DOE Solar Energy Technologies Program Peer Review

Technical Track: III-V & Concentrators

Project Name: High-Efficiency Cascade Solar Cells (NM)

Principal Investigators: Shuguang Deng (New Mexico State University),
Seamus Curran (University of Houston), **Igor Vasiliev** (New Mexico State University)

Denver, Colorado

March 9-10, 2009

Research Team

Shuguang Deng, Associate Professor, Chem. Eng., New Mexico State Univ.

Advanced materials: synthesis, characterization and applications

42 journal papers and book chapters, 10 patents/applications, 7 years industrial R&D

1 postdoc with 10^+ years of experience on CNT synthesis and characterization

3 graduate students (materials and devices fabrication, characterization)

Seamus Curran, Associate Professor, Physics, Univ. of Houston

Photovoltaic, nanocomposite fabrication & spectroscopic study of nanomaterials

72 journal papers, book chapter and proceedings, over 1350 citations, h=16

2 postdocs, 6 graduate students, 3 undergraduate students (7 involved in this project)

8 patent applications (at various stages) and 1 granted based on photovoltaics

Igor Vasiliev, Associate Professor, Physics, New Mexico State Univ.

Computational materials science and nanotechnology

36 journal papers and book chapters, over 800 citations

10+ years experience in modeling and simulations of nanoscale materials

1 graduate student involved in this DOE project (Ab initio calculations)

Relevant Research Facilities (Deng's Lab, NMSU)

- Renishaw inVia Raman microscope (with 5 laser beams)
- Veeco Aurora-3 NSOM and a new Caliber atomic force microscope
- Perkin Elmer SPECTRUM 400 MIR/NIR DTGS with in-situ capability
- Perkin Elmer LAMBDA 35 UV-vis
- Perkin Elmer Elan-DRC-e ICP-MS and HPLC-MS
- Rigaku MiniFlex II X-ray diffractometer
- Kevex Omicron X-ray florescence spectrometer
- Micromertics ASAP-2020 adsorption apparatus (BET, pore size)
- Brewer Science Cee200 spin-coater
- Solar cell current-voltage measurement unit (Sun simulator AM1.5, Keithley 2400 source meter, Keithley 2000 multimeters, load regulator)
- Two chemical vapor deposition reactors (1" and 4" tube)
- Rubotherm magnetic suspension balance (0-500 bar, 77-573K, TGA)

Relevant Research Facilities (Curran's Lab, UH)

General Lab Equipment: 3 Cole-Parmer Stir-Hot Plate, Sartorius Chemical Balance, Cole-Parmer Sonicator, Gas Vacuum Motor, Micropack Light-source, Corning Hotplate, Buchi Rotavapor RII, Welch dry fast chemical-duty vacuum pump 2034B, Fisher Scientific Isotemp economy vacuum oven, Fisher Scientific Centrific 225A centrifuge.

Characterization Facilities: 3 Ocean Optics Spectrometer with 2 Research Electro-optics helium-neon tunable laser (3 lines), tunable Ar+ ion laser (4 lines), Ocean Optics fluorescence Spectrometer, Terahertz technology inc. photodiode amplifier.

Device Fabrication Facilities: Laurell Spin Coater, Denton II Sputtering, 2 Terrra Universal glove box's, Denton Sputering unit II and V, Sciencope microscope, Probe station JR-2727, 2700 Keithley Multimeter, Keithley Source-meter, Microfab Jetlab 4 printing system.

Relevant Research Facilities (Vasiliev's Lab, NMSU)

Computer Facilities

17 node / 136 CPU Intel Xeon computer cluster (E5430 Harper Town 2.66 GHz Quad-Core processors, 272 Gb of memory, 8 TB of storage space, ultrafast InfiniBand network)

16 node / 32 CPU Intel Xeon 2.4 GHz computer cluster

8 node / 32 CPU AMD Opteron 2.4 GHz computer cluster

Major Accomplishments (Deng’s Lab, 8/2008-12/2008)

1. Built two chemical vapor deposition reactors for making carbon nanotubes (SWNT, DWNT, MWNT, and B-, N- doped CNTs)
2. Restored a Raman microscope and acquired a Veeco Caliber AFM
3. Synthesized single-walled carbon nanotubes in a 1” CVD reactor and characterized the CNT samples with SEM/TEM, EDS, and Raman
4. Purified the SWNT samples with acid washing to remove amorphous carbon and residual catalyst particles
5. Analyzed effects of CVD process parameters on CNT yield and purity
6. Established a micro-fabrication lab and explored the feasibility of replacing metal and insulation layers of inorganic solar cells with suitable polymers
7. Built a solar cell performance test unit
8. DWNT, MWNT and B-, N-doped CNTs are being synthesized
9. Will characterize CNT and composites with Raman, NOSM, AFM, UV-vis
10. Submitted two papers and are preparing another one

Major Accomplishments (Curran’s Lab, 8/2008-12/2008)

1. Hired 2 Postdocs (Chemistry and Physics)
2. Built a team of 7 students around the solar and materials program
3. Can now print controlled arrays of conductive and semiconductive nanocomposites
4. Carried out initial Raman and FTIR studies of nanocomposites
5. Carried out initial conductive (transport measurements) of nanocomposites
6. Produced transparent composite as a replacement of PEDOT (one of the major project milestones)
7. Started characterization work on hybrid nanocomposites (Raman, UV-Vis and Z-Scan)
8. Generated 3 patent applications
9. Submitted 1 paper and 3 in preparation based on composites for the project

Major Accomplishments (Vasiliev's Lab, 8/2008-12/2008)

1. Acquired a new Beowulf computer cluster (launched in September 2008).
2. Carried out computational studies of functionalized carbon nanotubes. A paper based on these studies was submitted to the Journal of Physical Chemistry C.
3. Initiated theoretical studies of B/N-doped carbon nanotubes.
4. Initiated theoretical studies of optically active nanoparticles adsorbed on nanotubes and embedded in polymers.

Resources, Budgets and Accomplishments

1. Total project budget: $1,220K for 2008-2010, $654K in 2008-2009
2. Spent $172K (DOE:$137K, Cost-share:$35K) 7/2008-12/2008
3. Will spend $482K in 2008-2009 and $566K in 2009-2010
4. $90K on restoring Raman and acquiring a new Caliber AFM (trade-in)
5. $30K on 2 CVD reactors, $10K on a spin-coater, $30K on a test unit
6. 30^+$K on chemicals, other supplies, and travels
7. Support 3 Co-PIs, 3 postdoctoral researchers, 9 students
8. DOE funding and cost-share have greatly improved research facilities and enhanced productivities in this project.

Scientific/Technical Approach

Project Objectives

Develop organic nano-electronic-based photovoltaics by using composites formed between nano-molecular structures (from quantum dots to fullerenes) and organic conjugated polymers. Identify materials suitable for use in cascade solar cells, and predict the properties of organic photovoltaic materials from theoretical calculations. Fabricate a suitable new active semiconductor material and form two distinct device architectures: a) thin film coating and b) cascade solar cell fiber.

Main Tasks

Material Fabrication: Functionalizing nanotubes and forming mesoscale nanocomposites

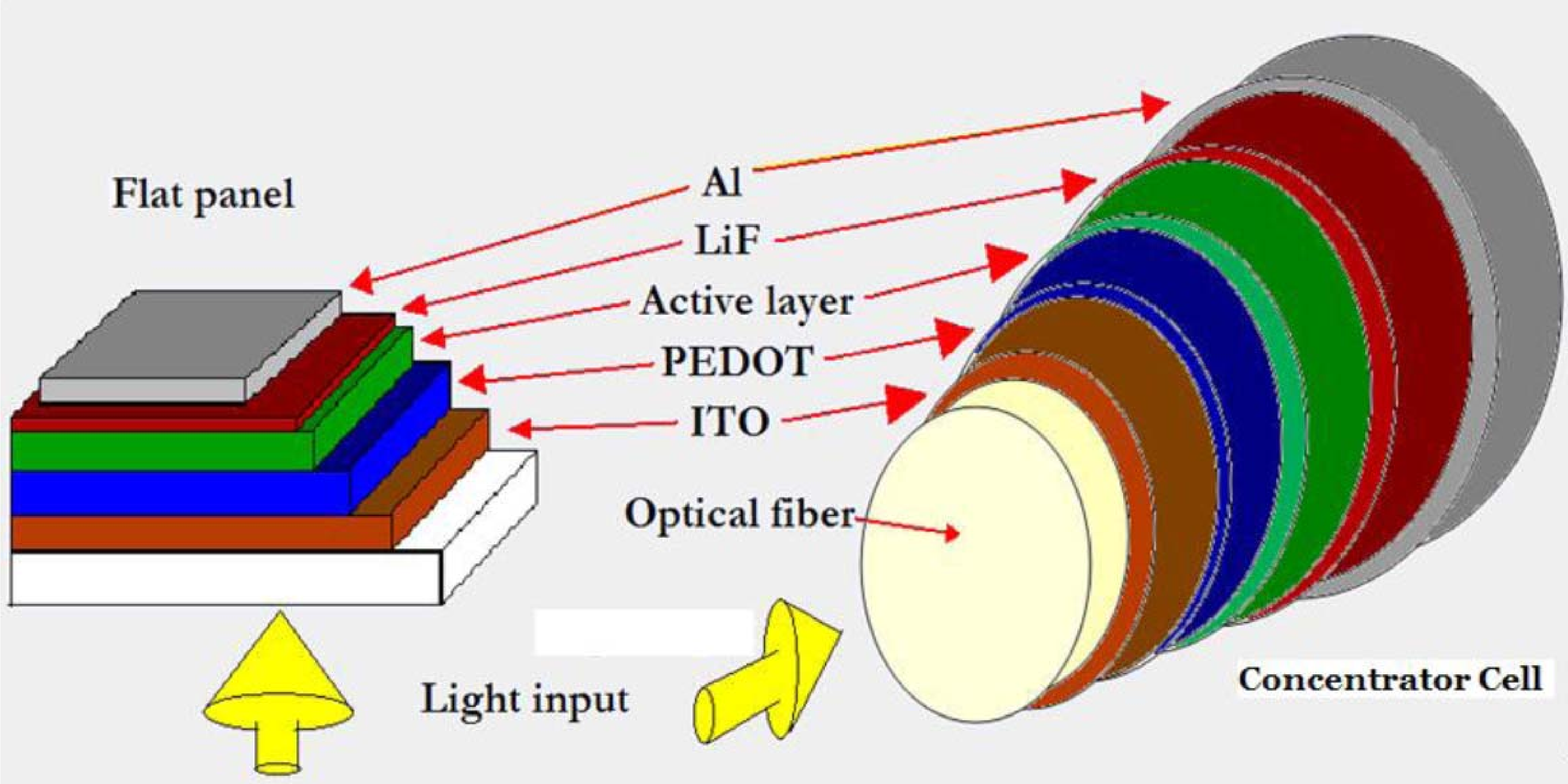
Spectroscopic and Morphological Control: Using proximal probes, AFM, Spectroscopic Control of Composite Formation and NSOM to understand the materials assembled

Ab initio Calculations: Perform charge transport calculation to assist design and production of materials and devices

Nanodevice Fabrication: Produce both of the thin film architectures to optimize the nanomaterial configuration and the cascade fiber solar cell

Device Testing: Test solar-cell devices produced and obtain independent validation

Scientific/Technical Approach



S. Curran, J. Talla, S. Dias and J. Dewald, ‘Micro-Concentrator Photovoltaic Cell (the m-C Cell): Modeling the Optimum Method of Capturing Light in an Organic Fiber Based Photovoltaic Cell’, J. Appl. Physics104,064305 (2008)
S.Curran, D.L. Carroll and J. Dewald, ‘Cascade solar cell increases efficiency’, SPIE,DOI: 10.1117/2.1200608.0324 (July; 2006)

Patent Applications

S. Curran, James Dewald and David Carroll, ‘Cascade Waveguide Photovoltaic’, [PCT (2008)]
S. Curran and James Dewald, ‘Cascade Solar Cell Fabrication and Production –the fiber weave system’, [PCT 2008)]

Catalytic CVD Growth of Carbon Nanotubes

1” CVD Reactor

- 50-1200 C
- 0-1000 ml/min
- Gas or liquid carbon sources
- Small scale production (<1g/day)

4” CVD Reactor

- 50-1200 C
- 0-10,000 ml/min
- Gas or liquid carbon sources
- Large scale production (10g/day)
- Scale-up studies

Catalytic CVD Growth of Carbon Nanotubes

Process Parameters

- Carbon sources
- Reaction temperature
- Reaction pressure
- Flow rate
- Reactor type (fix bed, fluidized bed, and etc.)
- Types of metal catalyst, particle size, and deposition methods
- Additives (sweep gas, reducing gas)
- Modifying agents (NH_3, CH_3CN, BCl_3)

CNT quality

CNT yield (growth rate)

CNT growth mechanism

CNT purification

Catalytic CVD Growth of Single-Walled Carbon Nanotubes

Carbon Source:	Acetylene (C_2H_2)
Reducing gas:	Hydrogen
Sweep gas:	Argon
Catalyst:	Nickel nitrate deposited on a silicon wafer substrate
Temperature:	750-800 C
Pressure:	Ambient pressure
CVD Reactor:	1” pipe reactor

Catalyst concentration (0.05M – 1M) effect was studied in the preliminary runs. Significant amorphous carbon and residual catalyst particles present in the SWNT powder obtained in the CVD reactor.

Purification of Carbon Nanotubes

Impurities to be removed

Amorphous carbon (selective oxidation)

Residual catalyst particles (dissolution in mineral acids)

Purification method

Acid reflux in a shaker or ultrasonic bath

Microwave heating-assisted acid washing

Mineral Acids

HCl

HNO_3

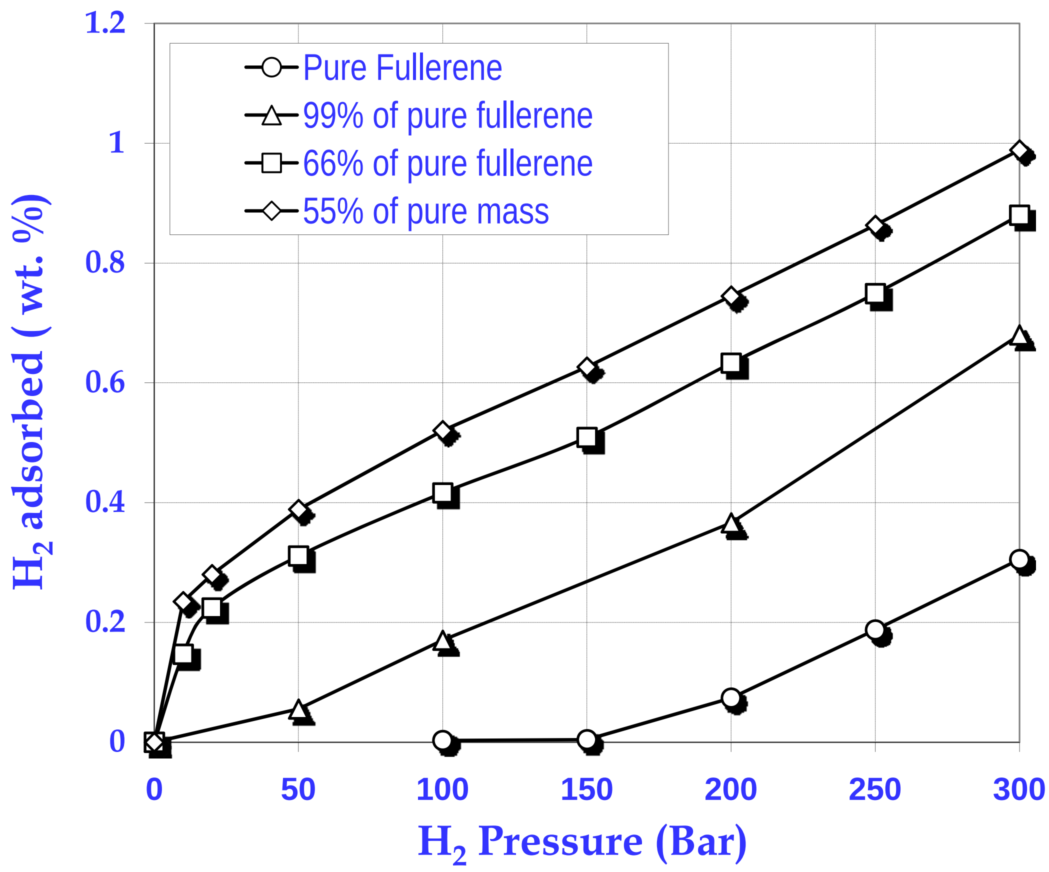
Side Effects of Purification

Generate more amorphous carbon

Generate defects

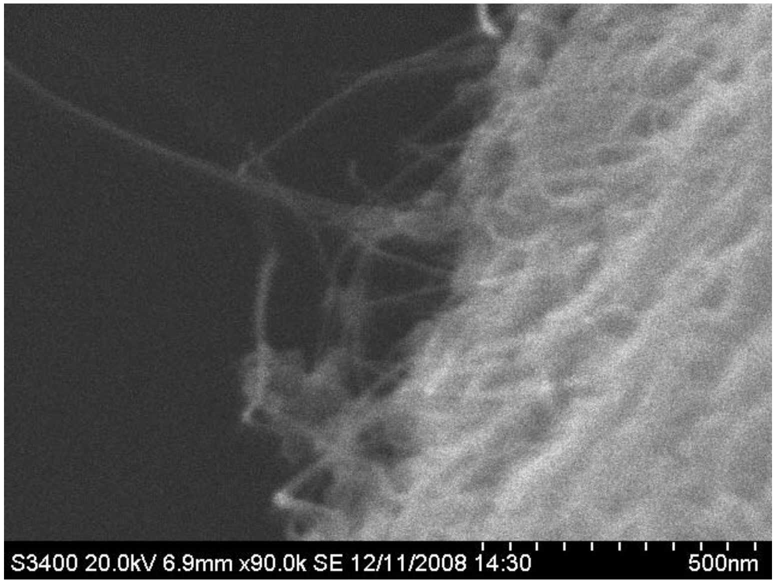
Functionalize the CNTs

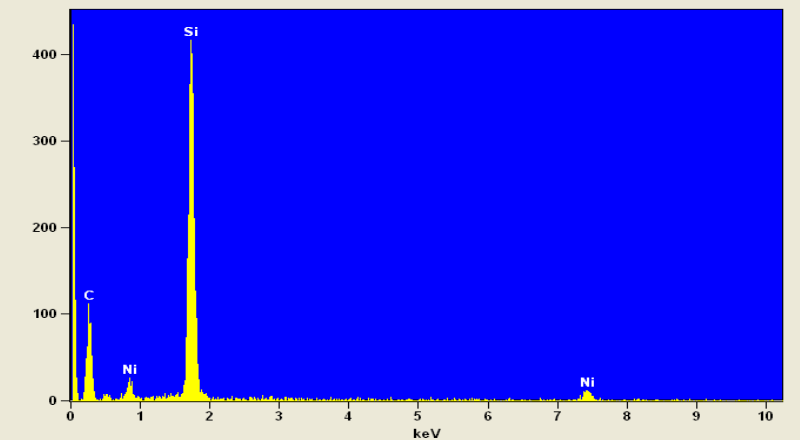
Controlled Oxidation of C60 Fullerene

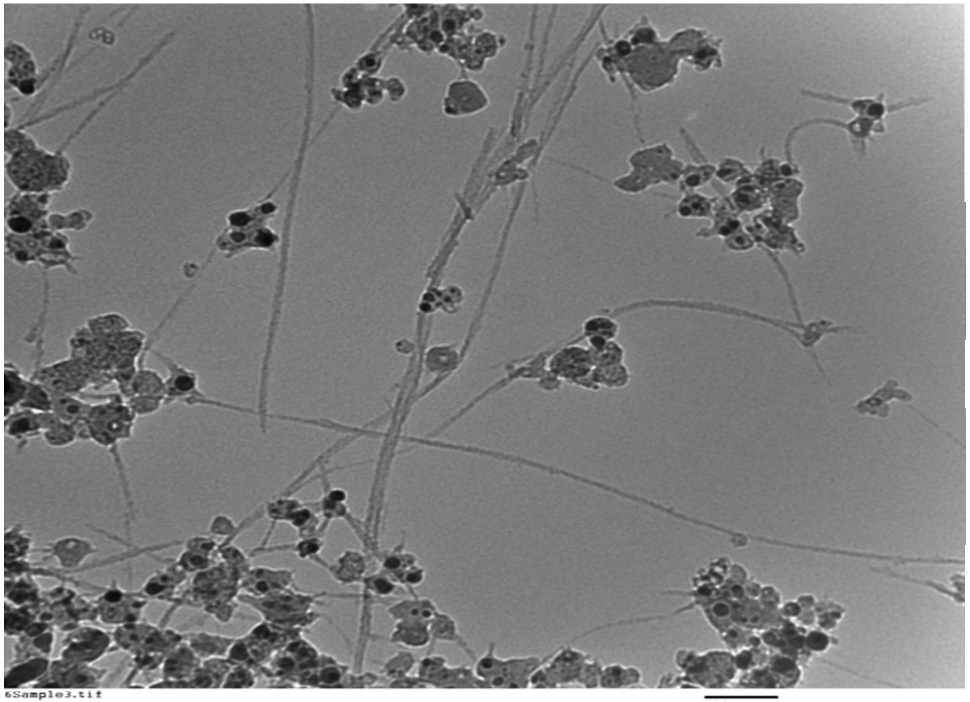


Saha and Deng "H_2 Adsorption on Partially Oxidized C_{60}Fullerene" in preparation, 2009.

