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| **Abstract:** |  |
| In this work, the Solar Cell Capacitance Simulator (SCAPS-1D) is employed to evaluate the characteristics of CdTe thin films with ZnTe as the Back Surface Field (BSF) layer and estimate the effective copper doping ratio at both the atomic scale and the device operational response perspective. The electrical characteristics of ZnTe, at varying levels of copper doping, were derived using density functional theory (DFT) by applying the generalized gradient approximation (GGA) and Hubbard U corrections (DFT+U). The performance of ZnTe with different Cu concentrations as a BSF layer was evaluated by analysing the values of four key parameters that are open circuit voltage (VOC), short circuit current density (JSC), fill factor (FF), and conversion efficiency (η). The results indicate that an increase in Cu concentration from 0% to 3%, 6%, 10%, and 12% resulted in a reduction of the energy band gap. Specifically, the energy band gap decreased from 2.24 eV to 2.10 eV, 1.98 eV, 1.92 eV, and 1.88 eV, respectively. Optimal Cu doping promotes the favourable shift in the valence band maxima (VBM) and formation of p + -ZnTe, lowering thermionic emission and improving carrier lifetime, which results in an improved ohmic contact, η = 18.73% for 10% of Cu content. Excessive doping in contrast degraded the overall device performance by forming an unmatched carrier band offset at the front interface with CdS, increasing the acceptor type defect and CdTe compensation rate. Overall, the findings suggest that incorporating a controlled level of Cu, which in this case is around 10%, promotes the efficiency and stability of the proposed CdTe device configuration to a certain extent. | |