Polymer Solar Cells Research at NSU

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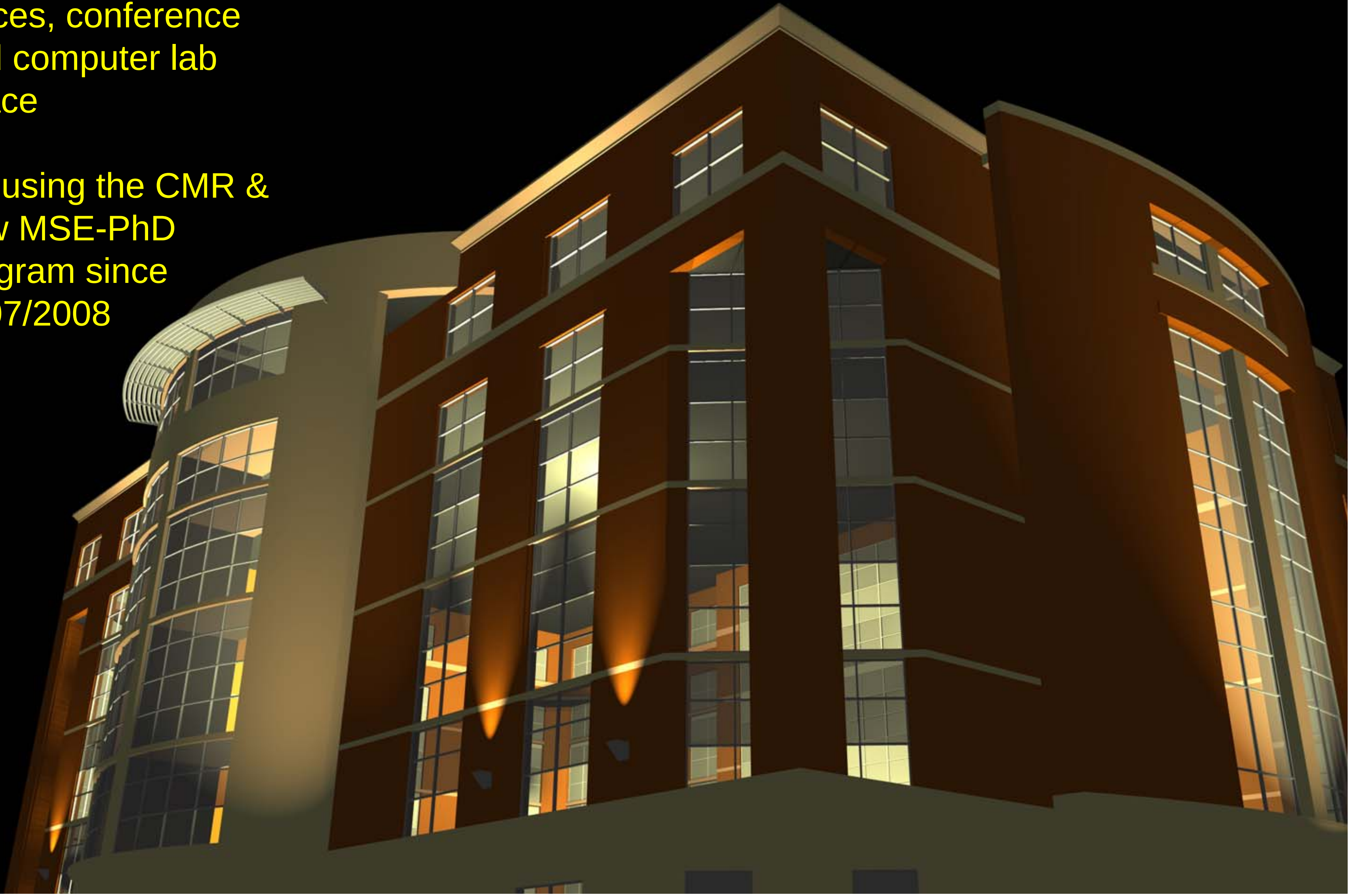
Marie V. McDemmond Applied Research Center (RISE

- 135,000 sq. ft. of research labs, offices, conference and computer lab space

- Housing the CMR & new MSE-PhD program since 2007/2008



Educational Objectives

- A PhD program in Materials Science and Engineering (PhD-MSE) has been established since 2007 (About 10 PhD students currently enrolled): the program admit and support graduate students majoring in physics, chemistry and engineering who are interested in obtaining advanced graduate degrees in materials science and engineering, particularly in advanced optoelectronic, photonic, spintronic, and nano materials and engineering.

