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FEM Analysis and Optimisation of High-Performing MXene Integrated Tandem $MAPbI_3$/ $MASnI_3$ Perovskite Solar Cell

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Venue: FST 414, 3rd Floor Natural Sciences Building

Zoom link: https://sta-uwi-edu.zoom.us/j/97128198187?pwd=Sfhb2JkkGFVKQD7yczif9fQFpK1CpC.1

ABSTRACT

Integration of MXene materials into the structure of solar cells has gained much attention in recent years due to their high electrical conductivity and tunable work function. In addition, modelling and simulation of novel device architectures have proven to be a valuable approach to developing highly efficient solar cells. As a result, this study investigates the performance enhancement via MXene-integrated double perovskite tandem solar cells using the finite element method (FEM) implemented in COMSOL Multiphysics. By applying appropriate boundary conditions and solving the coupled semiconductor governing equations, the optical, electrical, and thermal behaviour of the device was characterised. Six experimentally reported MXene materials were first identified from the literature and incorporated into a double perovskite tandem architecture by substituting the electron transport layer (ETL) and absorber layers to determine the most effective configuration. Among the candidates, TiO_2-Ti_3C_2 employed as the ETL produced the best baseline performance, achieving an efficiency of 28.60%. The TiO_2-Ti_3C_2 MXene-based electron transport layer (ETL), combined with a methylammonium lead iodide ($MAPbI_3$) / methylammonium tin iodide ($MASnI_3$) tandem absorber structure and a Spiro-OMeTAD (2,2′,7,7′-tetrakis(N,N-di-p-methoxyphenylamine)-9,9′-spirobifluorene) hole transport layer (HTL) device was then systematically optimised by tuning layer thicknesses and doping concentrations, yielding a maximum power conversion efficiency (PCE) of 39.90% with a fill factor (FF) of 88.60%, an open-circuit voltage (V_{OC}) of 1.0397 V, and a short-circuit current density (J_{SC}) of 43.196 mA cm^{-2}. Performance gains were interpreted through analysis of absorbance and photogeneration rates, thermal loss mechanisms (Joule heating and non-radiative recombination heating), and key electrical factors including Shockley-Read-Hall (SRH) recombination and energy level alignment. The improvements are attributed to the high theoretical efficiency ceiling of dual-absorber tandem devices (~46%) and enhanced charge transport and extraction enabled by the TiO_2-Ti_3C_2 MXene acting as conductive nanowire-like pathways. These findings provide practical design guidance for the next generation of high-performance perovskite tandem solar cells and indicate that the proposed optimised devices are feasible to fabricate using existing manufacturing methods.

Keywords: MXene, Perovskite Solar Cell, Finite Element Method (FEM), COMSOL Multiphysics, Optimisation.