Volatile Organic Compounds are Ghosts for Organic Solar Cells

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All our efforts to demonstrate a multifunctional device – photovoltaic gas sensor (i.e. solar cell which show photovoltaic action depending on the gas / volatile organic compounds (VOC) in the surrounding atmosphere) yielded negative results. Photovoltaic performance of the organic solar cells under study degraded – almost permanently by exposing them to volatile organic compounds (VOCs). Although, the proposed multifunctional device could not be demonstrated; Present investigations yielded very *important result* that organic solar cells have problems not only with oxygen and humidity (known facts) but also with many VOCs and hazardous gases – making lamination / encapsulation step mandatory for their practical utilization.

Keywords: Organic solar cell, Lamination, Volatile organic compounds.

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Recently, we demonstrated a multifunctional device by combining photovoltaic action and pressure sensing i.e. Pressure dependent photovoltaic action [1]. The device can be used as a solar cell, a pressure sensor or a photovoltaic pressure sensor. Motivated by this, we started with a novel idea of demonstrating a multifunctional device - Photovoltaic Gas Sensor - which is proposed to show photovoltaic action depending on the analyte in the surrounding atmosphere - and which can be used as a solar cell, as a gas sensor or a photovoltaic gas sensor. The 'analyte' can be either volatile organic compounds (VOCs) or hazardous gases. Heterojunction devices, n-Si / P3OT (incorporated with either double walled carbon nanotubes or multiwalled carbon nanotubes) are exposed to VOCs and their photovoltaic performance is measured. All my efforts yielded negative results irrespective of the type of the gas (electron donor or acceptor). Photovoltaic performance of the solar cells degraded - almost permanently. We could not realize the proposed multifunctional device; however, present investigations yielded very important results that organic solar cells have problems not only with oxygen and humidity (known facts) but with all (at least many) kinds of VOCs and hazardous gases - making the lamination / encapsulation step mandatory for their practical utilization.

Carbon nanotubes (CN) are attracting interest for application in photovoltaic energy conversion devices [2-12]. Incorporation of CN in organic/organicinorganic heterojunction solar cells is shown to improve the device performance by many folds [2-12]. In the present study, we used the same device which we have reported earlier in references [11, 12]. Double walled carbon nanotubes (DWCN) were incorporated in the polymeric layer of the *n*-Si/regioregular Poly(3octylthiophene) (P3OT) heterojunction solar cell. The device structure is *n*-Si/P3OT + DWCN / Au. Cell is illuminated from the semi-transparent Au (25 nm) side whereas n-Si makes a direct electrical contact with the conducting stainless steel stage. Thickness of the P3OT + DWCN layer was approximately 900 nm. Current-voltage (I-V) characteristics were measured in dark and under AM 1.5 simulated solar radiation at room temperature (25 °C) using a JASCO SS-200 W solar simulator. Current-Voltage (I-V) characteristics measured in air are taken as reference. Cells were also exposed to the saturated vapor (s) of the analyte and the I-V characteristics of such cells in dark and under illumination were recorded. Solar cells were soaked considerably (10 min.) in the saturated vapor of the analyte before taking the I-V measurements. After measurement of the photovoltaic performance in presence of analyte gas / vapor, the cells were exposed to air and the I-V measurements were recorded after every fixed pre-determined interval of time so as to understand recovery process. New solar cell is used every time for every analyte separately. Solar cells were also fabricated incorporating the multi-walled carbon nanotubes in the polymer layer of n-Si / P3OT heterojunction solar cells (Cell configuration: n-Si/MWCN+P3OT/Au) and tested in the similar manner. Vapors of ethanol, isopropyl alcohol (IPA), toluene are used as analytes.

