

Supplementary information

for

[NH₃(CH₂)₆NH₃]PbI₄ as Dion-Jacobson Phase Bifunctional Capping Layer for 2D/3D Perovskite Solar Cells with High Efficiency and Excellent UV Stability

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Experimental Details

Materials and reagents: PbBr₂ (99.999%) was purchased from TCI Chemicals. SnCl₂·2H₂O (dihydrate, ACS, 98%) and PbI₂ (99.9985%) were purchased from Alfa Aesar. HC(NH₂)₂I (FAI), CH₃NH₃Br, 1,6-diaminohexane ammonium iodide (HDADI) were purchased from Xi'an Polymer Light Technology Corp. N, N-dimethylformamide (DMF, anhydrous, 99.8%), dimethyl sulfoxide (DMSO, anhydrous, 99.9%), 2-propanol (99.5%), chlorobenzene (99.8%), CsI (99.999%), acetonitrile and 4-tert-butylpyridine (TBP, 96%) were purchased from Sigma-Aldrich. Spiro-MeOTAD was purchased from Borun New Material Technology Co., Ltd. Lithium bis-(trifluoromethylsulphonyl) imide (99.95%), and FK 209 Co (III) TFSI salt were purchased from Dyesol.

Preparation of [NH₃(CH₂)₆NH₃]PbI₄ (2D, n=1) film: 186 mg HDADI and 230.5 mg PbI₂ were added in 1 mL DMF (Sigma-Aldrich), followed by stirring for 3 hr at 60 °C. After cooling and filtered, it was spin-coated on top of FTO substrate at 2000 rpm for 60 s.

UV testing method: The prepared perovskite films were placed under the UV lamp with a light intensity of 6.9 mW cm⁻² for irradiation for a certain time.

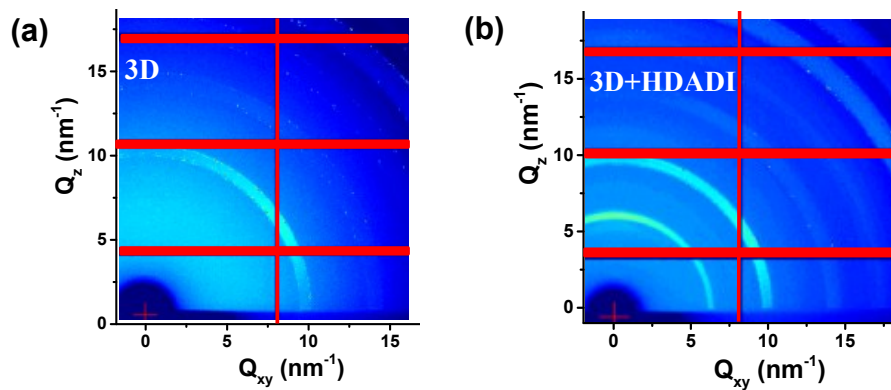


Figure S1. Grazing incidence wide-angle X-ray scattering images of 3D (a) and 3D+HDADI (b) film samples.

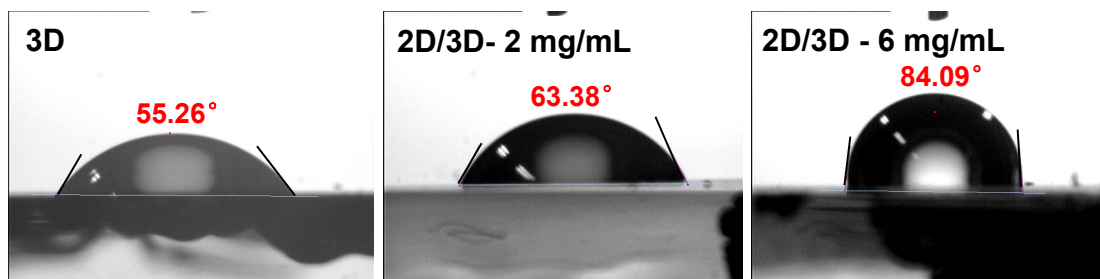


Figure S2. Water contact-angle test of 3D and 2D/3D based perovskite films, where 2 mg/mL and 6 mg/mL represent the concentrations of the HDADI isopropanol solution.