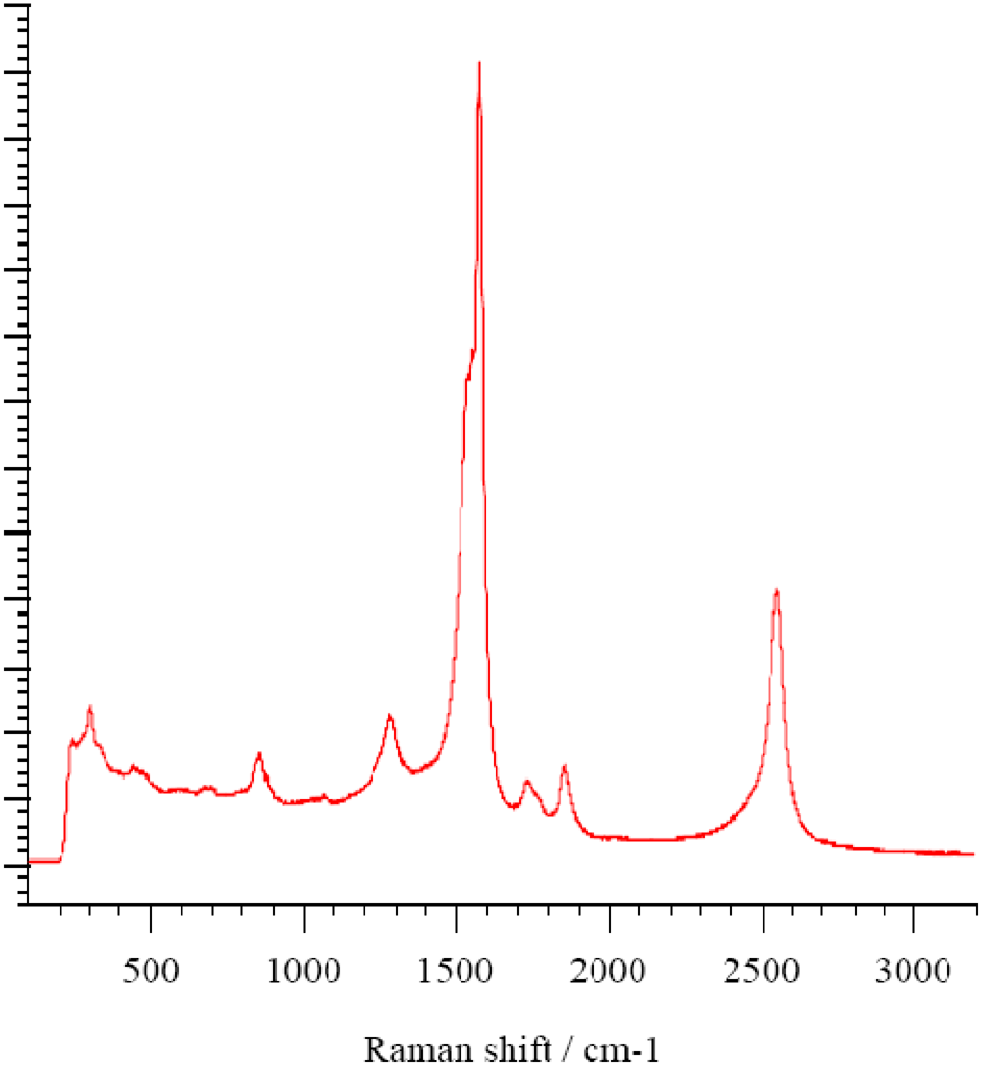
Characterization of Purified SWNTs with SEM/TEM, EDS







Characterization of Purified SWNTs with Raman



Scientific/Technical Approach

Ab Initio Calculations

Dispersion of nanostructures in emissive polymers improves performance of organic photovoltaic materials. Our theoretical research focuses on the properties of carbon nanotubes and nanoparticles embedded in electroactive polymers.

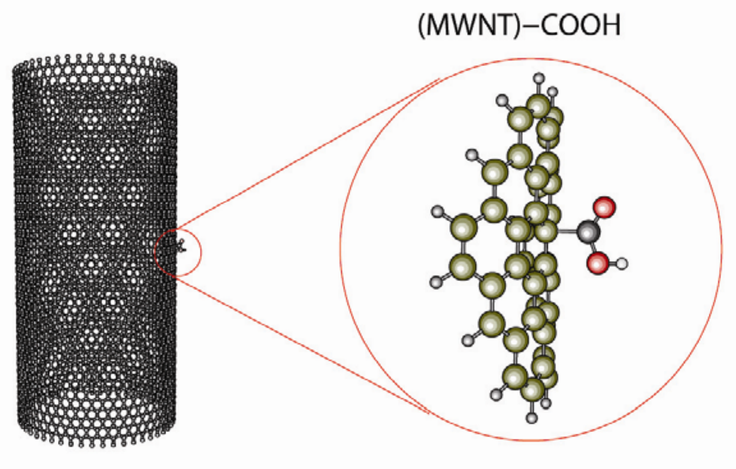
Objectives:
- Study the mechanism of interaction between nanostructures and polymer matrices.
- Examine the possibility of self-assembly of optically active molecules and chemical groups on the surface of nanoparticles and carbon nanotubes.
- Identify nanocomposites suitable for use in cascade solar cells.

Methods:
- Density functional theory combined with pseudopotentials.
- High-performance parallel computational algorithms.
- Efficient electronic structure codes (PARSEC, SIESTA).
- Optical properties are computed in the framework of time-dependent density functional theory.

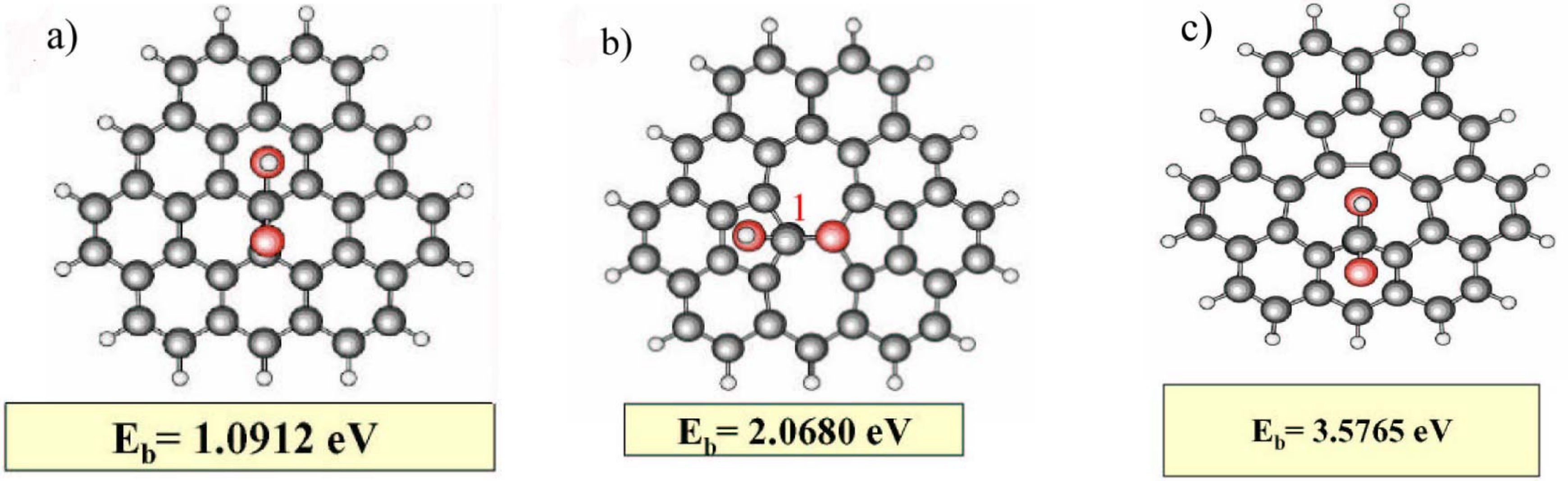
Scientific/Technical Approach

Covalent functionalization of carbon nanotubes:

Ab initio density functional study of carboxylated MWNTs using the PARSEC electronic structure code and the GGA exchange-correlation functional.



Theoretical model for a carboxylated MWNT



E_b= 1.0912 eV

E_b= 2.0680 eV

E_b= 3.5765 eV

Functionalization of MWNTs by COOH groups: (a) defect-free MWNT, (b) MWNT with a Stone-Wales defect, (c) MWNT containing a vacancy.

Scientific/Technical Approach

MWNT-COOH

Structure	Site	E_b(eV)	$d_{c\text{-}c}$(A)
No defects	--	1.09	1.55
Stone-Wales defect	C1	2.06	1.50
	C2	0.69	1.54
	C3	1.42	1.56
Vacancy	--	3.57	1.48

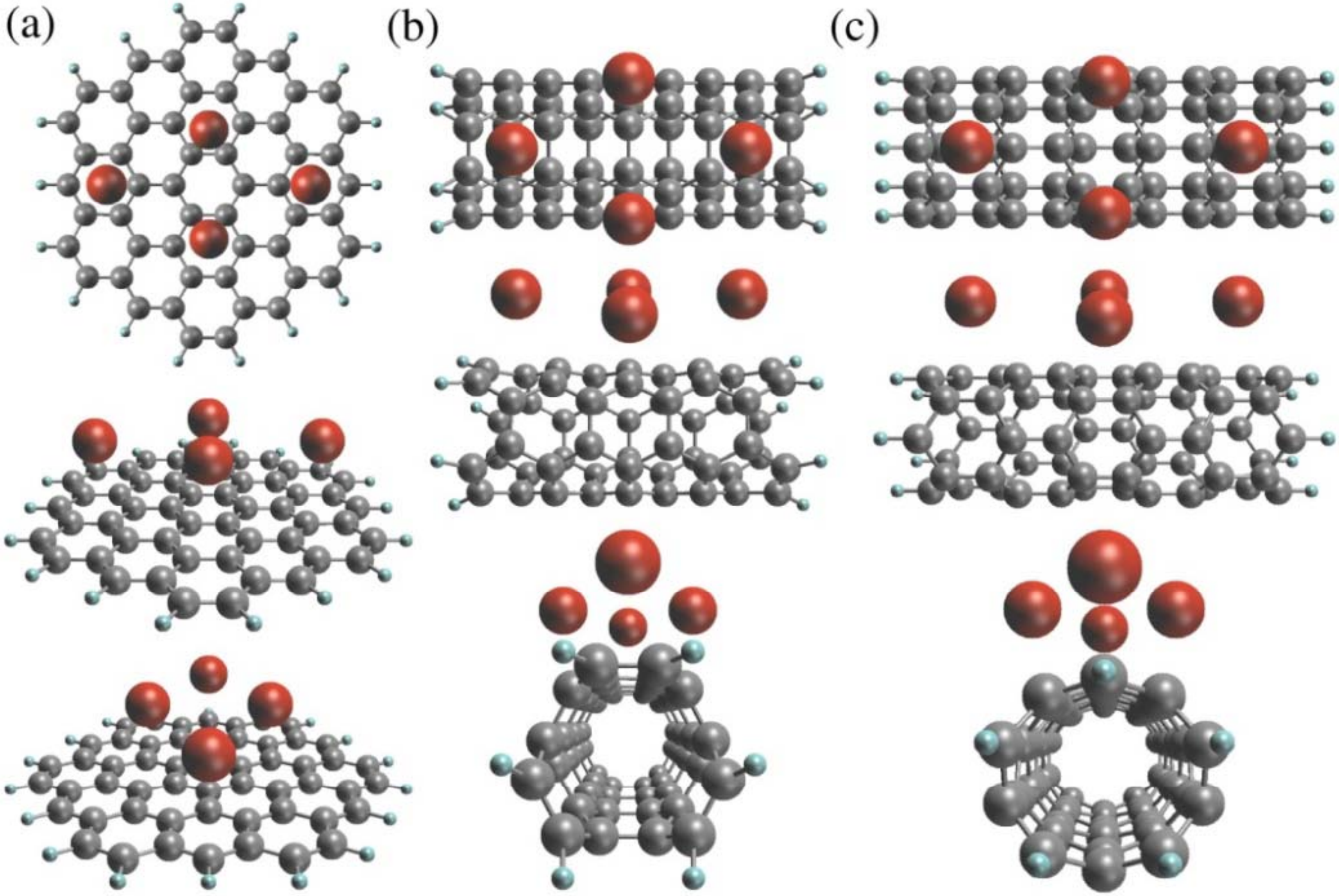
Binging energies and inter-atomic bond lengths for COOH groups attached to SWNTs.

- Chemical functionalization provides the mechanism for self-assembly of optically active molecules and chemical groups on the surface of carbon nanotubes.
- Our study indicates an important role of surface defects in chemical functionalization of carbon nanotubes.
- Surface defects on MWNTs increase the strength and stability of MWNT-COOH bonds.

Scientific/Technical Approach

Adsorption of metal clusters on graphene and carbon nanotubes:

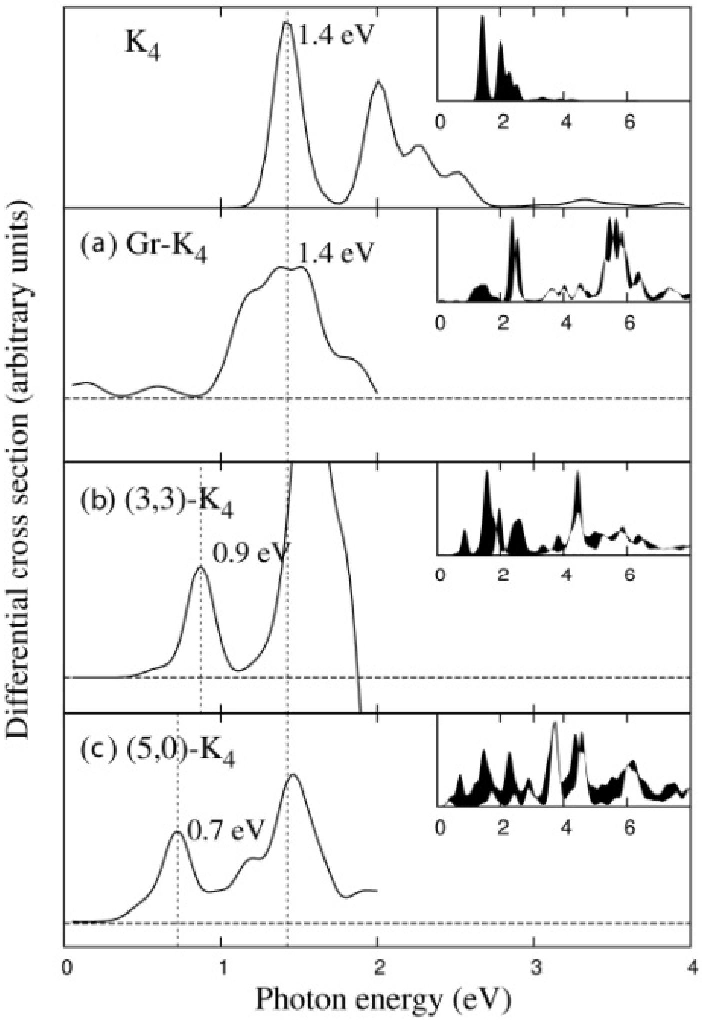
Ab initio density functional calculations using the PARSEC and SIESTA electronic structure codes. Optical spectra are computed using the TDDFT formalism.



Structures of K_4 clusters adsorbed on (a) graphene, (b) (3,3) SWCNT, and (c) (5,0) SWCNT.

