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| **Title:** | Cu2FeSnS4-based heterojunction solar cells with MxOy (M=Cu, Ni)-back surface field layers: Impact of defect density states and recombination | | |
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| **Abstract:** |  |
| Copper-based chalcogenide quaternary semiconductors have emerged as promising candidates for next-generation photovoltaic (PV) devices, owing to their unique electronic and photonic properties coupled with environmentally friendly compositions. This study explores the potential of copper-based absorber materials, specifically Cu2FeSnS4 (CFTS), as an absorber in heterojunction solar cells with Cu-/Ni-metal oxides back surface field (BSF) and SnS2 buffer layers using the SCAPS-1D Simulator. Initially, we assess the performance of CFTS-absorber solar cells and compare the key photovoltaic metrics with those of other Cu-based semiconductors including CuInxGa(1-*x*)Se2 (CIGS), Cu2ZnSnS4 (CZTS), Cu2CoSnS4 (CCTS), Cu2NiSnS4 (CNTS), Cu2BaSnS4 (CBTS), Cu2MnSnS4 (CMTS), to identify the most promising absorber. Subsequently, we optimize the layer properties, including active layer thickness, free-carrier concentration, bulk and interface defect density, and carrier recombination in potential CFTS. Further, we examine the impact of defects, and carrier recombination, including radiative, Shockley-Read-Hall (SRH), and Auger recombination. These detailed studies yield improved and competitive photoconversion efficiency, (*PCE*) of 27.31% (compared to 24.68%, without BSF) with open circuit voltage, (*V*OC) of 1.36 V, short-circuit current density, (*J*SC) of 22.28 mA/cm² and fill factor, (*FF*) of 90.47% for Cu2O, whereas the *PCE* of 26.97% with *V*OC of 1.07 V, *J*SC of 28.82 mA/cm² and *FF* of 86.91% for NiO*x* BSF layer in Au/Mo/BSF(Cu2O and NiO*x*)/CFTS/SnS2/ZnMgO/ZnO:Al/Pt configurations under optimized conditions. The enhanced charge separation and carrier collection efficiencies reveal the strong potential of CFTS absorber heterostructures with Cu2O/NiO*x*, SnS2, and bi-layer ZnMgO/ZnO:Al as BSF, buffer, and window layers, repectively, providing insights and resources for developing high-efficiency CFTS-based photovoltaic devices. | |