Material Perspectives for Organic Photovoltaics

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Outline

- ⌘ CNMS Macromolecular Group
- ⌘ Organic Photovoltaics
  - ✧ Why organic photovoltaics?
  - ✧ How does it work?
  - ✧ What are the challenges (and opportunities)?
- ⌘ Our effects on conjugated polymers
- ⌘ Outlook

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Center for Nanophase Materials Sciences

1. One of 5 DOE nanoscience centers
2. Integrates Nanoscale Science with 3 Synergistic Research Thrusts:

⌘ Neutron Science

Use unique capabilities of neutron scattering to understand nanoscale materials and function

⌘ Synthesis Science

Science-driven synthesis: nanoscale synthesis as enabler of new functionality

⌘ Theory and Modeling

Use theory and modeling to understand and design new nanomaterials

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Macromolecular Nanomaterials Group

Design & control nanoscale assembly of macromolecular materials to achieve novel properties & functionality.

- Dedicated in synthesis and characterization of well-defined polymers
  - Anionic polymerization: towards branched, block, graft polymers and copolymers
  - Controlled radical polymerizations: RAFT, ATRP, NMRP
  - Capabilities in synthesis of bio-inspired, optoelectronic polymers.

  - Self-assembly in confined spaces and in solution
- Additional expertise includes
  - Synthesis of deuterated monomers and their polymers
  - Fine characterizations of polymers

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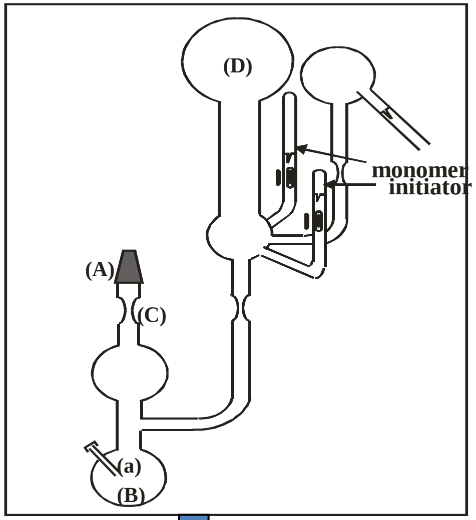
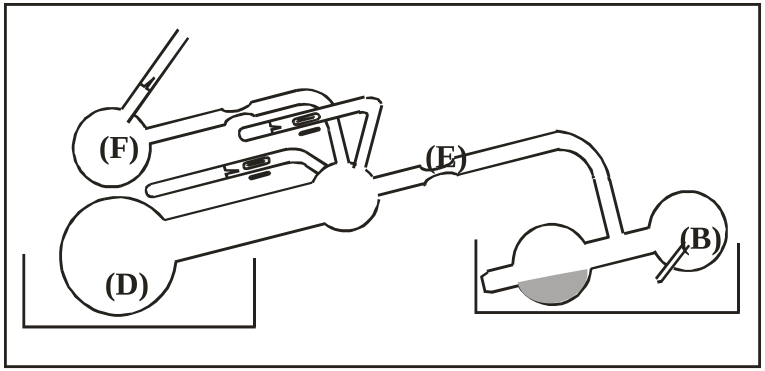
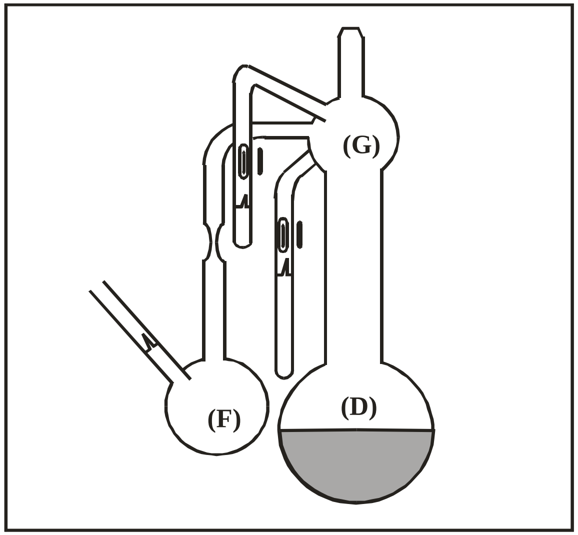
Custom Glass Blowing