Typical as prepared n-Si / P3OT heterojunction solar cell containing DWCN (*n*-Si / P3OT + DWCN / Au) shows (in air) the open circuit voltage (V_{oc}), shortcircuit current density (Isc), fill factor and white light conversion efficiency of approximately 0.53 V, 5.9 mA/cm², 0.15 and 0.49 %, respectively. This performance (in air) is considered as a reference value. I-V curve in dark goes through origin and shows rectification. After exposing such device to saturated vapor of isopropyl alcohol (IPA), the performance of the device decreases and becomes steady. Such device under illumination shows V_{oc} , I_{sc} , FF and % η approximately as 0.3935 V, 0.2689 mA/cm2, 0.1726 and 0.018 %, respectively. The response time (time taken by the device to saturate at its performance after exposed to analyte) is observed to be approximately 7 min whereas the recovery is almost absent. In fact, the device did not recov-

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ered its performance at all even after 48 hours in air atmosphere indicating thereby that it has undergone irrecoverable damage. Fast response and recovery is usually required for sensor applications. Long response time (in mins) observed which might be due to the fact that top surface (P3OT + DWCN) of the device is covered by the gold electrode (but not completely) whereas silicon is present at the bottom surface which prevents analyte molecules to interact with the active organic material (i.e. P3OT + DWCN film). We believe that in the present device, P3OT and DWCN are mainly the sensing materials and the interaction of volatile organic molecules with them should be considered. Hence, interaction and diffusion of IPA molecules inside the P3OT + DWCN film occurs mainly through the side edges of the device which are not protected. Further, the IPA molecules should diffuse throughout the film volume so as to saturate the performance of the device. Hence, it was expected that such device will show longer response times. Similar is the case for recovery of the device. Original performance of the device could only be achieved if all the IPA molecules somehow come out of the device - leaving the device microstructure intact. The only space through which they can come out of the active materials (P3OT + DWCN) film is again the side edges of the device. Hence, the smaller area of the side edges results in longer response and recovery time for the device. Nevertheless, the solar cell changes (more specifically, decreases) in its photovoltaic performance when exposed to the vapor of volatile organic compound, IPA. Similar decrease of the photovoltaic performance is also observed when the device is exposed to vapors of other volatile organic compounds such as ethanol and toluene. It is to be noted here that IPA and ethanol are polar organic compounds whereas toluene is a non-polar organic compound. Similar effect (decrease in the photovoltaic performance when exposed to the vapors of volatile organic compounds) is also observed in the devices incorporating MWCN (device structure : n-Si / MWCN + P3OT / Au). We believe that the irrecoverable damage to the device performance is due to the destruction of the organic active layer microstructure. Even annealing the devices in air / in nitrogen could not recover their performance.

In conclusion, we started with a novel idea of demonstrating a multifunctional device – *Photovoltaic* Gas Sensor – which can act as a gas sensor, a solar cell or a photovoltaic gas sensor. However, we got only negative results that the photovoltaic performance of the heterojunction solar cells i.e. n-Si / P3OT (containing DWCN or MWCN) decreases by exposing these devices to the vapors of volatile organic compounds. Type of the gas/vapor (polar/non-polar; electrondonating / accepting) seems to be irrelevant and only decreases the photovoltaic performance of the organic solar cells. The irrecoverable, almost permanent damage to the device performance might be due to destruction of the device microstructure and internal connecting / percolating paths for transfer of charge carriers to respective electrodes. However, present investigations yielded very important result that organic solar cells have problem not only with oxygen and humidity but also with all / many kinds of VOCs and hazardous gases - making lamination / encapsulation step almost mandatory for their practical utilization.

Solar Cell Structure: n-Si / P3OT + DWCN / Au					
Sr. No.	Description	V_{oc} (V)	I_{sc} (mA/cm ²)	\mathbf{FF}	$\% \eta$
1	Reference (in air)	0.53	5.9	0.15	0.49
2	Ethanol	0.4642	0.4423	0.1763	0.0362
3	Isopropyl Alcohol	0.3935	0.2689	0.1726	0.0182
4	Toluene	0.3656	0.2149	0.1702	0.0133

 $\label{eq:Table 1-Solar cell performance in air and when exposed to different VOC vapors.$

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