MXene Doped Perovskite Solar Cell Simulation For Enhanced Efficiency

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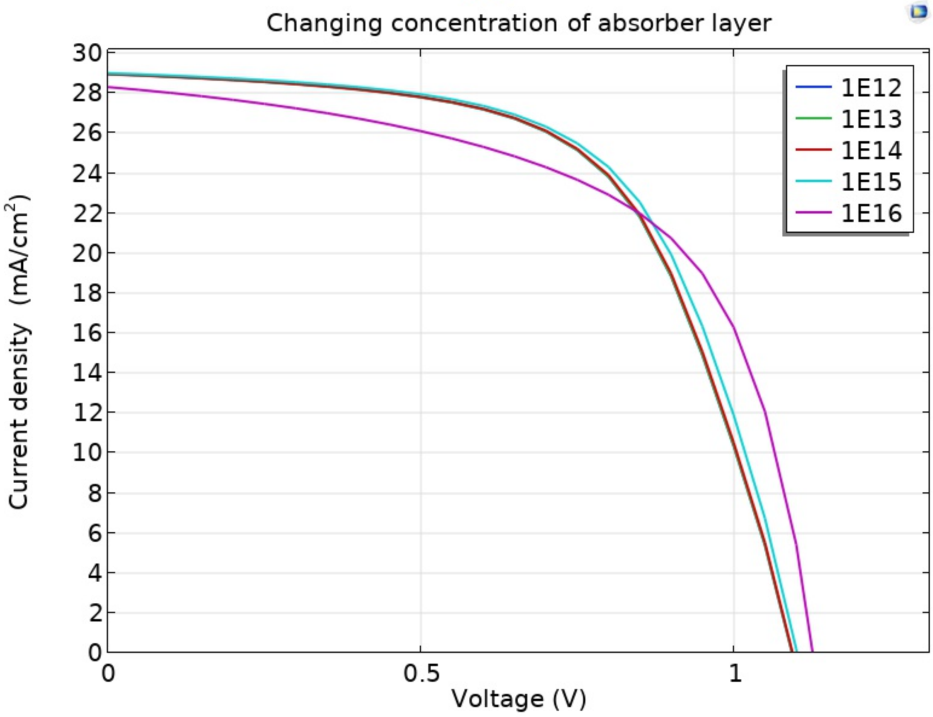
Abstract

The incorporation of two dimensional MXenes with perovskite solar cells have garnered much attention in recent years. MXenes of the form Ti3C2Tx have shown unique electrical capabilities due to its surface terminating functional group, Tx. Additionally, the inclusion of this material to perovskite solar cells has resulted in enhanced efficiency and improved optoelectronic performances. In the present work, COMSOL Multiphysics was used to simulate MXene doped perovskite solar cells consisting of an electron transport layer (ETL), absorber layer consisting of perovskite (MAPbI3) and MXene (Ti3C2Tx) and hole transport layer (HTL) with a configuration of ETL/MAPbI3+MXene/HTL. For the materials, TiO2 (120 nm) was used as the ETL and Sprio-OMeTAD (140 nm) was used as the HTL. The impact of both thickness and doping concentration of the absorber layer (MAPbI3+MXene) were thoroughly studied to boost its efficiency. The ideal variation in thickness and doping concentration was then used to inform the design of an optimal solar cell structure which achieved a maximum efficiency of 19.46%, a fill factor of 0.61, open-circuit voltage (Voc) of 1.11V and short-circuit current density (Jsc) of 29.03 mA/cm2. To the best of our knowledge, this is the first time COMSOL Multiphysics was used to simulate perovskite solar cells which contained 2D Ti3C2Tx MXene materials. The results therefore give meaningful guidance and insight into the fabrication and further study of MXene doped perovskite solar cells.

Figures used in the abstract

(a)



(b)