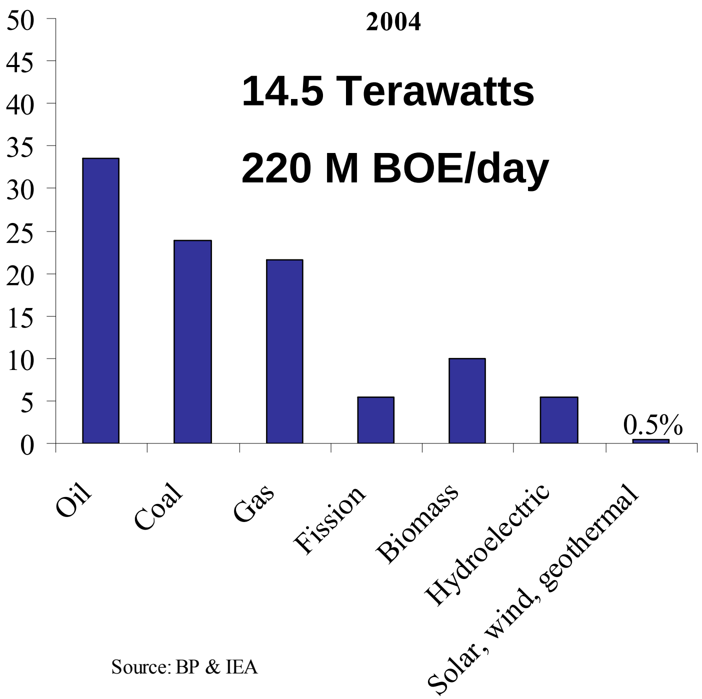
- We train students with critical and state of the art knowledge and skills in chemistry and solid state physics relevant to materials science and engineering, these include materials design/modeling, synthesis, processing, characterizations, spectroscopy, device fabrications, *etc*.

Research Focus

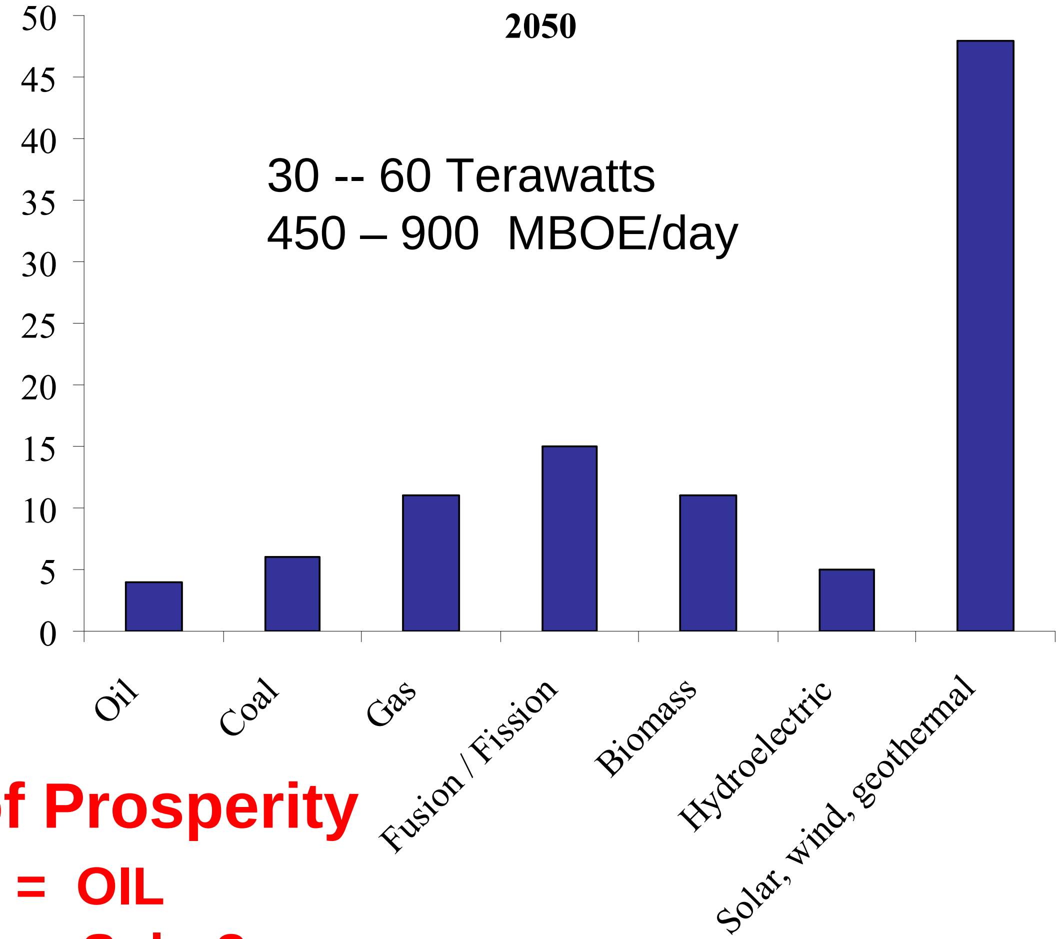
- Investigate and develop supramolecular and nano structured polymeric electronic and opto-electronic materials for future generation cost effective, lighter weight, more compact size, higher efficiency, and higher capacity opto-electronic (particularly photovoltaic or solar energy) device applications.

