

Supporting Information

Role of Water in Suppressing Recombination Pathways in CH₃NH₃PbI₃ Perovskite Solar Cells

Ankur Solanki^{1,†}, Swee Sien Lim^{1,2,†}, Subodh Mhaisalkar^{3,4} and Tze Chien Sum^{1,}*

¹Division of Physics and Applied Physics, School of Physical and Mathematical Sciences,
Nanyang Technological University, 21 Nanyang Link, Singapore 637371, Singapore

²Energy Research Institute @NTU (ERI@N), Interdisciplinary Graduate School, Nanyang
Technological University, Singapore 637553, Singapore

³Energy Research Institute @NTU (ERI@N), Research Techno Plaza, X-Frontier Block, Level 5,
50 Nanyang Drive, Singapore 637553, Singapore

⁴School of Materials Science and Engineering Nanyang Technological University Nanyang Avenue,
Singapore 639798, Singapore

[†]These authors have equal contribution to this work.

*Corresponding author. Tze Chien Sum: Tzechien@ntu.edu.sg

Results

X-ray Diffraction pattern

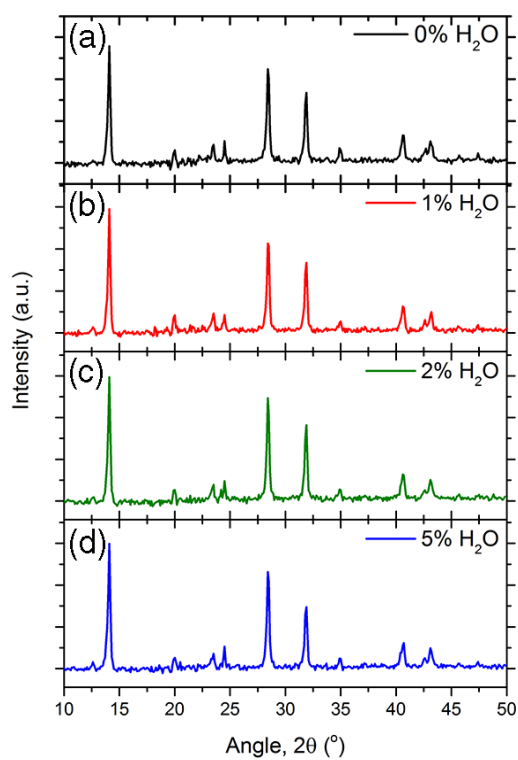


Figure S1. X-ray diffraction spectra of the different samples with varying H₂O additive concentrations: (a) 0%, (b) 1%, (c) 2% and (d) 5 vol% H₂O.

Scanning electron microscopy images

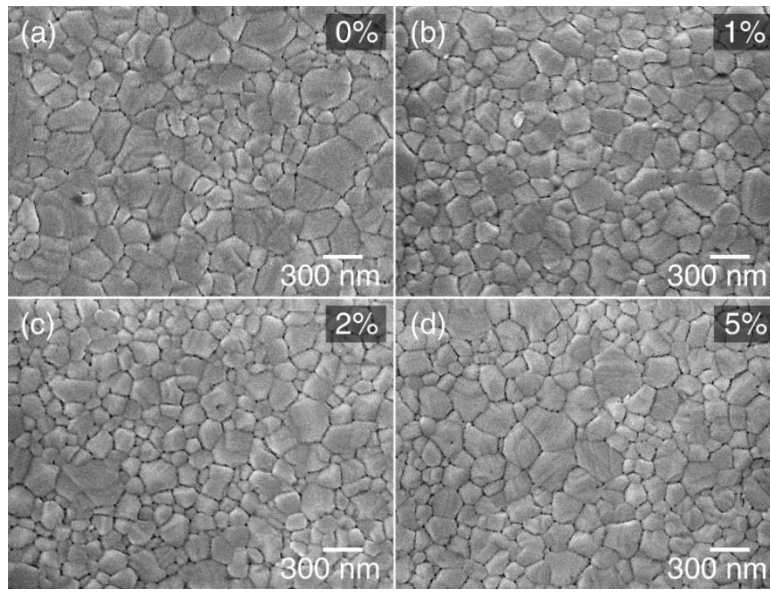


Figure S2. SEM images of perovskite films prepared from solutions with varying water additive concentration (a) 0%, (b) 1%, (c) 2% and (d) 5 vol% H₂O; 1% indicates perovskite solution with 1 vol% H₂O additive.

