Supporting information

Supramolecular Interactions Using β-Cyclodextrin in Controlling Perovskite Solar Cell Performance

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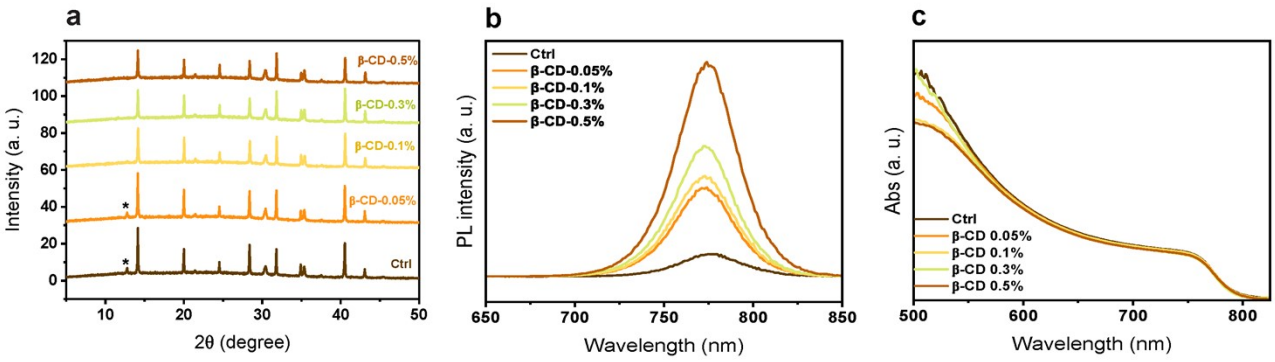

Figure S1. XRD pattern on ITO substrates covered by a SAM layer (star marks the XRD peak of PbI_2), (b) steady-state PL spectra (ITO/ MeO-2PACz/Perovskite), and (c) absorption spectra (Glass/Perovskite) of control (ctrl) and treated sample by various concentrations of β-CD.

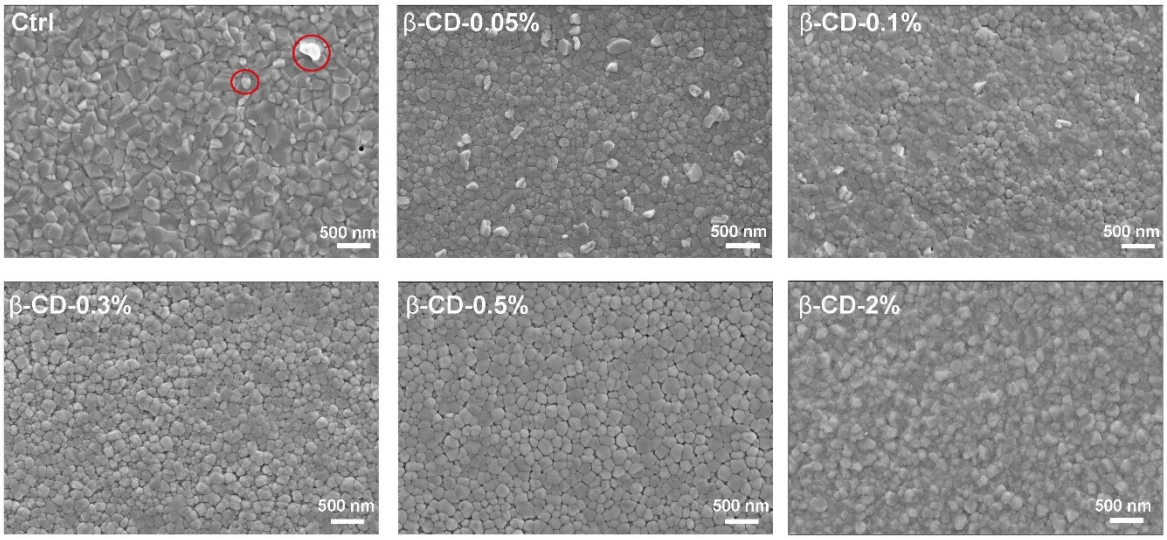

Figure S2. Top view SEM images of control (ctrl) and treated perovskite films with varying concentrations of β-CD. Red circles represent PbI_2 crystals.