- Processing, fabrication, and characterization of organic, polymeric, and inorganic/organic hybrid nano-structured thin film OE devices.

The ENERGY REVOLUTION (The Terawatt Challenge)



Source: BP & IEA



The Basis of Prosperity

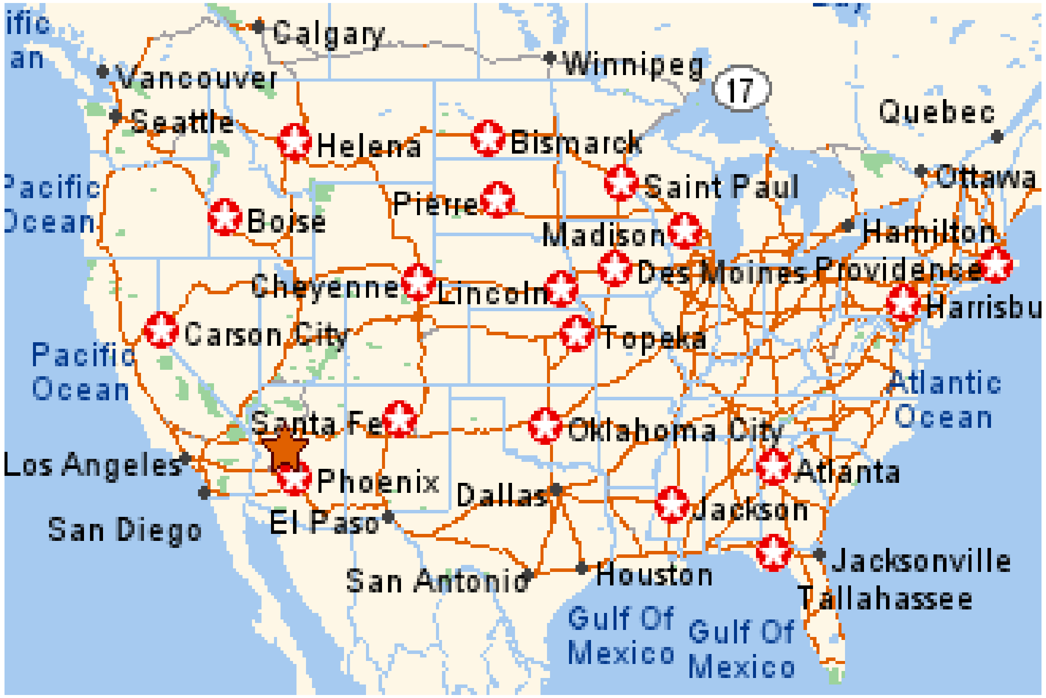
20st Century = OIL

21st Century = Solar?