Scientific/Technical Approach

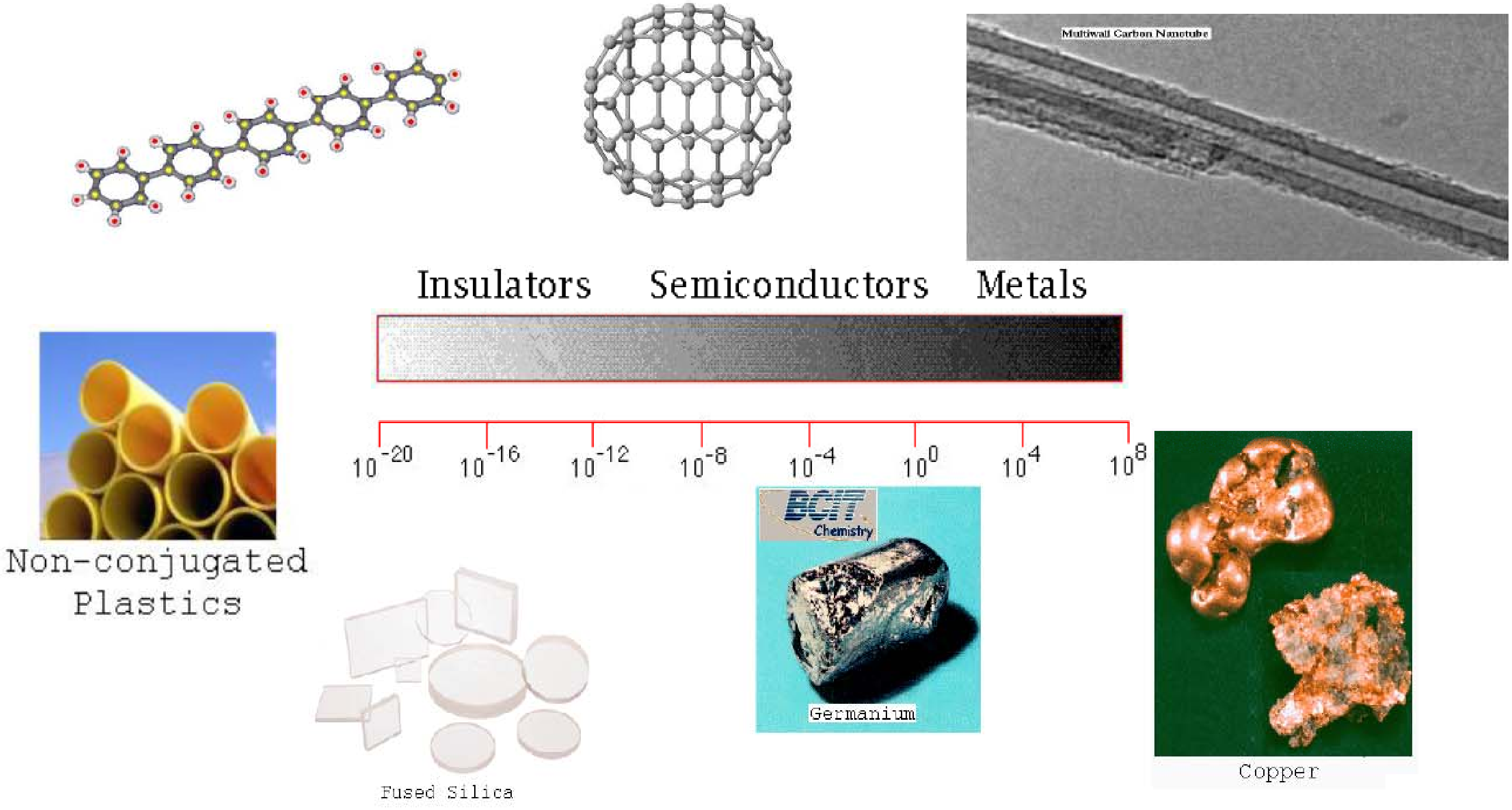
- We observe significant differences between the optical spectra of isolated alkali metal clusters and those adsorbed on graphene and carbon nanotubes.
- Large dipole moments and low-energy absorption bands in the spectra of K_4-graphene and K_4-SWCNT structures indicate charge transfer from potassium clusters to graphene/SWCNTs.
- Differences in the absorption spectra of K_4-graphene and K_4-SWCNT structures suggests a different mechanism of interaction of alkali metal clusters with graphene and SWCNTs.
- Calculations for larger metal & semiconductor clusters are in progress.



Optical spectra of K_4 clusters adsorbed on (a) graphene, (b) (3,3) SWNT, and (c) (5,0) SWNT

Scientific/Technical Approach

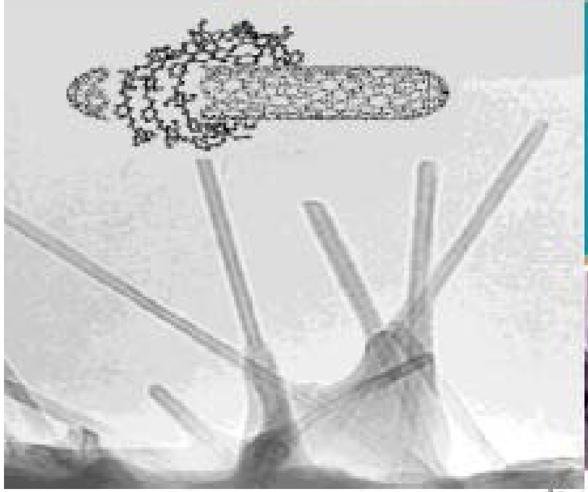
All about managing the charge ...

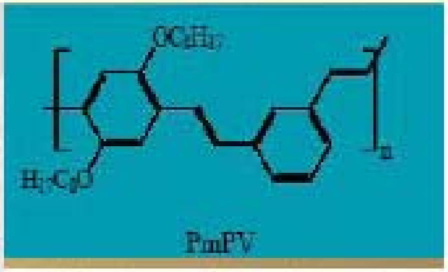


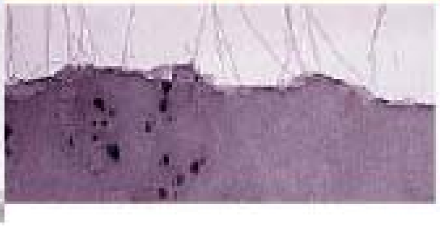
Scientific/Technical Approach

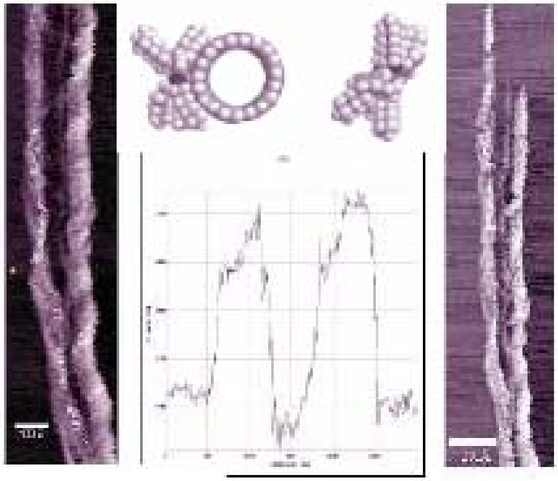
The First Polymer-Nanotube Composite Device

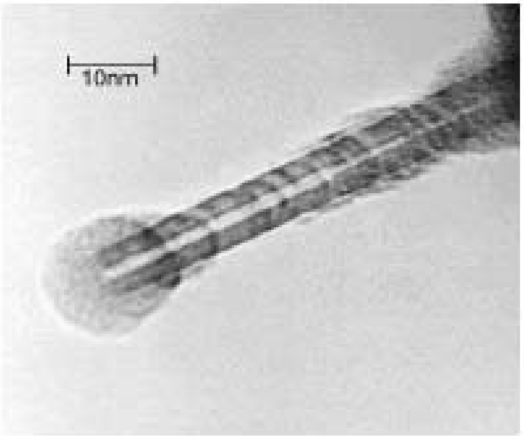
S. Curran, P.M. Ajayan, W. Blau, D.L. Carroll, J. Coleman, A. Dalton, A.P. Davey, B. McCarthy, and A. Strevens, *Advanced Materials*, 10, No. 14, (1998) 1091 (cover feature of this journal)

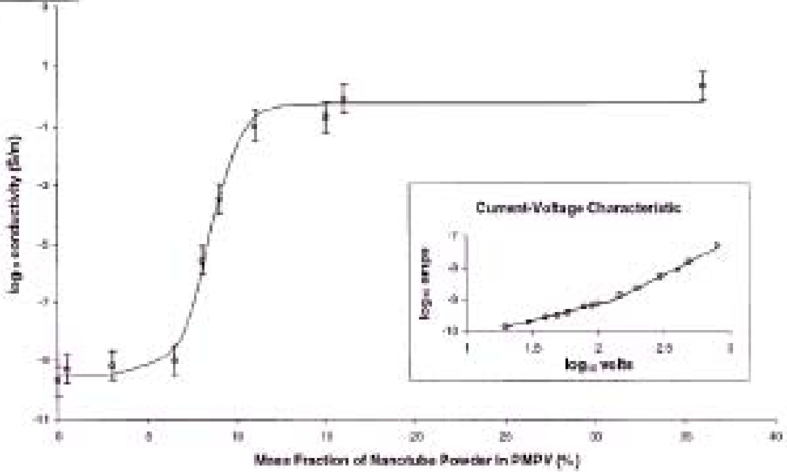


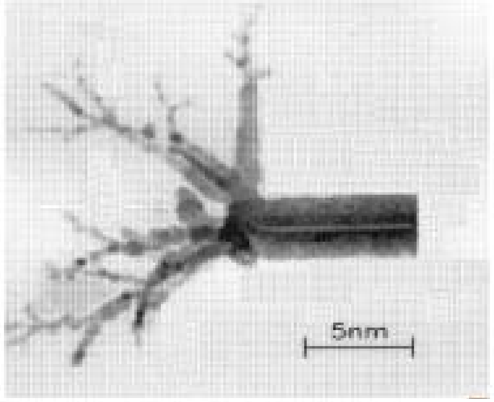






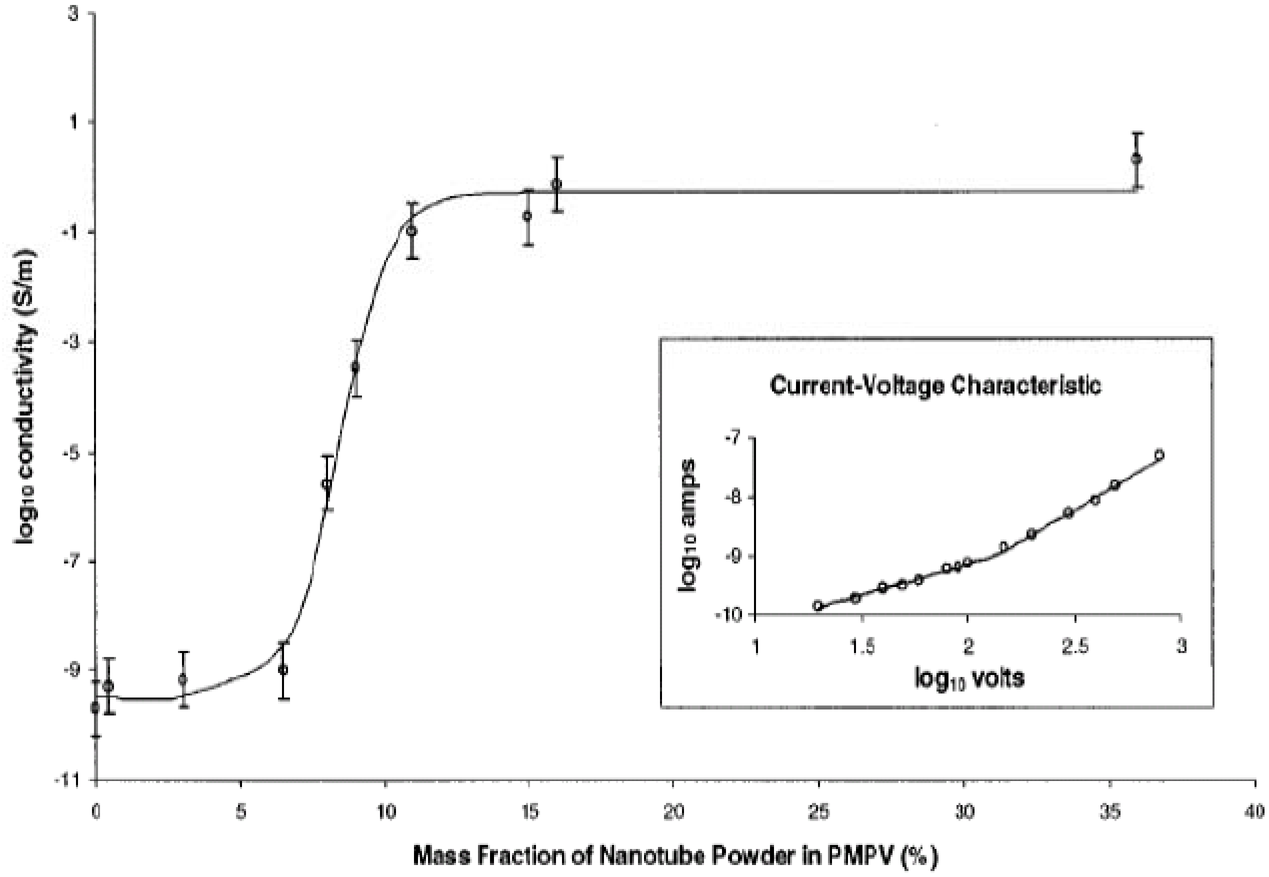


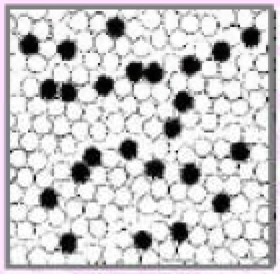




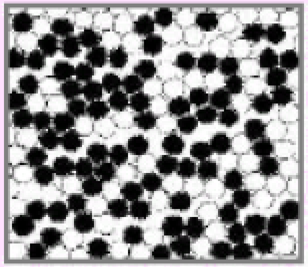
Patent: A Nanocomposite by *Curran et al*, Granted June 2003, Patent Number US 6,576,341, 3rd most cited nanopatent (S. Walsh, MANCEF 2006)

Scientific/Technical Approach

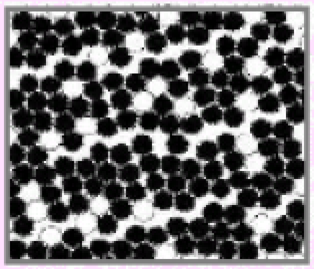




$p < p_c$



$p \simeq p_c$



$p > p_c$.

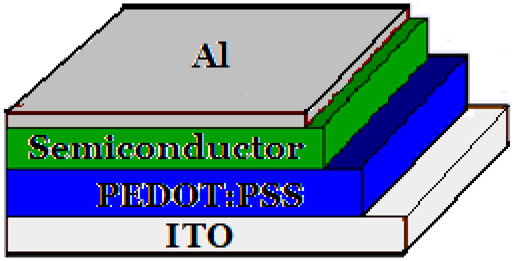
S. Curran, A.P. Davey, J. Coleman, A. Dalton, B. McCarthy, S. Maier, D. Gray, M.Brennan, K. Ryder, M.L. de la Chapelle, C. Journet, P. Bernier, H.J. Byrne, D. Carroll, P.M. Ajayan, S. Lefrant, and W.J. Blau, '*Evolution and Evaluation of the Polymer Nanotube Composite*' **Synthetic Met.** 103, 2559 (1999)

J.N. Coleman, S. Curran, A.B. Dalton, A.P. Davey, B. McCarthy, W. Blau, and R.C. Barklie, '*Percolation-dominated Conductivity in a Conjugated-polymer-carbon-nanotube Composite*', **Physical Rev. B**, 58, 7492, (1998)

Scientific/Technical Approach

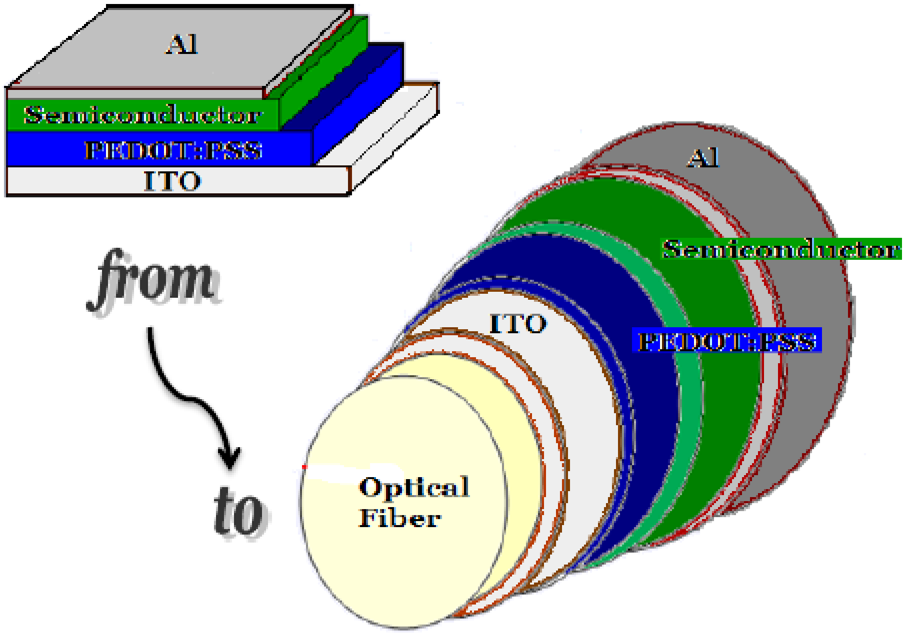
University of Houston's Program Challenge: Examining the composition of organic photovoltaic's in terms of materials and architecture

Material development



1. n-type semiconductor design
2. PEDOT:PSS replacement

Architecture change



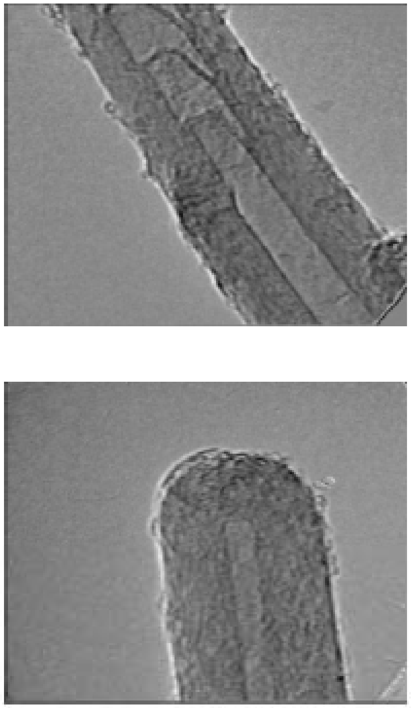
A concentrator architecture

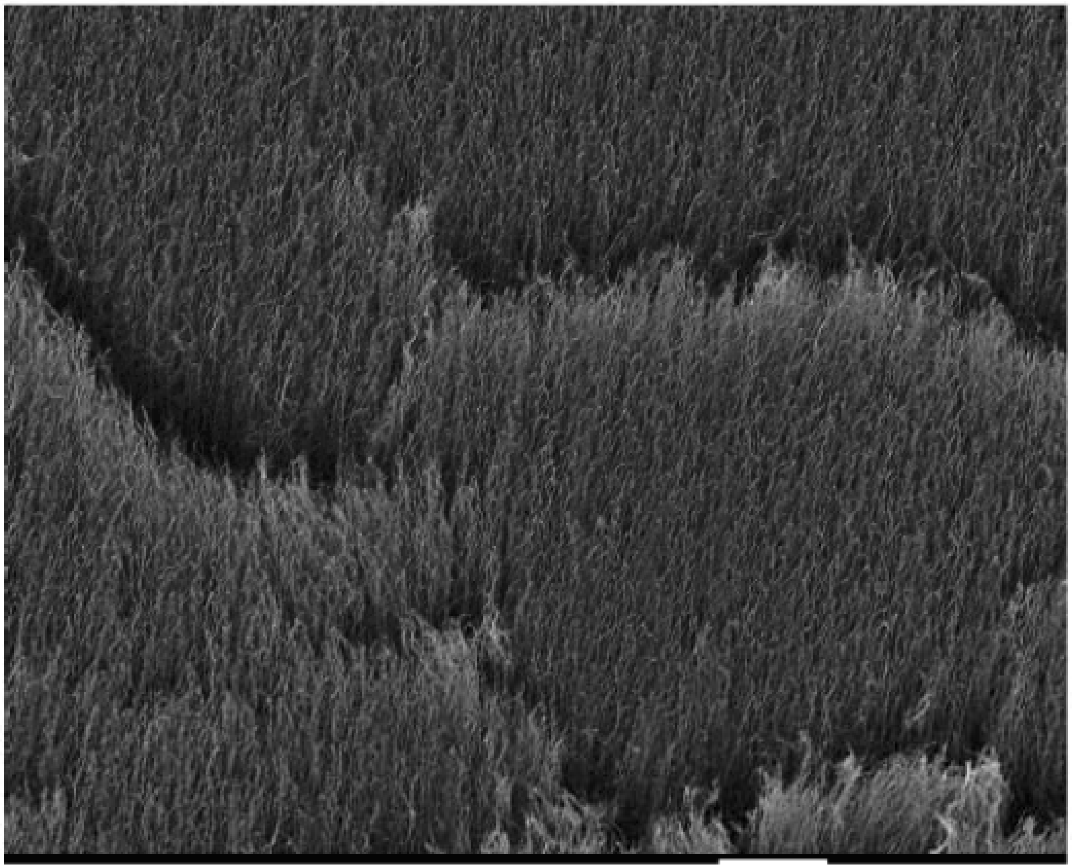
Scientific/Technical Approach

1. Gaining a spectroscopic and morphological understanding of the materials

Scientific/Technical Approach

Gaining an insight into defect formation using Raman and resonance Raman Spectroscopy





