Simulation Insights on Experimental Dark Recovery in Perovskite Solar Cells

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Perovskite solar cells continue to show great potential in photovoltaic applications due to their high efficiency and low manufacturing costs. However, their long-term stability remains a critical challenge. While degradation processes have been widely investigated [1], [2], less attention has been given to recovery dynamics. Gaining deeper insights into these processes is key for understanding metastable behaviors and improving the overall long-term stability of the cells.

In this work, we explore recovery during dark phases through a novel simulation framework that couples optical and drift-diffusion models with a genetic algorithm. This algorithm enables the statistical reproduction of experimental JV characteristics, serving as a basis to simulate degradation and recovery mechanisms. Each mechanism is simulated by varying a single material parameter (e.g., charge carrier mobility, defect density, doping level) independently.

To interpret these mechanisms, we employ a correlation space approach that maps the evolution of key electrical parameters (Voc, Jsc, FF) during recovery. These simulated trajectories are compared to those extracted from experimental JV data, allowing us to discriminate which physical mechanisms best align with observed behavior.

Our approach focuses on distinguishing recovery mechanisms active in the dark and assessing their reversibility. By comparing these to processes occurring under illumination, we aim to better disentangle the complex interactions governing perovskite solar cell behavior. This understanding can help guide strategies to enhance device stability by targeting critical irreversible degradation.

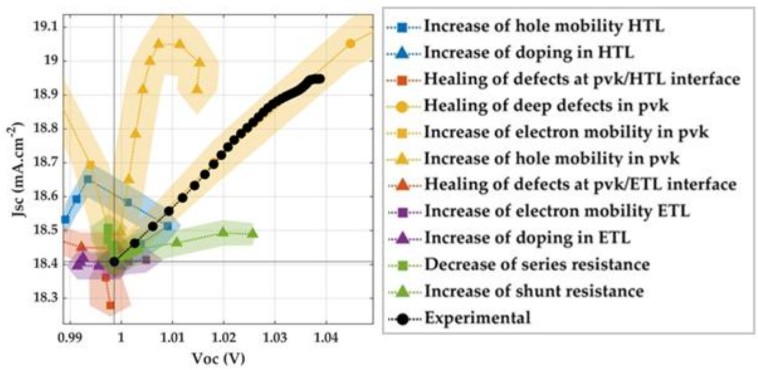

Figure 1. *Correlation plot of a recovery example indicating that simulated deep defect healing in the perovskite aligns with experimental recovery behavior.*

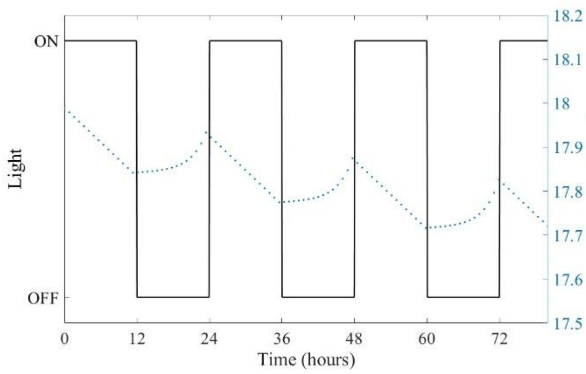

Figure 2*. Schematic of synthetic data illustrating perovskite solar cell recovery during dark-light cycling.*

[1] Boyd, C. C., Cheacharoen, R., Leijtens, T., McGehee, M. D. (2019). *Understanding Degradation Mechanisms and Improving Stability of Perovskite Photovoltaics*, Chem. Rev., 119(5), 3418–3451.

[2] Dunfield, S. P. et al. (2020). *Mechanistic Understanding of Degradation in Perovskite Devices*, Adv. Energy Mater., 10, 1904054.