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Strategy of improving photovoltage and efficiency of FeS_2 based heterojuction solar cell through absorber, buffer and window layers optimization with SCAPS-1D software

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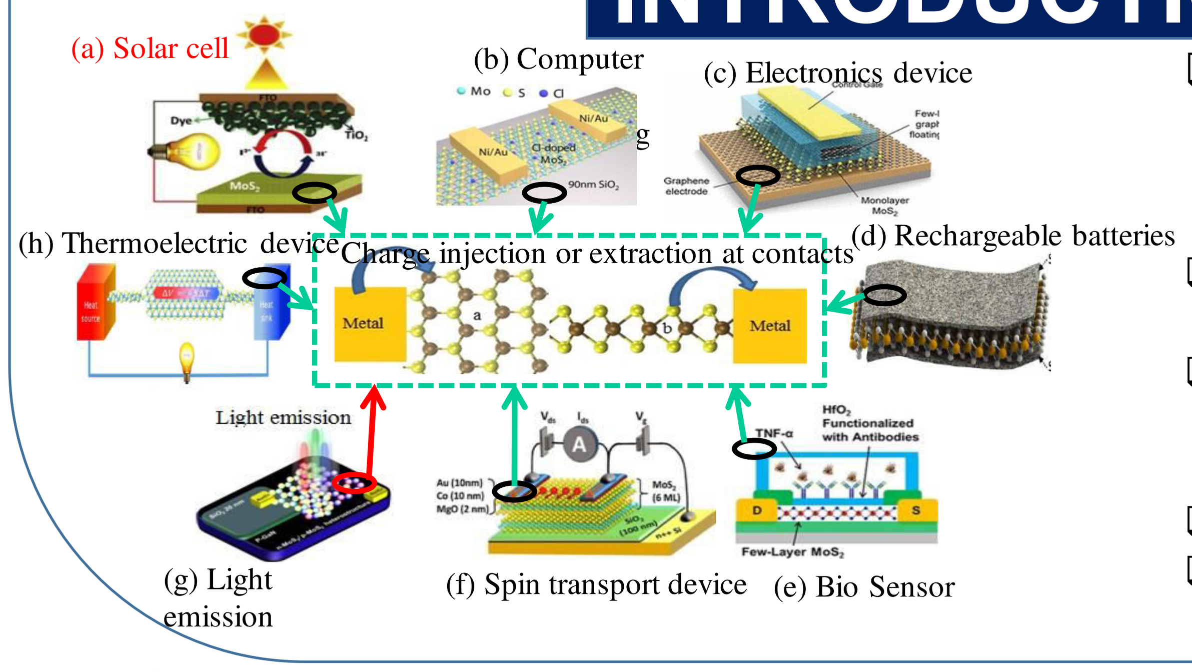
ABSTRACT: In this work, we proposed glass/FTO/ZnO:Al/CdS/FeS_2/MoS_2 solar cell architecture where MoS_2 layer is used to make heterojuction FeS_2(n)/MoS_2(p) along with buffer layer CdS. The photovoltage and the efficiency of iron pyrite (FeS_2) based solar cell have been improved through the component layers optimization. The CdS and MoS_2 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 FeS_2 and HTM-MoS_2 layers gave distinct photovoltaic properties to designing the proposed solar cell device. The results show that MoS_2 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 FeS_2, MoS_2, CdS and ZnO:Al layers with a thickness of 1.40, 0.80, 0.10 ad 0.20 µm heterojunction solar cell showed, η=36.60%, J_{SC}=50.20 mA/cm^2, V_{OC}=0.842 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 FeS_2 and MoS_2 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, FeS_2 outstands all of them in terms of the highest availability that may potentially lead to lower costs than Si-solar cells.
- A ~10^5 cm^{-1} for hν > 1.4 eV), mobility~ 360 cm^2 V^{-1} s^{-1} and diffusion length (100-1000 nm).
- Nontoxic, robust, earth abundance and biocompatible elements. Indirect E_g =0.95–1.38 eV and direct E_g=1.10-3.19 eV.
- J_{SC}=30−42 mA/cm^2), QE~90%.
- V_{OC}< 0.2 eV and PCE never exceeded 2.8%.

METHODOLOGY

- Solar cell capacitance simulator (SCAPS)-1 dimensional (1D) software.
- Baseline parameters for different layers of FeS_2 based solar cell.

