

Cite this: DOI: 10.1039/c0xx00000x

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Interface Design to improve stability of polymer solar cells for potential space applications

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Supplementary Information

This supplementary information consists of 1 table and 4 figures.

Radiation Tests at AFRL: The cells were mounted flat in an ARACOR 4100 X-ray irradiation system (W target) equipped with W probes to contact the In pads on the cell and probed electrically using a Hewlett Packard 4142 instrument. During irradiation, the anode and cathode were always short circuited to avoid the risk of charge buildup due to stray fields. Current–voltage measurements were made both in the dark and with a light source on. An uncalibrated halogen lamp (maximum 150 W) was used as the source and fiber fed into the ARACOR box so as to illuminate the solar cells edge on. The lamp was not used at full intensity and no effort was made to calibrate the intensity arriving at the solar cells. The lamp position was carefully fixed during the whole experiment to guarantee constant light intensity. This however, does not affect our measurements in any way as shown in Li *et al.* (Nanotechnology, 19, 424014 (2008)) and Kumar *et al.* (Adv. Funct. Mater. 20, 2729, (2010)).

Supplementary Table 1 summarizes the performance of baseline devices made at UCLA. These devices were shipped back “as is” from AFRL (without being subjected to radiation) and the efficiency loss was found to be less than 5%. (Note: These measurements were made under standard AM 1.5G illumination at 100 mW.cm^{-2} using an Oriel 96000 150 W solar simulator source. However, in-situ measurements in the text, as in figure 1, are made using the optically coupled uncalibrated halogen lamp mentioned above). Hence, the effect of oxygen and water during shipment could be neglected as causes for any probable changes in the devices.

The dark I-V curves (before and after radiation) for different interfaces are shown in **Supplementary Figure S1**. As mentioned in text, use of dark $I-V$ curves separates the effect of photo-generated current. Dark currents can give useful information about the built-in-potential in the device by looking at the injection barrier (the turn-on region). There is a negligible change in injection barrier for $\text{TiO}_2\text{:Cs/Al}$ and ZnO/Al interfaces compared to others. This is consistent with the $I-V$ measurements under light (Figure 1). Change in V_{oc} arises from a change in the built in potential of the devices, which is a direct result of change in electric field/energy alignment inside the device. It rules out the effect of any kind of photo-generated carriers.

Supplementary Figure S2 gives the series (R_s) and shunt (R_{sh}) resistances of the device calculated from the I-V curves measured in-situ during radiation exposure. Devices with $\text{TiO}_2\text{:Cs/Al}$ and ZnO/Al seem to be much more radiation tolerant than others.

R_s and R_{sh} were developed using a new software system that differs from the conventional method. The analysis of dark I-V curves was based on a commonly accepted one-diode circuit model. While the conventional methods normally fits the dark I-V curves and get the parameters

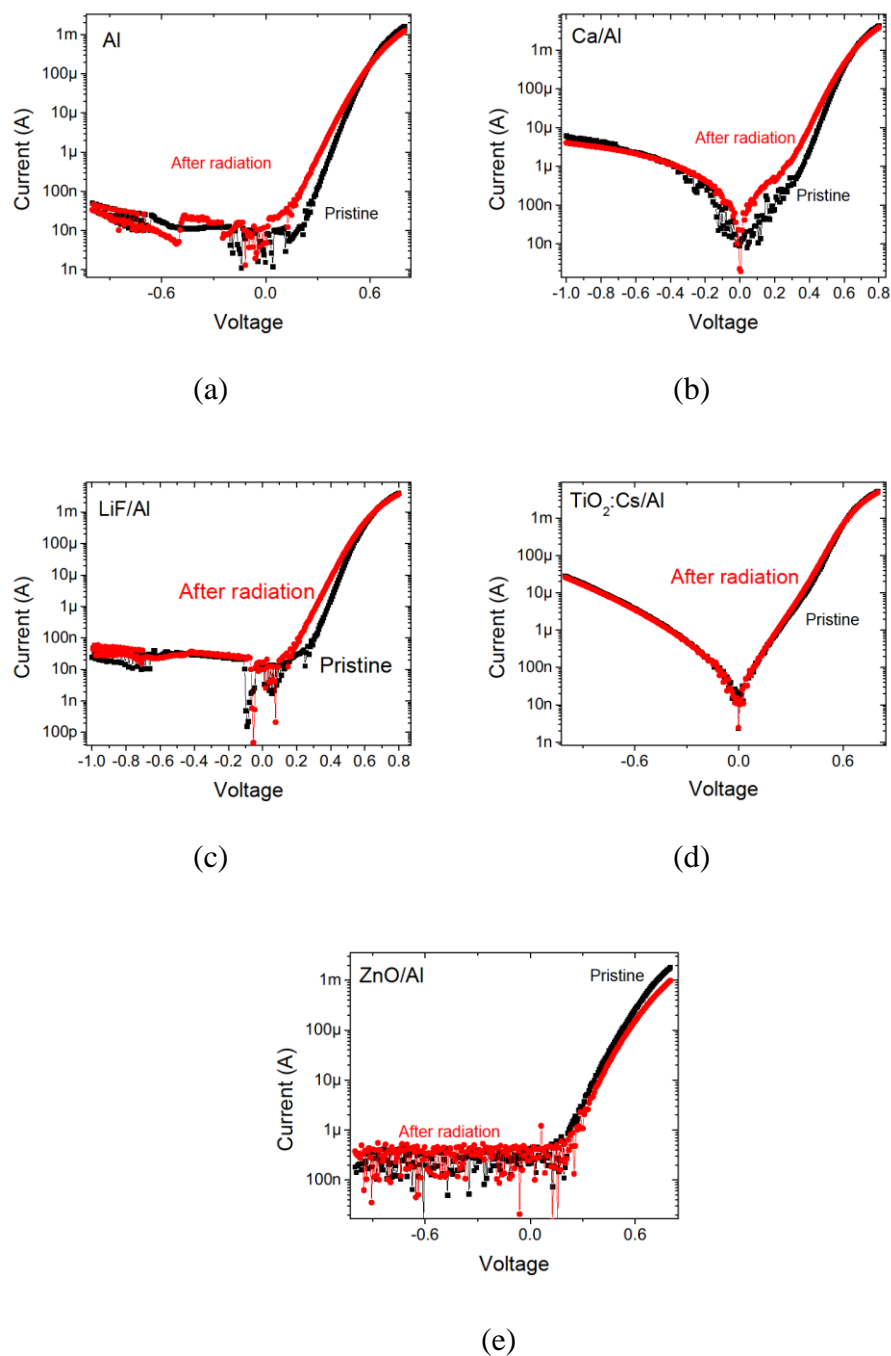
of the p-n junction and series (R_s)/shunt (R_{sh}) resistance directly, we first calculate the R_s based on the comparison between dark and light I-V curves. According to theoretical as well as experimental studies, the R_s extracted this way is more accurate compared to the one obtained by fitting the slope at the high voltage end, since it considers the different current flow patterns under dark and under illumination, and the multi-dimensional effect of R_s .