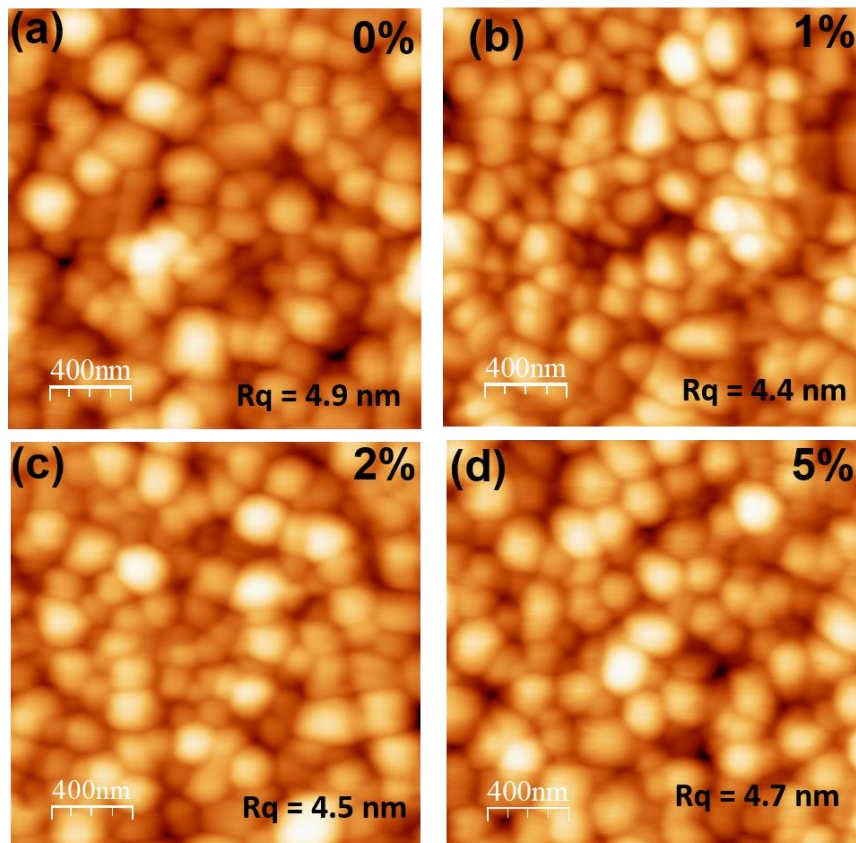


Figure S3: AFM images ($2\ \mu\text{m} \times 2\ \mu\text{m}$) of perovskite films prepared from solutions with varying water additive concentration with root-mean-square roughnesses of the various samples: (a) $Rq_{0\%} = 4.9\ \text{nm}$, (b) $Rq_{1\%} = 4.4\ \text{nm}$, (c) $Rq_{2\%} = 4.5\ \text{nm}$ and (d) $Rq_{5\%} = 4.7\ \text{nm}$ for the varying vol% H₂O-added perovskite films.