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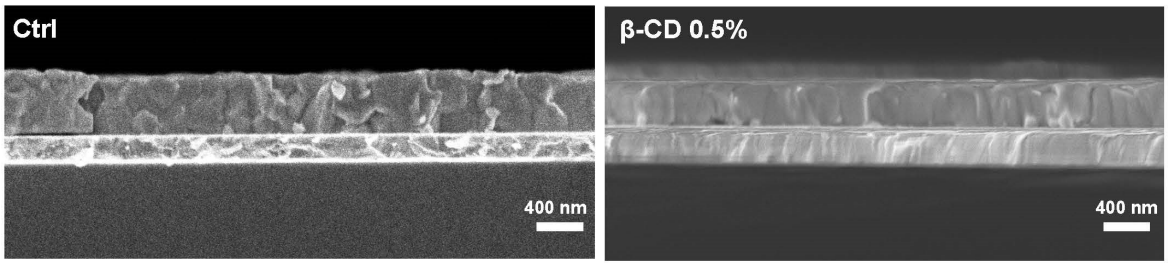

Figure S3. Cross section SEM images of control (left) and treated sample by 0.5% of β-CD (right).

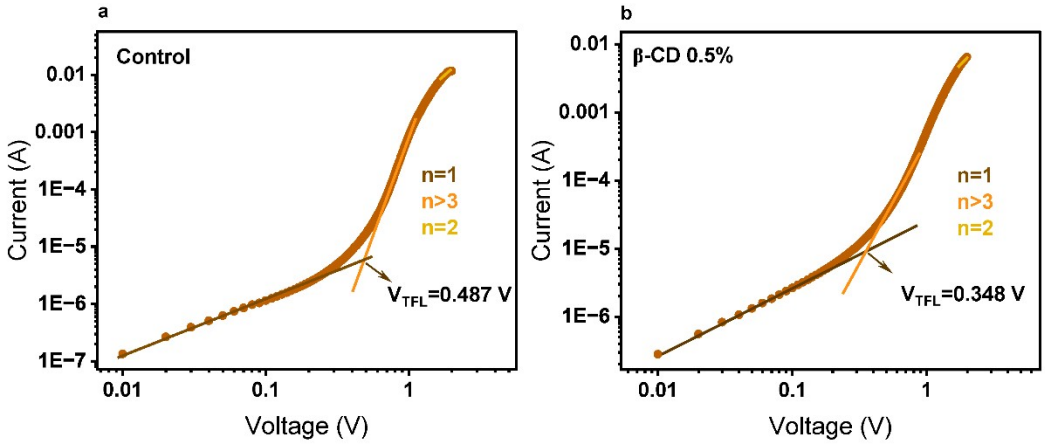

Figure S4. Space charge-limited current (SCLC) measurements of the electron-only devices (ITO/SnO_2/Perovskite (W/O or W/ β-CD)/PCBM/Ag).

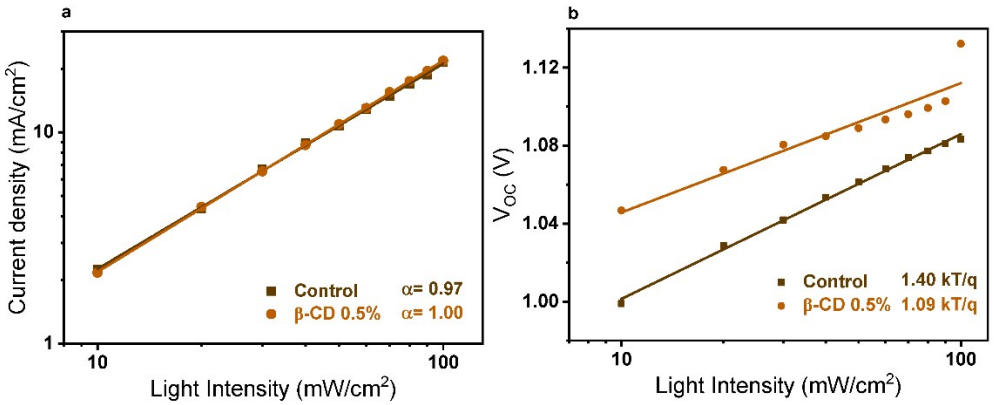

Figure S5. The dependence of a) J_{SC} and b) V_{OC} on the incident light intensity in case of (a) control and (b) treated sample by 0.5% of β-CD.

