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Analysing Instability Mechanisms of Perovskite Solar Cells with 2D/3D Interfaces Under Light- and Heat-Operational Condition

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Abstract

Two-dimensional/three-dimensional interfaces (2D/3D) are widely used in perovskite solar cells to obtain excellent optoelectronic properties. It improves long-term stability under mild conditions but becomes destructive in harsh aging conditions. Here, we show that the Ruddlesden-Popper (RP) perovskite is intrinsically unstable and gradually decomposes into PbI2 and metallic lead (Pb^0) under photo-thermal aging. The RP/3D structure collapse leads to a rise in vacancies that force iodide ions to migrate readily to the anode. The anode undergoes a redox reaction with iodide/polyiodide, leading to a decrease in mobility and doping concentration of the transport layer and a sharp increase in the series resistance. Dion-Jacobson (DJ)/3D is found to be much more structurally stable and effective in blocking the iodide migration process. However, its rebound of iodide causes iodide to form an interstitial defect in the bulk, exacerbating non-radiative recombination. Finally, introducing DJ to the 3D grain boundary rather than the top surface can confine the mobile ion inside the grain and suppress the cation phase segregation. As a result, the ultra-stable perovskite solar cells have an extrapolated T_{80} of over 1000 hours at 85 ℃ and 1 sun.

Keywords

Perovskite Solar Cells, Two-Dimensional, Operational Stability, Interfaces, High Temperature, Light-Soaking