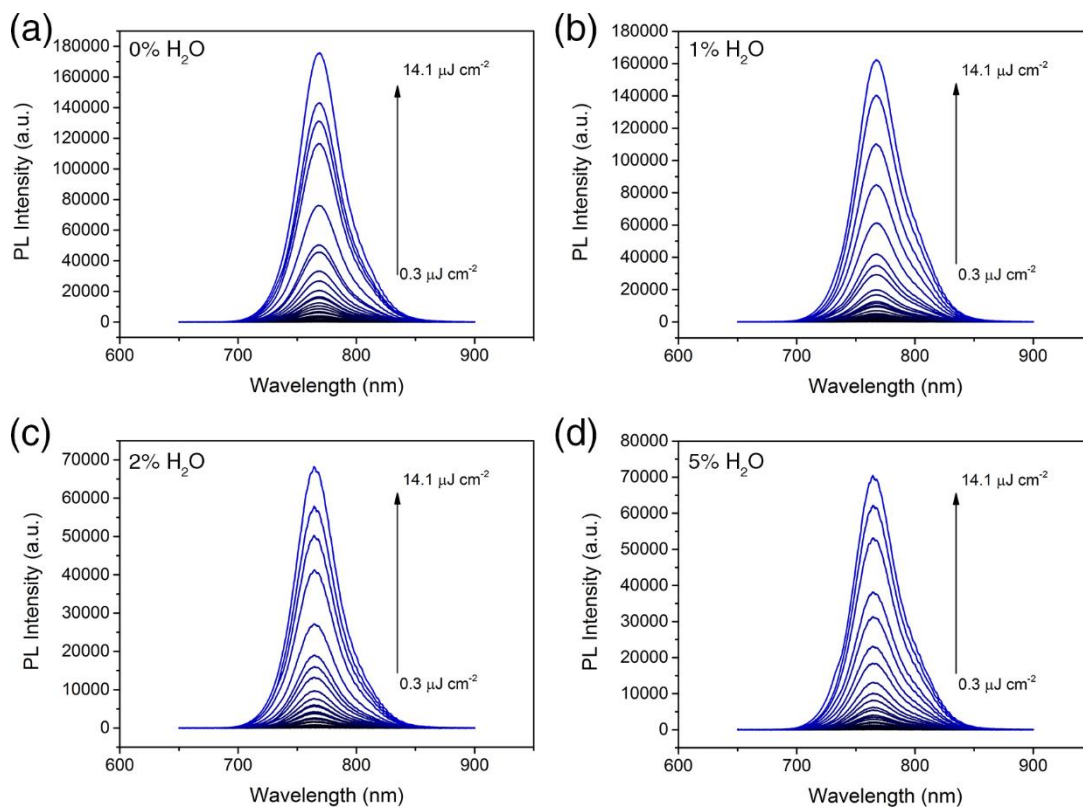


Figure S4. Power-dependent photoluminescence (PL) measured in the low fluence regime to extract trap densities in the perovskite films with varying H₂O additive concentrations: (a) 0%, (b) 1%, (c) 2% and (d) 5 vol% H₂O.