Reactor



Purging



Polymerization

Courtesy: Dr. David Uhrig

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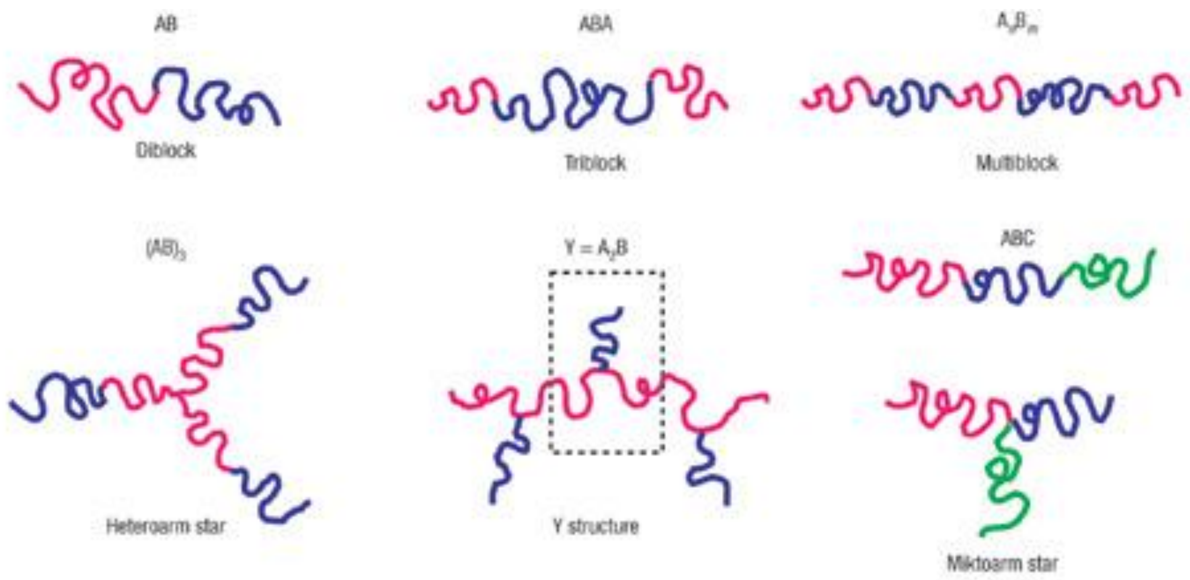
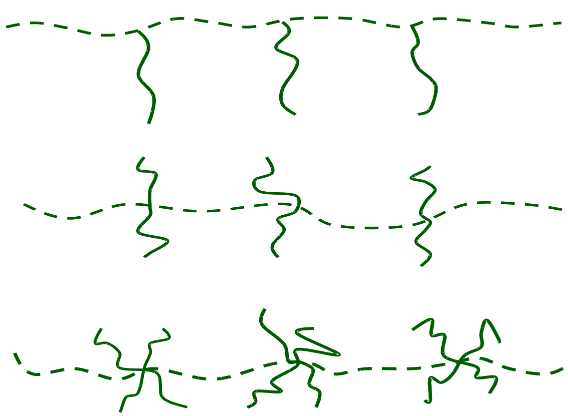
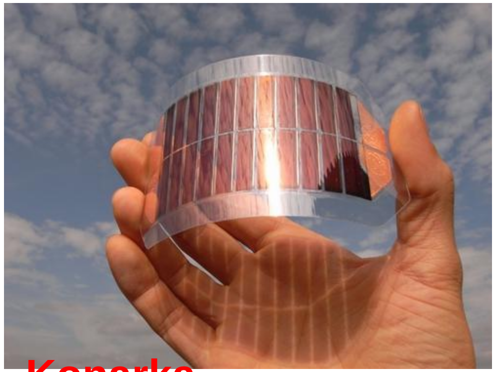
Polymers with Various Architectures





