Meso-Crowned Porphyrin as a Dual Cavity Hybrid Macrocycle for Improving the Efficiency and Stability of Perovskite Solar Cells

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Streszczenie

Perovskite solar cells (PSCs) have achieved remarkable power conversion efficiencies (PCEs) and cost-effective fabrication processes. However, defects in the bulk and interfaces of perovskite materials, as well as Li^+ migration (especially in n–i–p regular architecture), which are used to enhance the conductivity and hole mobility of spiro-OMeTAD, can significantly impact device performance and stability. Herein, we report a rationally designed *meso*-crowned porphyrin derivative (**[12]-C-4POR**) featuring dual macrocyclic binding sites, i.e., a porphyrin core for undercoordinated Pb^{2+} and a crown ether unit selective for Li^+ to suppress surface defects and mitigate lithium-ion migration simultaneously. The incorporation of **[12]-C-4POR** into perovskite films significantly reduced the trap-state density and suppressed non-radiative recombination, leading to improved charge-carrier dynamics. Devices treated with **[12]-C-4POR** delivered a champion PCE of 23.14%, surpassing the control device (21.6%), along with enhanced open-circuit voltage (V_{OC}) and fill factor (FF). More importantly, the passivated devices retained ∼95% of their initial PCE after 800 h of continuous operation, compared to ∼55% for the control. This study demonstrates a dual-site host–guest passivation strategy as an effective route to improve both efficiency and operational stability of PSCs.

Słowa kluczowe

host–guest complexation, meso-crowned porphyrin, passivation, perovskite solar cells, stability