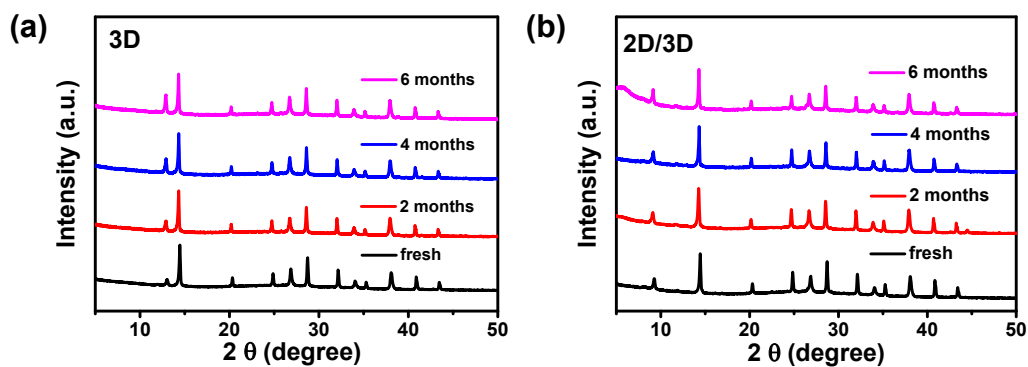


Figure S3. XRD patterns of (a) 3D, (b) 2D/3D. The sample was stored in $\approx 60\%$ RH humidity at ambient atmosphere in the dark condition without encapsulation.

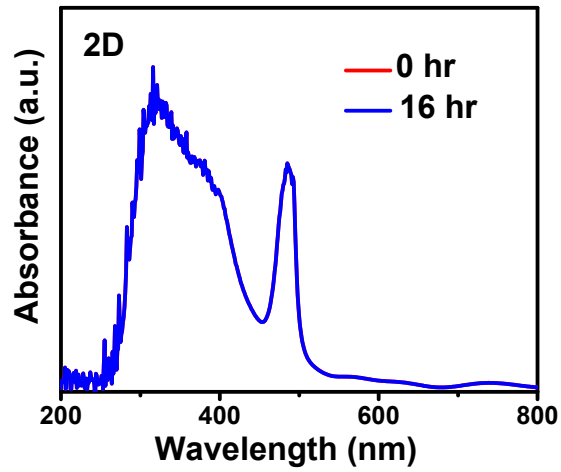


Figure S4. UV-vis absorption spectra of 2D perovskite films before and after exposing to the UV radiation for 16 hours.

