Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Highly stable of polymer solar cells employing highly conductive MoO_3 hole-transport layer

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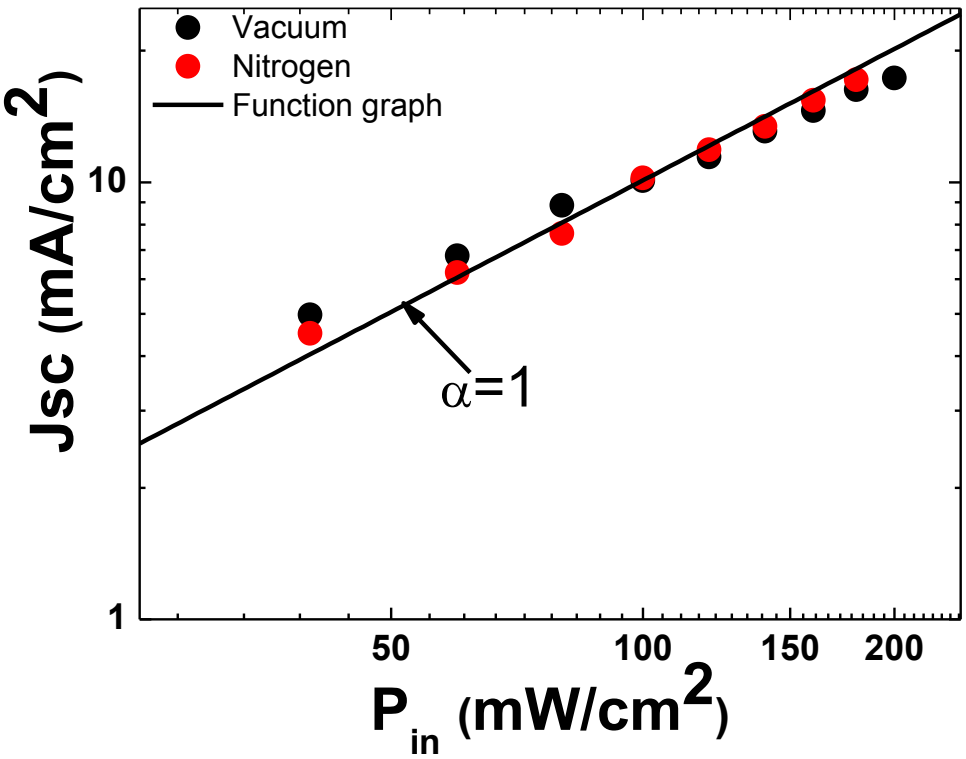
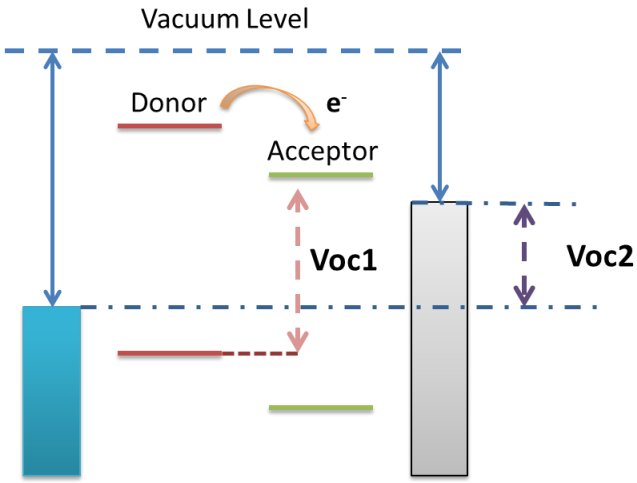
Supporting Information

S1

Scaling exponent (α) calculated using power-law for both devices.



