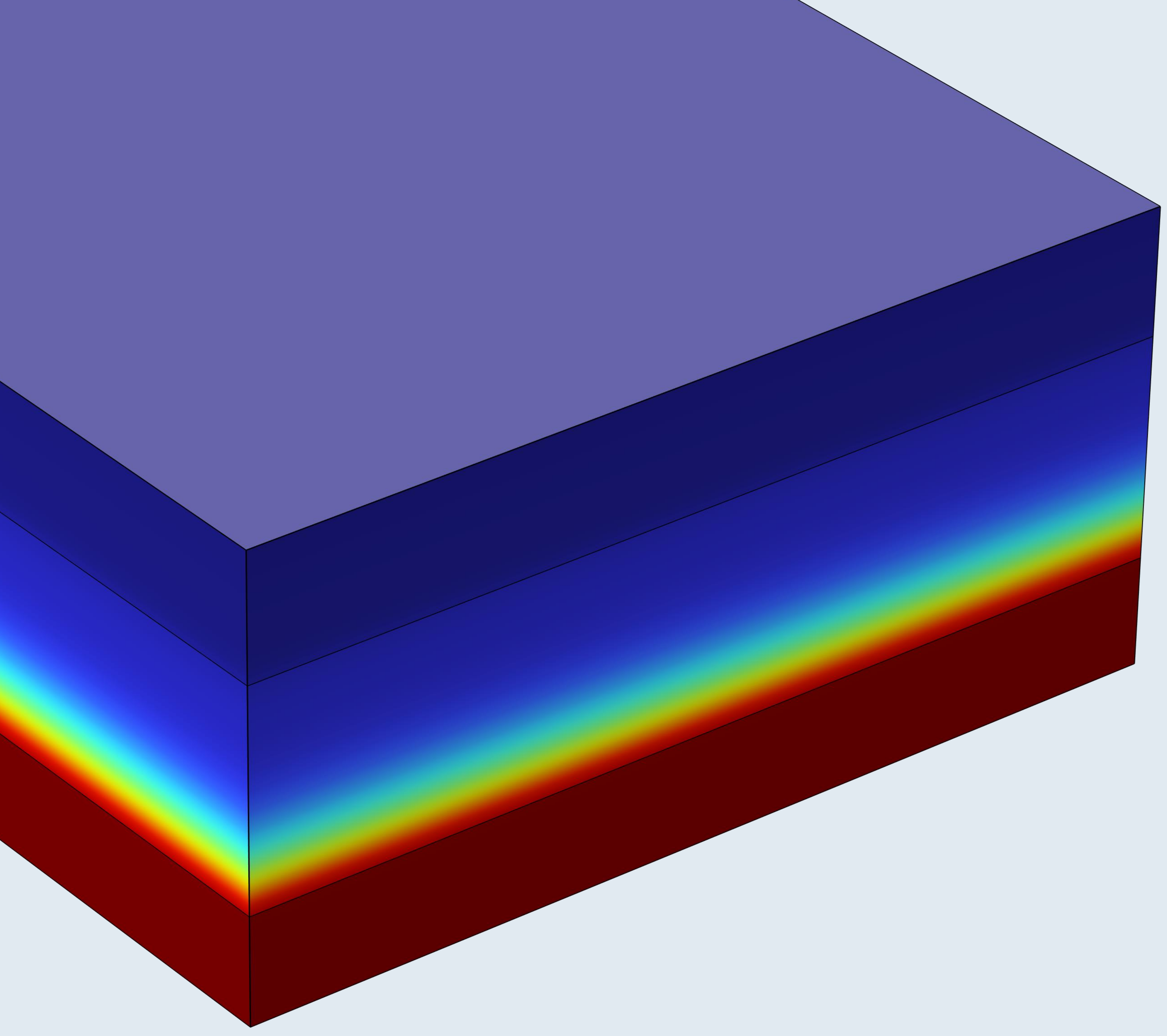

MXene Doped Perovskite Solar Cell Simulation for Enhanced Efficiency

MXene-doped perovskite solar cells, achieving 19.87% efficiency is simulated. Results offer insights into improvements and fabrication, highlighting Joule and nonradiative recombination heating effects.

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Abstract

MXene-doped perovskite solar cells with an ETL (TiO_2)/$MAPbI_3$ + MXene ($Ti_3C_2T_x$)/HTL (Spiro-OMeTAD) configuration were simulated. The study optimized the absorber layer's thickness and doping concentration, finding 500 nm and 1×10^{15} cm^{-3} to be ideal. This configuration achieved a maximum efficiency of 19.87%, a fill factor of 0.57, an open-circuit voltage (V_{OC}) of 1.10V, and a short-circuit current density (J_{SC}) of 31.97 mA/cm².

