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Exploration Of PV Potential Of $Sb_2(S_xse_{1-X})_3$/Znse Hetero-Junction Solar Cells Via Absorber Layer Engineering

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Extended Abstract

With contemplation of momentous potential of antimony sufide selenide compound semiconductor ($Sb_2(S_xSe_{1-x})_3$) towards absorber layer roles to solar cells, present work explores the optimization of photovoltaic (PV) performance of $Sb_2(S_xSe_{1-x})_3$/ZnSe hetero-junction devices by solar cell capacitance simulator-one dimensional (SCAPS-D) program. Due to tunable band gap in range of 1.1-1.8 eV, high absorption coefficient and earth abundance virtue, the $Sb_2(S_xSe_{1-x})_3$ compound is explored as promising light harvesting absorber layers while environmental friendly and non-toxic zinc selenide (ZnSe) is being utilized as window/buffer layer as a counterpart of hetero-junction. The PV analysis of modeled devices having architecture as glass/FTO/ZnSe/ $Sb_2(S_xSe_{1-x})_3$/Cu contact is carried by SCAPS-1D program via engineering of absorber layer parameters like thickness, defect density, doping concentration alongwith rare contacts. The optimization of absorber thickness is executed in 1-5µm range which showed the improvement in device performance viz. open circuit voltage (V_{oc}) from 254 mV to 341 mV and power conversion efficiency (PCE, η) from 5.49-7.99%. The performance of modeled devices is explicitly degraded as the defect density of $Sb_2(S_xSe_{1-x})_3$ layer is increased from 1×10^{13} cm^{-3} to 1×10^{15} cm^{-3} which resulted into short circuit current density (J_{sc}) from 34.63 mA/cm^2 to 33.37 mA/cm^2. Doping of suitable element and concentration to $Sb_2(S_xSe_{1-x})_3$ layer could be considered as effective tactic to boost the performance of designed devices. Presently the enhancement in acceptor concentration of $Sb_2(S_xSe_{1-x})_3$ layer from 10^{14} cm^{-3} to 10^{18} cm^{-3} resulted into significant augmentation in performance parameters viz. V_{oc} is enhanced from 341 mV to 740 mV and PCE from 7.99% to 20.98%. The efficient charge collection also depends upon the nature and work function of metal contact and PV performance is further improved when Ag is used as metal contact. The present detailed work shows that higher performance viz. Voc=829 mV, Jsc=33.375 mA/cm^2, fill factor=86.22% and η=23.87% of modeled devices could be achieved at optimization absorber conditions viz. thickness of 5 microns, defect density of 10^{13} cm^{-3} and acceptor density of 10^{18} cm^{-3}. Hence present numerical modeling study provides a substantial pathway towards realization of high performance, stable and environmentally friendly $Sb_2(S_xSe_{1-x})_3$/ZnSe hetero-junction solar cells.

Keywords: ($Sb_2(S_xSe_{1-x})_3$ compound, absorber layer engineering, solar cells, SCAPS-1D, power conversion efficiency acceptor concentration.

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