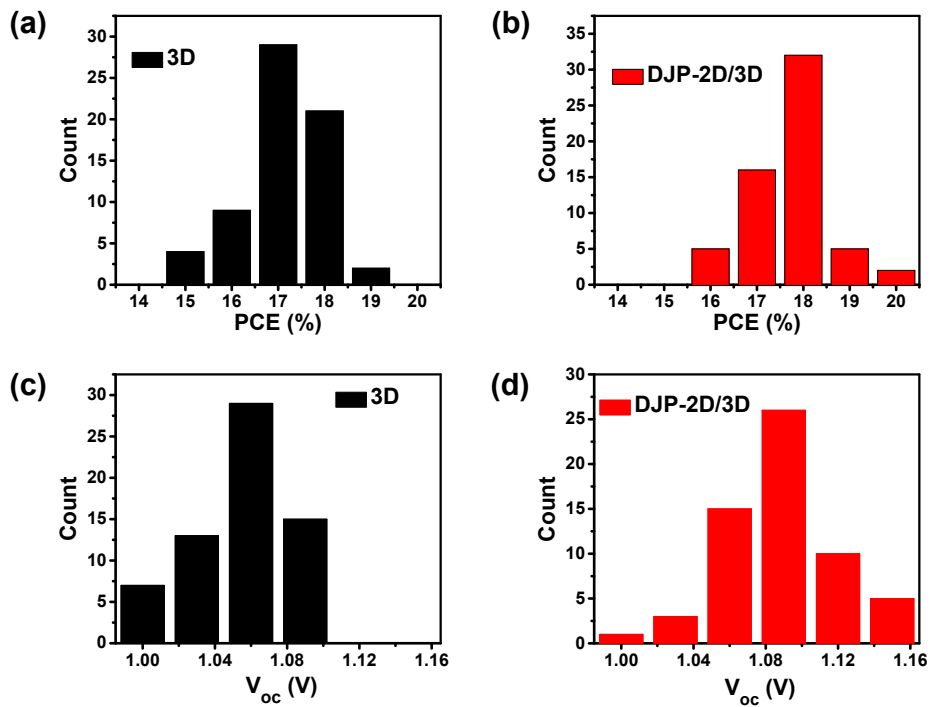


Figure S5. (a-b) Histogram of the number of cells as a function of PCE distributions under reverse scan direction of (a) 3D and (b) DJP-2D/3D based PSCs. (c-d) Histogram of the number of cells as a function of open-circuit voltage (V_{oc}) distributions under reverse scan direction of (c) 3D and (d) DJP-2D/3D based PSCs.

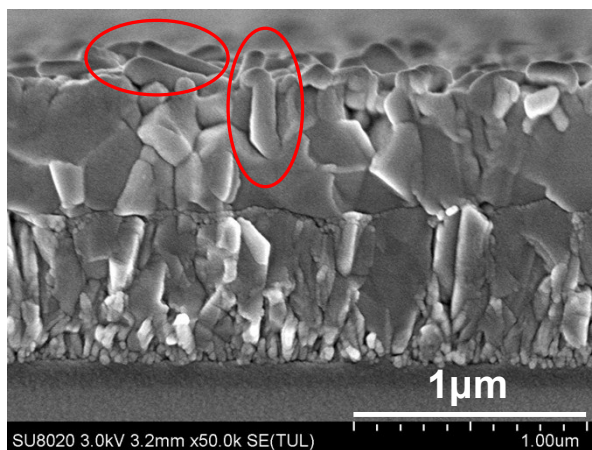


Figure S6. Cross-section SEM images of the DJP-2D/3D perovskite film deposited on FTO/SnO₂ substrate.

Table S1. Biexponential fitting decay profiles of 3D and DJP-2D/3D based Glass/Perovskite configurations.

Sample	τ_1 (ns)	A_1	τ_2 (ns)	A_2	τ_{avg} (ns)
3D	3.9	0.88	57.6	0.12	40
DJP-2D/3D	5.9	0.78	60.0	0.22	46

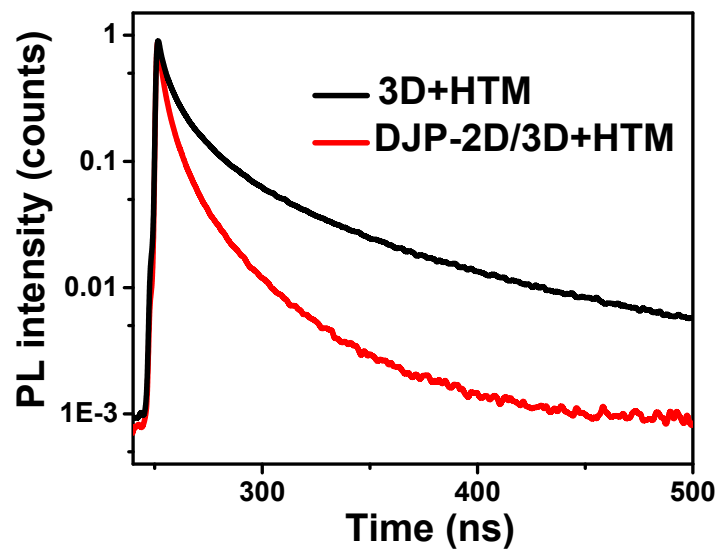


Figure S7. The time-resolved PL decay curves of the glass / Perovskite / HTM samples.