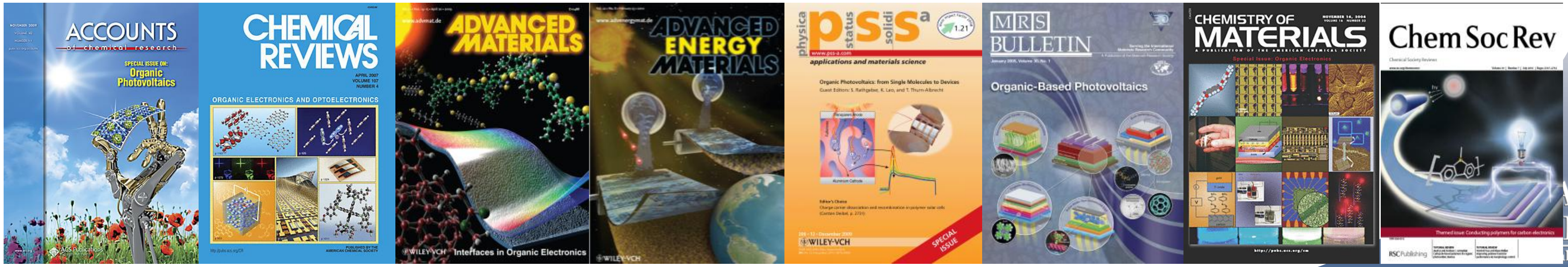


Konarka

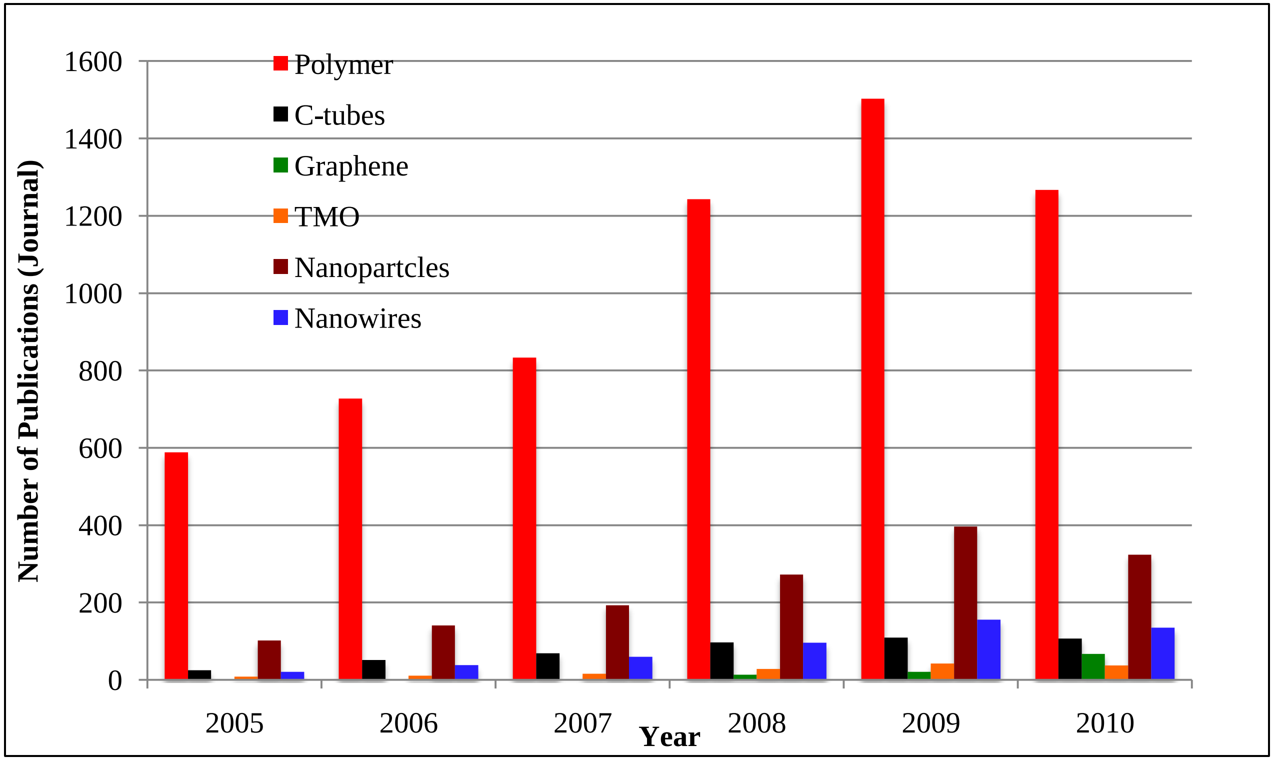
Why Organic PV

Heliatek

	Pros	Cons
Inorganic PV	High efficiency	High cost Materials shortage
Organic PV	Low cost, Flexible, light-weight; Easy processing (Low T/printing)	Low charge mobility Life time (3-5 years) Low efficiency
Hybrid PV	High charge mobilities	Low η (charge separation)



Nontraditional Photovoltaics (Journal publications since 2005)



2010: up to 09/03

Source: SciFinder (CAS services)

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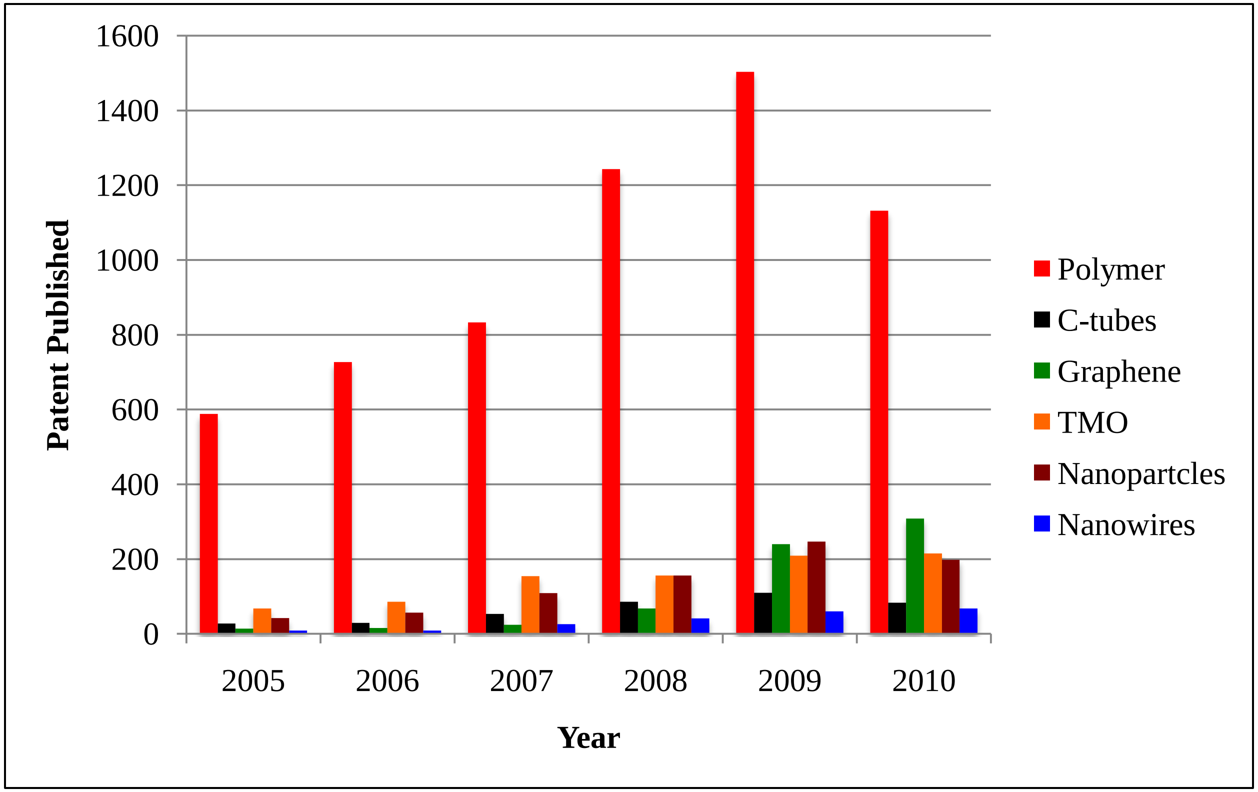
Nontraditional Photovoltaics (Patent published since 2005)



Year 2010: up to 09/03

Source: SciFinder (CAS services)

Strong growth continues worldwide for major classes of materials used in polymer/organic photovoltaics