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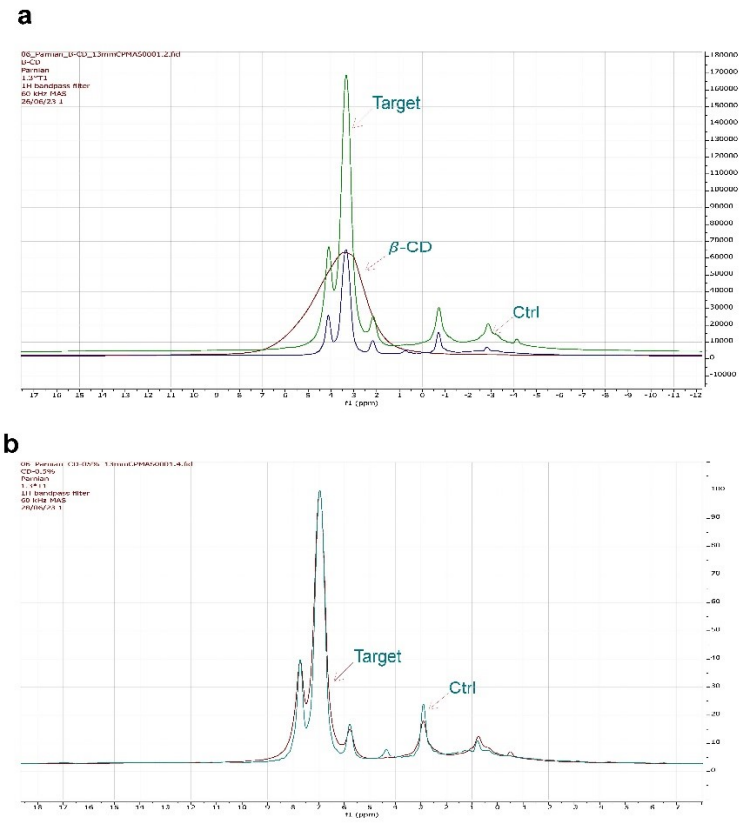

Figure S6. a) Solid-state NMR and b) normalized solid-state NMR of control, β-CD 0.5% treated perovskite and β-CD powders (Ctrl and target refer to pristine perovskite film and β-CD-treated perovskite film, respectively).

