JNPV 2025

Modelling of Ion Migration in Perovskite-based Solar Cells and Application to the Metastability Phenomena Observed in Luminescence

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Perovskite-based solar cells (PSCs) are among the most promising candidates for next generation photovoltaic technologies, attracting international researchers' attention. Despite achieving high efficiencies at the laboratory scale, their performance under real operating conditions -such as under different illuminations and electrical bias- remains unclear. In particular, PSCs exhibit changes in luminescence intensity over a wide range of different timescales, from minutes to several hours, indicating complex underlying mechanisms. In addition, the stability is still the Achilles heel of perovskite solar devices. One of the most detrimental degradation mechanisms is linked to ion migration [1]. The reorganization of ions, promoted by biassing, can induce corrosion by reacting with the metal electrodes [2],[3]. Hence, deeper understanding of the different degradation mechanisms and how the ions affect the perovskite performance under electrical excitation is necessary.

In the present study, we use one dimensional drift-diffusion modelling of PSCs considering both electronic and ionic moving carriers [4] to simulate current-voltage (*JV*) curves and electroluminescence (EL), tracking energy diagram and carriers' distribution evolution, to deeply understand the impact of physical and chemical parameters such as ionic concentration and ionic mobilities on the device's performance. In particular, transient regimes are investigated and linked to performance or degradation mechanisms in the device. Ultimately, the simulated results are compared to experimental *JV* and EL measurements to validate the accuracy of developed model. This combined analysis will provide deeper insights into device performance and further support the optimization of the fabrication protocols of PSCs.

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