

Supporting Information

Towards Efficient Carbon Nanotube / P3HT Solar Cells:

Active Layer Morphology, Electrical and Optical

Properties

Shenqiang Ren,^{†§} Marco Bernardi,^{†§} Richard R. Lunt,[‡] Vladimir Bulovic,[‡] Jeffrey C. Grossman[†], Silviya Gradečak[†]

[†] Department of Materials Science and Engineering and [‡] Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

§ These Authors contributed equally to this work.

1. List of materials

High purity semiconducting single-walled carbon nanotubes (s-SWCNTs) with nominal diameter in the range 1.2 – 1.7 nm and length in the range 300 nm – 5 μm (IsoNanotube-S from NanoIntegris, powder with 98% purity) were used in conjunction with regioregular P3HT (99% head-tail coupling, average molecular weight $MW \approx 50,000$, purchased from Rieke Metals). The SWCNT diameter and length were confirmed using transmission electron microscopy (TEM) and atomic force microscopy. An average diameter of 1.5 nm (Figure S1) was found by averaging over several nanotubes.

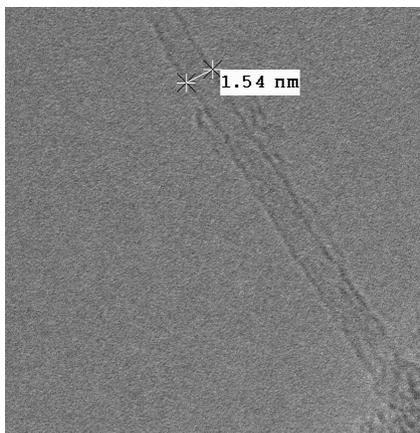


Figure S1. TEM image of a representative s-SWCNT used in this work.

2. Absorption spectrum of pristine s-SWCNTs

For absorption measurements, the SWCNT powder (as received from NanoIntegris) was dissolved in 1,2 dichlorobenzene. The observed S_{22} transitions fall in the interval 800–1200 nm, as predicted by the Kataura plot. The onset of the S_{11} transitions at wavelengths >1400 nm was also observed.

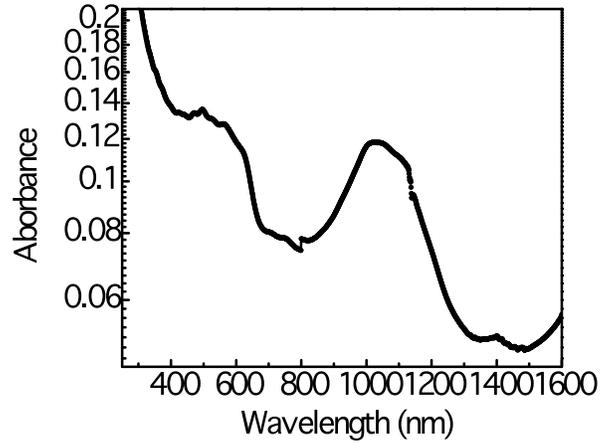


Figure S2. Absorption spectrum of s-SWCNT used in this work.

3. I - V Curve

I - V curve of the highest efficiency s-SWCNT/P3HT nanofilament device obtained using 3 wt.% s-SWCNTs, in dark and under 1.5AM illumination.

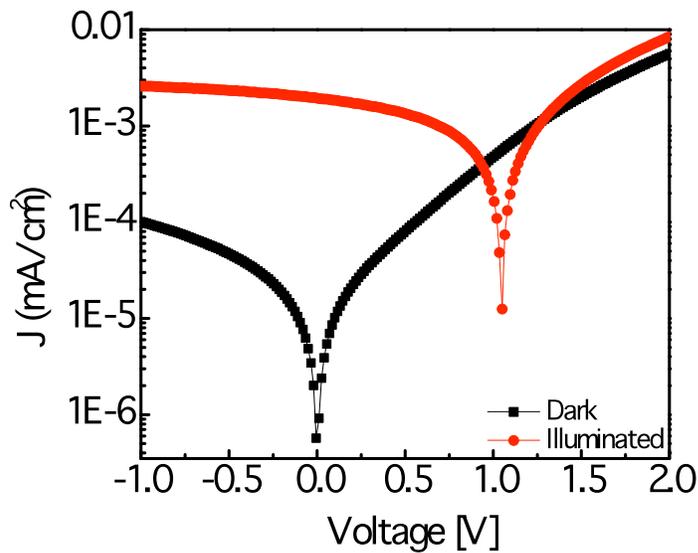


Figure S3. I - V curve for device with 0.72% efficiency.

4. Details of the quantum efficiency measurements

External quantum efficiency (EQE) measurements were collected in a glovebox using a monochromator, chopped locked-in, and an NREL calibrated Ge detector (Newport). Internal quantum efficiencies (IQE) were inferred by dividing the EQE by the absorption in the SWCNTs only. The SWCNT absorption was measured using a Cary Eclipse 5000 dual-beam spectrophotometer at an incidence angle of $\sim 6^\circ$, where the final device absorption (with SWCNTs in the active layer) was subtracted by a reference sample with similar P3HT-only device (without SWCNTs in the active layer).

5. s-SWCNTs with diameter in the range 1.2–1.7 nm

Shown below is a list of the chiral numbers (n,m) of s-SWCNTs with diameter d in the range of 1.2–1.7 nm similar to the nanotubes used in our solar cell devices. From the IQE and optical absorption measurements carried out in the paper we conclude that nanotubes with diameter in the range of 1.3 – 1.4 nm are expected to form type-II heterojunctions and contribute to the photovoltaic conversion. Such nanotubes are marked in bold in the list below.

(n,m) $d(\text{\AA})$		
(10,8) $d = 12.23$	(14,4) $d = 12.81$	(17,0) $d = 13.31$
(10,9) $d = 12.89$	(14,6) $d = 13.91$	(17,1) $d = 13.72$
(11,7) $d = 12.30$	(14,7) $d = 14.50$	(17,3) $d = 14.62$
(11,9) $d = 13.58$	(14,9) $d = 15.71$	(17,4) $d = 15.12$
(11,10) $d = 14.24$	(14,10) $d = 16.35$	(17,6) $d = 16.18$
(12,7) $d = 13.03$	(15,1) $d = 12.15$	(17,7) $d = 16.73$
(12,8) $d = 13.65$	(15,2) $d = 12.60$	(18,1) $d = 14.50$
(12,10) $d = 14.93$	(15,4) $d = 13.58$	(18,2) $d = 14.93$
(12,11) $d = 15.60$	(15,5) $d = 14.11$	(18,4) $d = 15.89$
(13,5) $d = 12.60$	(15,7) $d = 15.24$	(18,5) $d = 16.40$
(13,6) $d = 13.17$	(15,8) $d = 15.83$	(19,0) $d = 14.87$
(13,8) $d = 14.37$	(16,0) $d = 12.52$	(19,2) $d = 15.71$
(13,9) $d = 15.00$	(16,2) $d = 13.38$	(19,3) $d = 16.18$
(13,11) $d = 16.29$	(16,3) $d = 13.85$	(20,0) $d = 15.66$
(13,12) $d = 16.95$	(16,5) $d = 14.87$	(20,1) $d = 16.06$
(14,3) $d = 12.30$	(16,6) $d = 15.42$	(20,3) $d = 16.95$
	(16,8) $d = 16.57$	(21,1) $d = 16.84$