Electronic Supplementary Information

Title: Design and understanding of encapsulated perovskite solar cells to withstand temperature cycling

Rongrong Cheacharoen¹, Nicholas Rolston², Duncan Harwood³, Kevin A. Bush¹, Reinhold H. Dauskardt¹, Michael D. McGehee^{*1}

1. Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, United States

2. Department of Applied Physics, Stanford University, Stanford, California 94305, United States

3. D2 Solar, San Jose, 95131, United States

*Email: mmcgehee@stanford.edu



Linear Thermal Expansion Coefficient (x10⁻⁶/°C)

Figure S1: Literature reported values of linear thermal expansion coefficients of layers in perovskite solar cells in parenthesis.

	EVA RC02B-45T	Ionomer PV5400 (Surlyn)
Providers	Mitsui Chemicals	Dupont
Elastic Modulus(MPa)	10	394
WVTR(g/m^2.day) @38°C	20-30	0.66
Melting Point(°C)	66.8	87.8
Processing T (°C)	140	140
Transmittance(cured) %	93	93.4
Refractive Index	1.455	1.49

Table S1: Comparison and properties of encapsulants used in this study



Figure S2: XPS of fractured interfaces of initial unencapsulated perovskite film stack, or "ITO device".



Figure S3: Unencapsulated perovskite film stack after 250 temperature cycles between -40°C and 85°C.

a) ITO device initial



b) ITO device after 250 temperature cycles



Figure S4: Atomic force microscopy topography image of fractured surfaces from a) initial unencapsulated perovskite film stack or "ITO device" b) ITO device after 250 temperature cycles.



Figure S5: XPS of fractured interfaces of unencapsulated perovskite film stack after 250 temperature cycles between -40°C and 85°C.



Figure S6: Photographs of fractured perovskite devices: a) initial ITO device, b) ITO device after 20 minutes annealing at 140°C (the laminating condition), c) ITO device with EVA and glass laminated on top, and d) ITO device with Surlyn and glass laminated on top, whose fracture energies are plotted in Figure 2. The fracture interface is uniform and consistent across the entire sample in all cases within the $PC_{60}BM$.



Figure S7: Atomic percentage of carbon in the fractured perovskite devices laminated with no encapsulant (ITO), EVA, or Surlyn. In all cases, the surface contains >70% carbon, indicating that the fracture occurred uniformly in the PC₆₀BM layer.



Figure S8: Atomic force microscopy topography image of fractured surfaces from a) ITO device with ethylene vinyl acetate (EVA) laminated on top b) ITO device with ionomer Surlyn laminated on top.



Figure S9: Figures of merit of the perovskite solar cells encapsulated in ionomer Surlyn PV5400 packages as they went through the temperature cycling between -40°C and 85°C. Different colored lines represent five solar cells in the data set.



Figure S10: Perovskite solar cell encapsulated in ionomer Surlyn after 200 temperature cycles. The rectangular box highlights the delaminated area with noticeable interference fringes. The photocurrent map was taken from the rectangular box area.



Figure S11: EVA laminated perovskite solar cells after 225 temperature cycles.



Figure S12: Figures of merit of the solar cells encapsulated in EVA packages as they went through the temperature cycling between -40°C and 85°C. Different colored lines represent nine solar cells in the data set.



Figure S13: Load vs. displacement curve for a representative encapsulated perovskite film stack and the extracted fracture energy vs crack length using equation (1).

Glass-Glass encapsulation Optimization:

1. The vacuum time was varied to ensure that all the air bubbles were removed before the encapsulant completely melted in the first lamination stage.

2. Multiple pressing pressures were used. We gradually increased the pressure in steps from 100 \rightarrow 300 \rightarrow 650 mbar to make sure that the encapsulant adhered well and the package did not break during the second lamination stage. The temperature inside the package, measured by a thermocouple inserted between encapsulant and glass, immediately reached the required condition of 140°C, ensuring that it was processed correctly in the second lamination step.

A successful lamination occurred when the package was free of air bubbles and the edge seals were well pressed together with the expected bond width.

<u>Note:</u> The lamination temperature and duration is the standard 20 minutes at 140°C, suggested by the encapsulant provider, and it is the most commonly used industry standard.