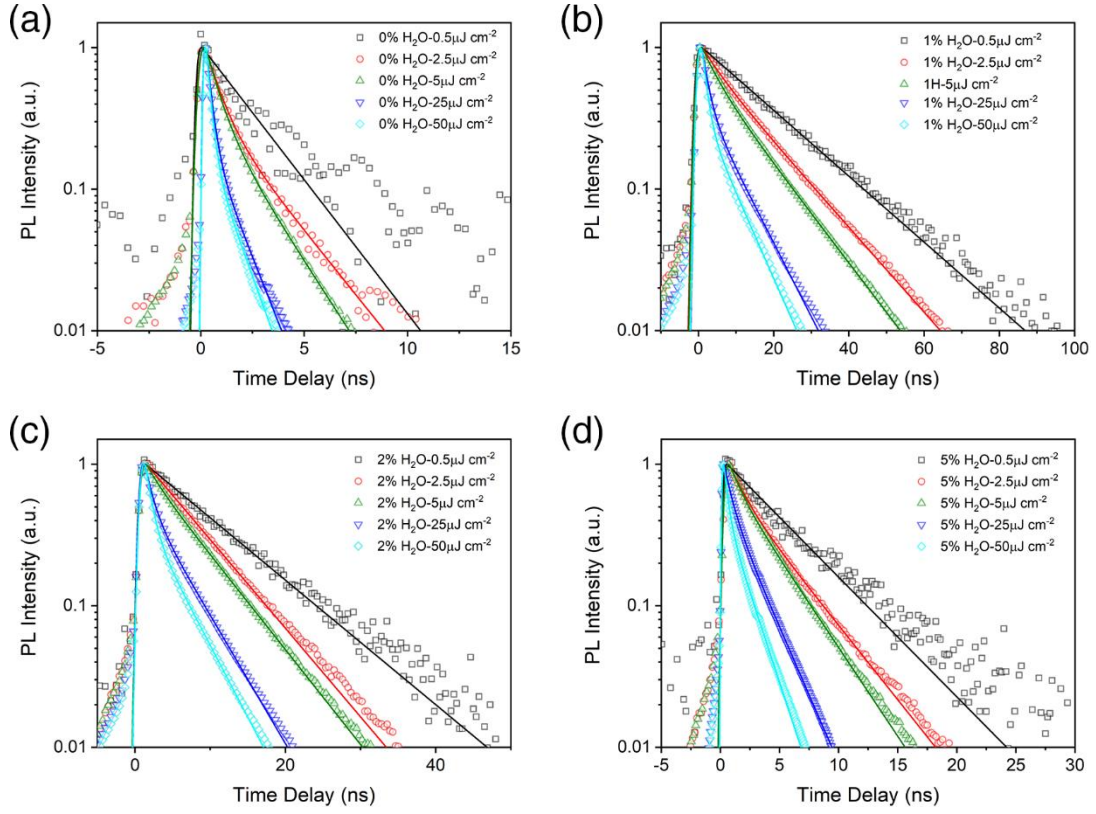


Figure S5. Power dependent time-resolved PL (TRPL) traces fitted with mono- or biexponential decay functions to extract the PL lifetimes and their associated amplitudes in the perovskite films with varying H₂O additive concentrations: (a) 0%, (b) 1%, (c) 2% and (d) 5 vol% H₂O.