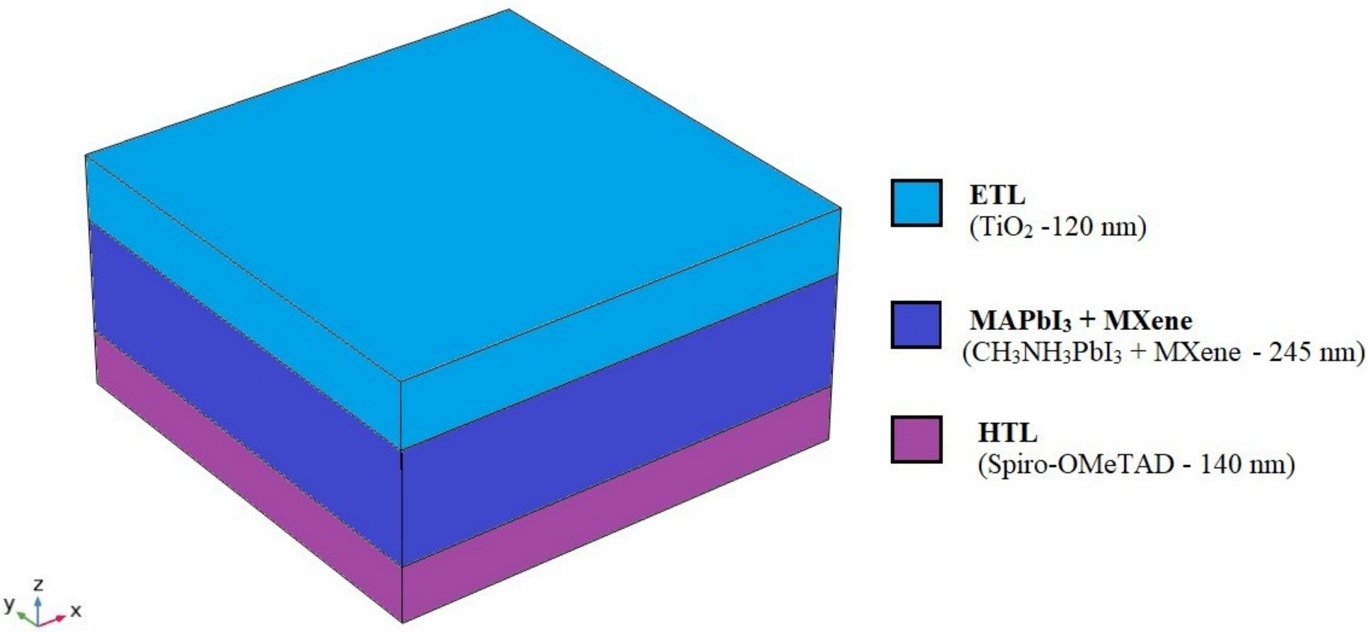


Figure 1 : (a) JV graph with various doping concentrations of the absorber layer. (b) Representation of the multijunction solar cell structure simulated.