un

165,000 TW
of sunlight
hit the earth

Solar Energy for National Electricity Needs



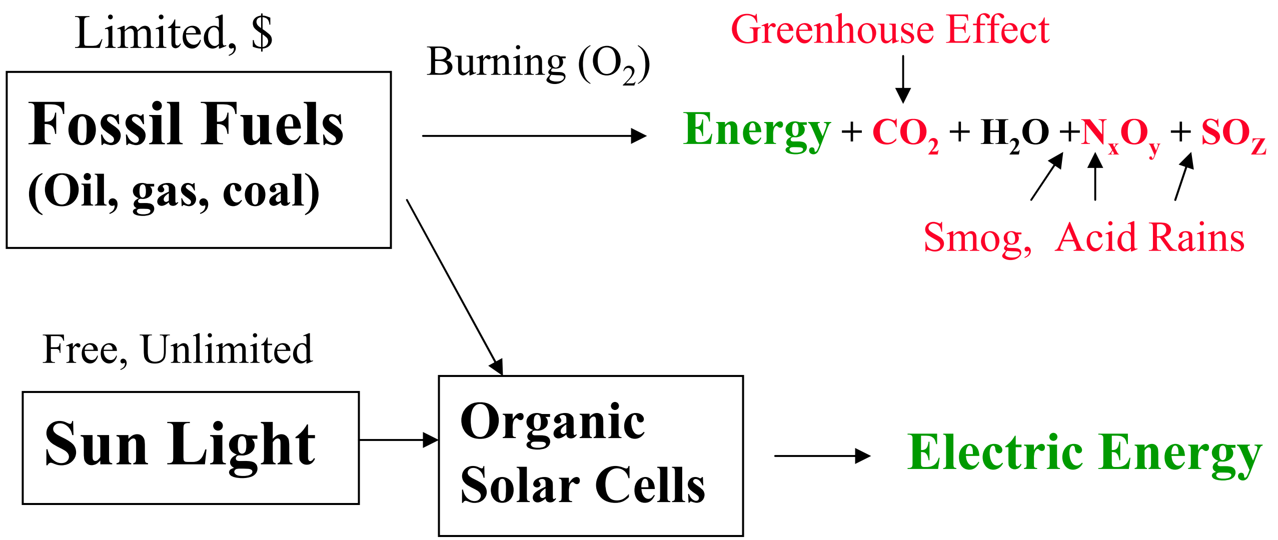
Electricity needs in the United States

≈ 10% Efficiency Solar Cell with a size of 70 x 70 miles

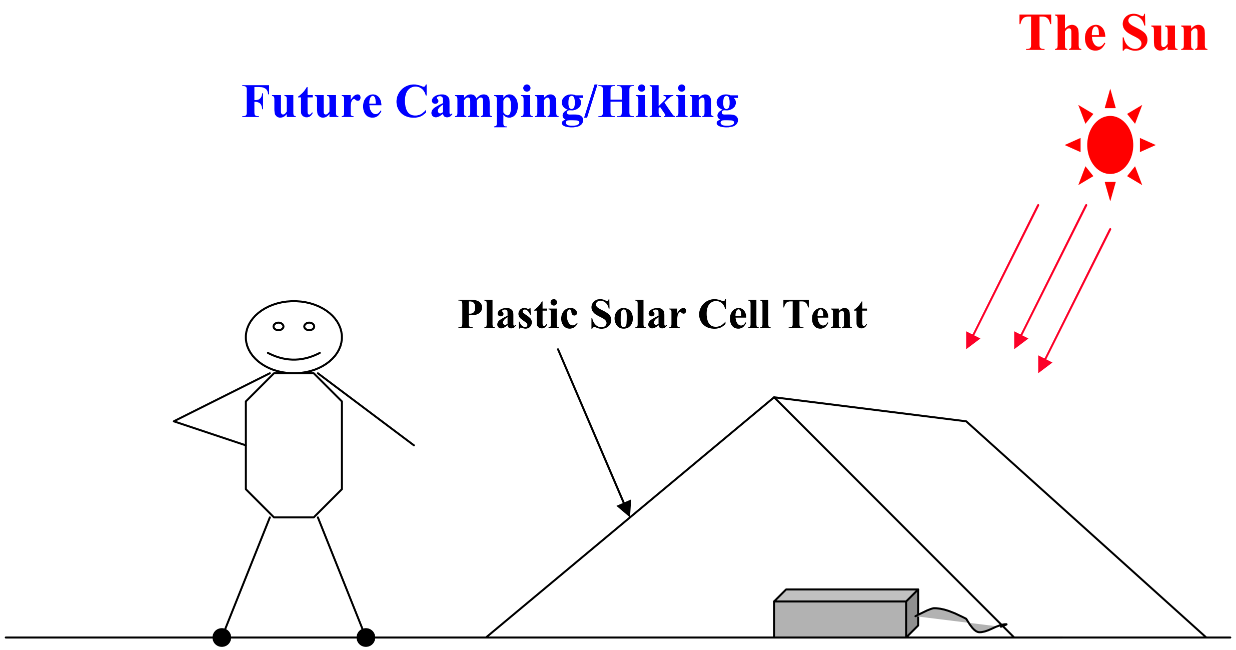
in a SW states (California, Arizona, New Mexico, etc.)

