Supporting Information

Air-stable hybrid perovskite solar cell by sequential vapor deposition in a single reactor

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UV-Vis Transmission Modelling

The transmission spectra were analysed with SCOUT[®] simulation software (<u>https://wtheiss.com</u>), employing an iterative method using Bruggeman Effective Medium Approximation¹ to mix quantities of PbI₂ and MAPbI₃ optical functions, such as the refractive index and extinction coefficient.^{2, 3} The experimental and modelled transmittance spectra of the PbI₂ and converted perovskite films are shown in Figure S2(c), with the fits depicting a good agreement between the experiments and simulations.

References

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Figure S1: (a) Schematic illustration of the home-built chemical vapour deposition system, (b) photographs of the deposited films with a yellow PbI_2 and the dark perovskites after different conversion times as labelled.



Figure S2: (a) Optical and (b) AFM micrograph of the as-deposited PbI_2 thin film on glass substrate showing high surface coverage and smooth grains. (c) Experimental and simulated transmittance spectra of the PbI_2 and perovskite films.



Figure S3: Scanning electron microscopy micrographs of the perovskite films after different conversion times, (a, b, c, and d) is 15, 30, 60, and 120 minutes, respectively. (e) Cross-sectional SEM micrograph of the 15-minute converted sample, depicting continuous grains across film thickness.



Figure S4: Optical micrographs of the perovskite films after different conversion times, (a) – (e) is 15 minutes – 120 minutes (scale is same in all) and (f - j) is AFM micrographs showing large perovskite grains (scale is same in all).



Figure S5: XPS measurements of the 90 minutes converted perovskite film, (a) XPS full survey, (b) XPS high resolution spectra of Pb(II) $4f_{7/2}$ and $4f_{5/2}$ transitions; (c) XPS high resolution spectra of I $3d_{5/2}$ and $3d_{3/2}$ transitions; (d) Pb/I atomic ratio depth profile; and (e) high resolution spectral depth profile of Pb(II) $4f_{7/2}$ and $4f_{5/2}$ transitions at different sputtering times showing the appearance of the metallic Pb (Pb⁰) peak.



Figure S6: Optical properties of the converted perovskites, (a) absorbance, (b) absorption coefficient, (c) refractive index, and (d) optical band extrapolation.



Figure S7: J-V characteristics measured at different days for (a) reverse and (b) forward scan.



Figure S8: Evolution of (a) open circuit voltage (V_{oc}), (b) short circuit current density (J_{sc}), (c) fill factor (FF) and the (d) power conversion efficiency (PCE) of the device measured for 21 days in reverse and forward scan.