The analysis included the heating profile caused by Joule heating and nonradiative recombination. In addition, Charge carrier generation and recombination were also examined.

These findings provide essential insights for constructing and further researching MXene-based perovskite solar cells, emphasizing key factors for optimizing efficiency and managing thermal effects.

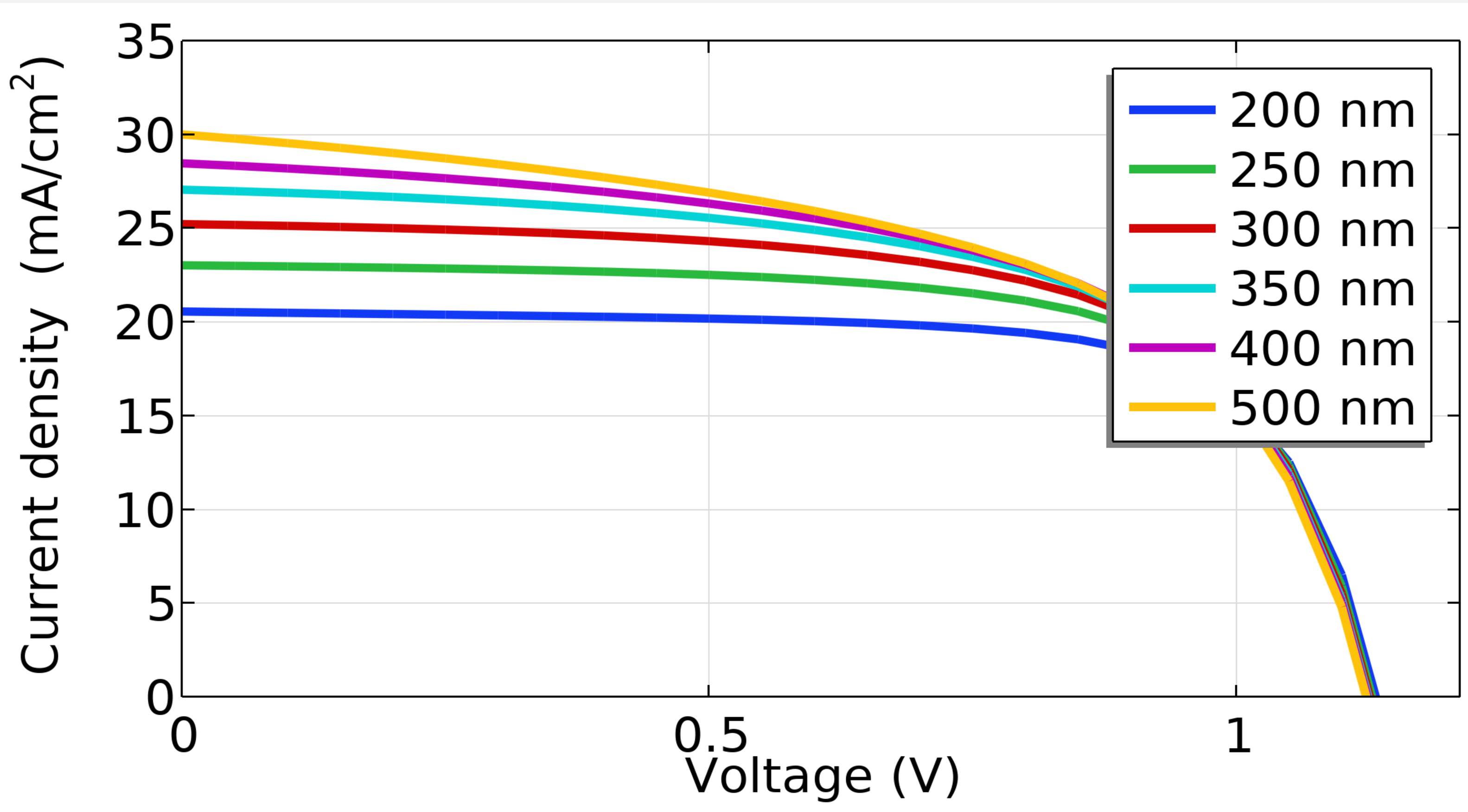

FIGURE 1. Varying thickness of the absorber layer.

Methodology

A 1D solar cell of cross-sectional area, 1cm² , was simulated using the *Semiconductor module*. The geometry, material properties, physics and mesh were applied and numerically analysed.