The effect of carboxylation (the current method of purification) needs to be addressedand the effect on conductivity will be examined in terms of defect formation

N. Chakrapani , S. Curran , B. Wei , P. M. Ajayan , A. Carrillo, and R. S. Kane, '*Spectral fingerprinting of structural defects in plasma-treated carbon nanotubes*', J. Mater. Res. **18, 2515** (2003)

Scientific/Technical Approach

Spectroscopic characterization of nanotubes and their defects

- Graphite belongs to the D^4_{6h} space group
- Irreducible representation can be described by:

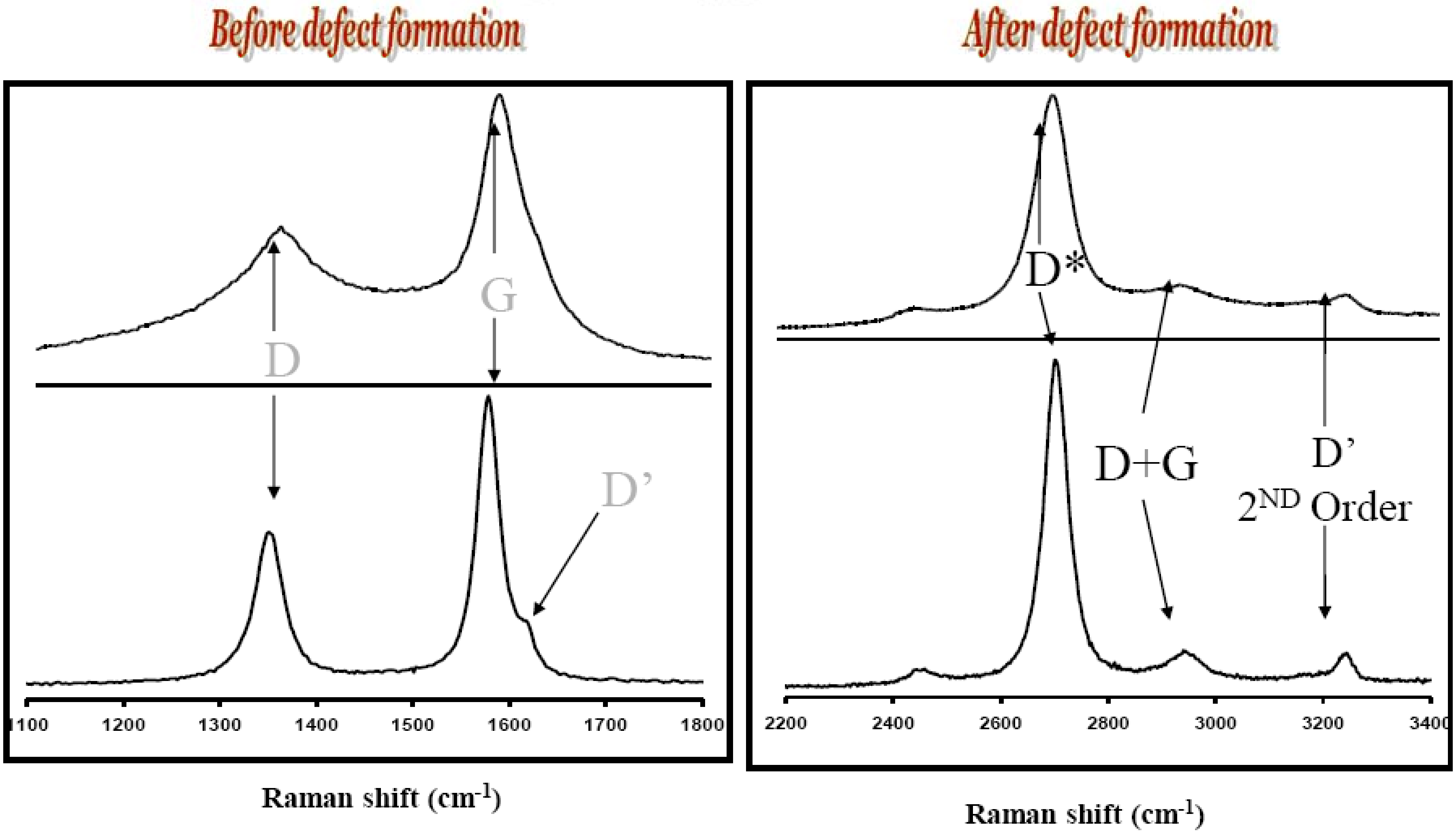
$$G = 2E_{2g} + E_{1u} + 2B_{2g} + A_{2u}$$

Initial analysis of NT showed that the following modes are Raman active

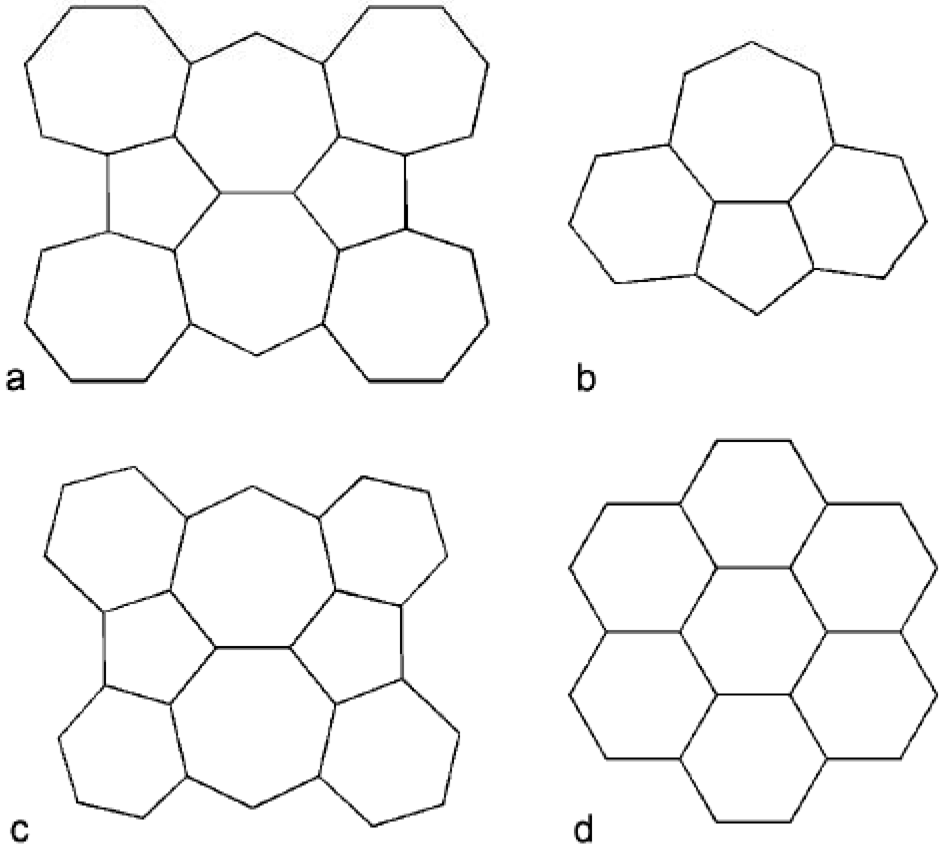
- E_{2g} in plane stretching mode and A_{2u} 'Breathing mode'

Scientific/Technical Approach

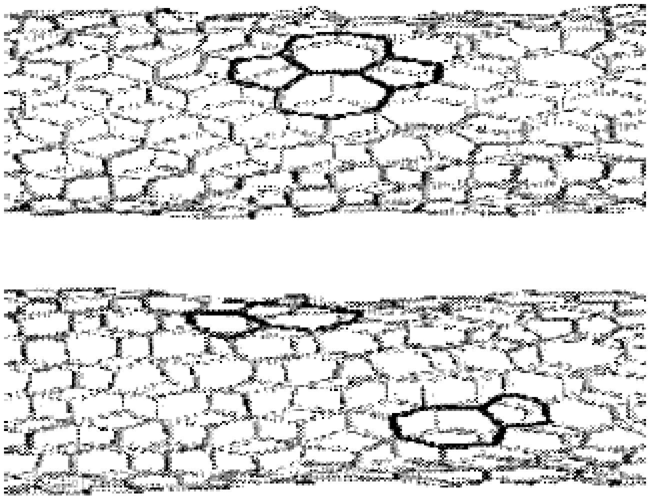
Typical Raman spectra of plasma treated nanotubes



With greater analysis, we can now characterize the defects as well



Graphic representation of three types of Haecklites in addition to graphite (a: $R_{5,7}$; b: $O_{5,6,7}$; c: $H_{5,6,7}$; d: graphite).



Defects in carbon nanotubes (CNT)

<u>S.A.Curran</u>, J.A.Talla, D. Zhang, and D.L.Carroll, *'Defect Induced Vibration Response of MWCNT using Resonance Raman Spectroscopy'*, **J. Mater. Res.,** Vol. 20, No. 12, *(2005)*

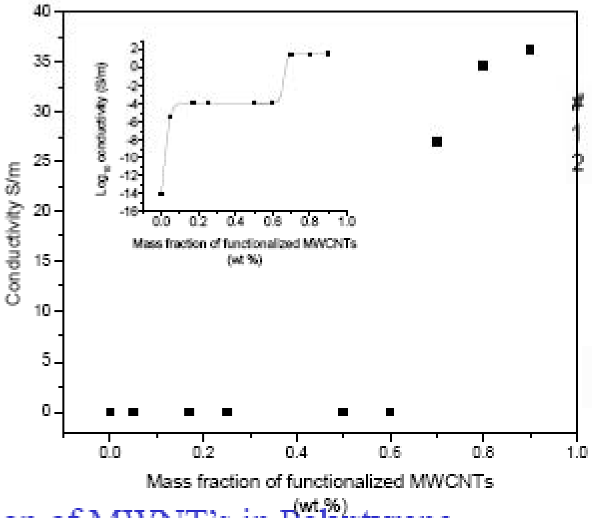
Scientific/Technical Approach

2. Looking for highly controllable conductive layers

Thin film composites
(addressing transparency
and high conductivity)

Scientific/Technical Approach

gRAFT Composite

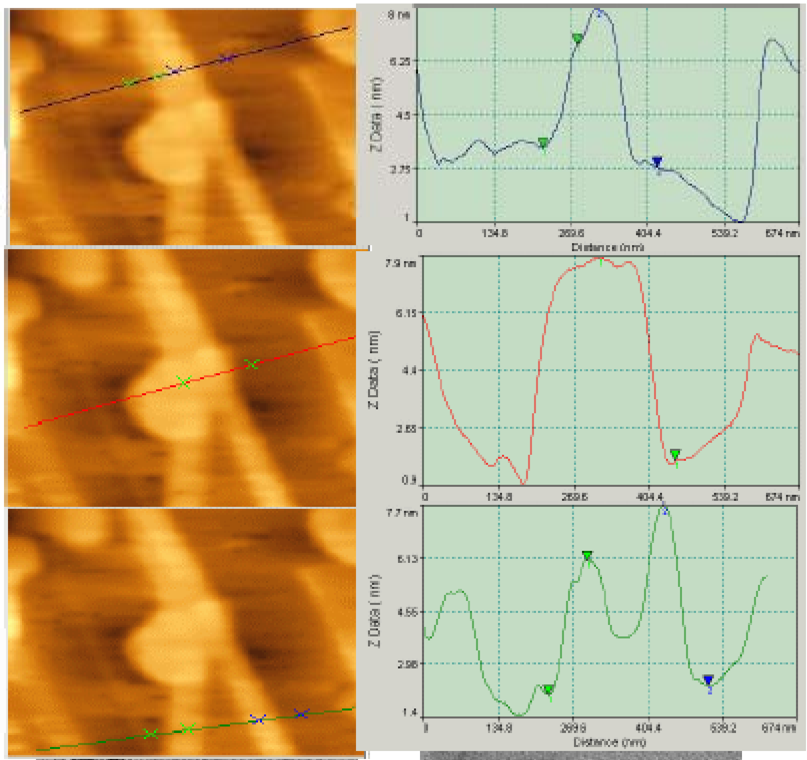


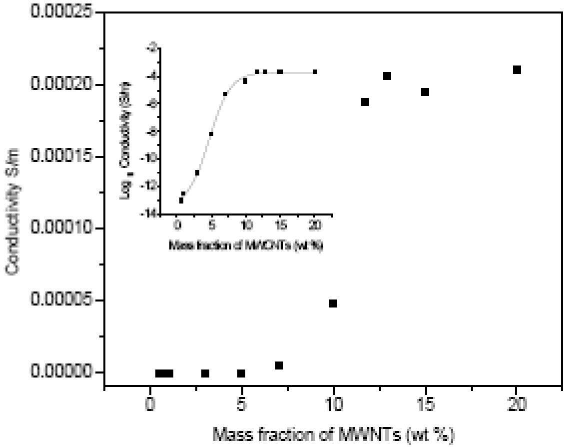
Mass fraction of MWNT's in Polystyrene

#	Distance	Height
1	60.80 nm	3.34 nm
2	104.7 nm	5.11 nm

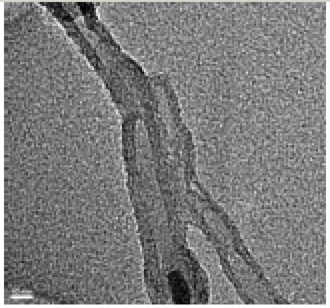
Distance	Height
136.5 nm	6.18 nm

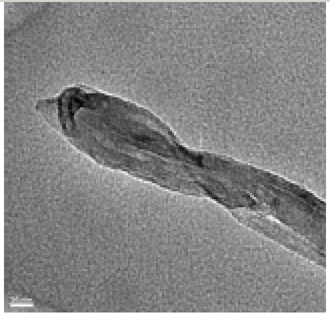
Distance	Height
70.84 nm	3.97 nm
81.20 nm	5.27 nm





Traditional Composite

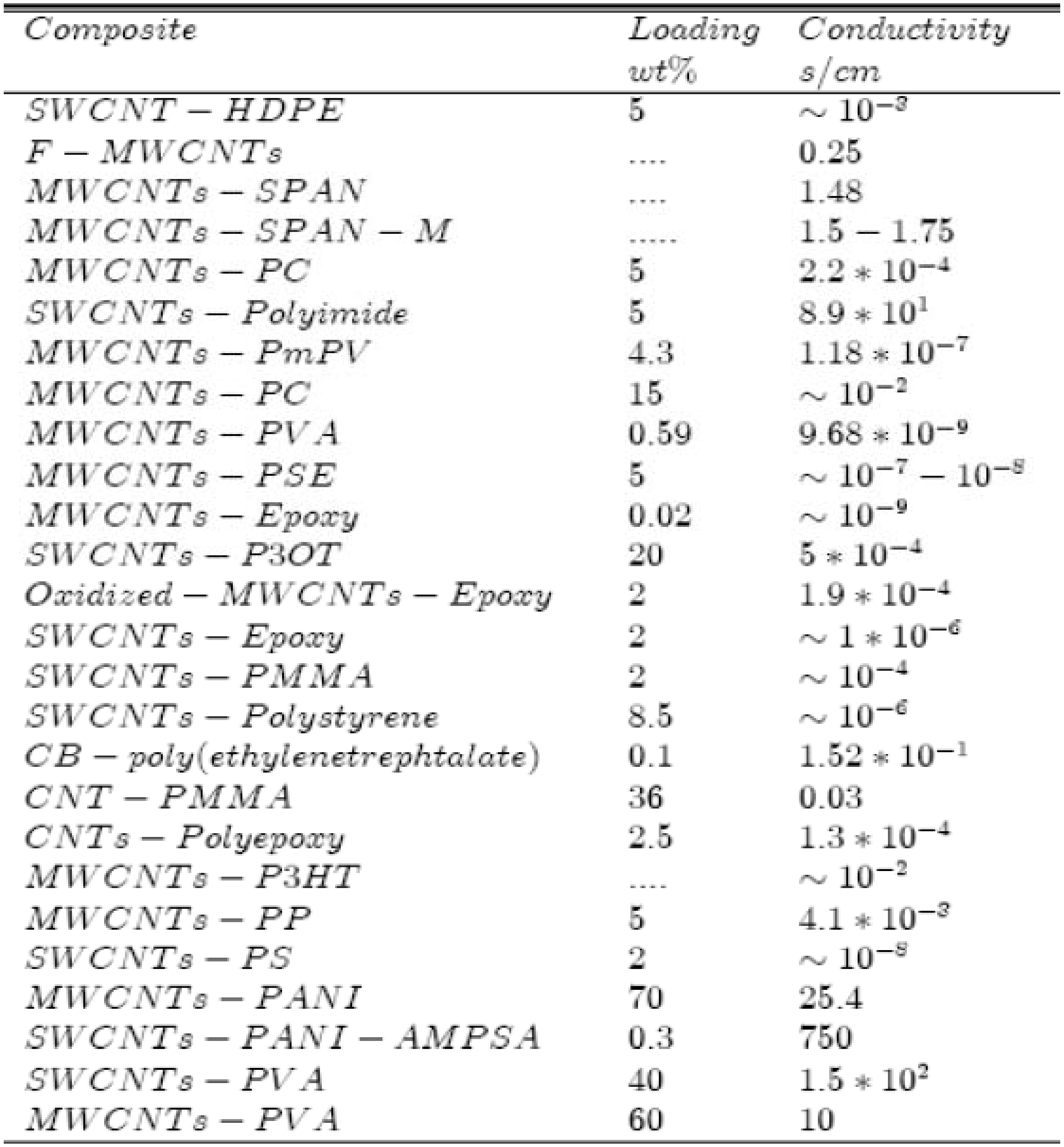




S. A. Curran, D. Zhang, W. T. Wondmagegn, A. V. Ellis, J. Cech, D. L. Carroll and S. Roth, '*Dynamic electrical properties of polymer Carbon Nanotube Composites: Enhancement through covalent bonding*', **Journal of Materials Research**, 21, 4, 1071 (2006)

S. A. Curran, J. Cech, D. Zhang, J. L. Dewald, A. Avadhanula, M. Kandadai and S. Roth, 'Thioation of Carbon Nanotubes and Sidewall Functionalization', **J. Mater. Res**., 21, 4, 1012 *(2006)*