Optimized Structure

Characterization

- J-V characteristics.
- PCE (η), J_{SC}, V_{OC} and FF.

Input Parameters: The baseline parameters for different layers of FeS_2 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 MoS_2 acts as hole transport and other layers act as electron transport medium

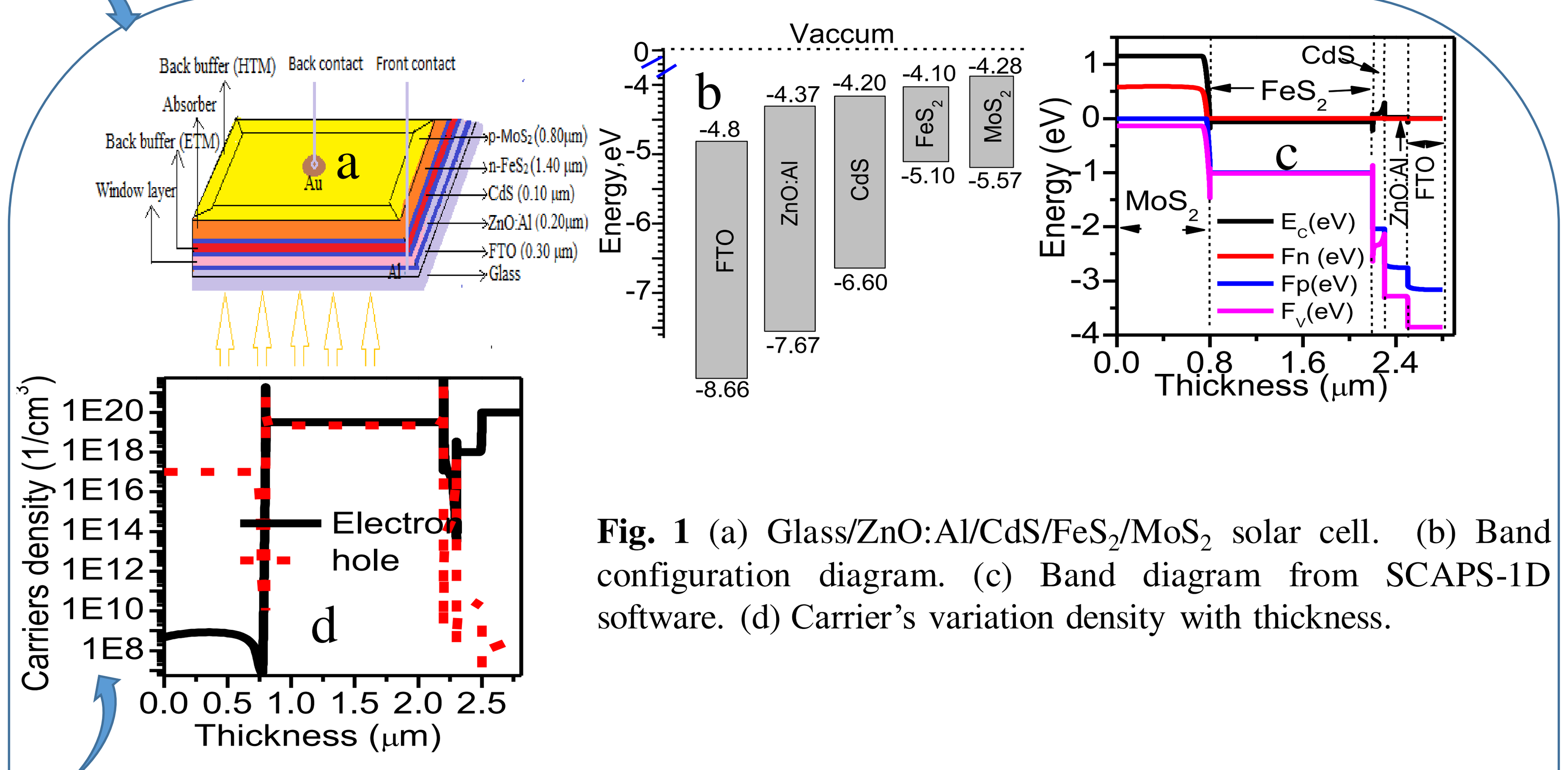


Fig. 1 (a) Glass/ZnO:Al/CdS/FeS_2/MoS_2 solar cell. (b) Band configuration diagram. (c) Band diagram from SCAPS-1D software. (d) Carrier's variation density with thickness.