“Solar House”

Energy from Fuels/Sun

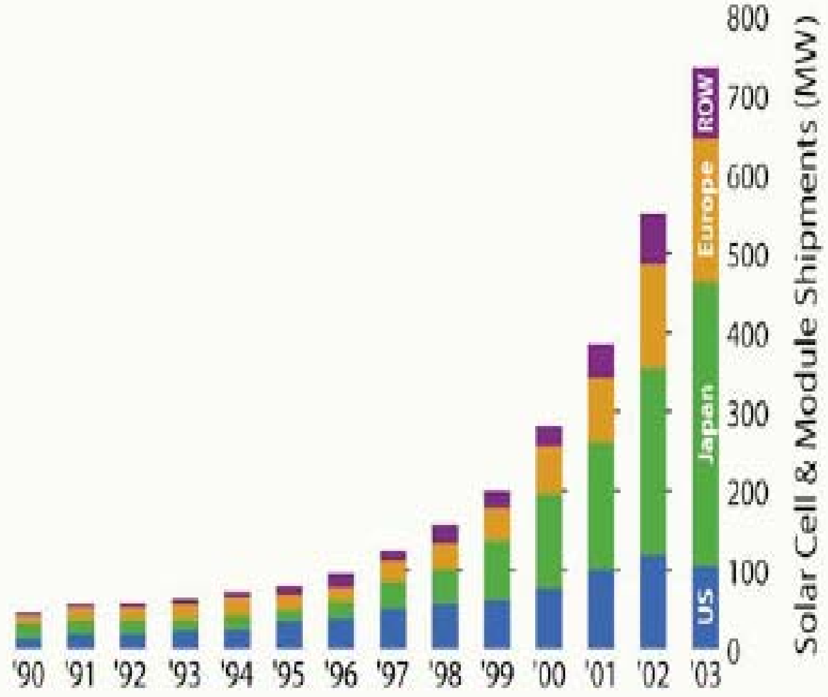


Plastic Solar Cells for Campers/Hikers



World PV Shipments

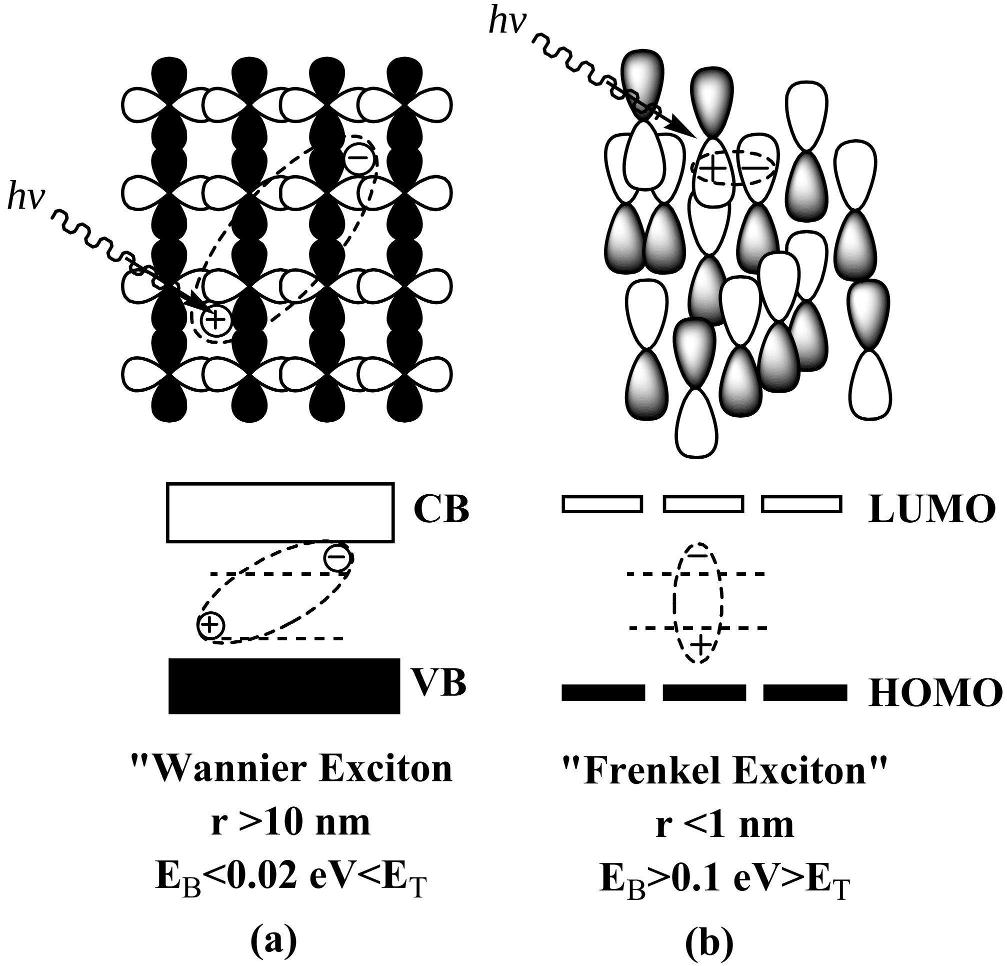
- 2004 PV Shipments
  - Over 1000 MW (47% Growt
- US 140MW
  - Sunpower, Evergreen
- EU 300MW
  - BP, Q-Cells, Shell
- Japan 500MW
  - Sharp, Sanyo, Kyocera
- $7B market in 2004
- **$30B in 2010**



