

Supporting Information for

“Tandem Solar Cells Efficiency Prediction and Optimization via Deep Learning”

1. Absorption Spectrum

Short circuit current is calculated from the simulated absorption spectra of the referenced and optimal tandem structure respectively. Fig. S1(a) and (b) shows the simulated absorption spectra of the reference solar cell [S1] and our optimal solar cell. Fig. S1(a) is the simulated absorption spectrum of the MAPbI₃/c-Si tandem solar cells we referenced except that the hole transport layer is PEDOT instead of Spiro-OMeTAD and the corresponding calculate short-circuit current ($I_{S, Re}$) is 17.72 mA/cm². Red line and blue line are the absorptances of top sub-cell and bottom sub-cell, respectively, the black line shows the total absorptance of tandem cells of referenced tandem solar cells. Fig. S1(b) shows the absorption spectrum of the optimal structure found by SA-D and the corresponding calculated short-circuit current ($I_{S, Op}$) is 20.28 mA/cm². Red line and blue line are the absorptances of top sub-cell and bottom sub-cell, respectively, the black line shows the total absorptance of optimal tandem cells.

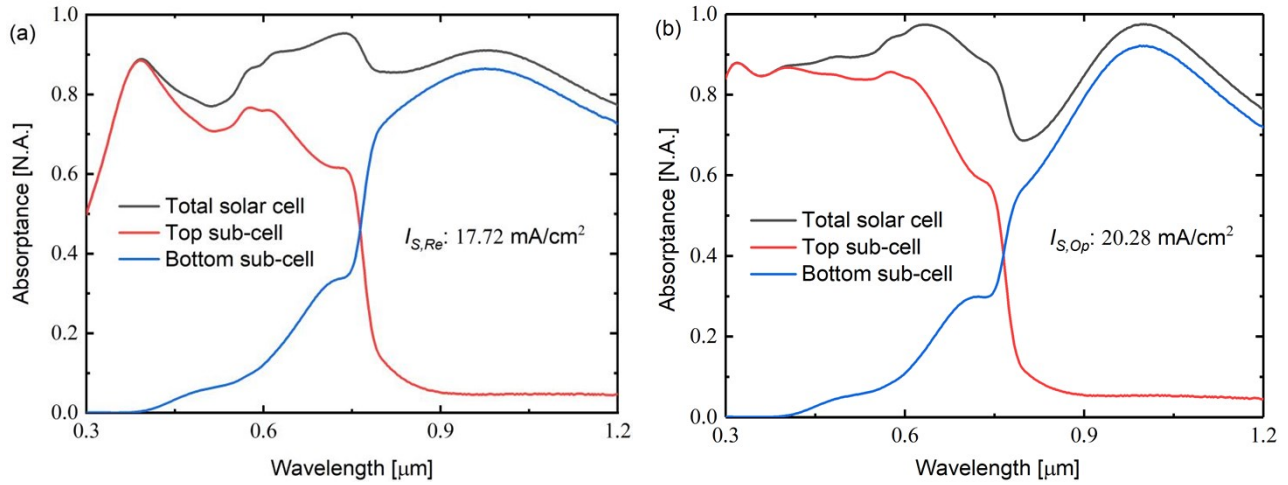


Fig. S1 Top sub-cell, bottom sub-cell and total cell absorption spectra of (a) the referenced tandem solar cell and (b) our optimal tandem solar cell.

In order to investigate the influence on absorption spectrum and short circuit current by replacing the hole transport layer of Spiro-OMeTAD with PEDOT of the reference tandem cell. Fig. S2 shows the absorption spectra and short-circuit current of MAPbI₃/c-Si tandem solar cells with hole transport layer as PEDOT and Spiro-OMeTAD respectively. These two structures show similar spectral response and the corresponding calculated short circuit current is 17.96 mA/cm² for PEDOT and 17.72 mA/cm² for Spiro-OMeTAD respectively. Small short-circuit current deviation of both tandem cells means that the influence of using PEDOT as the hole transport layer instead of using Spiro-OMeTAD is neglectable.

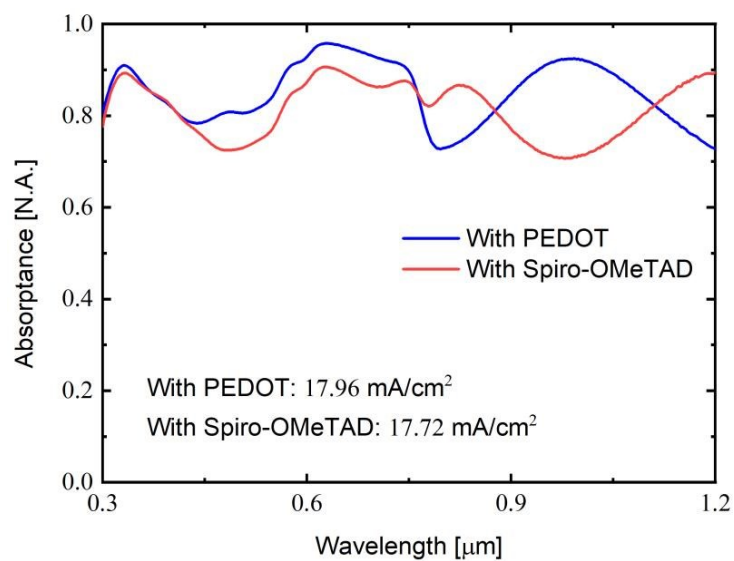


Fig. S2 Absorption spectra and short-circuit current of MAPbI₃/c-Si tandem solar cells with PEDOT and Spiro-OMeTAD respectively.

References

- [S1] J. Werner, et al, "Efficient Monolithic Perovskite/Silicon Tandem Solar Cell with Cell Area > 1 cm²", *J. Phys. Chem. Lett.*, vol. 7, no. 1, pp. 161–166, 2016.