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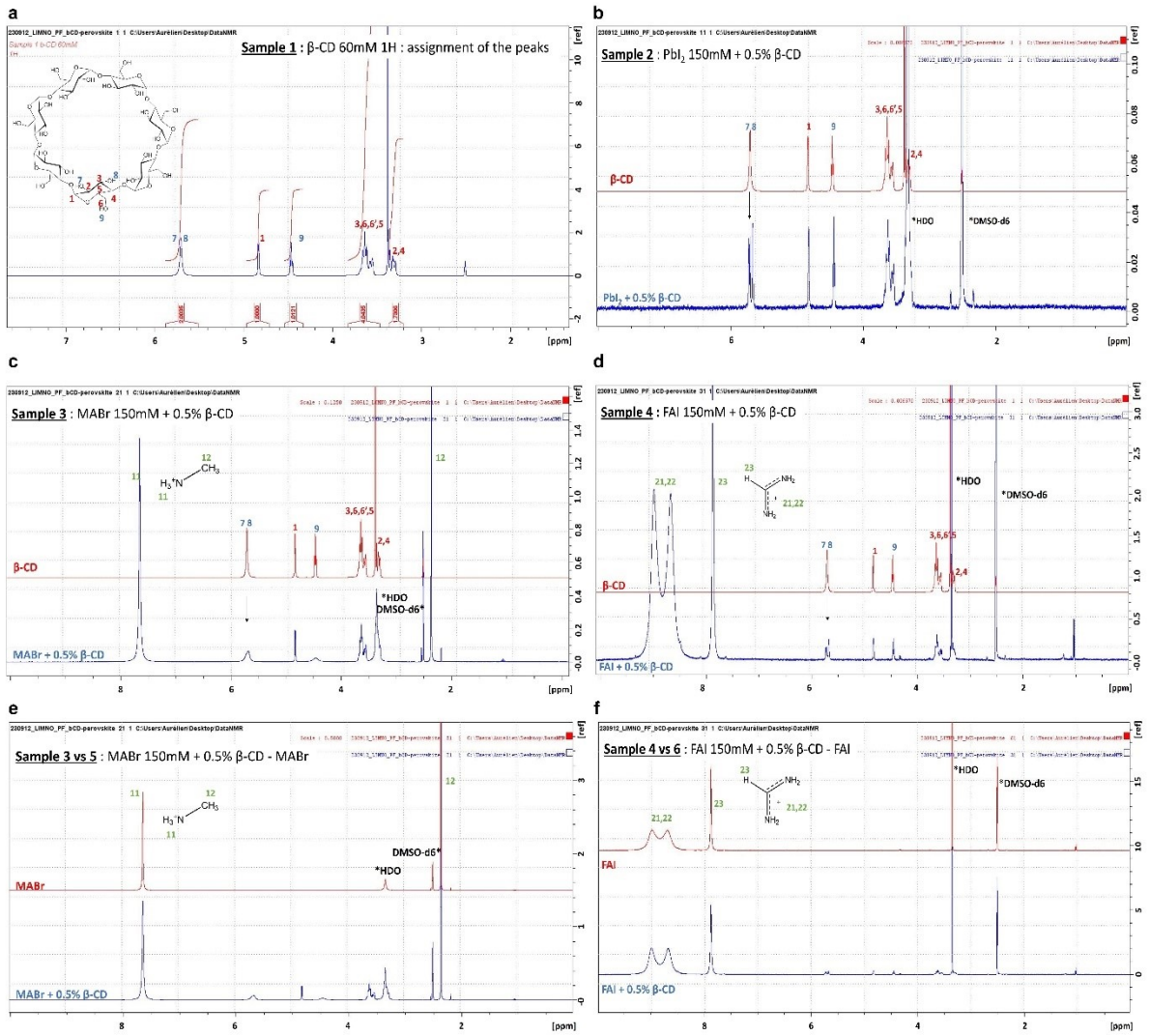

Figure S7. Solution ^{1}HNMR of a) β-CD, b) PbI_2 + 0.5% β-CD, c) MABr+ 0.5% β-CD, d) FAI + 0.5% β-CD, e) MABr + 0.5% β-CD-MABr, and f) FAI + 0.5% β-CD-FAI precursor solutions in DMSO-d6.

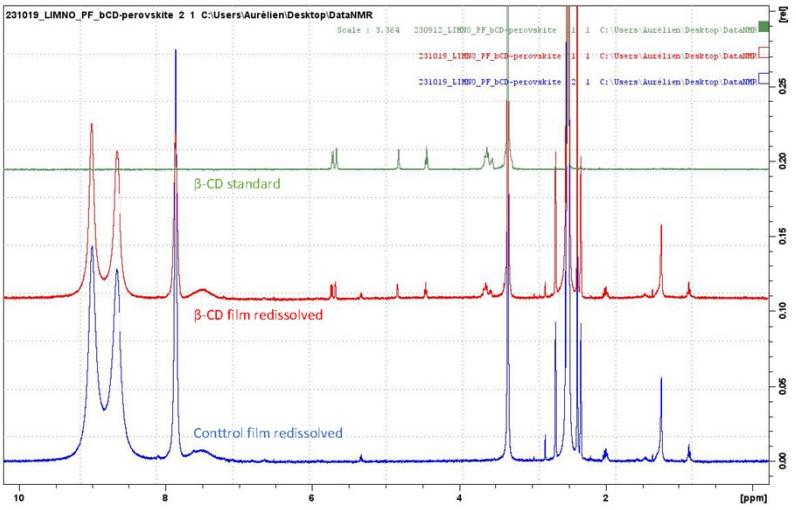

Figure S8. Solution ^{1}HNMR of β-CD and treated perovskite powder (0.5% β-CD) dissolved in DMSO-d6.

