Supplementary Information

Understanding the Role of Interface Layers in the Photostability of PM6:Y7-based Organic Solar Cells under Different Degradation Conditions

Magaly Ramírez-Como^a, Enas Moustafa^a, Mohamed Samir^a, Alfonsina Abat Amelenan Torimtubun^a, José G. Sánchez^b, Josep Pallarès *^a, and Lluis F. Marsal *^a

^{a.} Department of Electric, Electronic and Automatic Engineering, Universitat Rovira i Virgili, 43007 Tarragona, Spain. E-mail: josep.pallares@urv.cat; Iluis.marsal@urv.cat

b. Institute of Chemical Research of Catalonia, The Barcelona Institute of Science and Technology (ICIQ-BIST), 43007 Tarragona, Spain.



Figure S1. The current density-voltage (J-V) characteristics curves under illumination conditions of PM6:Y7 based NFA-OSCs under three different degradation conditions: (a) N_2 atmosphere, (b) encapsulated devices and (c) non-encapsulated both exposed under ambient environment over shelf storage time.

Standard	Time	V _{oc}	J _{sc}	FF	PCE _{avg}	PCE_{max}	R _s	R _{SH}
lifetime	[h]	[mV]	[mA/cm ²]	[%]	[%]	[%]	$[\Omega \text{ cm}^2]$	$[\Omega \text{ cm}^2]$
	N ₂ atmosph	ere						
T ₁₀₀	1	836 ± 5	31.30 ± 0.45	66.63 ± 1.07	17.43 ± 0.30	17.53	1.74 ± 0.14	359 ± 79
T ₉₅	288	839 ± 4	30.35 ± 0.47	64.65 ± 1.18	16.46 ± 0.41	16.71	2.46 ± 0.40	352 ± 120
T ₉₀	696	831 ± 4	30.84 ± 0.65	61.57 ± 0.82	15.78 ± 0.14	15.84	2.38 ± 0.21	278 ± 62
T ₈₈	1000	830 ± 2	29.78 ± 0.04	62.43 ± 0.40	15.43 ± 0.10	15.45	2.69 ± 0.04	309 ± 19
	Encapsulate	d devices						
T ₁₀₀	1	828 ± 7	31.25 ± 0.83	65.00 ± 1.54	16.80 ± 0.12	16.97	2.15 ± 0.63	296 ± 134
T ₈₀	336	745 ± 8	31.40 ± 0.06	57.99 ± 0.32	13.57 ± 0.16	13.63	2.39 ± 0.01	274 ± 26
T ₅₀	576	630 ± 2	28.92 ± 0.49	48.39 ± 0.82	8.82 ± 0.18	9.06	5.47 ± 0.23	156 ± 21
T ₃₄	1000	556 ± 5	27.57 ± 0.15	36.96 ± 0.39	5.67 ± 0.03	5.70	10.10 ± 0.12	71 ± 2
	Non-encaps	ulated devices						
T ₁₀₀	1	830 ± 2	30.59 ± 0.72	64.70 ± 0.97	16.43 ± 0.30	16.46	1.84 ± 0.02	337 ± 72
T ₆₀	24	659 ± 4	29.80 ± 0.34	53.30 ± 0.88	10.26 ± 0.22	10.52	3.56 ± 0.21	231 ± 22
T ₅₀	48	605 ± 5	29.06 ± 0.22	47.48 ± 3.08	8.35 ± 0.54	8.89	5.10 ± 0.82	159 ± 15
T ₃₀	744	479 ± 11	26.33 ± 0.21	38.09 ± 3.12	4.80 ± 0.35	5.30	13.89 ± 2.75	73 ± 16

Table S1. Device performance parameters of the NFA-OSCs measured under AM 1.5G with 100 mW/cm² intensity exposed to three degradation conditions: N_2 atmosphere, encapsulated and non-encapsulated devices under ambient conditions. The row displays the average and the standard deviation of the photovoltaic parameters obtained from over 8 devices.



Figure S2. Dark J-V characteristic of PM6:Y7-based devices under degradation different conditions: (a) N_2 atmosphere, (b) encapsulated devices, and (c) non-encapsulated devices both exposed to ambient conditions over storage time. T_{80} and T_{60} are the time the devices took to decay 20% and 40% from their initial power conversion efficiency (PCE), respectively.



Figure S3. Fitting *J-V* characteristic under AM 1.5 G illumination spectrum of fresh and degraded NFA-OSC at 1000 h exposed to degradation different conditions: (a) N_2 atmosphere, (b) encapsulated devices, and (c) non-encapsulated devices both exposed to ambient conditions over storage time. (d) the equivalent circuit proposed by García-Sánchez et al. ^{1,2} used in this work for the fitting of the *J-V* characteristic.

	J _L [mA/cm²]	n ₁	J ₀₁ [mA/cm²]	n ₂	J ₀₂ [mA/cm²]	n ₃	J ₀₃ [mA/cm²]	
N ₂ atmosph	iere							
Fresh	31.46	1.10	5.86 × 10 ⁻¹²	-	-	-	-	
T ₈₈	30.23	1.17	3.74 × 10 ⁻¹¹	1.00	9.19	1.00	8.89	
Encapsulate	Encapsulated devices							
Fresh	32.07	1.11	7.30 × 10 ⁻¹²	-	-	-	-	
T ₃₄	30.04	1.40	7.30 × 10⁻⁵	1.40	4.74	1.20	9.09	
Non-encapsulated devices								
Fresh	31.50	1.11	7.19 × 10 ⁻¹²	-	-	-	-	
T ₂₆	26.94	1.50	1.69 × 10 ⁻⁴	1.50	25.18	1.30	11.09	

 Table S2. The fitted parameters obtained from Circuital model shown in Fig. S3(d).



Figure S4. EQE spectra for NFA-OSCs exposed to (a) N₂ atmosphere, and (b) non-encapsulated cells.

Table S3. The fitted parameters, capacitance, and resistance values, of each layer for NF-OSCs exposed to N_2 atmosphere, encapsulated and non-encapsulated devices under ambient conditions. The IS measurement was carried out under AM1.5G at V_{OC} . The values were extracted by using the circuit model shown in Figure 4(f) of the main article.

	R_1	C ₁	R ₂	C ₂	R ₃	C ₃		
	[Ω]	[nF]	[Ω]	[nF]	[Ω]	[nF]		
N ₂ atmosphere								
Fresh	6	5	3	2.8	16	26.6		
T ₉₇	6.7	5	3.2	2.8	16.7	26.6		
T ₈₀	10.5	5	3.2	2.8	19	26.6		
T ₈₈	10.6	5	3.3	2.8	19.1	26.6		
Encapsulated devices								
Fresh	8	6	3.5	2.8	16	26.6		
T ₉₀	15	6.6	3.5	2.8	24	34.6		
T ₃₄	27	12	10	2.8	30	34.6		
Non-encapsulated devices								
Fresh	9	6	3	2.8	18	26.6		
T ₆₀	22	8	6	2.8	20.5	39.6		
T ₃₇	39.5	9	10	3.5	29.5	45.6		
T ₂₆	48	12.5	12.5	3.5	42	55.6		

SUPPLEMENTARY REFERENCES

- 1 F. J. García-Sánchez, D. Lugo-Muñoz, J. Muci and A. Ortiz-Conde, *IEEE J. Photovoltaics*, 2013, **3**, 330–335.
- 2 F. García-Sánchez, B. Romero, D. Lugo-Muñoz, P. Del, B. Arredondo, J. Liou and A. Ortiz-Conde, *Facta Univ. Ser. Electron. Energ.*, 2017, **30**, 327–350.