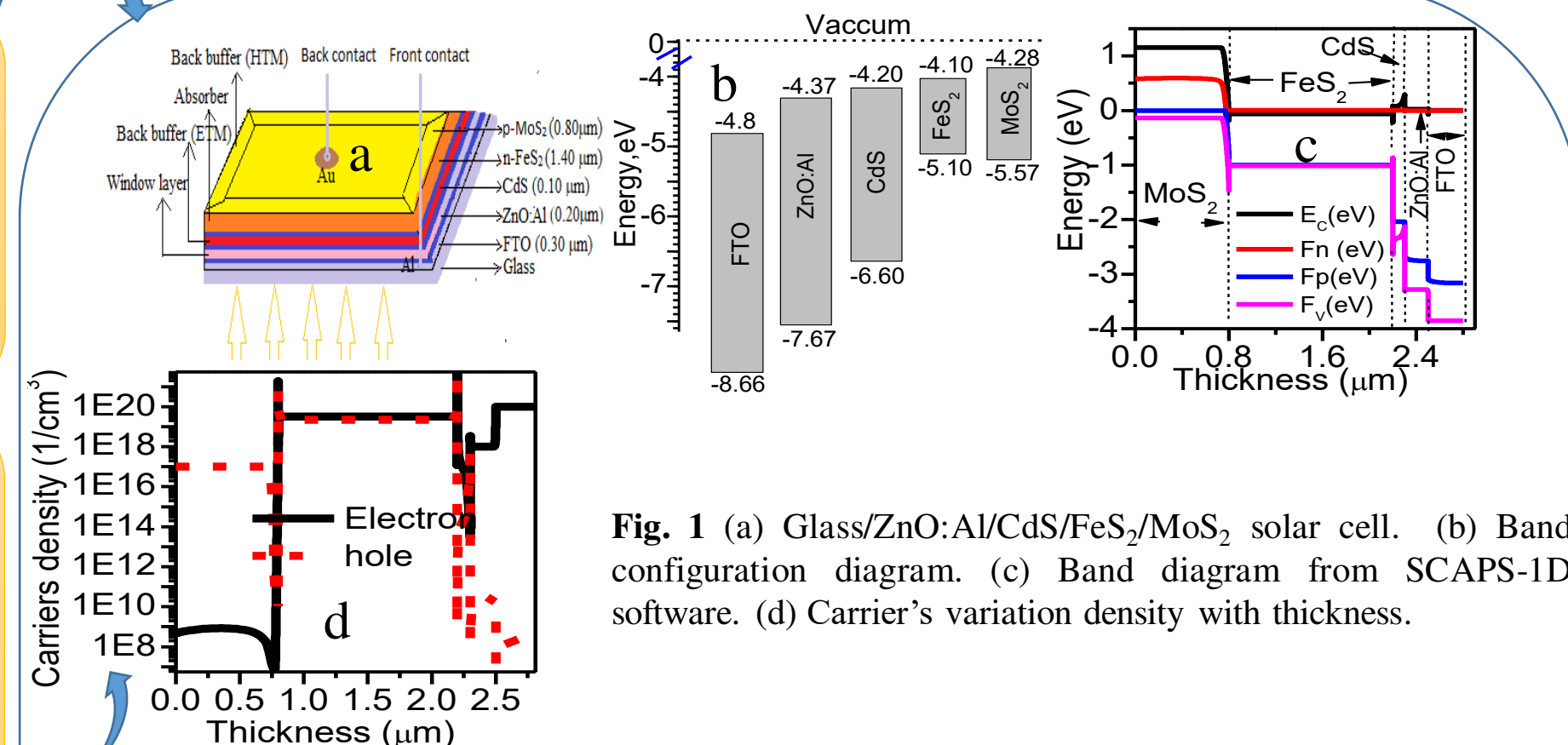


Fig. 1 (a) Glass/ZnO:Al/CdS/FeS₂/MoS₂ solar cell. (b) Band configuration diagram. (c) Band diagram from SCAPS-1D software. (d) Carrier's variation density with thickness.