Scientific/Technical Approach

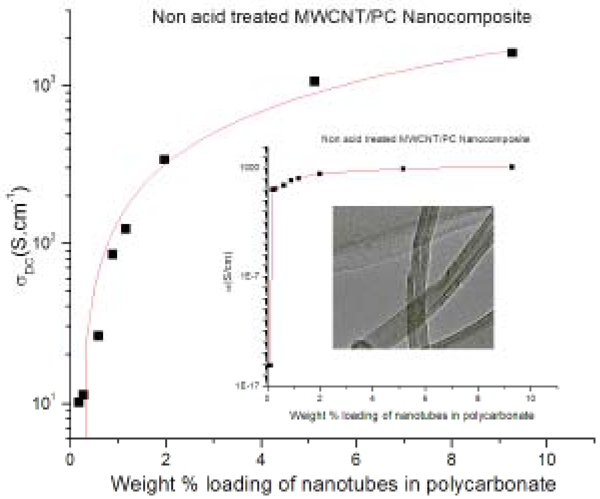


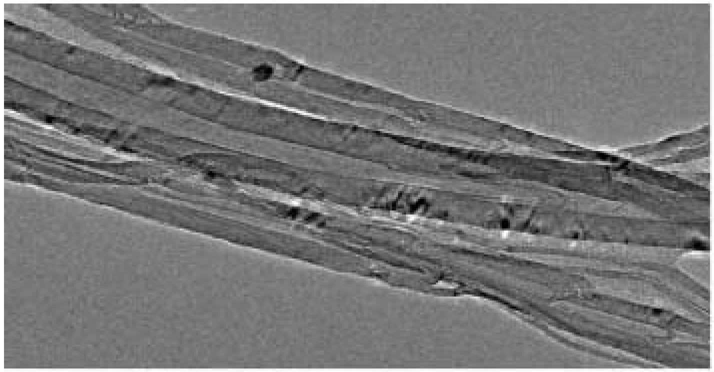
Composite	Loading wt%	Conductivity s/cm
SWCNT − HDPE	5	$\sim 10^{-3}$
F − MWCNTs	....	0.25
MWCNTs − SPAN	....	1.48
MWCNTs − SPAN − M	.....	1.5 − 1.75
MWCNTs − PC	5	$2.2 * 10^{-4}$
SWCNTs − Polyimide	5	$8.9 * 10^{1}$
MWCNTs − PmPV	4.3	$1.18 * 10^{-7}$
MWCNTs − PC	15	$\sim 10^{-2}$
MWCNTs − PVA	0.59	$9.68 * 10^{-9}$
MWCNTs − PSE	5	$\sim 10^{-7} - 10^{-8}$
MWCNTs − Epoxy	0.02	$\sim 10^{-9}$
SWCNTs − P3OT	20	$5 * 10^{-4}$
Oxidized − MWCNTs − Epoxy	2	$1.9 * 10^{-4}$
SWCNTs − Epoxy	2	$\sim 1 * 10^{-6}$
SWCNTs − PMMA	2	$\sim 10^{-4}$
SWCNTs − Polystyrene	8.5	$\sim 10^{-6}$
CB − poly(ethylenetrephtalate)	0.1	$1.52 * 10^{-1}$
CNT − PMMA	36	0.03
CNTs − Polyepoxy	2.5	$1.3 * 10^{-4}$
MWCNTs − P3HT	....	$\sim 10^{-2}$
MWCNTs − PP	5	$4.1 * 10^{-3}$
SWCNTs − PS	2	$\sim 10^{-8}$
MWCNTs − PANI	70	25.4
SWCNTs − PANI − AMPSA	0.3	750
SWCNTs − PVA	40	$1.5 * 10^{2}$
MWCNTs − PVA	60	10

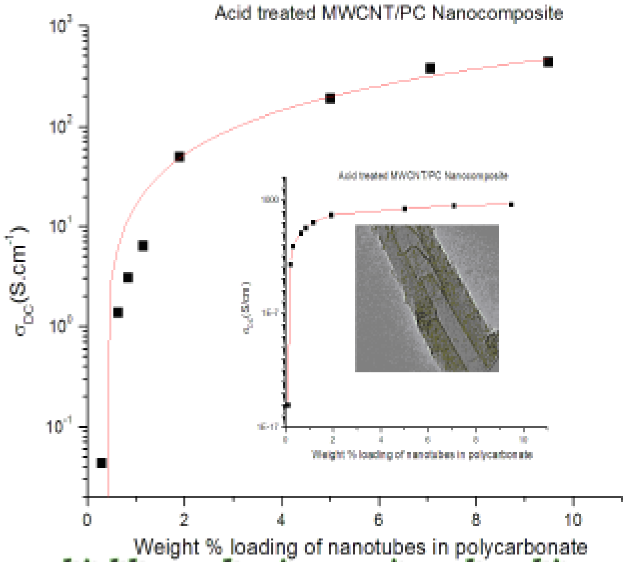
Situation a lot more complex: Not a trivial notion of mixing a conductive filler with a psudo-nonconducting matrix

More importantly, if nanotubes have conductivities in excess of metals why do we not see this manifest itself at the peak percolation threshold

Scientific/Technical Approach







Purified MWCNT/PC		Non-purified MWCNT/PC	
Loading %	σ_{DC} (S/cm)	Loading %	σ_{DC} (S/cm)
0.0	~10^{-16}	0.0	~10^{-16}
0.1	~10^{-16}	0.1	~10^{-16}
0.2	0.002 ± 0.00	0.19	11.29 ± 1.47
0.3	0.08 ± 0.01	0.28	12.98 ± 1.35
0.64	1.10 ± 0.09	0.6	26.68 ± 5.56
0.84	3.12 ± 0.14	0.89	77.45 ± 4.30
1.15	9.09 ± 0.10	1.17	122.03 ± 5.90
1.91	49.37 ± 2.00	1.98	317.8 ± 20.17
5.01	174.83 ± 9.27	5.13	896.58 ± 23.90
7.07	339.02 ± 6.40	-------	-------
9.49	408.8 ± 22.8	9.28	1312.93 ± 91.30

We can get highly conductive coatings, but this method precludes transparency

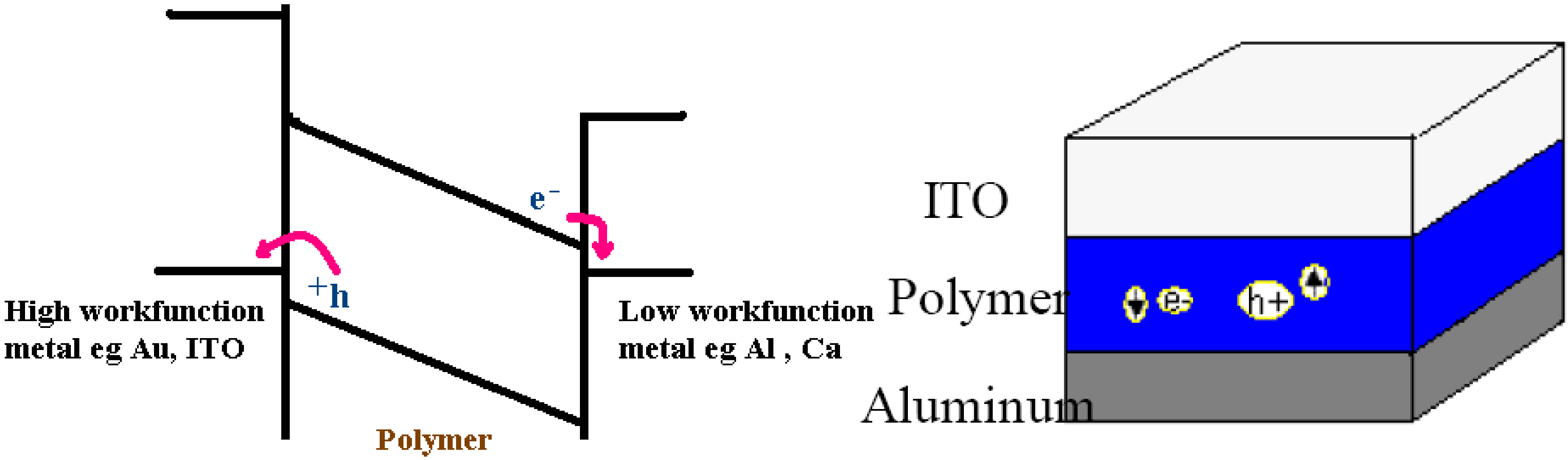
(Curran et al, JAP Spring 2009)

Scientific/Technical Approach

3. Forming organic photovoltaic's

Classical materials and architectures, and the continued developments

Semiconductor Devices - Schottky Junction



- This was the first architecture to be tried in the 1990’s
- Al replaced Ca as the Schottky contact
- Originally used for OLED device as an architecture
- Conjugated polymers from the polythiophene family were initially tried
- Best solar cell efficiencies of these devices was typically 1%
- Poor transport, oxidation and limited spectral absorption remain as the main drawbacks

Typical polymer Schottky solar cell

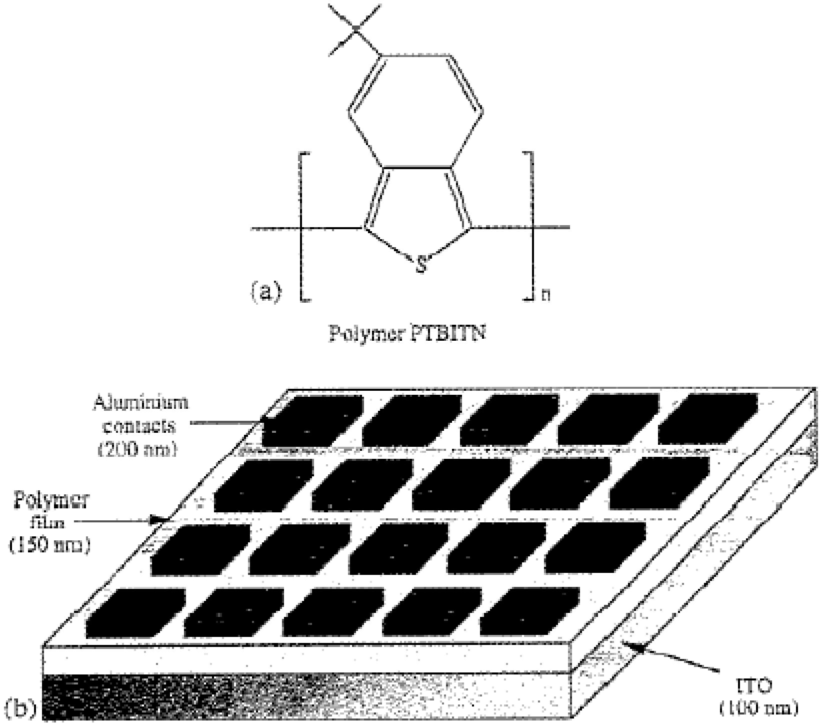


Fig. 1. Structure of (a) PTBITN and (b) typical diodes fabricated.

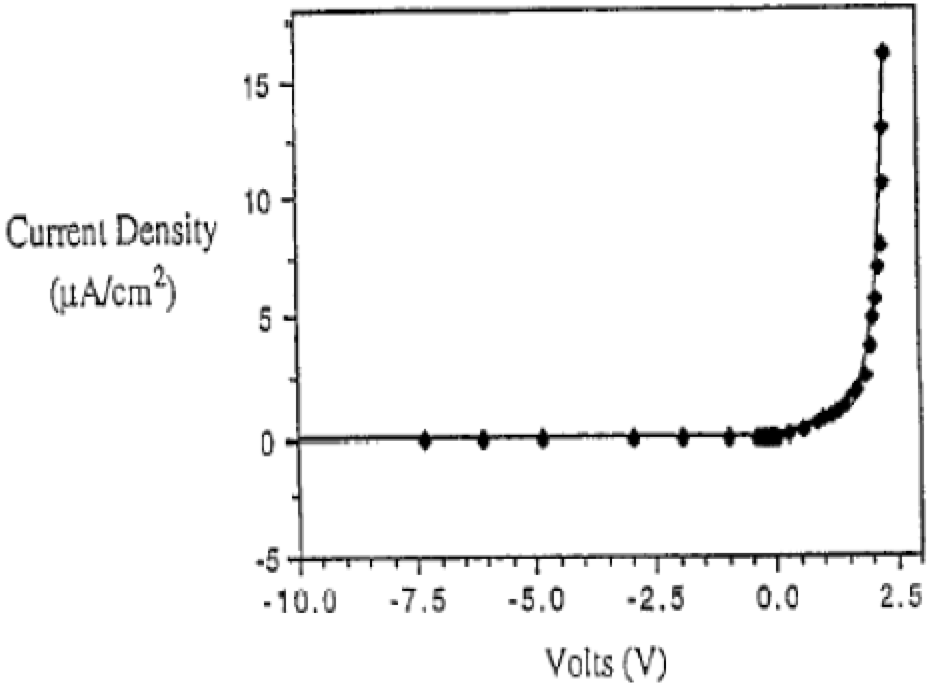


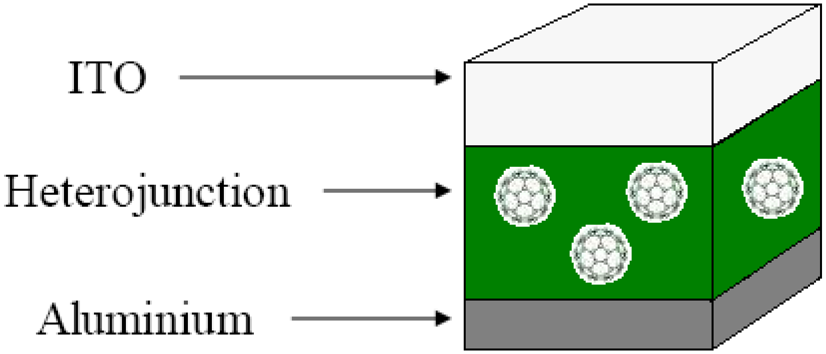
Fig. 2. Current density against applied voltage (in the dark) for both forward and reverse bias conditions.

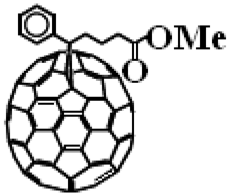
These polymers have been shown to be typically poor in terms of the power conversion efficiency

- S. Curran, S. Roth, A.P. Davey, A. Drury, and W. Blau. *Photoconduction and Photovoltaic Effects from a Conjugated Polymer Poly-Tert Butyl-Isothionaphthalene'*, **Synthetic Metals**, 83, 239, **(1996)**

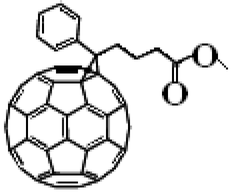
Organic Photovoltaics - the Heterojunction

Best polymer type found for these devices so far has been P_3HT

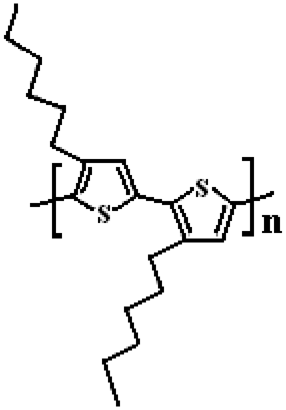




C_{70} - PCBM



C_{60} - PCBM



P_3HT

Using a functionalized fullerene has proven to be the best n type material found to date

Much research into using these materials has been done in the last 5-6 years and is the subject of over 1,000 journal publications

By varying the mix, device efficiencies have gone beyond 2 ½ %

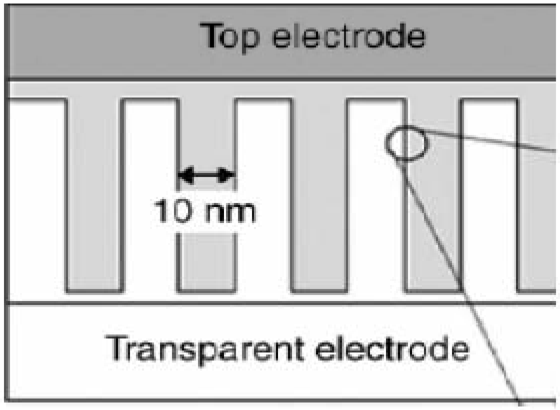
Thermal treatment for over an hour produces large fullerene crystals within the polymer mix – has led to efficiencies of 3 ½ %

Recent work on morphology has led to improvements in efficiency of beyond 5%

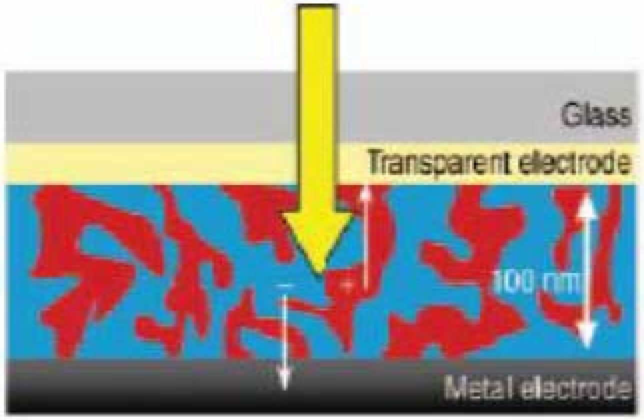
M. Reyes-Reyes, K. Kim, J. Dewald, R. López-Sandoval, A. Avadhanula, S. Curran and D. L. Carroll, *'Meso-Structure Formation for Enhanced Organic Photovoltaic Cells'*, **Organic Letters**, 7, 26, 5749-5752, *(2005)*

Scientific/Technical Approach

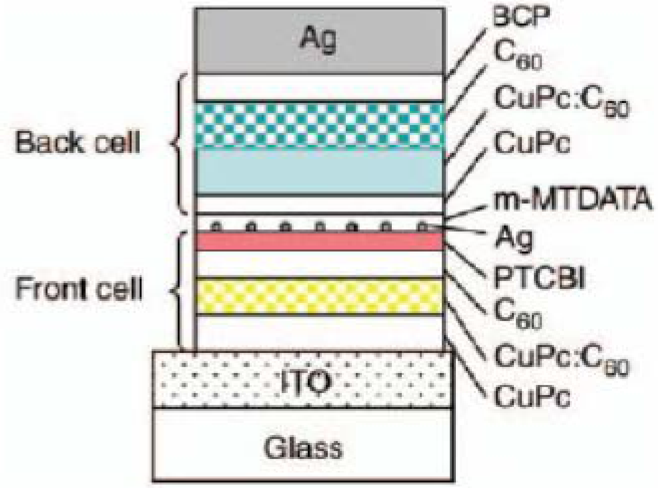
New Device Architectures being explored for the latest OPV cells



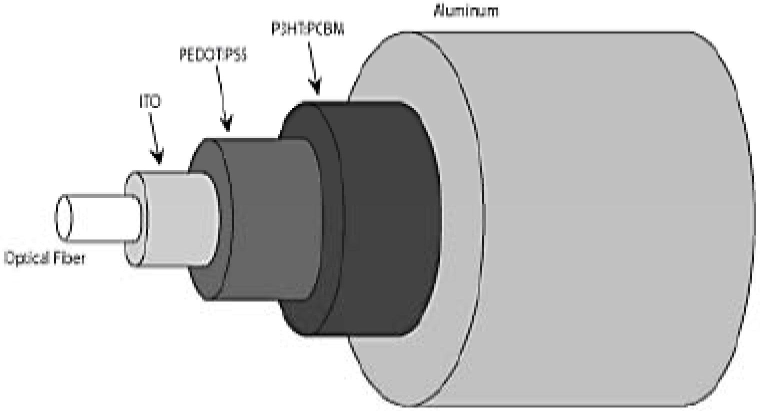
1. Hybrid Organic-inorganic bulk heterojunction