To remove the effect of ohmicity of the devices, the I-V curves obtained experimentally in-situ during radiation were corrected for $R_s=0 \Omega$ and $R_{sh}=1E10 \Omega$ using our new software. The resultant I-V curves are shown in **Supplementary Figure S3**.

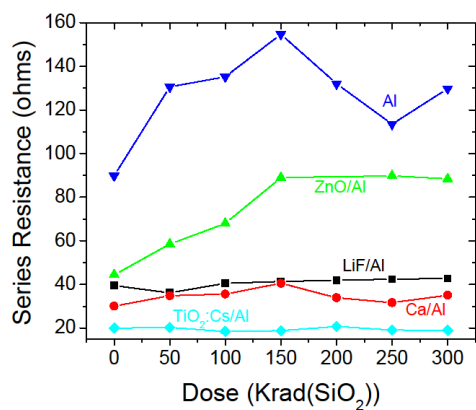
Transient photovoltage (TPV) measurements are performed with a “light bias” (a white light source) to generate a steady V_{oc} . We measured TPV transients over a range of light intensities corresponding to a V_{oc} range of 0.28–0.50V. The decay transient for P3HT:PCBM =1:1 for Ca/Al interface was found to be in excellent agreement with that reported earlier. In addition, as reported the τ was found to vary exponentially with V_{oc} for all measured V_{oc} values. **Supplementary figure 4** shows τ for P3HT:PCBM devices with different interfaces. The exponential curve was fitted to equation 2 (of the main manuscript) and the extracted parameters are shown in Table 1.

Supplementary Table 1: Device performance of pristine P3HT: PCBM photo cells corresponding to different interfaces.

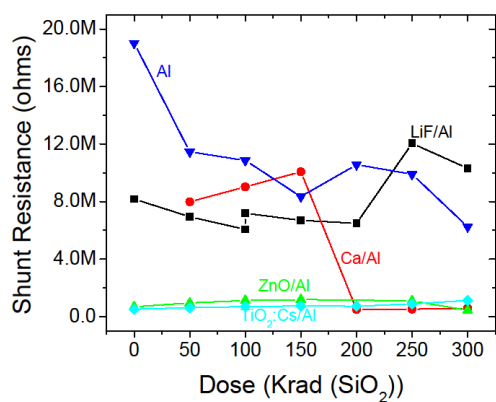
Interface	V_{oc} (V)	J_{sc} ($\text{mA}\cdot\text{cm}^{-2}$)	PCE (%)	FF (%)
Al	0.601	9.07	2.84	51.84
Ca/Al	0.596	8.84	3.65	68.78
LiF/Al	0.589	7.95	3.14	66.97
TiO ₂ :Cs/Al	0.576	8.58	3.2	64.93
ZnO/Al	0.607	8.49	3.47	67.46



Supplementary Figure S1: I - V curves under dark demonstrating the diode behavior of P3HT:PCBM based solar cells with different interfaces (a) Al only (b) Ca/Al (c) LiF/Al (d) TiO₂:Cs/Al and (e) ZnO/Al. The Figure shows I - V curves obtained before (black curve) and after (red curve) 0.3 Mrad (SiO₂) X-ray radiation.