Fig. 2 (a)-(b), solar cell parameters increased up to a specific thickness of FeS₂ and MoS₂. The conversion efficiency (η) and V_{OC} are increased significantly until thickness of MoS₂ and FeS₂ reached at ≤ 0.80 and $1.40 \mu\text{m}$. η is unchanged up to specific thickness of CdS and ZnO:Al (Fig.2c-d)

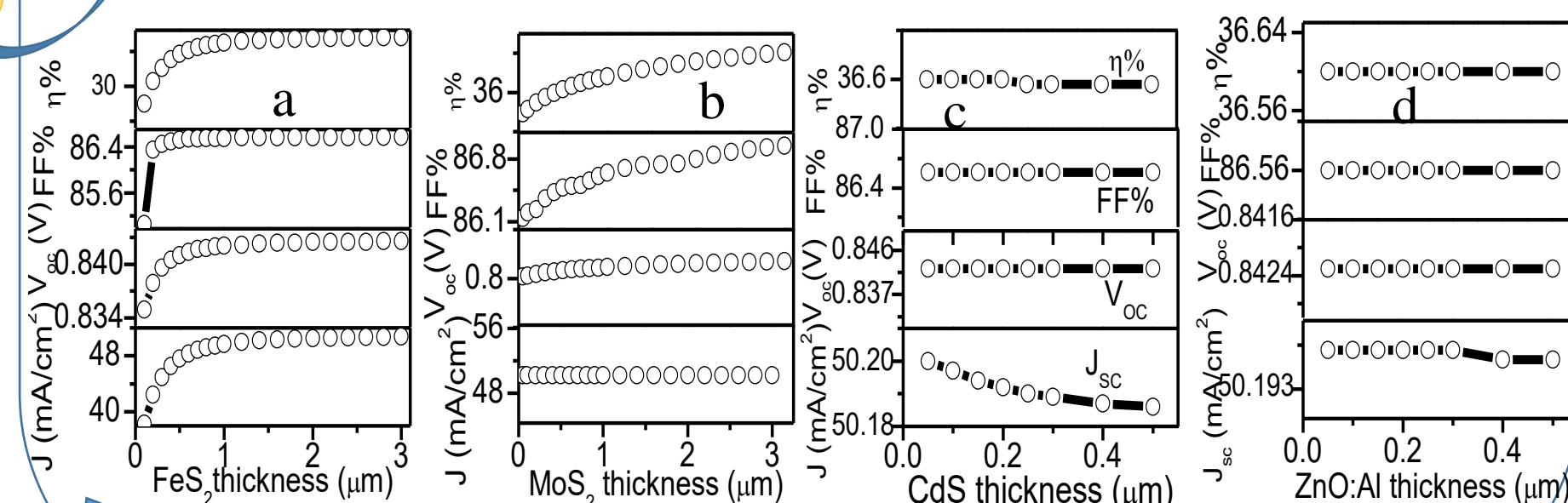


Fig. 2 Variation of J_{SC} , V_{OC} , FF and η as a function of (a) absorber FeS₂, (b) top MoS₂, (c) bottom buffer CdS and (d) window ZnO:Al layers thickness.

Efficiency is decreased with including resistances (Fig.3b) and temperature (Fig.3d). But there is no effect on QE% (Fig.3c).

Fig. 4 a-b, band gap of MoS₂ and FeS₂ layers were considerably affect solar cell performance which is coherent with operating temperature. By increasing R_s , V_{OC} is almost constant, but J_{SC} and FF are decreased which affects solar cell performance (Fig.4c). As R_{sh} is climbed (Fig.4d), J_{SC} and V_{OC} are increased which expresses leakage loss decreases with increasing R_{sh} .

