

# CHARGE TRANSPORT LAYERS ENGINEERING IN PEROVSKITE SOLAR CELLS

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Photovoltaic (PV) technology, which directly converts solar energy into electrical energy, is regarded as one of the most promising renewable and clean energy technologies. Currently, developing low-cost and highly efficient PV technology is a major research focus in both academia and industry. In this context, perovskite solar cells (PSCs), utilizing metal halide perovskites [ABX<sub>3</sub>, where A = CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> (MA<sup>+</sup>), CH(NH<sub>2</sub>)<sub>2</sub><sup>+</sup> (FA<sup>+</sup>), Cs<sup>+</sup>; B = Pb<sup>2+</sup>; X = Cl, Br, I] as light-harvesting materials, are gaining significant attention due to their simple fabrication process and high-power conversion efficiency (PCE).

In the coming days, eliminating non-essential charge carrier recombination in devices and enhancing device stability will be formidable challenges and key focuses of the next stage of research. In all different architectures, the charge carrier transfer processes at the interfaces—namely, the perovskite/electron transport layer (ETL) interface and the perovskite/hole transport layer (HTL) interface—along with the interfacial materials, play crucial roles in achieving high PCE and stability. Suitable ETL and HTL can enhance charge carrier extraction and reduce recombination. In this presentation, we briefly examine recent advances and provide a perspective on charge transport layer engineering for highly efficient and stable perovskite solar cells (PSCs).

The perovskite/ETL interface is crucial for electron extraction, transfer, and charge recombination dynamics, thereby significantly influencing PSC performance. Some researchers focus on optimizing the energy level alignment at the perovskite/ETL interface to enhance electron extraction and transport efficiency. Common strategies to achieve optimal energy alignment include designing novel ETLs with more suitable energy levels, tuning energy levels through doping, and inserting an interlayer between the ETL and perovskite layer. This work reports the influence of atomic layer deposition (ALD) using its variants as thermal ALD, remote plasma ALD (RPALD), and direct plasma ALD on the physical parameters of the as-deposited SnO<sub>x</sub> films. The deposition process and chemical composition are related to their electronic band structure such as valence band maximum, conduction band minimum, band gap, and work function [1].

As crucial as the ETL, the HTL is responsible for efficient hole extraction at the perovskite/HTL interface, hole transport within the HTL bulk, and the prevention of undesired charge recombination processes, all of which contribute to exceptional

photovoltaic performance. Our focus is on identifying the optimal oxidizing agent to achieve the best electronic band structure of Ni<sub>1-x</sub>O films for use as an efficient hole transport layer (HTL) in perovskite solar cells (PSCs). X-ray photoelectron spectroscopy (XPS) confirms the non-stoichiometric nature of Ni<sub>1-x</sub>O films synthesized by PEALD in both thermal and plasma-enhanced modes. Specifically, Ni<sub>1-x</sub>O films synthesized using O<sub>2</sub> as a co-reactant in PEALD mode exhibit a high density of Ni<sup>3+</sup> (18 at. %), associated with nickel vacancies (VNi), which confirms their p-type conductivity. Moreover, ultraviolet photoelectron spectroscopy (UPS) indicates that the work function ( $\phi$ ) and the depth of the valence band maximum (VBM) can be modulated depending on the co-reactant employed, allowing variations of up to 1 eV between TALD and PEALD synthesis. Our results suggest a better energy band alignment between Ni<sub>1-x</sub>O and perovskite when PEALD is employed.

[1] M.A. Martínez-Puente, J. Tirado, F. Jaramillo, R. Garza-Hernández, P. Horley, L.G. Silva Vidaurri, F.S. Aguirre-Tostado, E. Martínez-Guerra, Unintentional Hydrogen Incorporation into the SnO<sub>2</sub> Electron Transport Layer by ALD and Its Effect on the Electronic Band Structure, *ACS Appl. Energy Mater.* 4 (2021) 10896–10908. <https://doi.org/10.1021/acsaem.1c01836>.