JV, thermal, and generation recombination graphs were analysed. The experiment was repeated by varying the thickness (200-500 nm) and doping concentration (1×10^{12} cm^{-3} to 1×10^{16} cm^{-3}) of the $MAPbI_3$ + MXene absorber layer. The photogeneration equation used was:

$$G(z) = \int_0^\infty \alpha(\lambda)\phi(\lambda)\exp(-\alpha(\lambda)z)d\lambda$$

Results

The study optimised the absorber layer's thickness and doping concentration, identifying 500 nm and 1×10^{15} cm^{-3} as ideal. This configuration achieved a maximum efficiency of 19.87%, a fill factor of 0.57, an open-circuit voltage (V_{OC}) of 1.10V, and a short-circuit current density (J_{SC}) of 31.97 mA/cm².

The heating profile, including Joule heating and nonradiative recombination, was analysed. Joule heating primarily occurred at the absorber layer's start, while nonradiative recombination heating was concentrated in each layer's midsection. Charge carrier generation and recombination were examined, with generation occurring at photon incidence sites and recombination within each layer.

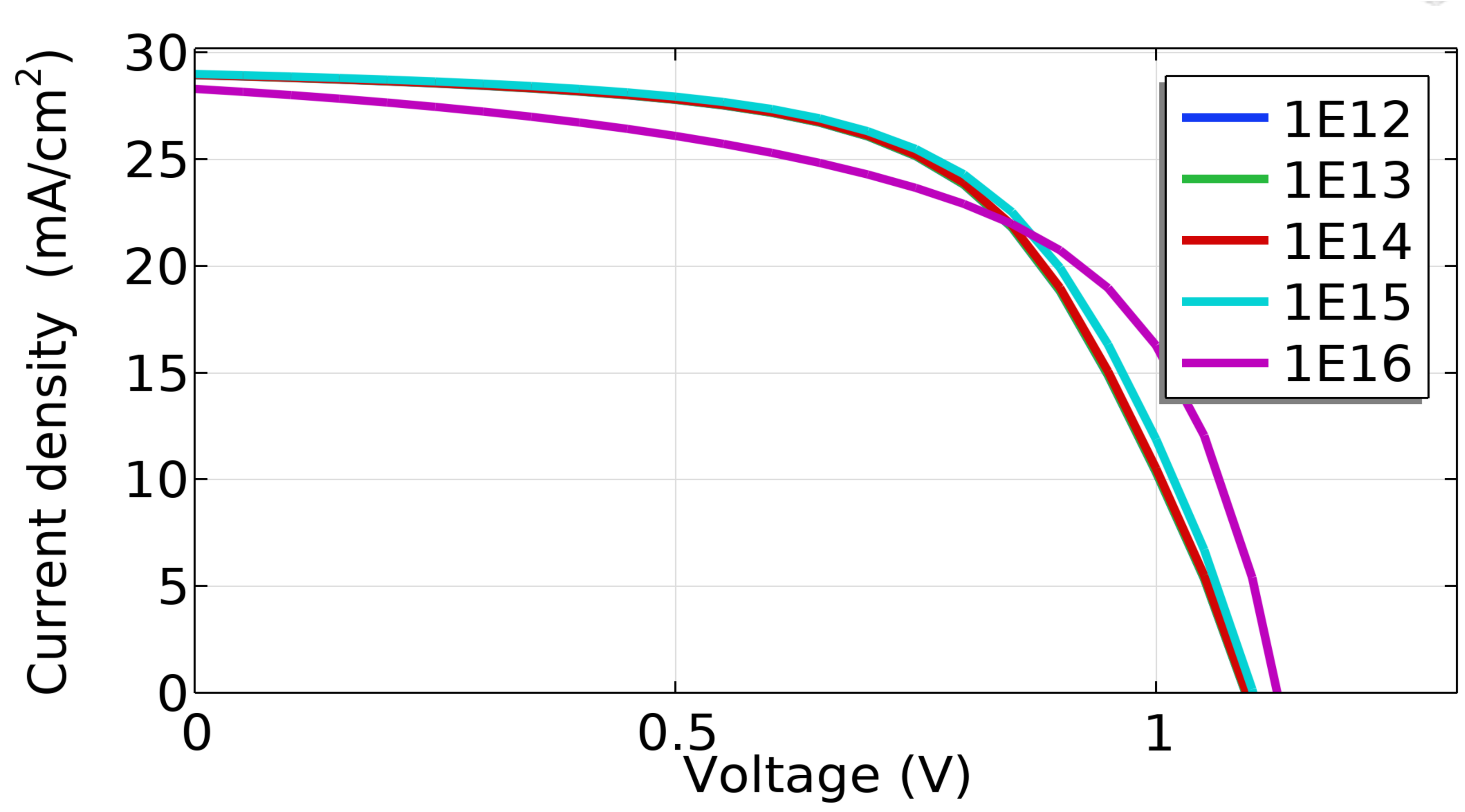

FIGURE 2. Varying doping concentration of the absorber layer.

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