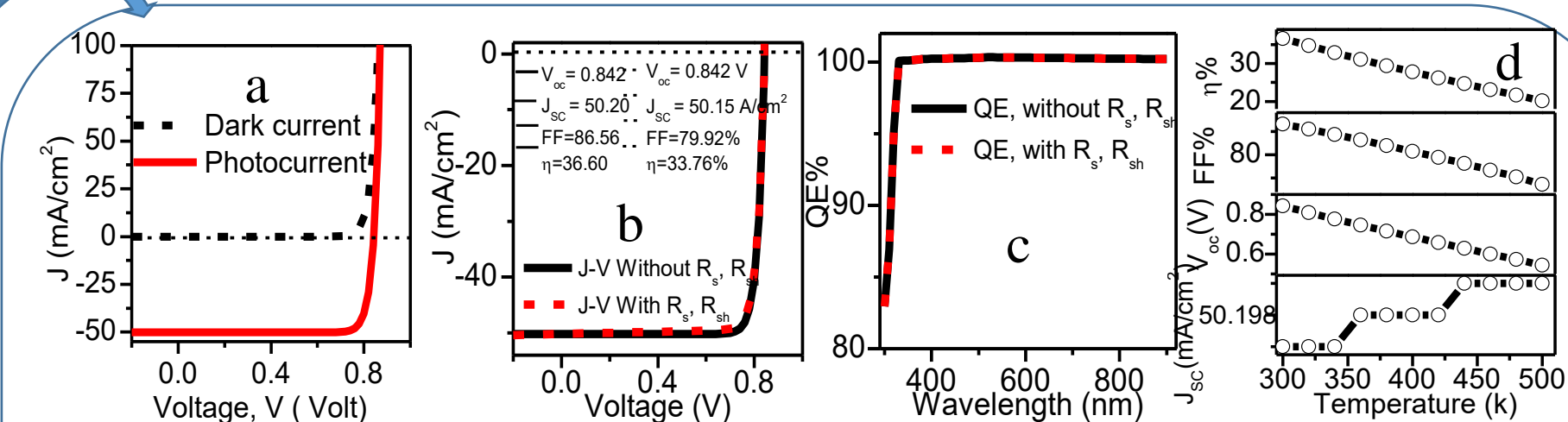


Fig.3. (a) J-V of optimized solar cell in dark and under light. (b) J-V characteristics and (c) quantum efficiency with and without of R_s and R_{sh} . (d) Performance as a function of operating temperature.

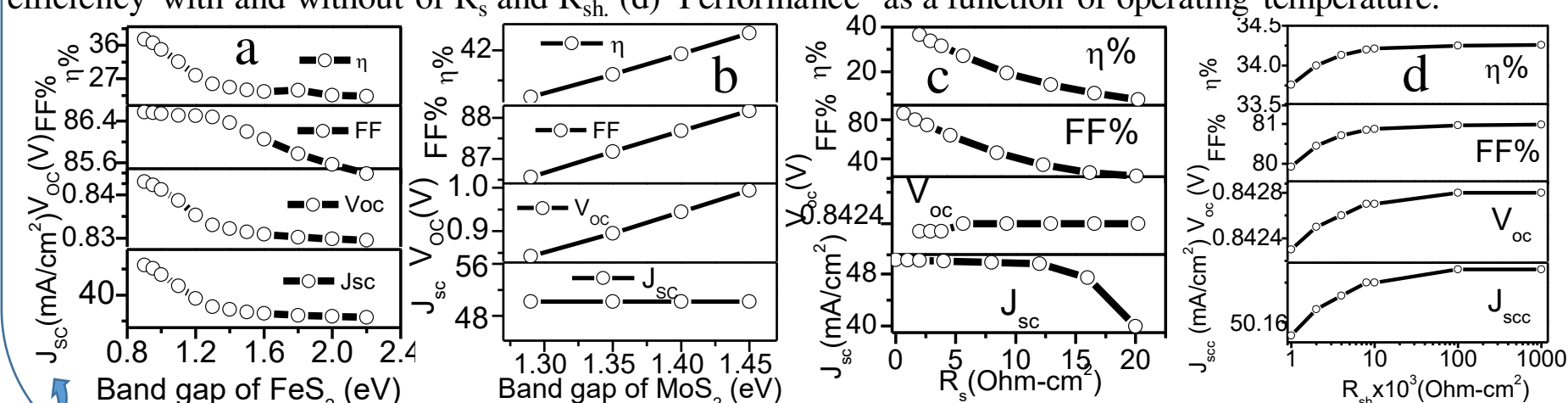


Fig. 4. Effect of band gap of (a) FeS₂, (b) MoS₂ layers and of (c) series and (d) shunt resistances.

CONCLUSIONS

- The optimal values are found out to improve the performance of glass/FTO/ZnO:Al/CdS/FeS₂/MoS₂ solar cell.
- By including MoS₂ and CdS layers, the photovoltage and efficiency are improved significantly.
- η was increased significantly up to ≤ 0.80 & $1.40 \mu\text{m}$ of MoS₂ and FeS₂ layers thickness.
- Band gap of MoS₂ and FeS₂ were considerably affect the solar cell performance.
- η was deteriorated at a temperature coefficient of $-0.083\%/K$ which insights the better stability. The optimized solar cell parameters were observed as: efficiency- 36.60%, FF-86.56%, J_{SC} -50.20mA/cm² and V_{OC} -0.842 V.
- Our findings can lead to develop efficient FeS₂ based heterojunction solar cells for practical application.