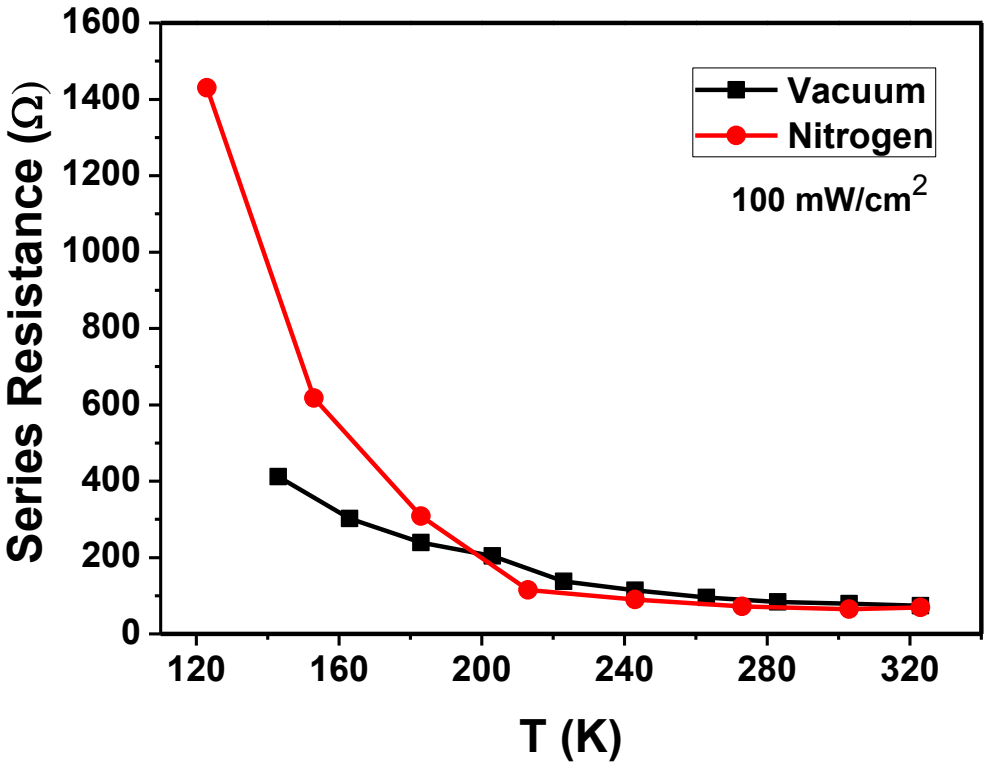
S2



Voc1 – Voc determined by Eg difference in donor and acceptor
Voc2 – Voc determined by workfunction difference between the electrodes

S3

Series Resistance



In both the vacuum and nitrogen annealed devices, the series resistance increases with decrease in temperature. The trends of the I-V curve beyond the Voc from the figure 2a and figure 2b shows that the series resistance do not vary similarly with respect to temperature for both devices. The change in series resistance with respect to temperature is a combination of bulk and contact resistance. In this case, both the devices have similar architecture except for the annealing conditions; therefore the bulk resistance should not differ much between the devices.

The pronounced increase in series resistance in the case of device N can be attributed to higher contact resistance at the P3HT/MoO_3 interface as well as decreased charge transport pathways existing within the MoO_3 interlayer. The band bending existing at the interface, which favours the hole extraction, decreases with decrease in temperature. Moreover reduction in temperature also reduces the diffusion co-efficient leading to reduction in the

band bending. This eventually changes the diffusion current at the interface. [1]These factors results in increased surface charge recombination leading to lowering of fill factor.

Moreover the oxygen vacancies are comparatively lesser in the case of device N, which denotes that the MoO_3 interlayer in this device is more stoichiometric while compared with device V.[2] Hence when the temperature is lower the thermal energy applied to the electrons is also lowered thereby their transport is purely dependent across the already existing pathways within the MoO_3 buffer layer. In stoichiometric MoO_3 the defect states are lesser; it means the resistance for charge transport is higher as there are fewer pathways for the charge transport to occur. The device V annealed in vacuum conditions has more charge transport pathways (defect states) compared to device N. Hence when the temperature is lowered the series resistance is significantly lower than that of the device V.

[1] P. Kumar, S. C. Jain, H. Kumar, S. Chand, and V. Kumar, "Effect of illumination intensity and temperature on open circuit voltage in organic solar cells," *Applied Physics Letters*, vol. 94, pp. 183505-183505, 2009.

[2] M. T. Greiner, M. G. Helander, Z. B. Wang, W. M. Tang, J. Qiu, and Z. H. Lu, "A metallic molybdenum suboxide buffer layer for organic electronic devices," *Applied Physics Letters*, vol. 96, 2010.