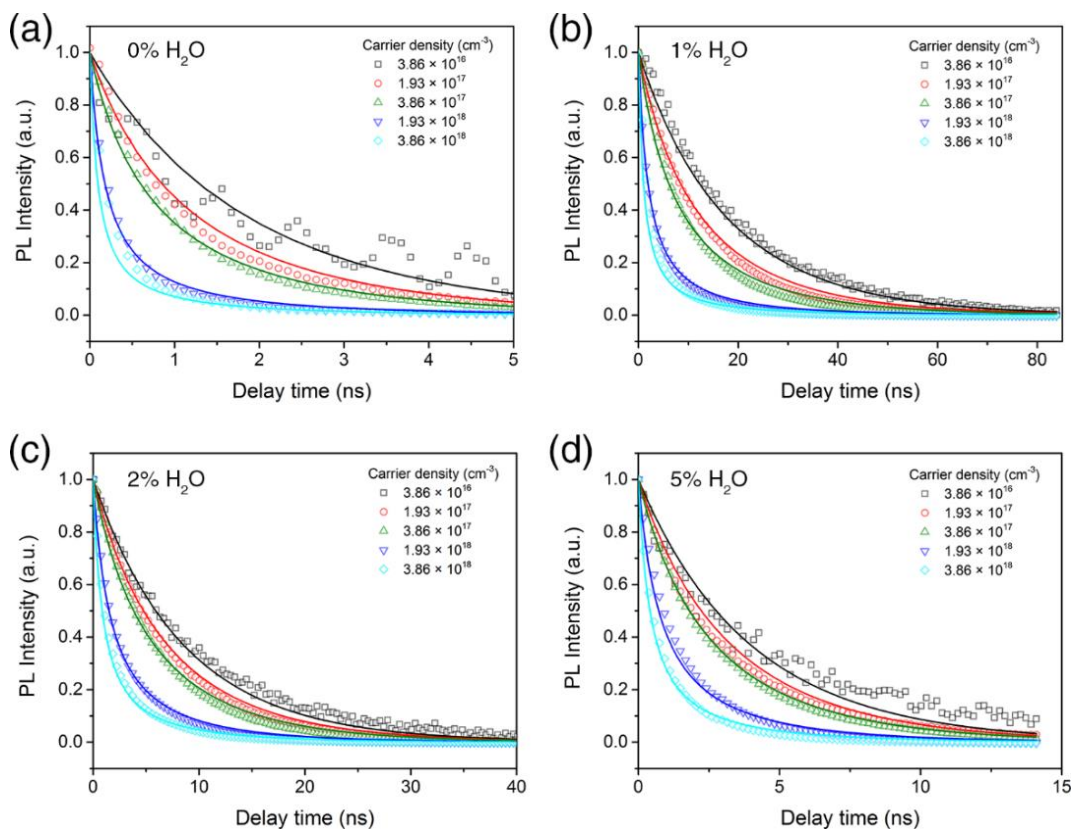


Figure S6. Power dependent TRPL traces fitted with the recombination rate equation (see main text) to extract the monomolecular and bimolecular recombination rate constants in the perovskite films with varying H₂O additive concentrations: (a) 0%, (b) 1%, (c) 2% and (d) 5 vol% H₂O.