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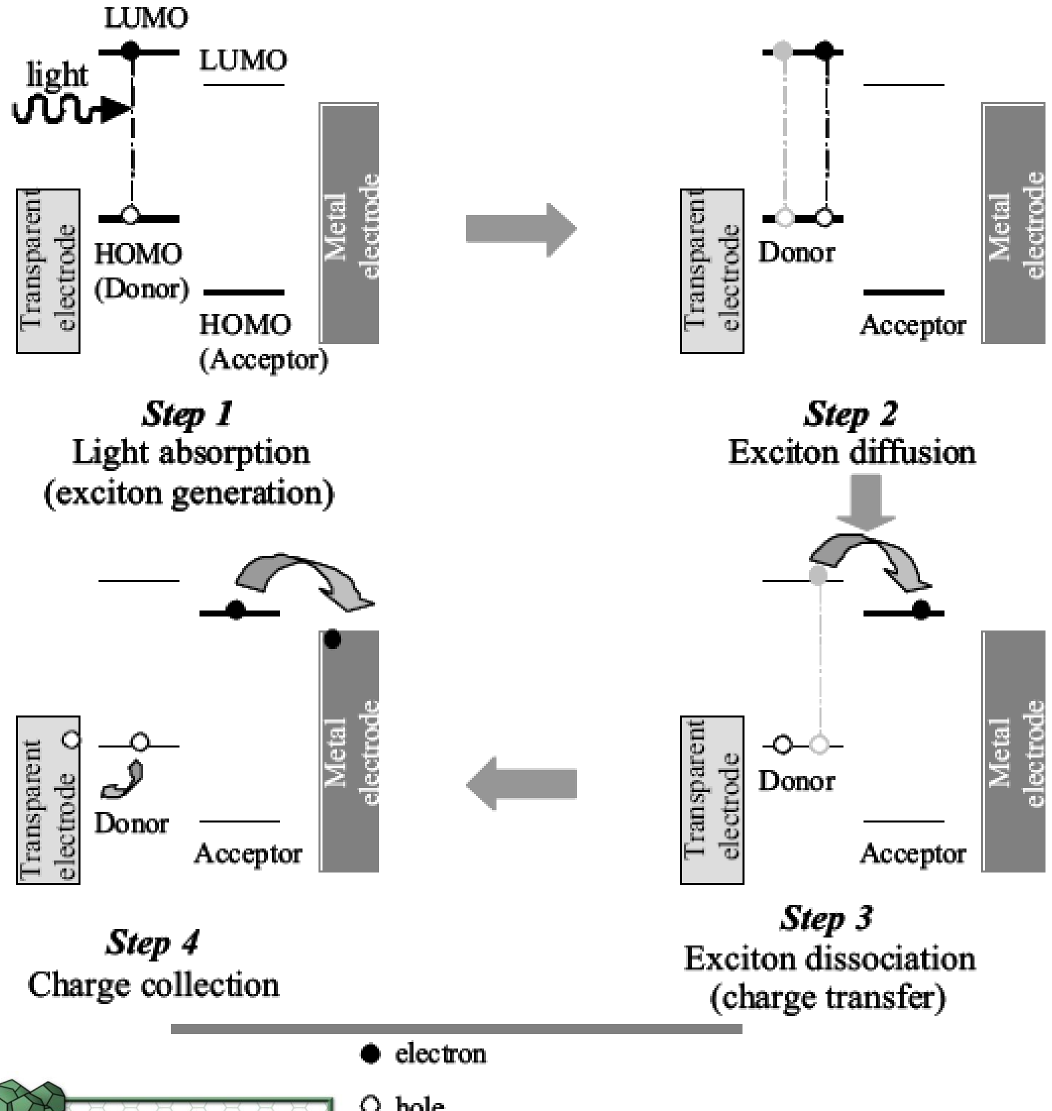
OPV Mechanism



- **Overall Efficiency**

  $\eta = \eta_A \times \eta_{ED} \times \eta_{CT} \times \eta_{CC}$

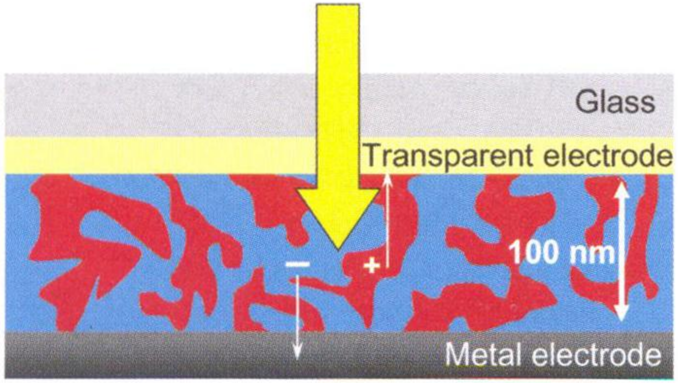
Key Parameters:

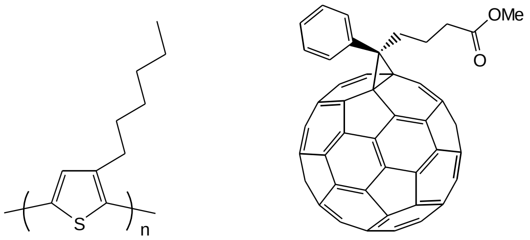
1. *Interfaces*
2. *Morphology*
3. *Energy levels*
4. *Domain purity*

Thompson & Frechet *Angew. Chem. Int. Ed*, 45, 77(2007)

OPV Architectures

Single layer; double layer, BHJ, tandem cell…





P3HT

PCBM

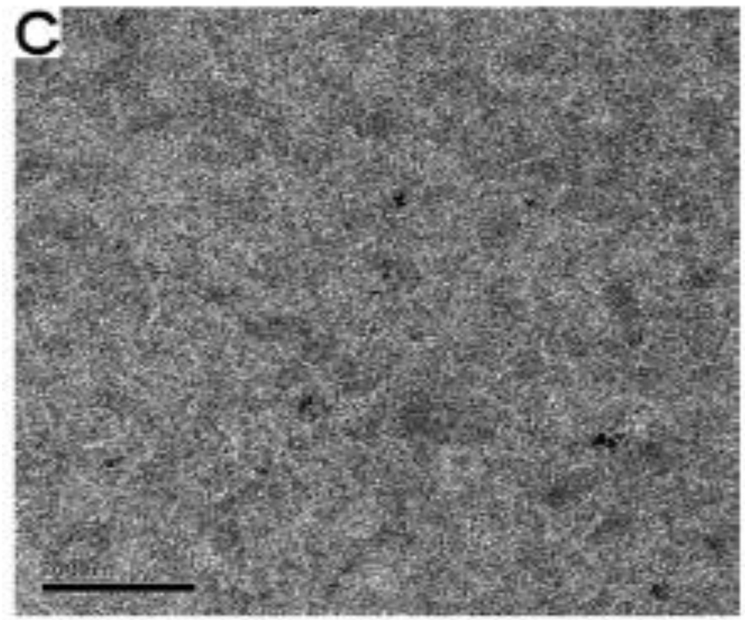
Bulk Heterojunction configurations: *Bicontinuous interpenetrating network of donor and acceptor*