Fig. 2 (a)-(b), solar cell parameters increased up to a specific thickness of FeS_2 and MoS_2. The conversion efficiency (η) and V_{OC} are increased significantly until thickness of MoS_2 and FeS_2 reached at ≤0.80 and 1.40 µm. η is unchanged up to specific thickness of CdS and ZnO:Al(Fig.2c-d)

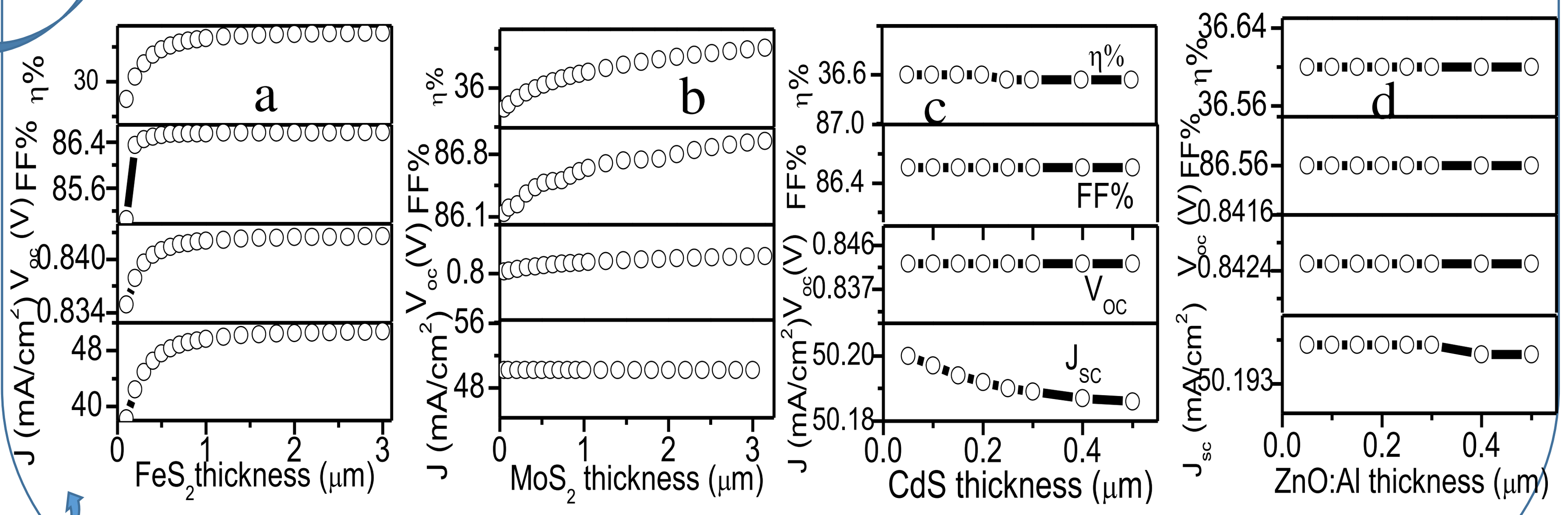


Fig. 2 Variation of J_{SC}, V_{OC}, FF and η as a function of (a) absorber FeS_2, (b) top MoS_2, (c) bottom buffer CdS and (d) window ZnO:Al layers thickness.