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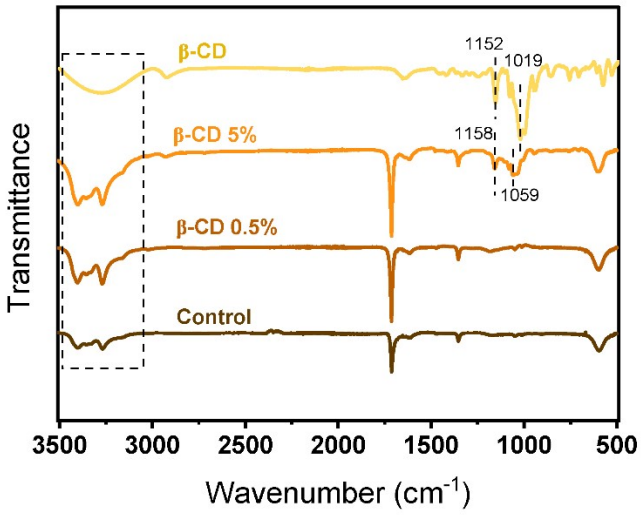

Figure S9. ATR-FTIR spectra of pure β-CD as powder, perovskite films without β-CD (control), and perovskite films treated by with 0.5% of β-CD and 5% of β-CD.

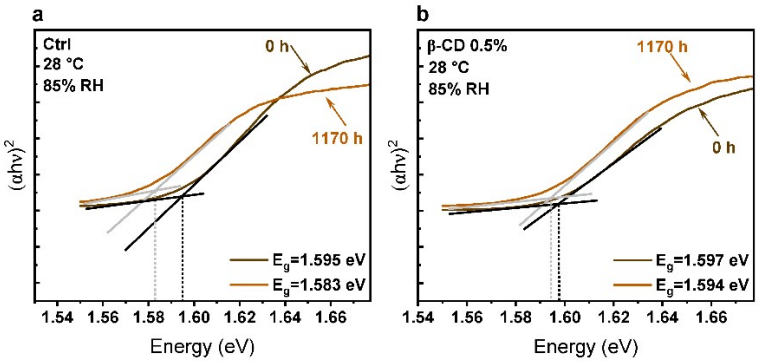

Figure S10. Plot of $(\alpha h\nu)^2$ as a function of photon energy for a) control and b) treated sample by 0.5% of β-CD before and after exposure to humidity stress.

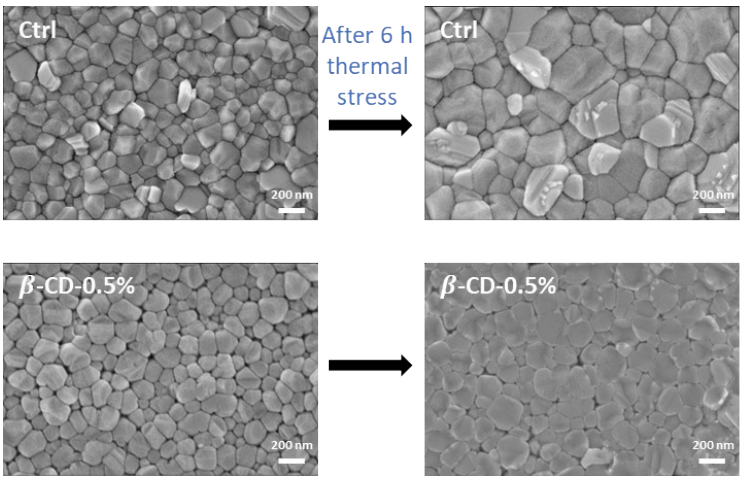

Figure S11. Top view SEM images of the control and β-CD 0.5% treated perovskite films before and after 6 hours aggressive thermal stress.