Organic Photovoltaics: Materials, Device Physics, and Manufacturing Technologies", Wiley-VCH (2008)

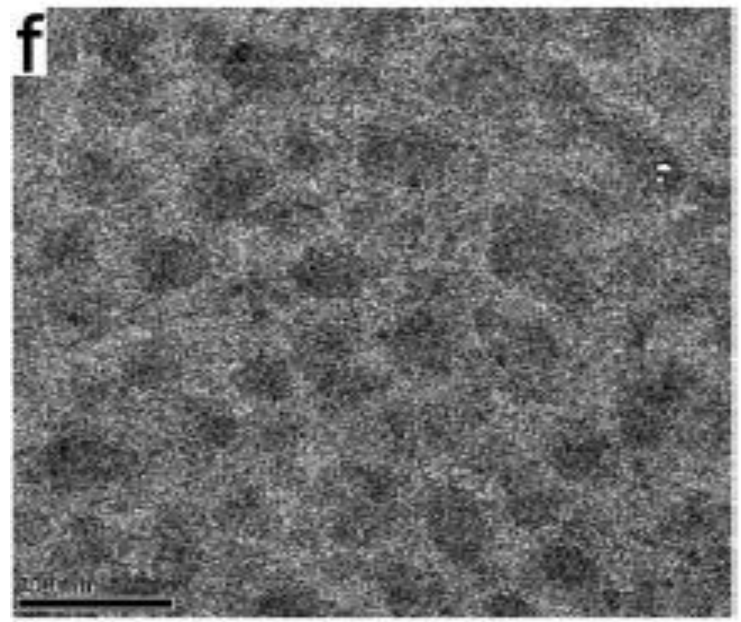
Self-assembled nanoscale material with charge-separating junctions everywhere!

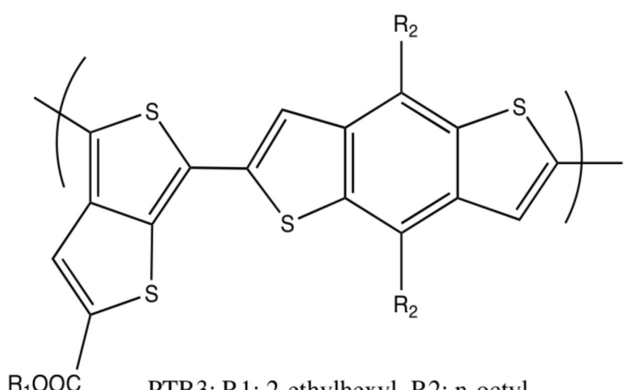
The Power of New Materials

PTB3 (PCE: 5.53%)



PTB6 (PCE:2.26%)





PTB3: R1: 2-ethylhexyl, R2: n-octyl

PTB6: R1: n-butyloctyl, R2: n-octyl

TEM of PTB3 & PTB6; Yu et al J. Am. Chem. Soc. **131**, 7795(2009)

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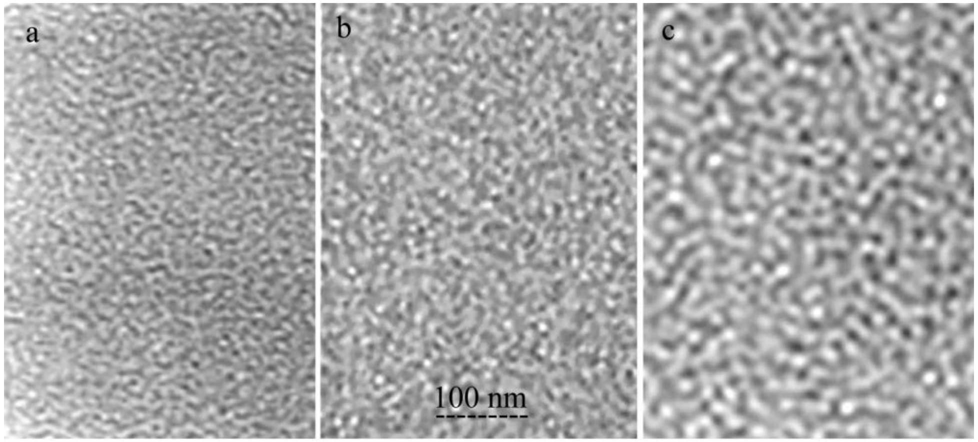
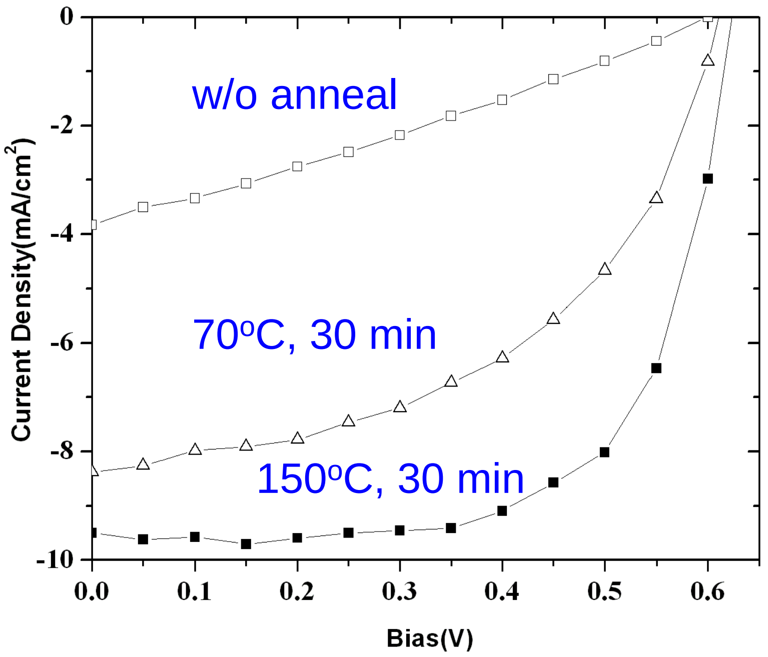
The Power of Engineering