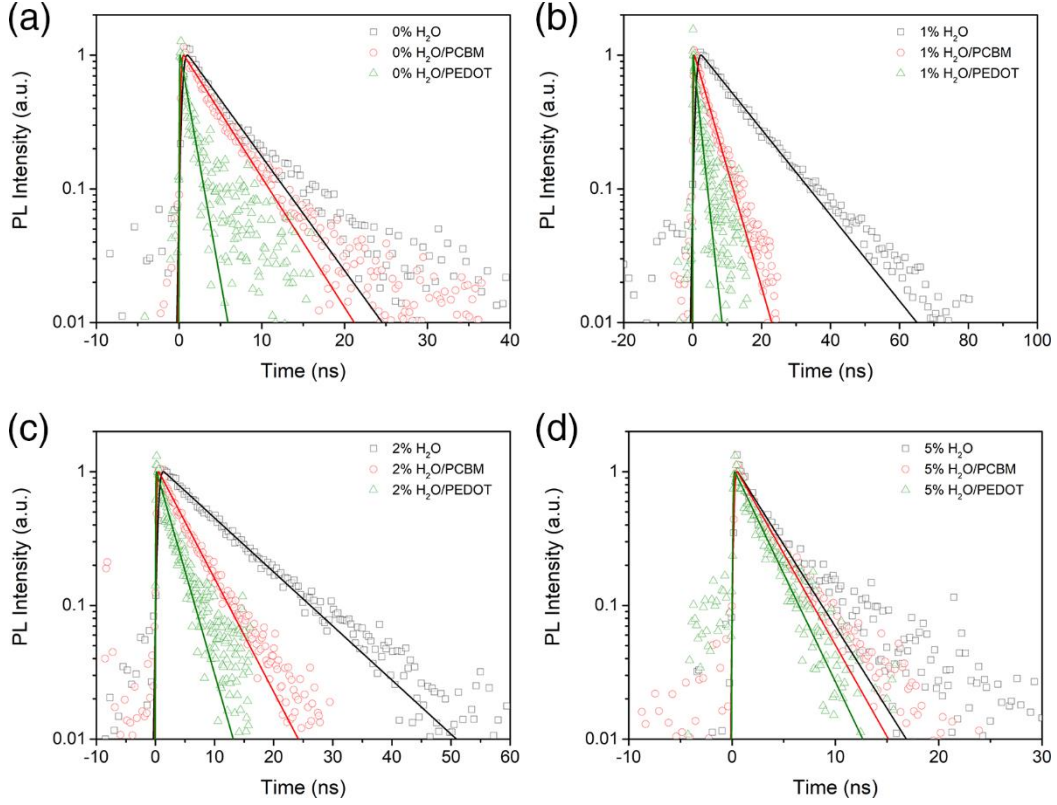


Figure S7. Diffusion length measurements of the in the perovskite films with varying H₂O additive concentrations: (a) 0%, (b) 1%, (c) 2% and (d) 5 vol% H₂O with the respective quencher (black: neat film, red: PCBM layer, green: PEDOT layer) measured at a fluence of 0.5 $\mu\text{J cm}^{-2}$. Symbols are the data obtained from PL measurements, solid lines are exponential fits.

Trap density calculation: Initial photogenerated carrier density in different perovskite films were estimated using Plank Equation ($\alpha E = nhc/\lambda$) (Equation S1), where α is the absorption coefficient at 600 ($=\lambda$) nm while E , n , h , c are excitation pump fluence, charge carrier density, plank constant and light velocity, respectively. α is calculated using equation $\alpha = I/L$ (Equation S2) where I is the absolute absorption intensity at 600 nm and L represents the film thickness (~ 275 nm). In order to estimate the defects density, the integrated steady state PL intensity for the different perovskite films was fitted with the model:

$$n_c(0) = \sum n_{TP}(0)(1 - e^{-k_1 I_{PL}}) + k_2 I_{PL} \quad \text{Equation S3}$$

where $n_c(0)$ and n_{TP} represent photogenerated charge carrier density and trap density, respectively while k_1 , k_2 are the constants.

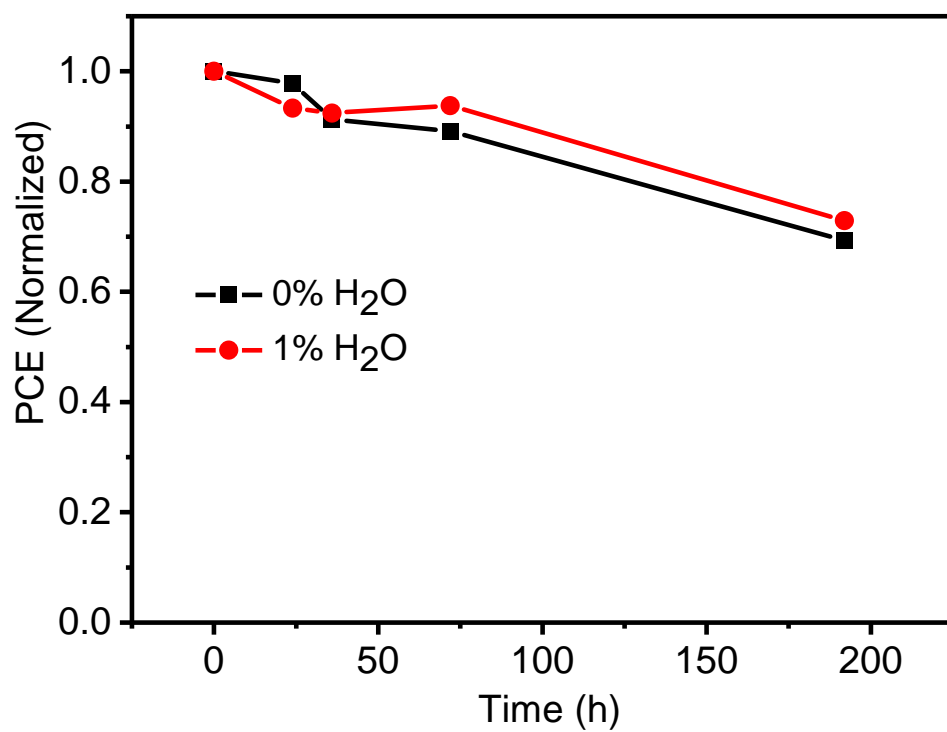


Figure S8: Comparative study of device degradation of 0% and 1% H₂O added solar cell devices.