2. Organic-organic bulk heterojunction



3. Multilayered OPVs



4. micro-Concentrator solar cell

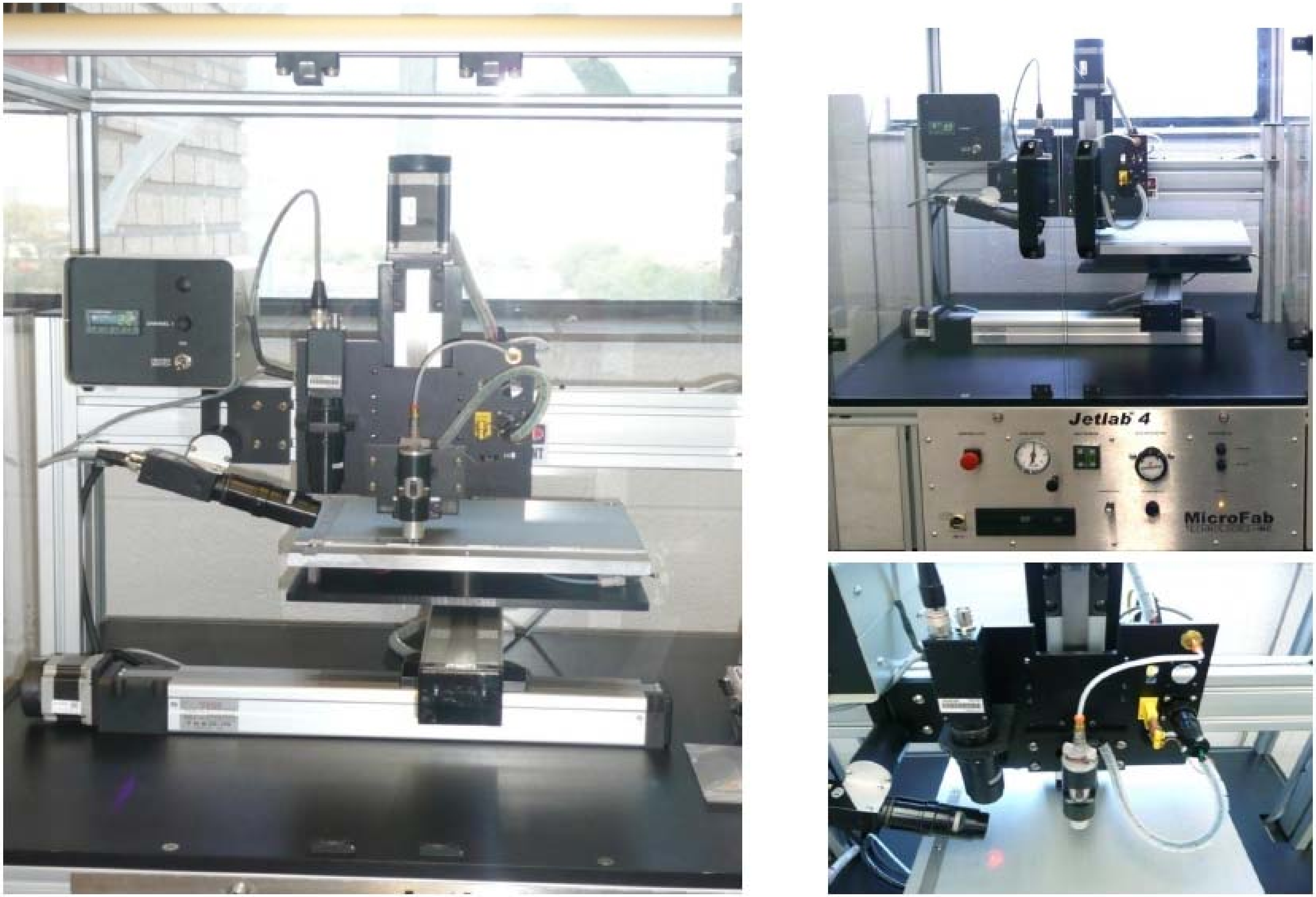
P. Peumans, A. Yakimov, and S.R. Forrest, *J. Appl. Phys.* **93** (2003) p. 3693.3. Y. Liu, K.M. Coakley, and M.D. McGehee, *Proc., SPIE: Organic Photovoltaics IV* **5215** (2004), S.Curran, *et al*, *'Cascade solar cell increases efficiency'* **SPIE,** DOI: 10.1117/2.1200608.0324 (2006)

Scientific/Technical Approach

4. Looking for composite formations

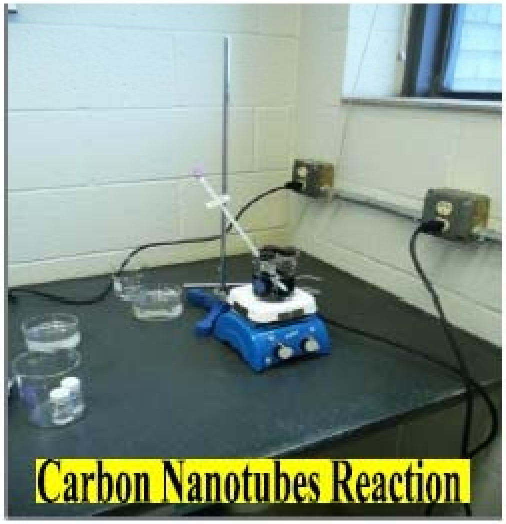
Scientific/Technical Approach

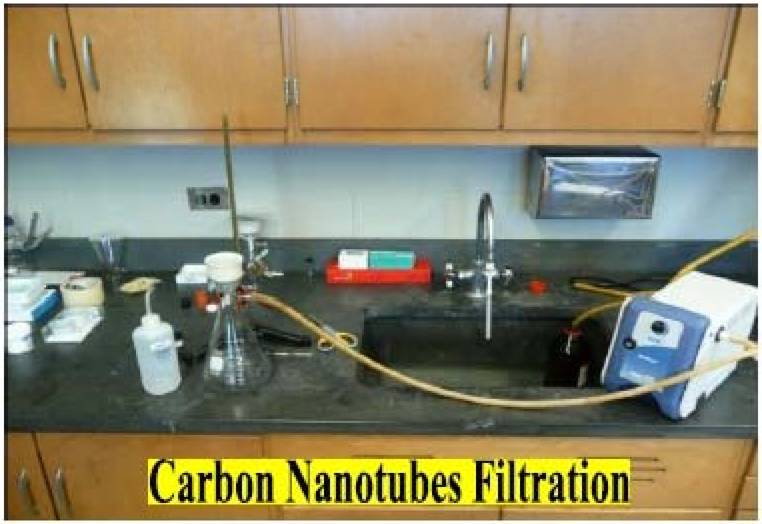
New print system for controlled nanomaterial deposition

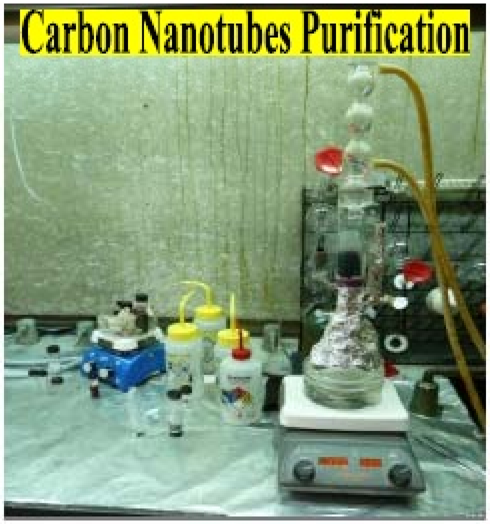


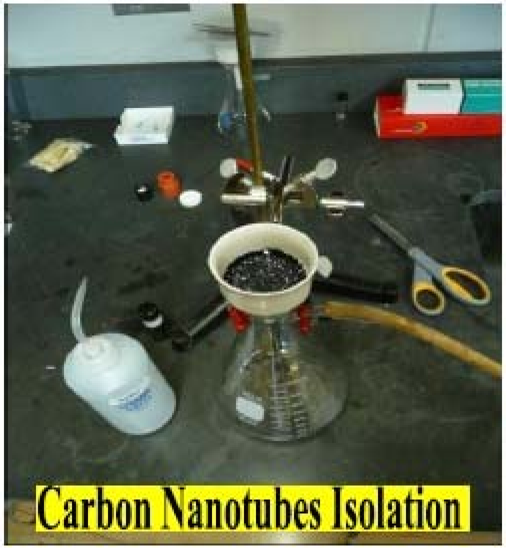
Scientific/Technical Approach

Carbon Nanotube processing for ink and doped materials


Carbon Nanotubes Reaction

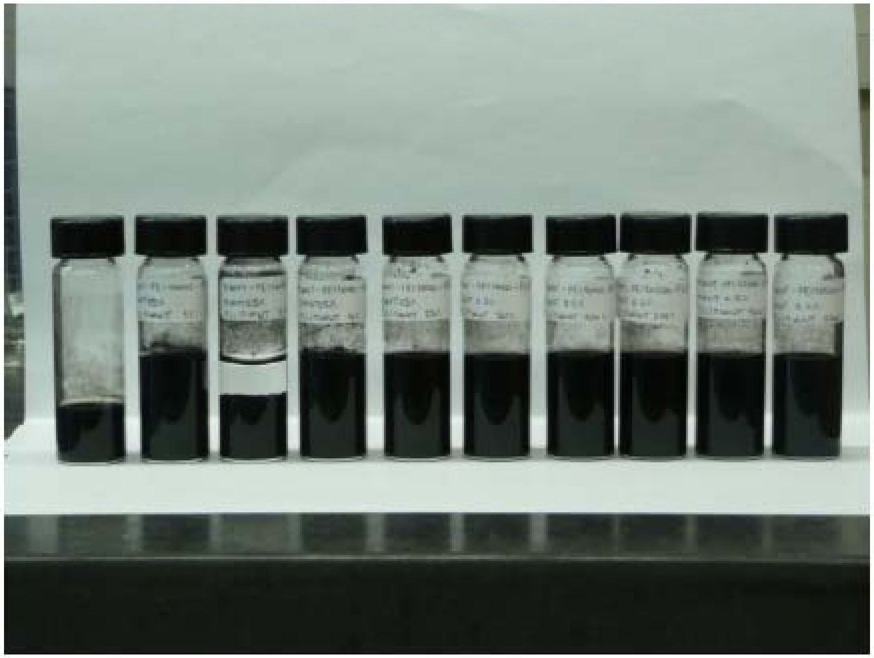

Carbon Nanotubes Filtration

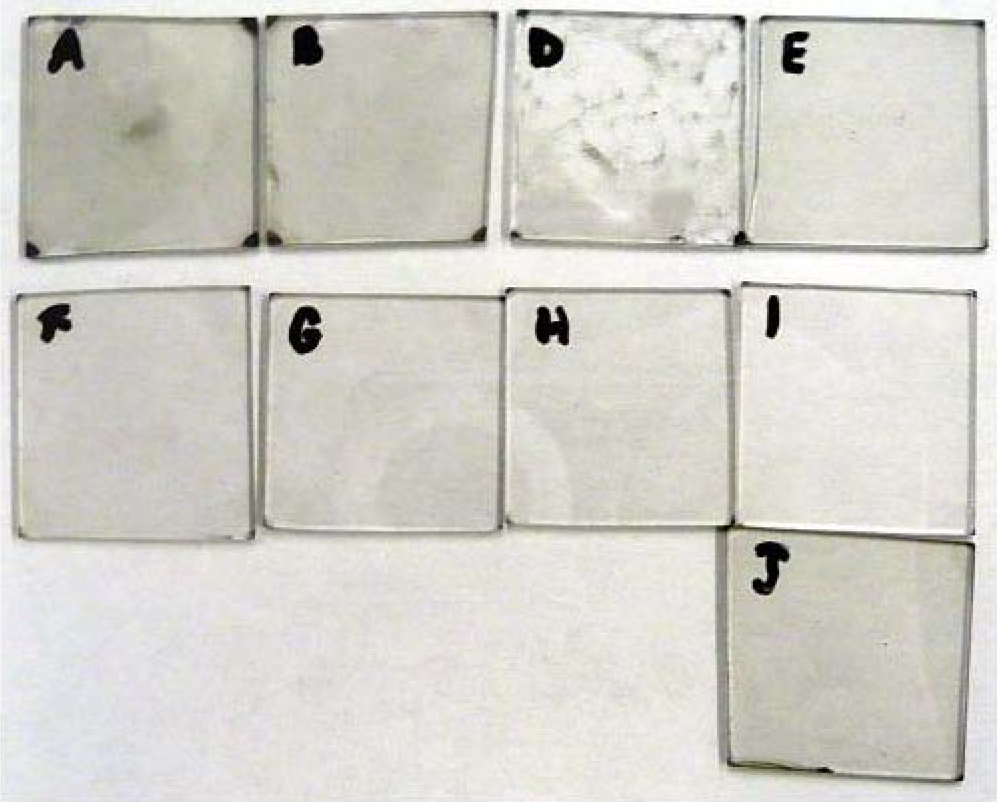

Carbon Nanotubes Purification


Carbon Nanotubes Isolation


Carbon Nanotubes Products

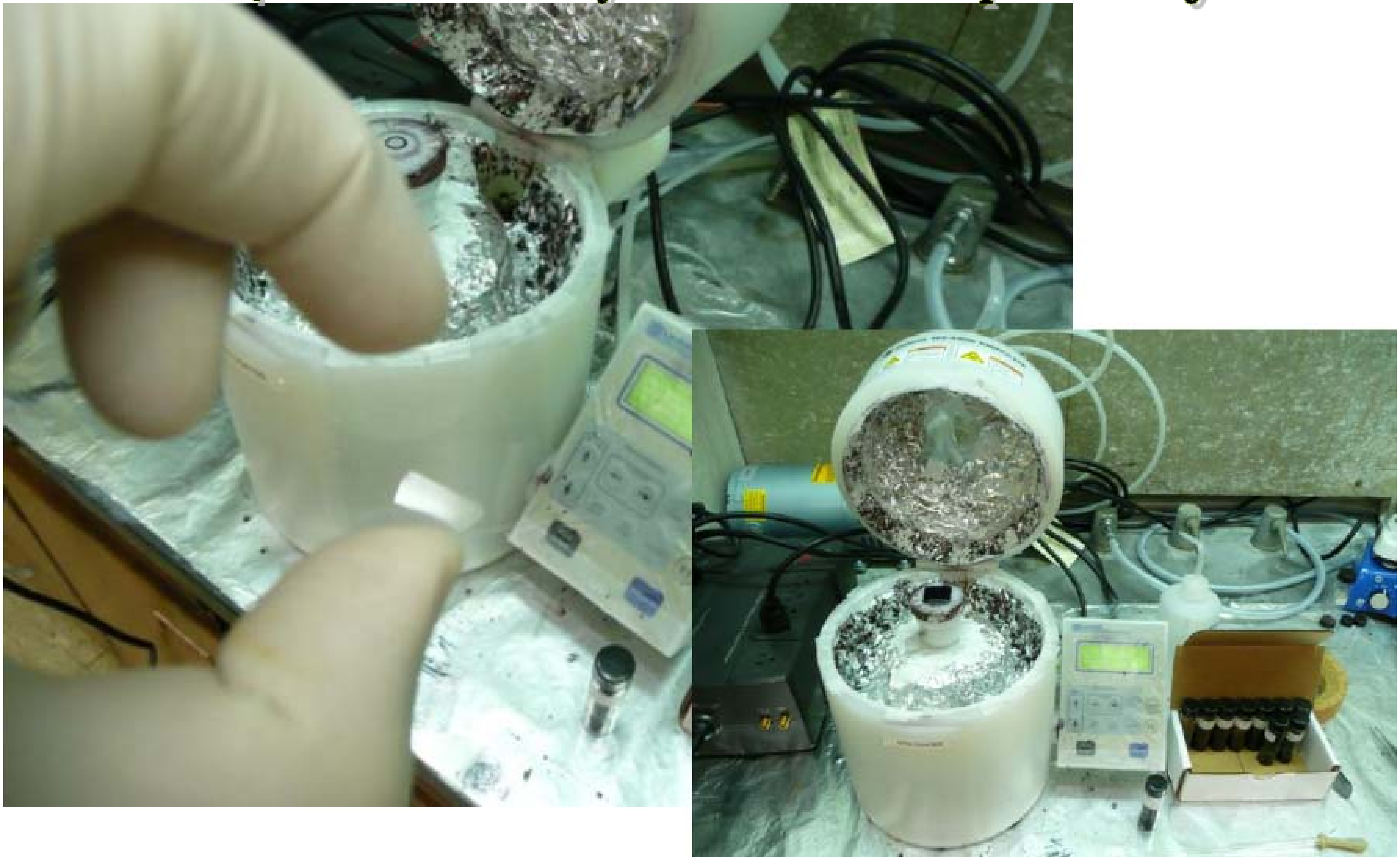
4a. Initial ink formulations





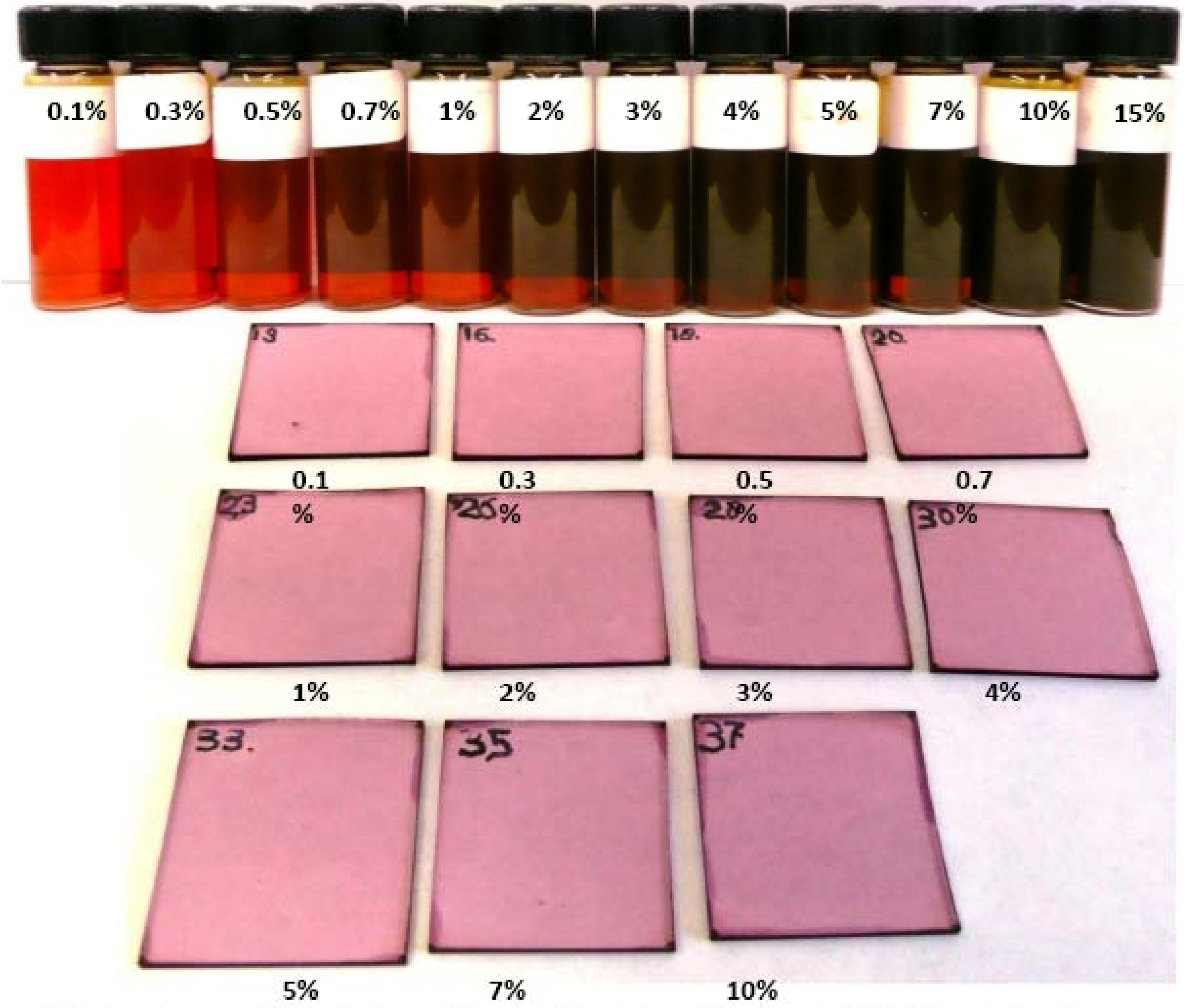
K.S Liao, E. Andreoli and S.A Curran, 'Water soluble nanocomposite ink formulation', UH Patent Application (2009)

