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TCAD-Based Design and Optimization of Flexible Organic/Si Tandem Solar Cells

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Abstract: In order to surmount the Shockley–Queisser efficiency barrier of single-junction solar devices, tandem solar cells (TSCs) have shown a potential solution. Organic and Si materials can be promising candidates for the front and rear cells in TSCs due to their non-toxicity, cost-effectiveness, and possible complementary bandgap properties. This study researches a flexible two-terminal (2-T) organic/Si TSC through TCAD simulation. In the proposed configuration, the organic solar cell (OSC), with a photoactive optical bandgap of 1.78 eV, serves as the front cell, while the rear cell comprises a Si cell based on a thin 70 μm wafer, with a bandgap energy of 1.12 eV. The individual standalone front and bottom cells, upon calibration, demonstrate power conversion efficiencies (PCEs) of 11.11% and 22.69%, respectively. When integrated into a 2-T organic/Si monolithic TSC, the resultant tandem cell achieves a PCE of 20.03%, indicating the need for optimization of the top organic cell to beat the efficiency of the bottom Si cell. To enhance the performance of the OSC, some design ideas are presented. Firstly, the OSC is designed by omitting the organic hole transport layer (HTL). Consequently, through engineering the front contact work function, the PCE is enhanced. Moreover, the influence of varying the absorber defect density of the top cell on TSC performance is investigated. Reduced defect density led to an overall efficiency improvement of the tandem cell to 23.27%. Additionally, the effects of the variation of the absorber thicknesses of the top and rear cells on TSC performance metrics are explored. With the matching condition design, the tandem efficiency is enhanced to 27.60%, with V_{OC} = 1.81 V and J_{SC} = 19.28 mA/cm^2. The presented simulation results intimate that the OSC/Si tandem design can find applications in wearable electronics due to their flexibility, environmentally friendly design, and high efficiency.

Keywords: organic; silicon; two terminal; tandem solar cell; power conversion efficiency; TCAD

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1. Introduction

Solar energy is a key renewable energy source with the potential to meet global energy demands sustainably [1]. To reduce carrier thermalization losses and improve the efficiency of solar cells beyond the theoretical constraints of single-junction solar devices, tandem cells have emerged as an auspicious solution [2]. Tandem cells stack multiple photoactive materials with different bandgaps, enabling broader spectrum absorption and higher efficiencies. Various tandem solar cell (TSC) configurations have been researched