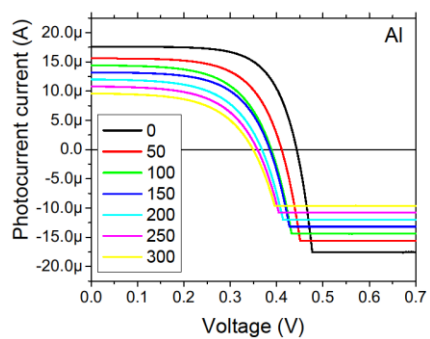


(a)

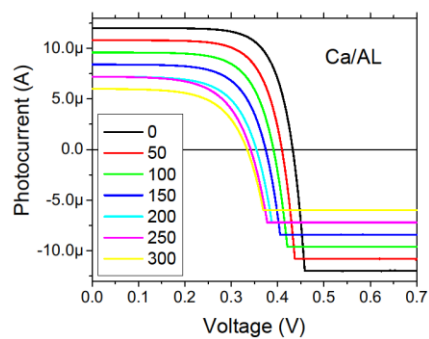


(b)

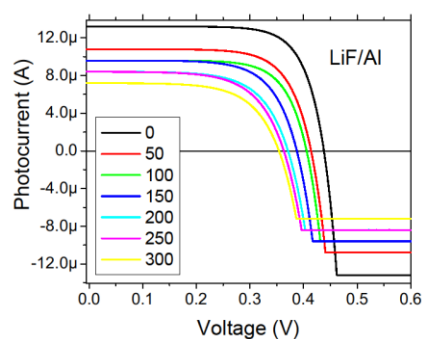
Supplementary Figure S2: Series Resistance R_s and (b) Shunt resistance R_{sh} as a function of degradation time under X-ray radiation. The different curves correspond to different interfaces Al (dark blue inverted triangle), Ca/Al (red circle), LiF/Al (black square), TiO₂/Cs/Al (cyan rhomboids) and ZnO/Al (light green up triangle).



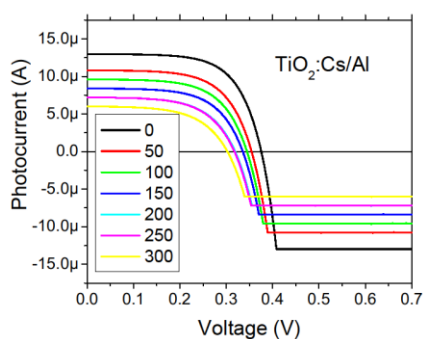
(a)



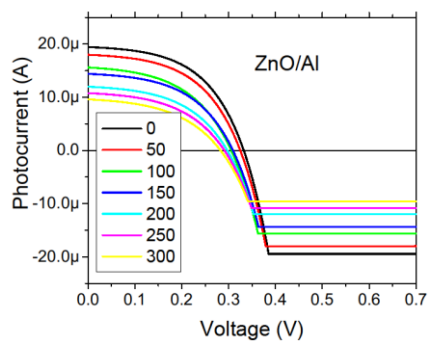
(b)



(c)

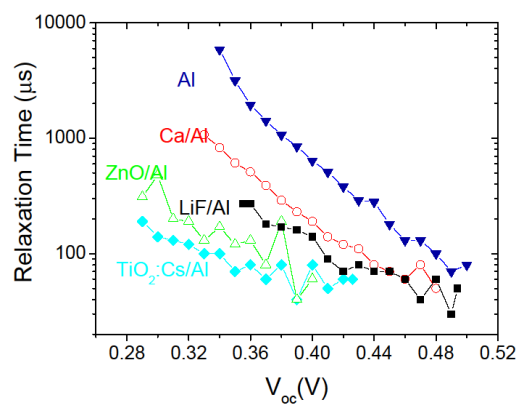


(d)



(e)

Supplementary Figure S3: Light I-V curves after correction for $R_s=0 \Omega$ and $R_{sh}=1E10 \Omega$ for P3HT: PCBM based solar cells with different interfaces a) Al only (b) Ca/Al (c) LiF/Al (d) TiO₂:Cs/Al and (e) ZnO/Al. The label shows the amount of X-ray radiation in Krad (SiO₂) to which the cells were exposed.



Supplementary Figure S4: Carrier lifetime (τ) measured using transient photo-voltage as a function of V_{oc} (changed by changing the light intensity) for pristine P3HT:PCBM based solar cells with different interfaces Al (dark blue inverted triangle), Ca/Al (red open circle), LiF/Al (black square), TiO₂:Cs/Al (cyan rhomboidal) and ZnO/Al (green up triangle).