4a. Initial ink formulations and spin coating



Scientific/Technical Approach

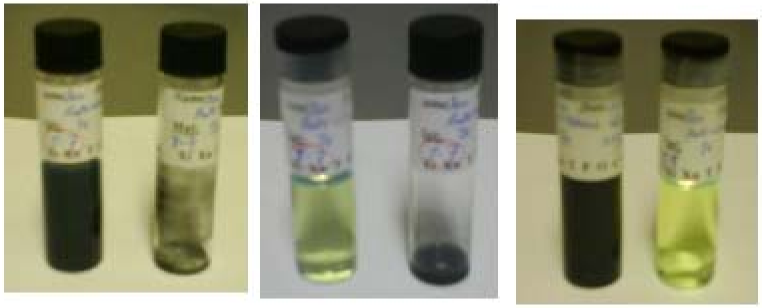
Polymer-Nanotube Composites (P3HT and NT of different loadings)

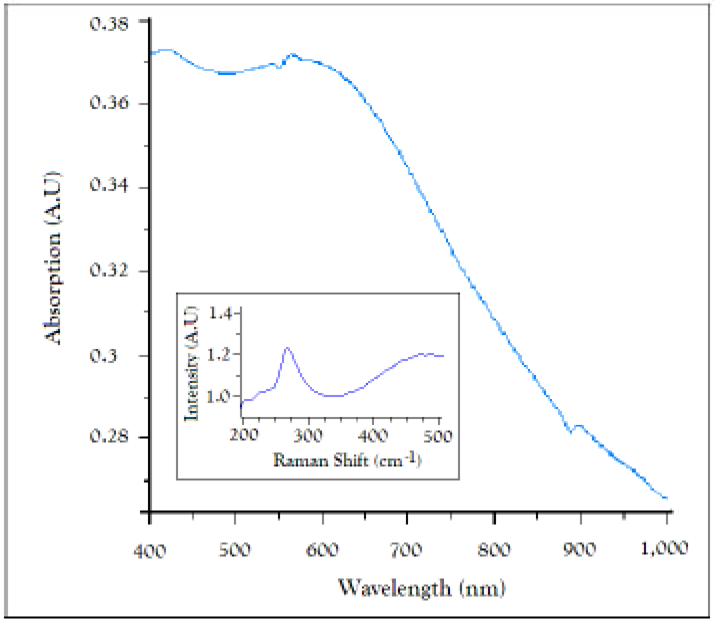


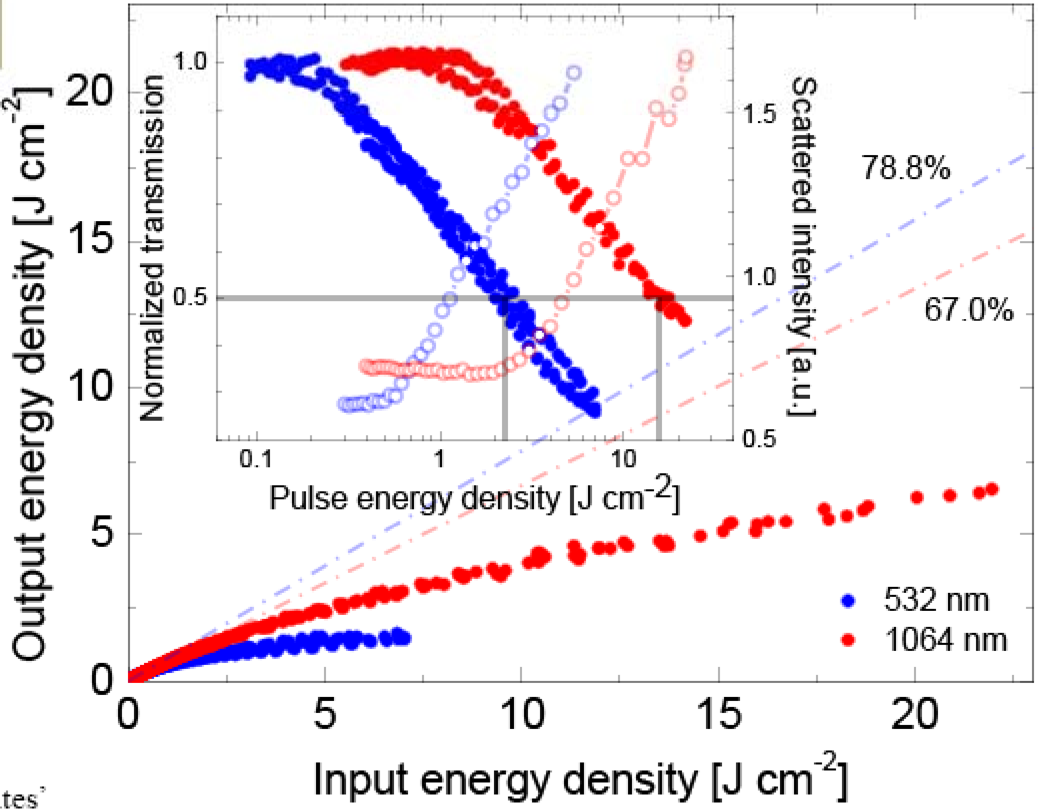
K.S Liao, E. Andreoli and S.A Curran, ‘Nanotube-Fullerene functionalization’, UH Patent Application (2009)
K.S Liao, E. Andreoli and S.A Curran, ‘Nanotube-dye functionalization’, UH Patent Application (2009)

Scientific/Technical Approach

Polymer-Hybrid Composites (PmPV and NT of Te)





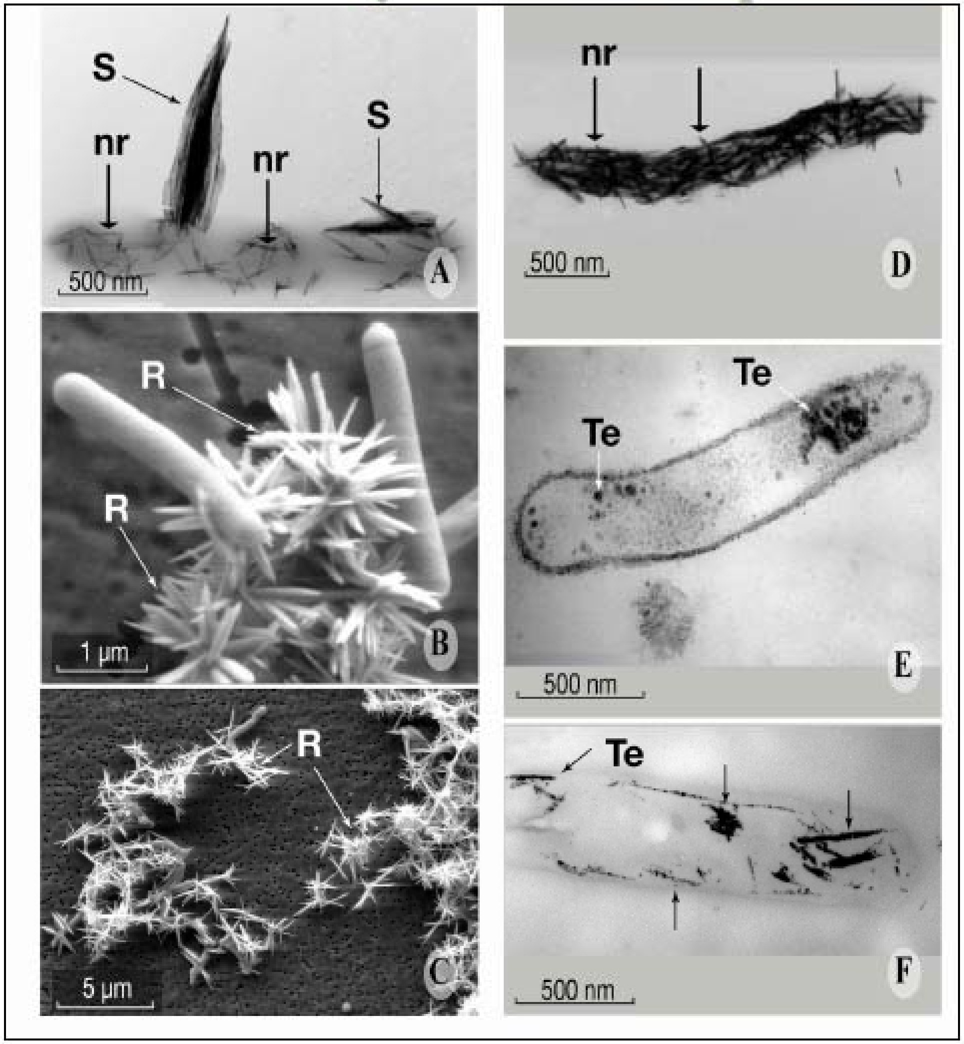


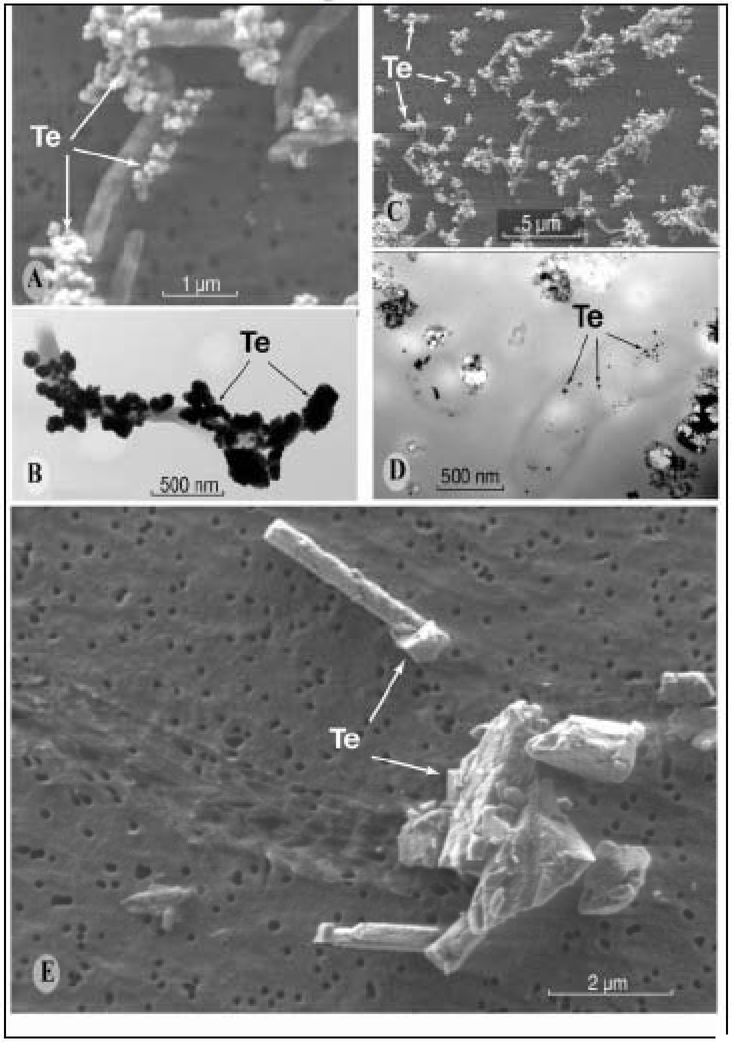
S.Curran et al, 'Strong Non-linear Photonic Responses from Microbiologically Synthesized Tellurium Nanocomposites' submitted (2009)

S.Curran, S.Dias, R. Oremland, S. Baesman, J.Wang and W.Blau, 'Biologically inspired nanocomposites using hybrid Te nanorods and polymers' Patent Application (2008)

Scientific/Technical Approach

Te fabrication: bio respiration rather than chemical synthesis





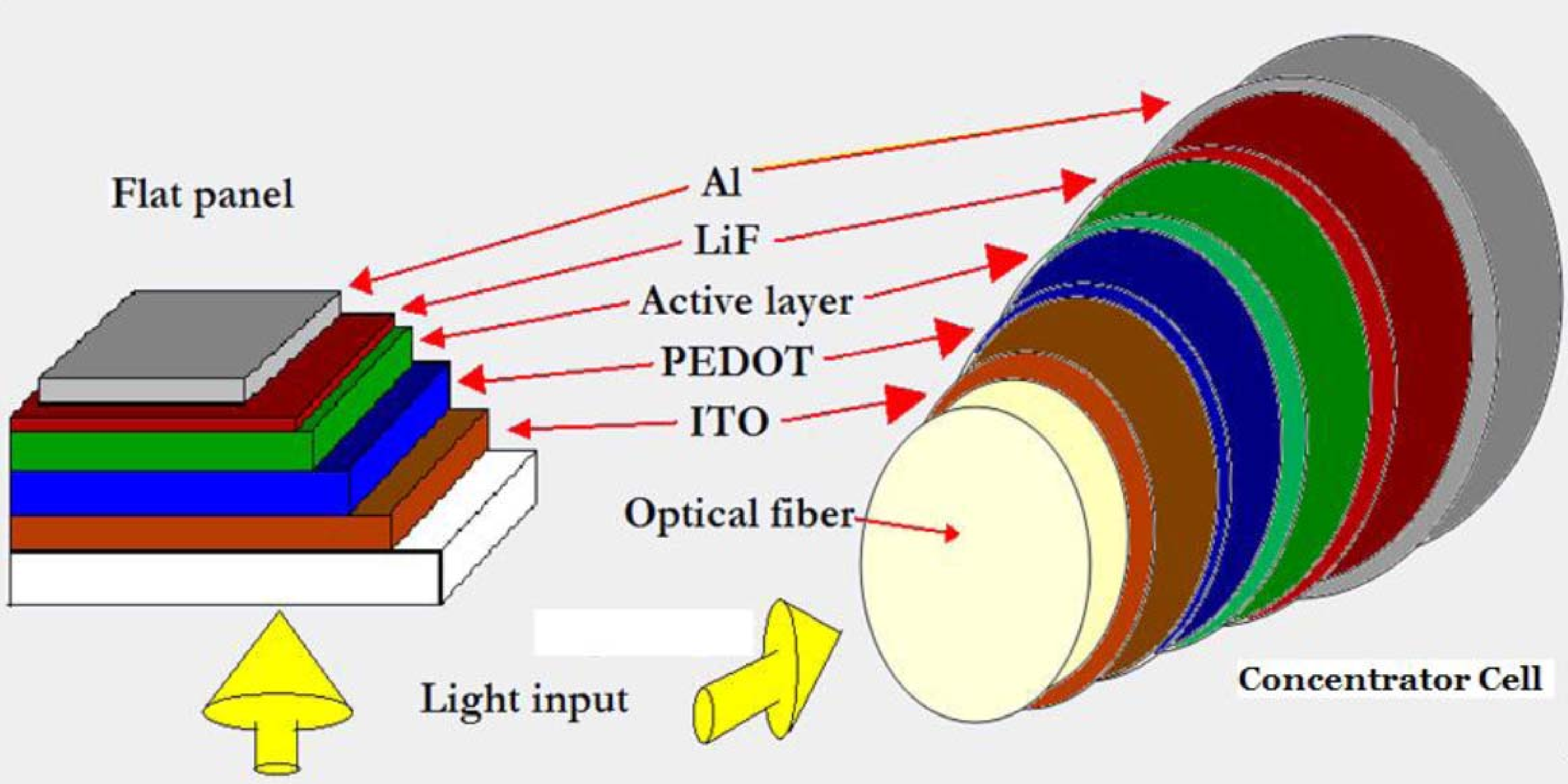
S. M. Baesman *et al*, '*Formation of Tellurium Nanocrystals with Anaerobic Growth of Bacteria that use Te-Oxyanions as Respiratory Electron Acceptors*', **Applied and Environmental Microbiology**, 73, 7, 2135 (2007)

Scientific/Technical Approach

5. Architectural Management

Initial phase of device fabrication – examining the concentrator effect

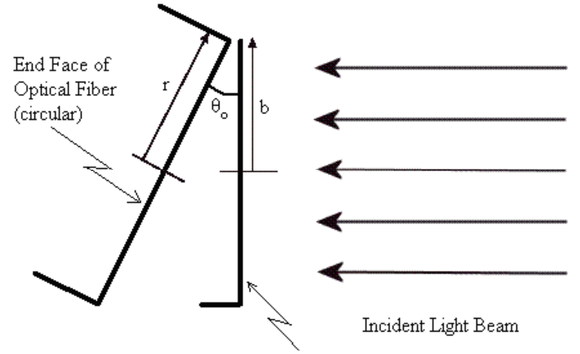
Scientific/Technical Approach

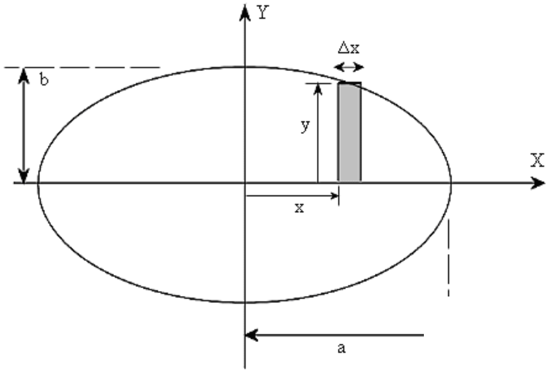


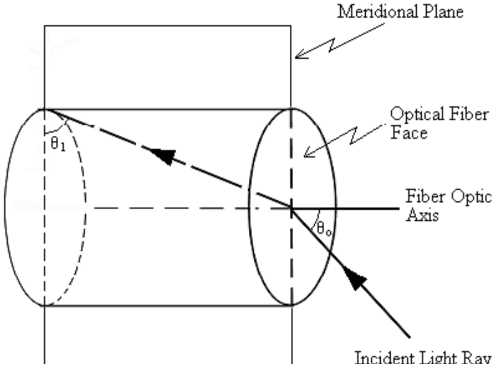
S. Curran, J. Talla, S. Dias and J. Dewald, ‘Micro-Concentrator Photovoltaic Cell (the m-C Cell): Modeling the Optimum Method of Capturing Light in an Organic Fiber Based Photovoltaic Cell’, J. Appl. Physics104,064305 (2008)
S.Curran, D.L. Carroll and J. Dewald, ‘Cascade solar cell increases efficiency’, SPIE,DOI: 10.1117/2.1200608.0324 (July; 2006)

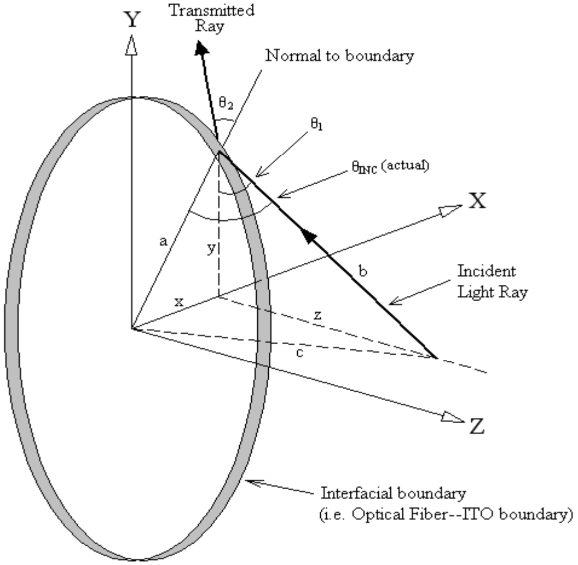
Patent Applications
S. Curran, James Dewald and David Carroll, ‘Cascade Waveguide Photovoltaic’, [PCT (2008)]
S. Curran and James Dewald, ‘Cascade Solar Cell Fabrication and Production –the fiber weave system’, [PCT 2008)]

