Efficient and stable perovskite solar cells: new materials and modeling

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Perovskite solar cells (PSCs) have attracted widespread attention in academia and industry due to their high-power conversion efficiency (PCE) and potential for low-cost, sustainable, and large-scale manufacturing. We have incorporated two-dimensional (2D) materials to enhance the performance of double-cation mixed halide perovskite (Cs0.17FA0.83Pb(I0.83Br0.17)3) solar cells. We developed a Nb2O5 ETL layers adding Ti3C2Tx MXene into a solution processable ink [1]. The addition of MXene increased the PCE (19.46% for the champion device) and the stability (96% of its original PCE after 500 hours) compared to pristine devices. The improved performance of the Nb2O5–Ti3C2 is attributed to the alignment of the energy bands between perovskite and the ETL layer. In inverted or p-i-n PSCs we used an ultra-thin poly(methyl methacrylate) (PMMA) layer to passivate interfacial defects between the perovskite and the ETL layer [2]. With the addition of Ti3C2Tx MXene resulted in improvement of the PSC photovoltaic parameters, boosting their efficiency to 21.30 ± 0.51% (22.1% for the benchmark PSC). The enhanced performance is attributed to a reduction of trap state densities accompanied by mitigation of non-radiative recombination. The PMMA:MX based devices maintained 95% of their original PCE after 3000 h (ISOS-D-1I) and took 3X longer to reach T80 compared to the control PSC under heat and light soaking (ISOS-L-2). In another study [3], the deposition of Nb2O5 as an electron transport layer via slot die coating was systematically investigated. These Nb 2 5 layers were used as electron transport layers in n-i-p perovskite devices. Current density versus voltage scans were utilized to evaluate the device performance, alongside transient analysis. Under optimal coating conditions, efficiencies up to 12 % were obtained. We will also present a conceptual framework for characterizing photovoltaic devices by integrating cyclic voltammetry (CV) and impedance spectroscopy (IS) [4]. This framework is constructed from a microscopic, multi-mode perspective that explicitly accounts for drift, diffusion, displacement, and memory contributions. We derive comprehensive analytical expressions for current-voltage relationships and complex admittance. Our model reveals the inseparable connection between hysteresis behaviors in current-voltage characteristics observed in CV and the apparent capacitive and inductive behaviors seen in IS spectral analysis.

The authors acknowledge FAPESP (Projects: 2020/12356-8 and 2013/07296-2), FINEP, CAPES and CNPq (INCT NanoVida) for financial support.

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