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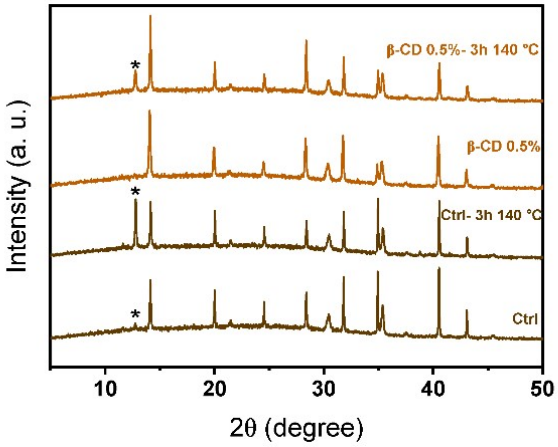

Figure S12. XRD pattern of control (ctrl) and treated sample by 0.5% of β-CD on ITO substrates covered by a SAM layer (star marks the XRD peak of PbI_2).

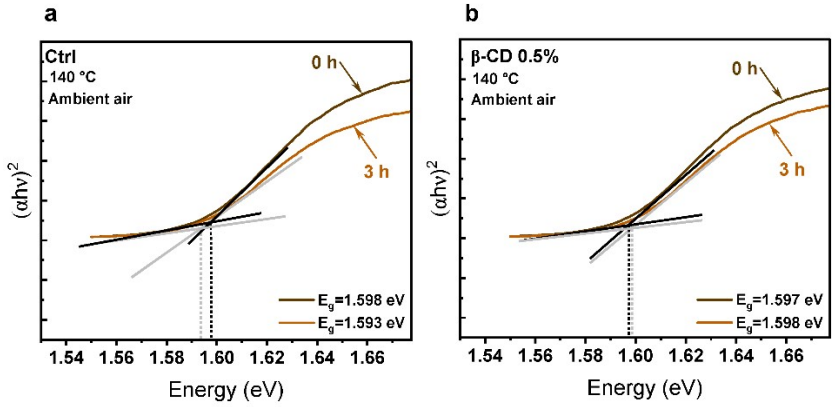

Figure S13. Plot of $(\alpha h\nu)^2$ as a function of photon energy for a) control and b) treated sample by 0.5% of β-CD before and after exposure to aggressive thermal stress.

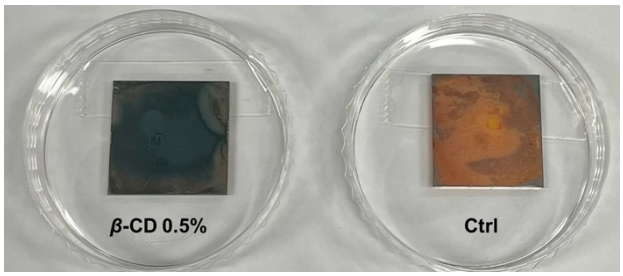

Figure S14. Images of control (ctrl) and treated sample by 0.5% of β-CD on ITO substrates after 5 months at a controlled environment with a temperature range of 18-20℃ and humidity between 40 to 45%.

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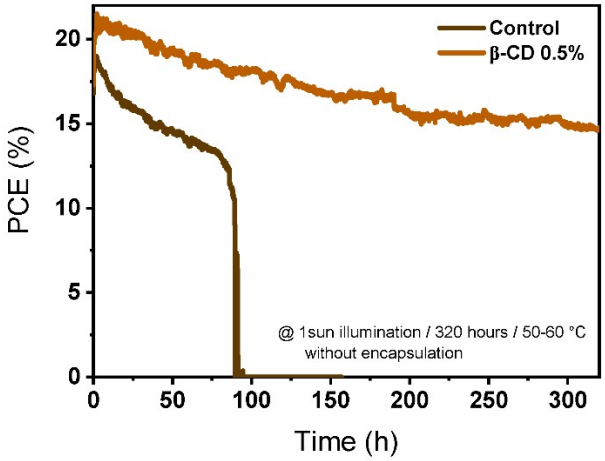

Figure S15. Long-term stability of control and β-CD 0.5% treated devices under constant 1-sun illumination without encapsulation, maintaining temperatures between 50 to 60°C.