Before 150°C anneal	150°C anneal 30 min	150°C anneal 2 hours



TEM images of the P3HT/PCBM interpenetrating network



Heeger A. et al. *SPIE*, 6336 U139-U148 (2006)

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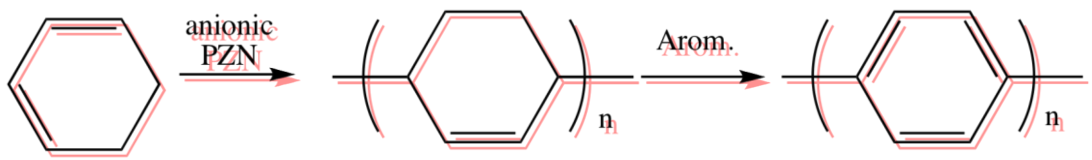
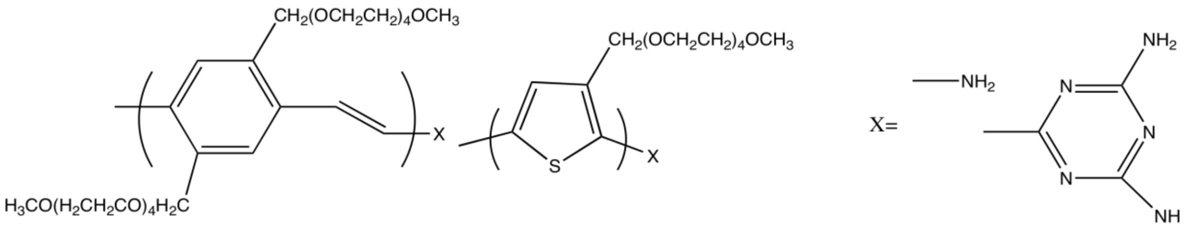
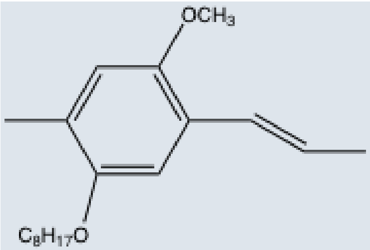
Conjugated Polymers Activities at CNMS

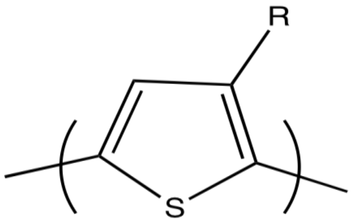




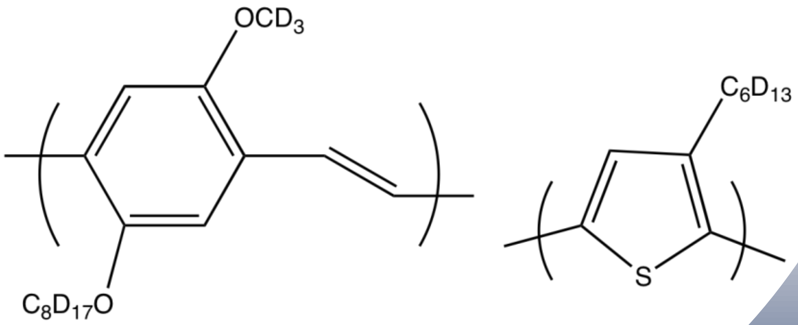
Hydrogen production and mimic LCHII (with Hugh O'Neill), biosensors (with Deli Wang (UCSD)