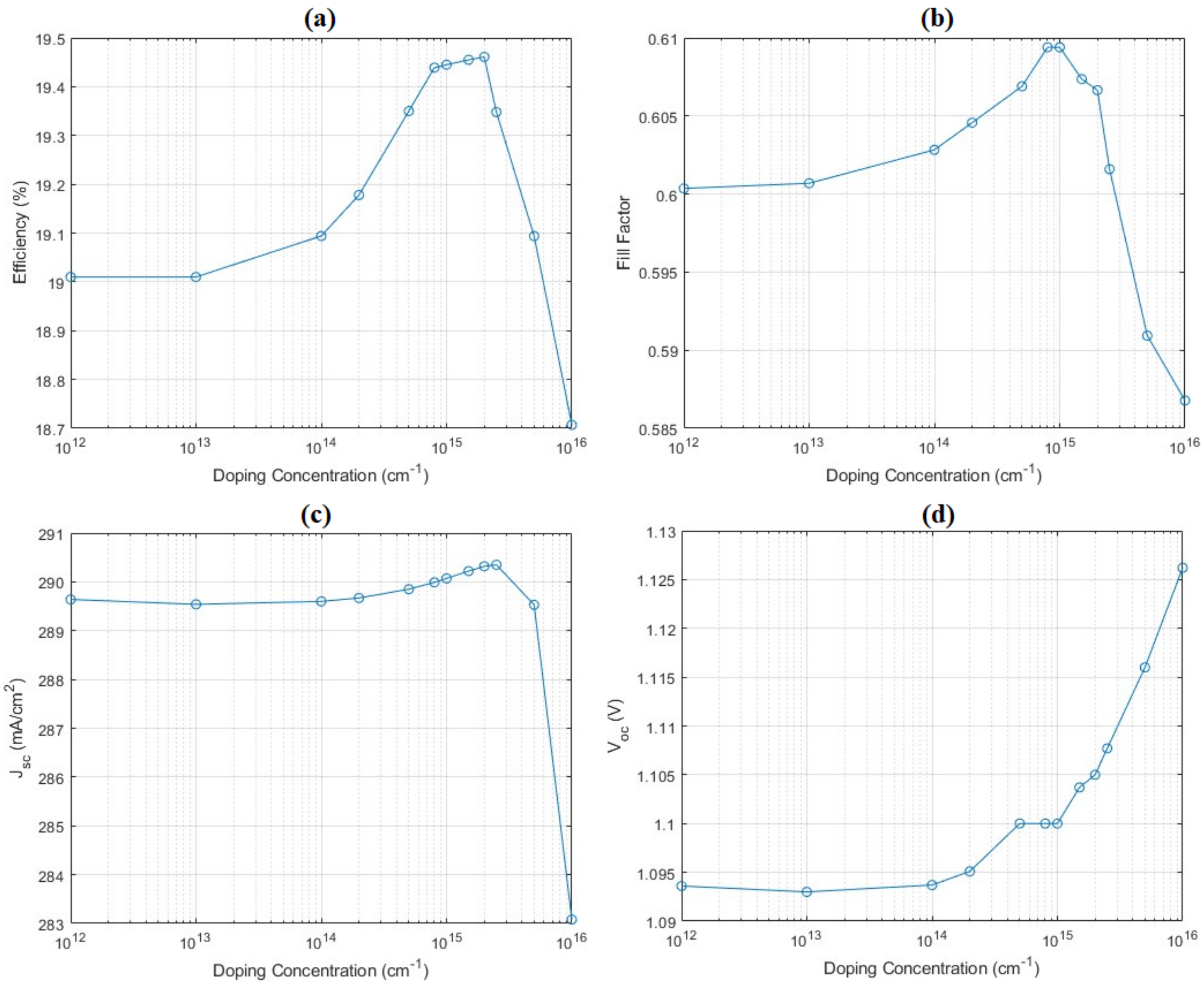


Figure 2 : (a) Efficiency vs. Doping concentration (b) Fill factor vs. doping concentration (c) Short circuit current density vs doping concentration (d) Open circuit voltage vs. doping concentration graphs for the simulated multijunction structure.

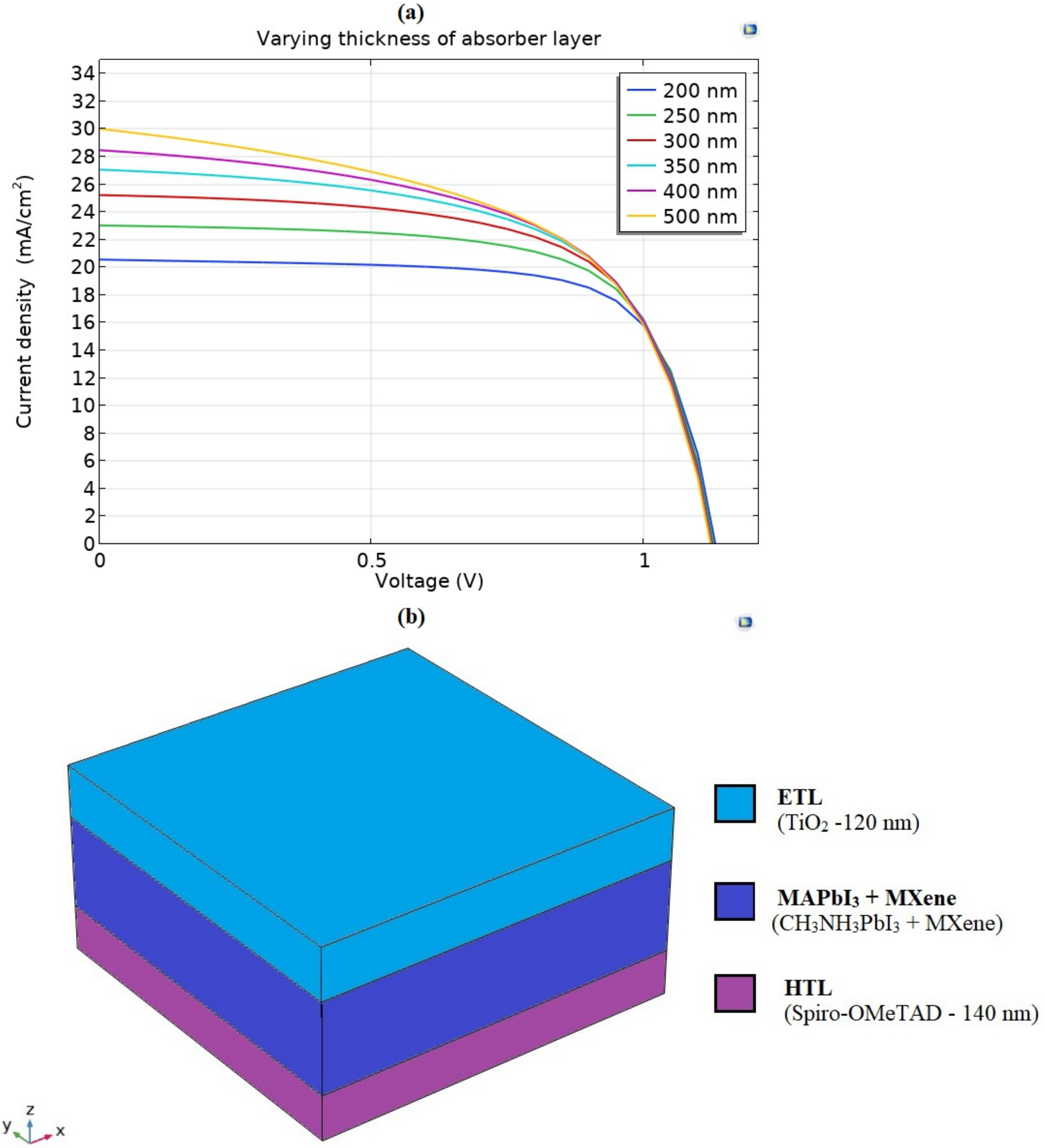


Figure 3 : (a) JV graph with various thicknesses of the absorber layer. (b) Representation of the multijunction solar cell simulated.

