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First-principles investigation on the impact of copper concentration on zinc telluride as the back contact for cadmium telluride solar cells

Abstract

Cadmium telluride (CdTe) solar cells have attracted a lot of interest in recent years, attributed to their low cost and eco-friendly fabrication technique. However, the back contact is still the key issue for further improvement in device performance due to the work function difference between p-CdTe and metal contacts. In this study, the interatomic characteristics of zinc telluride (ZnTe) and Cu-doped ZnTe (ZnTe:Cu) as a back surface field (BSF) in CdTe structure is investigated using first-principles density functional theory (DFT) to overcome the Schottky barrier in CdTe solar cells. The incorporation of different doping levels of copper (Cu) in ZnTe on an atomic scale, where $Zn_{1-x}Te:Cu_x$ (x = 0, 2, 4, 6, 8, and 10) as the potential back surface field layers is investigated. The effect of doping concentration on electrical characteristics such as bandgap structure and density of states (DOS) were examined via ab initio with the Hubbard U (DFT + U) correction. The results showed an interesting gradual decrease in the bandgap energy of ZnTe from 2.24 eV to 2.10 eV, 1.98 eV, 1.92 eV, 1.88 eV, and 1.87 eV for the incremented value of Cu content of 3.13%, 6.25%, 9.38%, 12.50%, and 15.63%, respectively. Accordingly, it has been found that controlling of the effective copper doping, i.e., concentration, is crucial for developing efficient back contact junctions for high-efficiency CdTe thin-film solar cells.

Keywords

Back surface field (BSF); Cadmium telluride (CdTe); Density functional theory (DFT); Energy; Solar cell; Thin films