Dynamics in solutions



P3HT Related polymer



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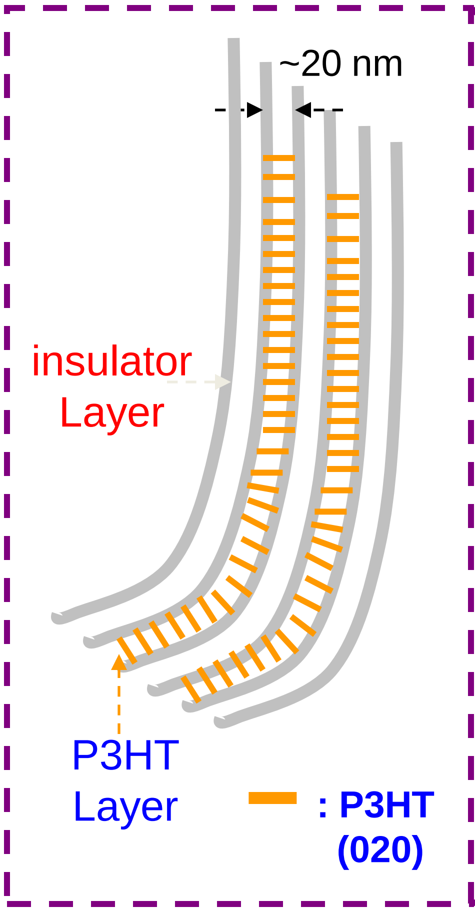
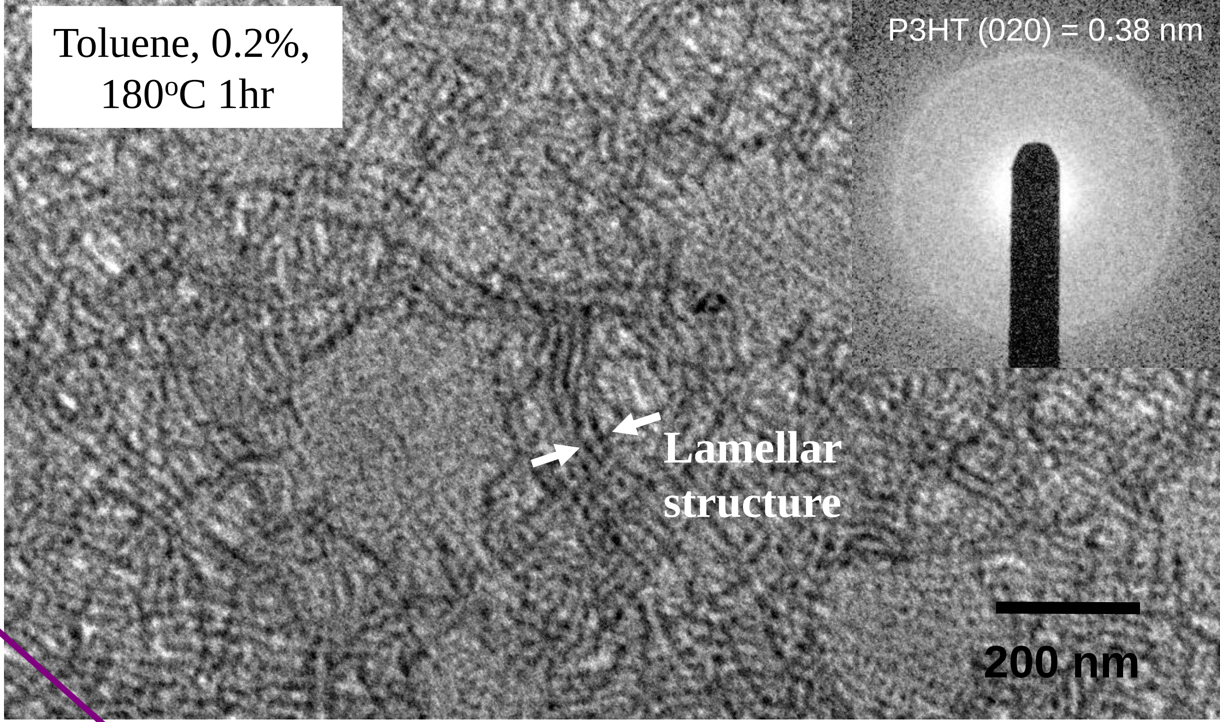
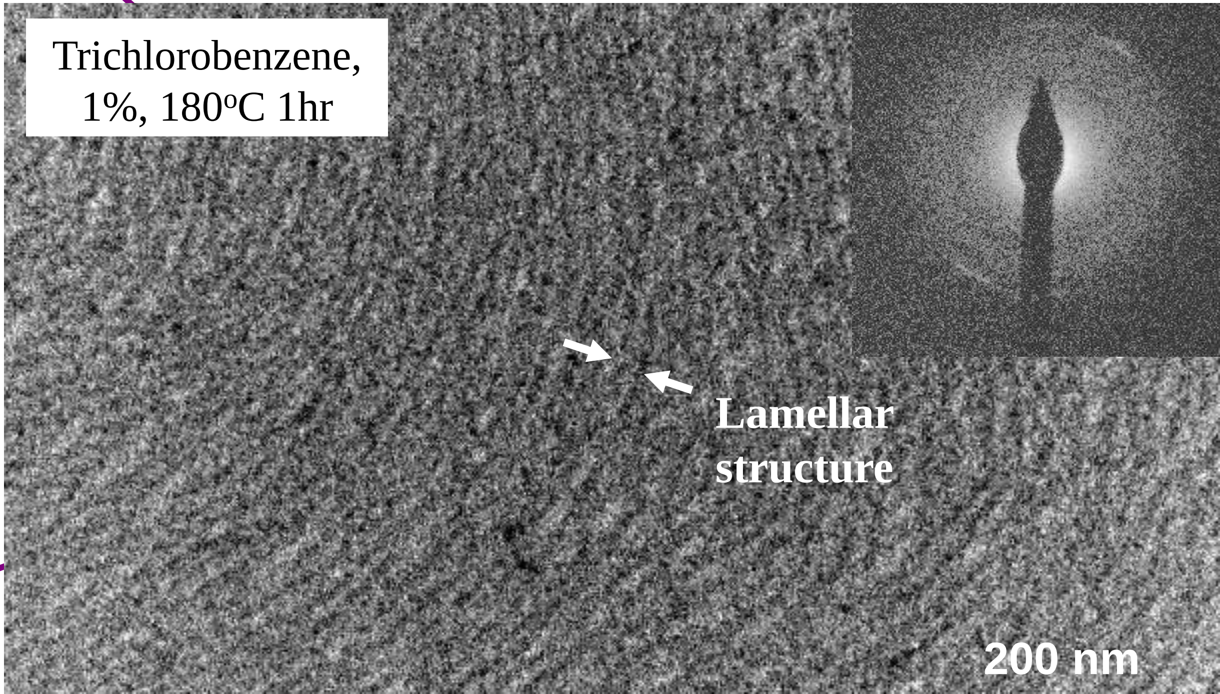
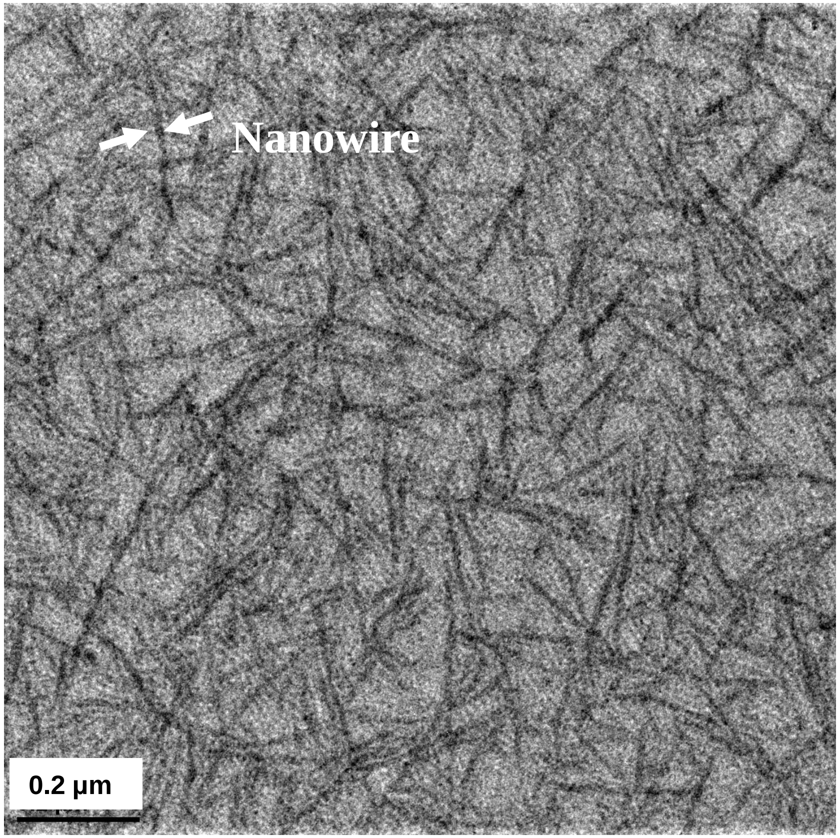
Lamellar Structures of Drop-Cast Films (a P3HT copolymer w/ 67%P3HT)