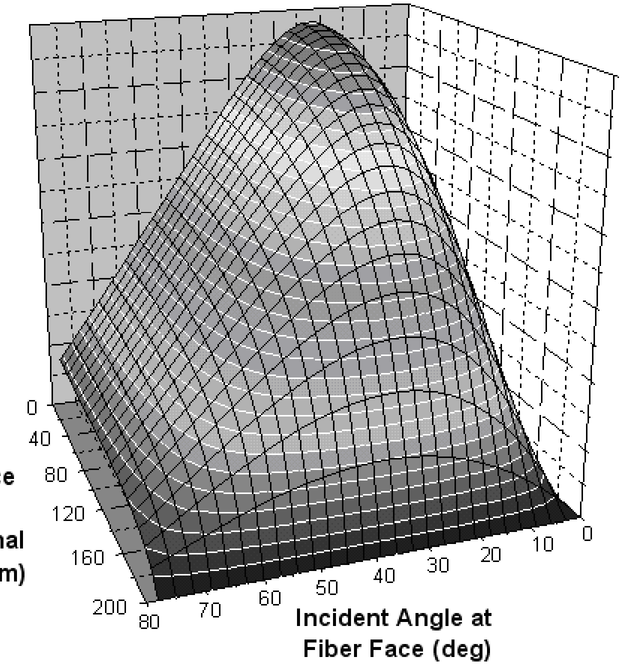
Scientific/Technical Approach







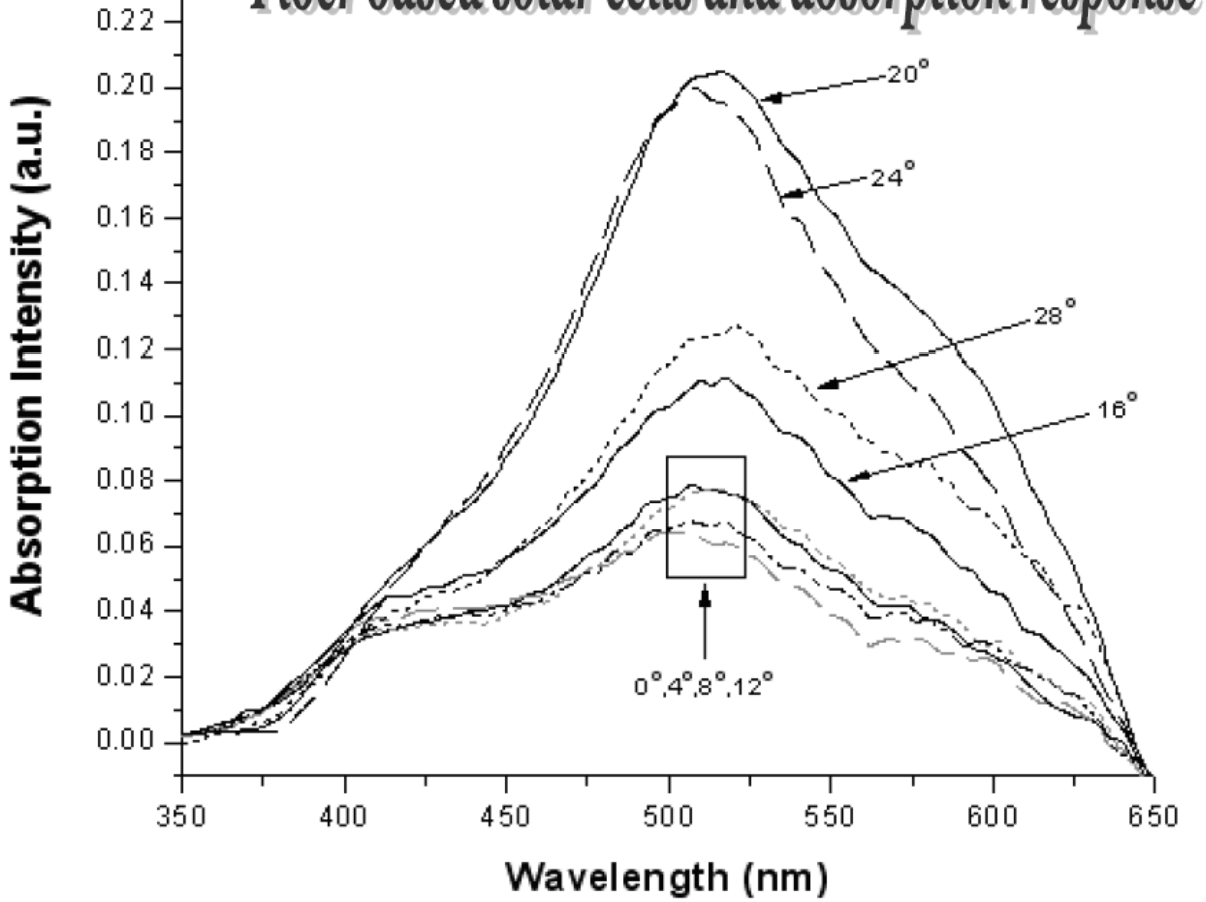




S. Curran, J. Talla, S. Dias and J. Dewald, ‘Micro-Concentrator Photovoltaic Cell (the m-C Cell): Modeling the Optimum Method of Capturing Light in an Organic Fiber Based Photovoltaic Cell’, *J. Appl. Physics* **104**, 064305 (2008)

Scientific/Technical Approach

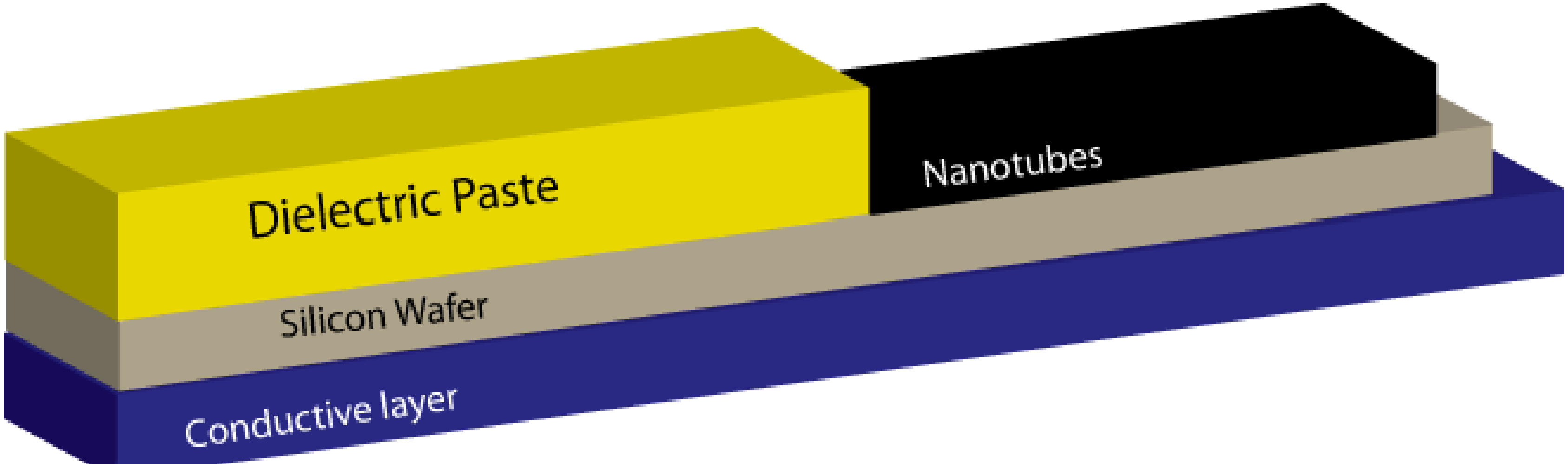
Fiber based solar cells and absorption response

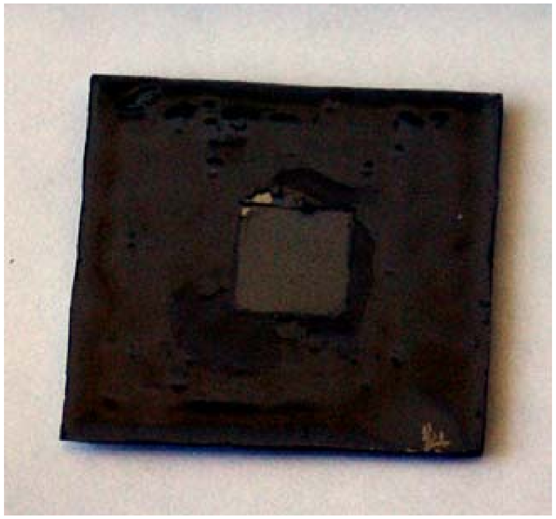


Initial tests using P3HT only as the semiconductor – understanding and modeling the optical response

Patent Applications
S. Curran, ‘Multi-tandem linear organic photovoltaic’, Patent Application UHID 2008018 (2008)
S. Curran, J. Dewald, S. Dias and J. Talla,‘Micro-Concentrator Photovoltaic Cell (the m-C Cell) Modeling the optimum method of capturing light in an organic fiber based photovoltaic’, Patent Application UHID 2008025 (2008)

Silicon Nanotube Heterojunction Solar Cells

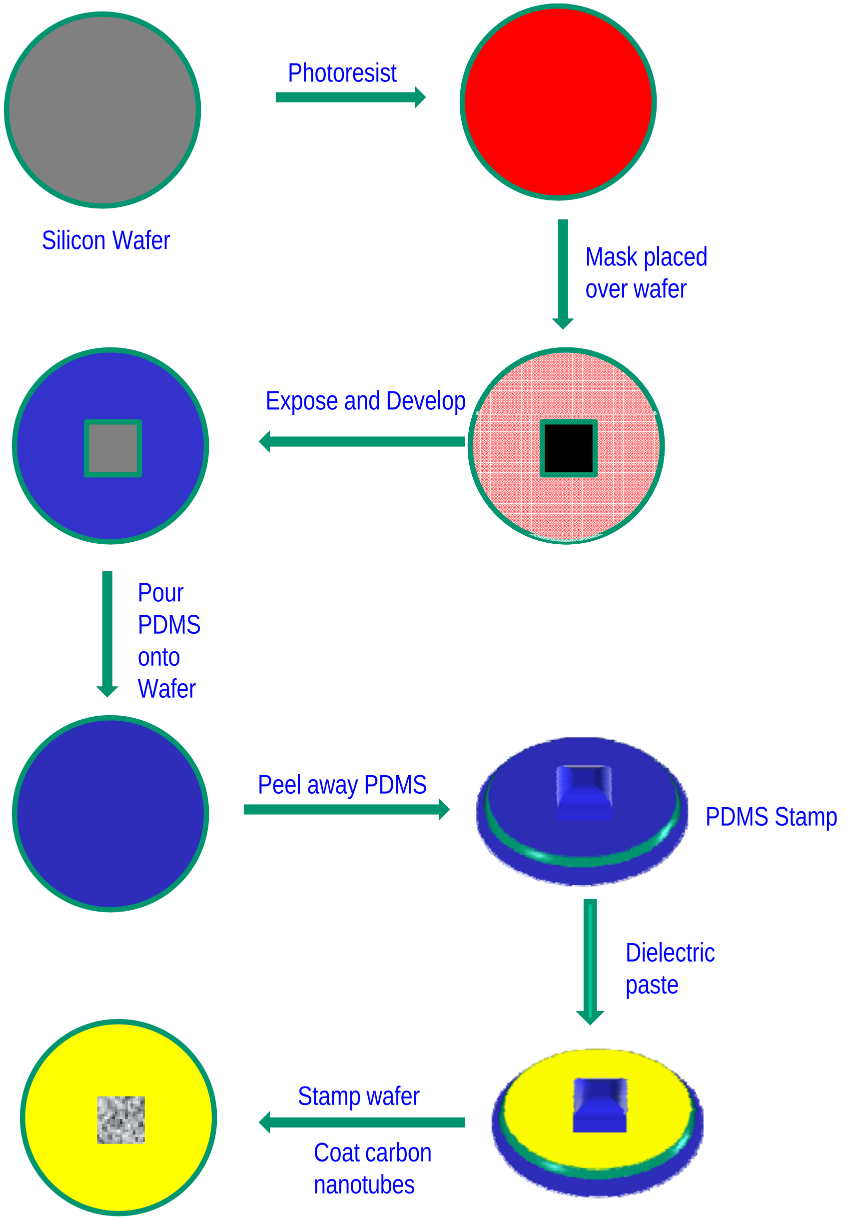




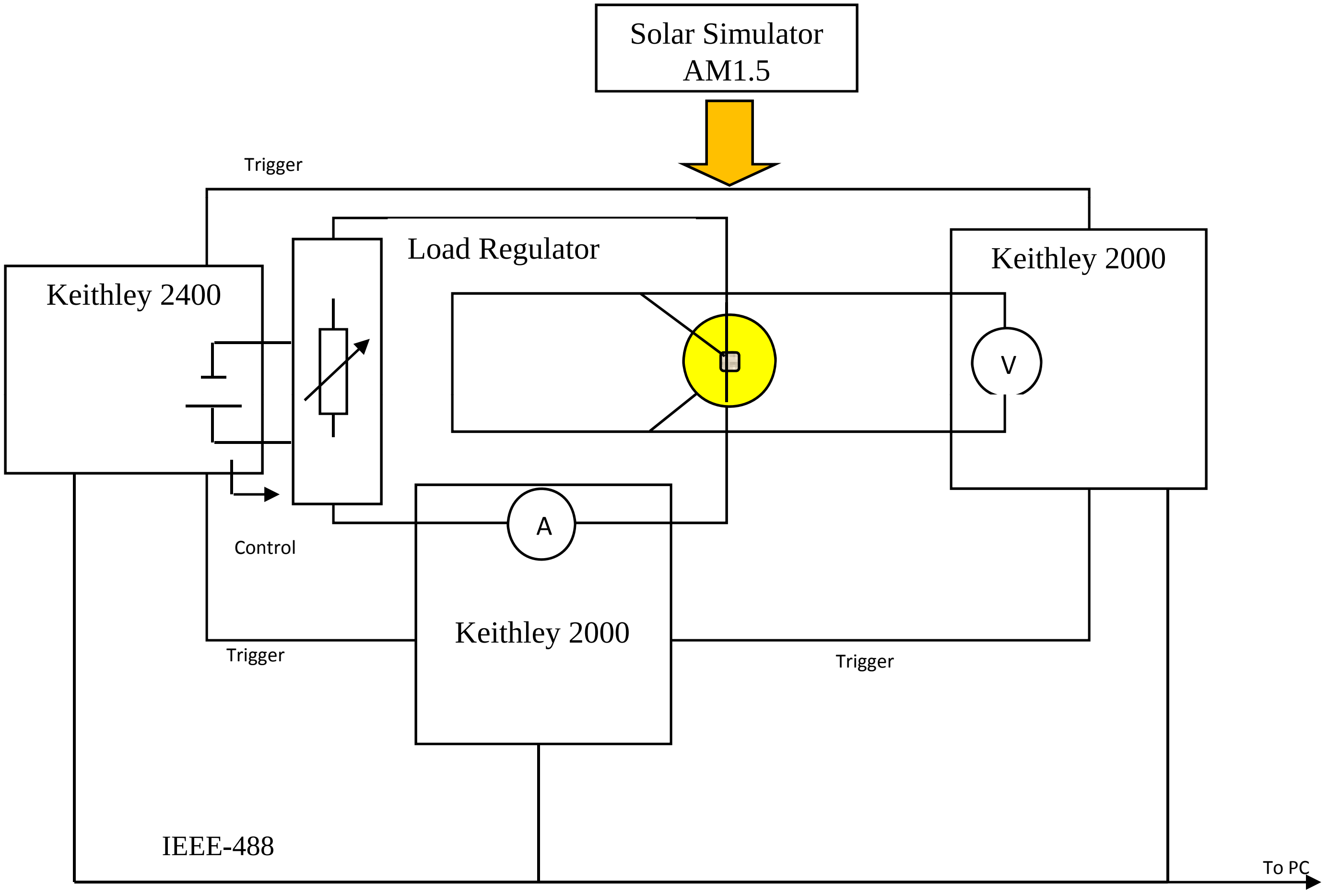
Scientific/Technical Approach

Photolithography Process

- Initially, pattern the top surface of the silicon wafer using a stamp fabricated in polydimethyl siloxane (PDMS)
- Coate the wafer with a photoresist
- Place a specially designed film mask on the wafer and subsequently expose it.
- After exposure, develop the wafer with a design patterning
- Coat PDMS onto the patterned wafer, peal off the PDMS after, obtain the PDMS stamp.
- Coat the stamp with a dielectric paste (insulator), stamp onto another wafer, and coat the exposed silicon surface with CNTs.



Solar Cell Performance Test Unit



Relevance/Impact of Research

High-performance, light-weight, flexible, low-cost, sustainable and green solar electricity systems

1. Closely aligned with the DOE Solar Energy Technologies Program (photovoltaics sub-program)
2. Could potentially increase efficiency for organic solar cells
3. Could potentially reduce cost of solar cells
4. Light weight, flexible, possible long service time
5. Could significantly simplify the fabrication process
6. Less impact to the environment and energy-saving production process
7. Use of sustainable and nontoxic species

Future Directions

1. Synthesize double-walled, multiwall, B- and N-doped carbon nanotubes with catalytic CVD growth
2. Develop 1-(3-methoxycarbonyl)propyl-1-phenyl-[6,6]-methanofullerene (PCBM) materials that optimize electron transport within the composite device bilayers
3. Characterize doped carbon multi-walled nanotubes using spectroscopic and morphological techniques
4. Develop tunable quantum dots
5. Functionalized and characterize PEDOT:PSS replacement transparent nanomaterial (NT-Ink)
6. Study transport properties of NT-Ink
7. Develop thin film heterojunction layers with NT-Dye/P_3HT and NT-Fullerene/P_3HT
8. Develop thin film heterojunction layers with Te Nanorods/P_3HT and TeQD’s/P_3HT
9. Characterize the electronic and vibrational response
10. Analyze the surface (AFM) and bulk (NSOM) morphology of the thin films

Future Directions

11. TEM and EELS analysis of the functionalized nanotubers
12. DC and AC transport measurements, percolative analysis to obtain maximum filler n-type loadings in the active heterojunction
13. Determine optimum loading for NT-Ink in PV cells
14. Build single fiber cells with each individual semiconductor layer and characterize solar response
15. Apply the advanced tandem cell arrangement to construct the cascade solar cells (also known as the m-C Photovoltaics cells) and to maximize the efficiency of the photovoltaics
16. Study the properties of boron- and nitrogen-doped carbon nanotubes; examine the possibility of self-assembly of organic molecules on B/N-doped nanotubes
17. Study the electronic and optical properties of semiconducting nanoparticles; develop a realistic theoretical model for nanoparticles embedded in polymers
18. Develop a theoretical model for electroactive nanocomposite materials; apply this model to optimize the absorption properties and improve charge-carrier characteristics of organic photovoltaic materials

Acknowledgements

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New Mexico State University

University of Houston