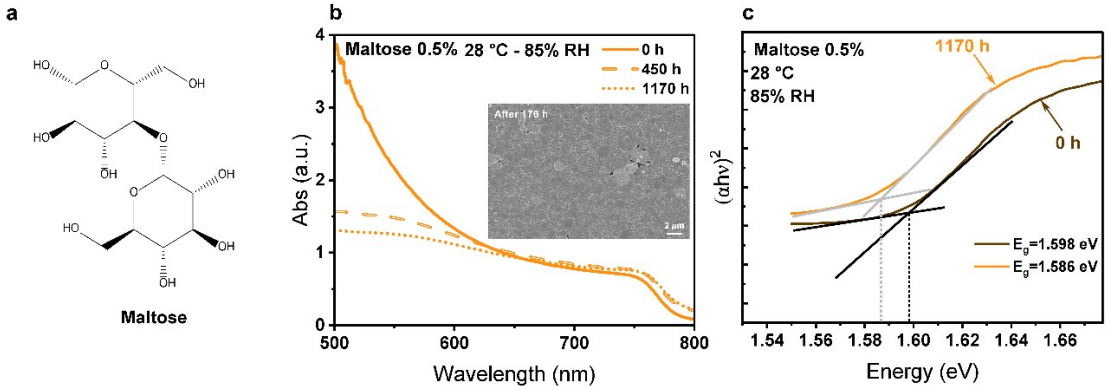

Figure S16. a) Chemical structure of Maltose and b) absorption spectra of Maltose 0.5% treated films under humidity environment (85% RH) at 27°C. Then inset shows top-view SEM image of film after 176-hour humidity exposure. c) Plot of $(\alpha h\nu)^2$ as a function of photon energy.

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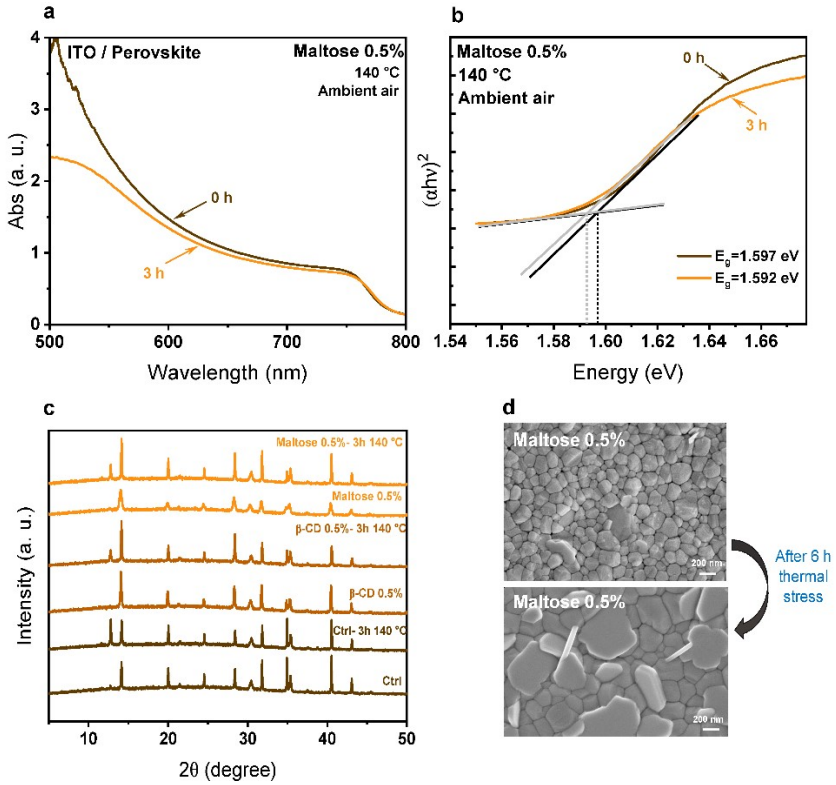

Figure S17. a) Absorption spectra of Maltose 0.5% treated films before and after exposure to aggressive thermal stress for 3 hours at 140°C, b) plot of $(\alpha h\nu)^2$ as a function of photon energy c) XRD pattern of control (ctrl) and treated sample by 0.5% of β-CD and Maltose on ITO substrates covered by a SAM layer, and d) top view SEM images of the Maltose 0.5% treated perovskite films before and after 6 hours aggressive thermal stress.

Table S1. Average value of trap-filled limit voltage and trap-state density from SCLC.

Sample	Average V_{TFL}(V)	Average N_{trap}(cm^{-3})
β-CD 0.5%	0.353	1.14358E+16
Control	0.455	1.47193E+16