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

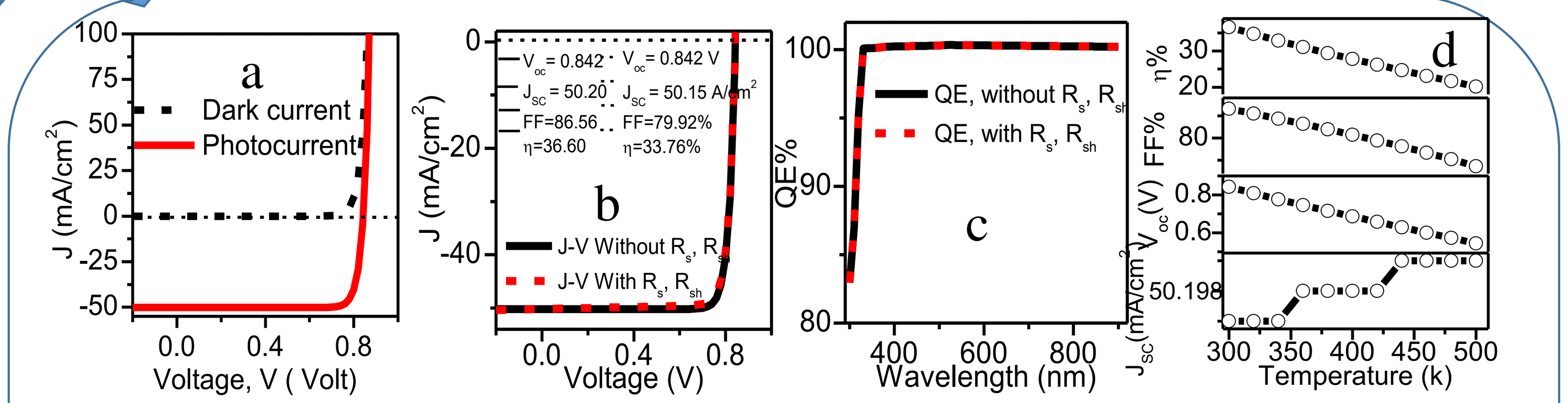


Fig.3. (a) J-V of optimized solar cell in dark and under light. (b) J-V characteristics and (c) quantum efficiency with and without of R_s and R_{sh} (d) Performance as a function of operating temperature.

Fig. 4 a-b, band gap of MoS_2 and FeS_2 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},

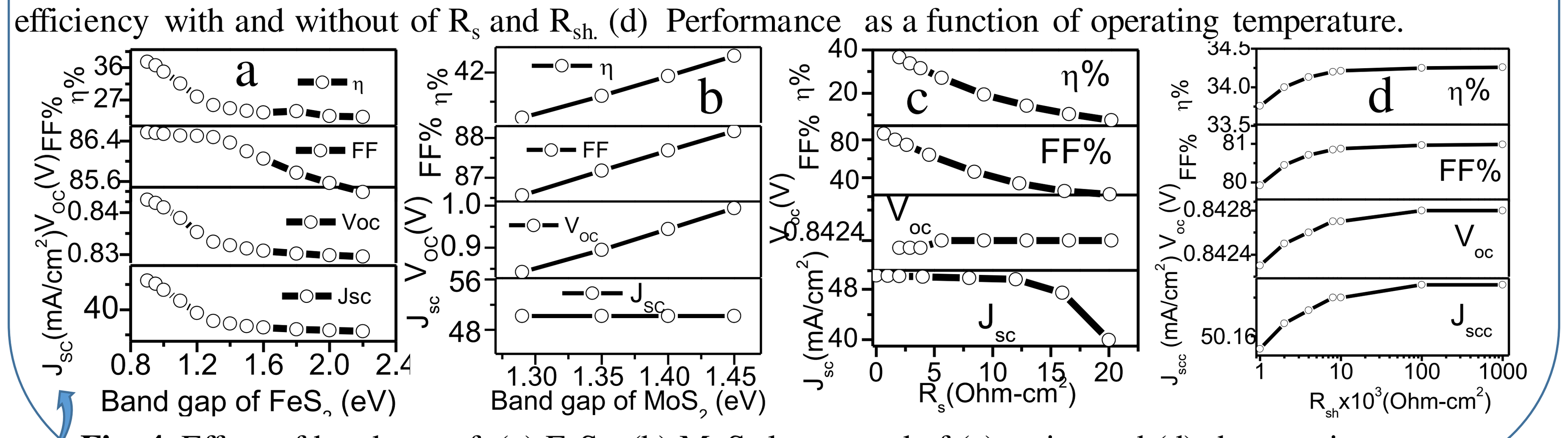


Fig. 4. Effect of band gap of (a) FeS_2, (b) MoS_2 layers and of (c) series and (d) shunt resistances.

CONCLUSIONS

- The optimal values are found out to improve the performance of glass/FTO/ZnO:Al/CdS/FeS_2/MoS_2 solar cell.
- By including MoS_2 and CdS layers, the photovoltage and efficiency are improved significantly.
- η was increased significantly up to ≤ 0.80 & 1.40 µm of MoS_2 and FeS_2 layers thickness.
- Band gap of MoS_2 and FeS_2 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/cm^2 and V_{OC}-0.842 V.
- Our findings can lead to develop efficient FeS_2 based heterojunction solar cells for practical application.

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