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Skillfully Deflected the Question: A Small Amount of Piperazine-1,4-diium Iodide

Radically Enhances the Thermal Stability of CsPbI₃ Perovskite

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Supporting information



Figure S1. TG analysis of the pristine CsPbI₃ film. Three weight loss stages at 250 °C, 540 °C and 770 °C, corresponding to the sublimation of dimethylammonium iodide (DMAI), PbI₂ and CsI, respectively. The ratio of DMAI/CsI is calculated to be about 8.2% in the film.



Figure S2. Top-view SEM images of the CsPbI₃·xPZDI₂ films with different x values.



Figure S3. Grain-size distributions that are taken from the corresponding SEM images and relationship of the average grain size with $PZDI_2$ contents (x < 25%).



Figure S4. AFM images of $CsPbI_3 \cdot xPZDI_2$ films: (a) x = 0, (b) x = 0.5%, (c) x = 1% and (d) x = 10%.



Figure S5. Steady-state PL spectra of the CsPbI₃·xPZDI₂ films deposited on glass side.



Figure S6. XPS spectra of (a) C 1s and (b) N 1s for CsPbI₃, CsPbI₃ $\cdot 0.5\%$ PZDI₂ and CsPbI₃ $\cdot 100\%$ PZDI₂ films.



Figure S7. Comparison of XPS spectra of the CsPbI₃, CsPbI₃ \cdot 0.5%PZDI₂ and CsPbI₃ \cdot 100%PZDI₂ films: (a) Cs 3d, (b) I 3d and (c) Pb 4f.



Figure S8. FTIR and Raman spectra of the $CsPbI_3 \cdot xPZDI_2$ samples: (a) FTIR spectra of $CsPbI_3 \cdot xPZDI_2$ and $PZDI_2$ powder and (b) Raman spectra of $CsPbI_3 \cdot xPZDI_2$ film. The traces are shifted vertically for clarity.



Figure S9. Distributions of the (a) V_{oc} , (b) J_{sc} and (c) FF obtained from CsPbI₃, CsPbI₃·0.5%PZDI₂ and CsPbI₃·3%PZDI₂ C-PSCs.



Figure S10. *J*-*V* curves of the CsPbI₃ \cdot 0.5%PZDI₂ C-PSCs under forward and reverse scans. The hysteresis index is calculated to be 8.5%.



Figure S11. XRD patterns of the corresponding perovskite samples after heating at 100 °C for different duration: (a) CsPbI₃, (b) CsPbI₃·0.5%PZDI₂, (c) CsPbI₃·3%PZDI₂ and (d) MAPbI₃. The δ represents the yellow CsPbI₃ phase, while the P denotes the photoactive CsPbI₃ perovskite phases.



Figure S12. Data of the thermal stability tests of $CsPbI_3 \cdot xPZDI_2$ C-PSCs: Change of PV parameters with storage time at 85 °C in a dry air (RH ~ 10-20%): (a) $CsPbI_3$, (b) $CsPbI_3 \cdot 0.5\%PZDI_2$ and (c) $CsPbI_3 \cdot 3\%PZDI_2$.