MXenes for Interface Engineering in Halide Perovskite Photovoltaic

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Perovskite solar cells (PSCs) have emerged as one of the most promising next-generation photovoltaic (PV) technologies due to their high efficiencies and simple solution-based fabrication processes, comparable to conventional PV systems. Interface engineering plays a critical role in multi-layered PSCs by controlling many properties of the overall system. We previously demonstrated that graphene and other 2D materials, such as MoS_2, can effectively tune interface properties and improve cell efficiency.[1,2] In this talk I will present the discuss about the $Ti_3C_2T_x$ and other MXenes with different surface terminations (T_x) as an effective strategy to modulate the work function (WF) of both the perovskite absorber and the electron transport layer (ETL), thus optimizing the perovskite/ETL interface and enhancing cell performance and stability.

Using ultraviolet photoemission spectroscopy and Density Functional Theory (DFT) calculations, we demonstrate that incorporating $Ti_3C_2T_x$ into halide perovskite and ETL enables WF tuning without altering other electronic properties. We establish a nonlinear correlation between the terminal group composition and the resulting WF for both standalone MXenes and MXene/perovskite composites. Our results [3] show that the dipole moment induced by $Ti_3C_2T_x$ at the perovskite/ETL interface can modify the band alignment between these layers, leading to significant performance improvements. Specifically, MXene-modified PSCs in a direct (nip) configuration show a 26% increase in power conversion efficiency (PCE) and reduced hysteresis compared to reference cells. Similarly, for the inverted (pin) configuration using a NiO/perovskite+MXenes/PCBM stack, comparable enhancements were observed.[4] Specifically, using MXenes on the n-side of a pin cell structure (NiO/perovskite/C60/BCP/Cu) significantly enhances cell stability, achieving T90 > 2000 h under continuous light soaking at Maximum Power Point in ambient conditions and T80 > 1000 h under thermal stress at 85 °C.[5]

I will also show as MXenes combined with other 2D materials can be effectively used in perovskite/silicon tandem cell [6], modules and panels paving the way for possible industrialization of the MXene-Perovskite PV.

References

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