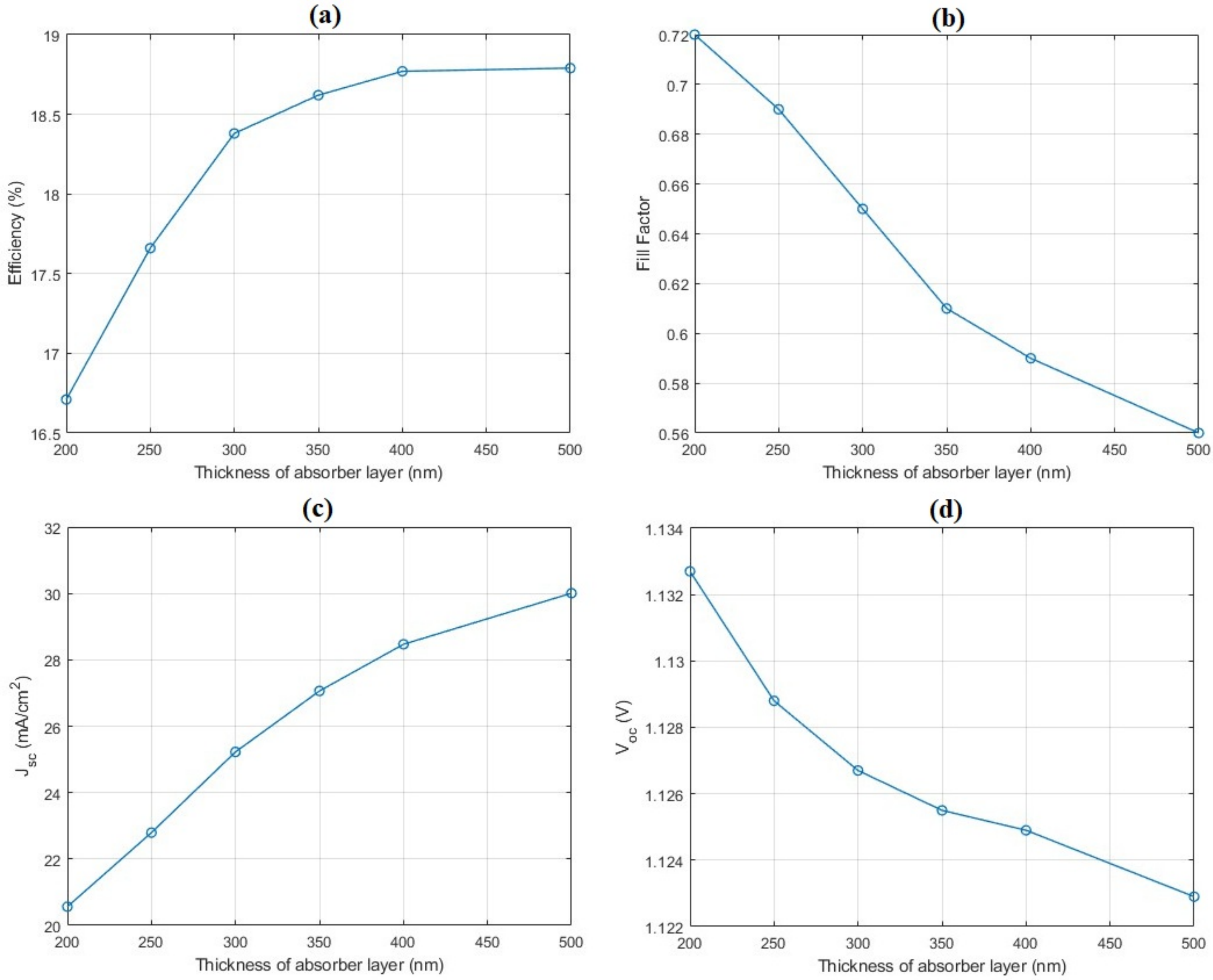


Figure 4 : (a) Efficiency vs. thickness of absorber layer (b) Fill factor vs. thickness of absorber layer (c) Short circuit current density vs thickness of absorber layer (d) Open circuit voltage vs. thickness of absorber layer graphs for the simulated multijunction