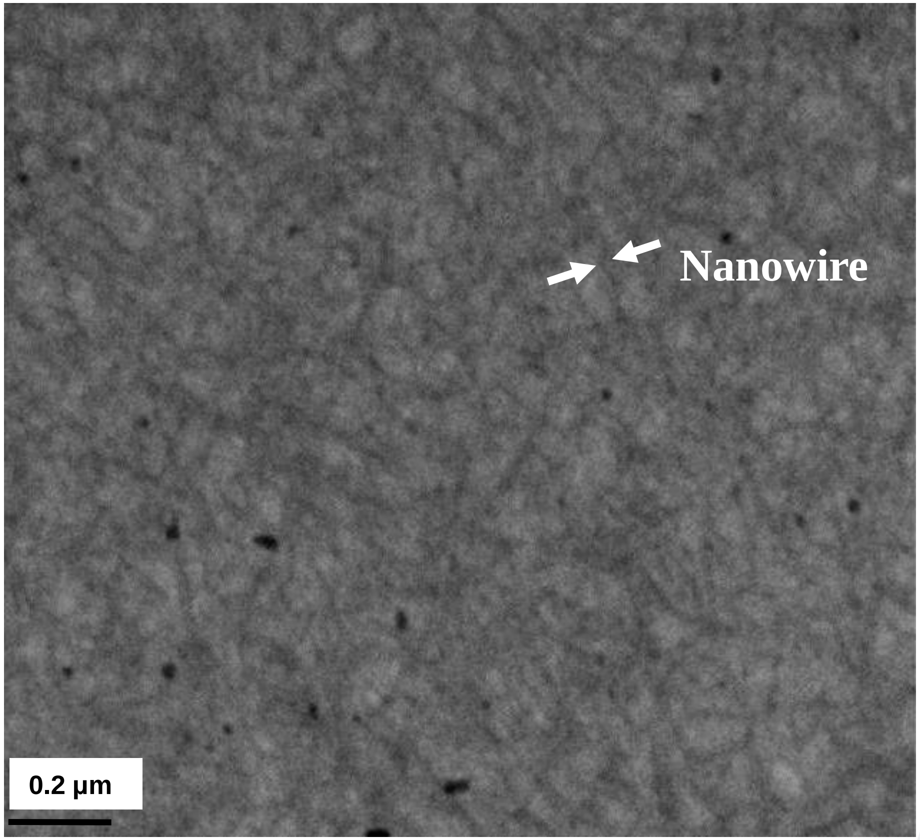






Nanowire Structures (Drop-Cast Films)





A P3HT copolymer w/ 67%P3HT
(Toluene, thicker film, 180^{o}C 1hr)

P3HT-copoymer (85% P3HT)
(Trichlorobenzene, 1%, 180^{o}C 1hr)

Enhanced hole mobility (0.065 cm^2/Vs)
as compared to 100% P3HT (0.041 cm^2/Vs)

Bright Future for OPV

Polymer photovoltaiv: Present status--- 8.13%
What can we expect to achieve?? --- ***Eff ≈ 20%***

New Architecture --- optical spacer --- 50% improvement

Current materials' band gap too large --- missing half the solar spectrum; Opportunity: Potential for 50% improvement using polymer with smaller band gap

Increase open circuit voltage ---
Opportunity: Potential for 50% improvement

Materials! Materials!! Materials!!!

Summary and Outlook

- OPV has a bright future!
  - Material development holds the key!!!!

- Challenges abound (they are also opportunities)

Acknowledgement

- Dr. Xiang Yu (CSD) and Jun Yang (CNMS);
- Drs. Ilia Ivanov; Kai Xiao; Jihua Chen (CNMS)
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THANKS FOR YOUR ATTENTION!

Questions?