Worldwide solar power shipments in 2003 totaled 744 MW, with the U.S. share at only 14%.

Inorganic vs. Organic Excitons

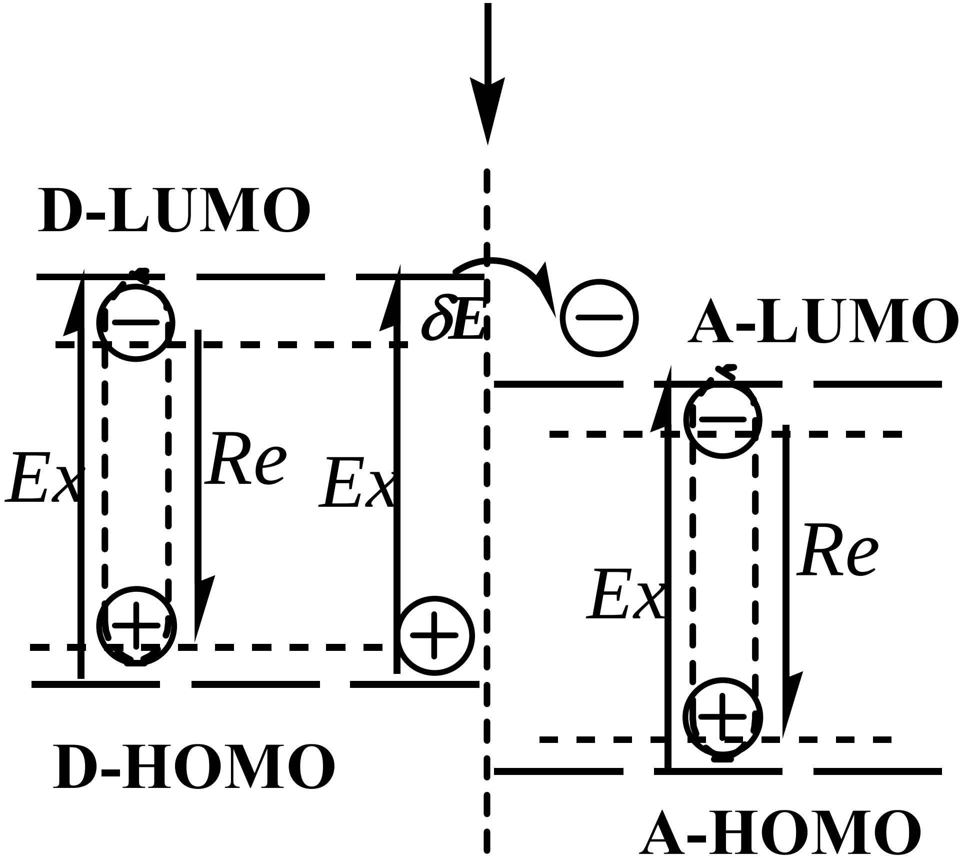
(Sun, S. "Organic and Polymeric Solar Cells", in *Handbook of Organic Electronics and Photonics*, edited by S. H. Nalva, American Scientific Publishers, Los Angeles, California, **2008,** Vol. 3, Chapter 7) .



Comparison of Inorganic vs. Organic: Double Layer Solar Cell Energy Levels

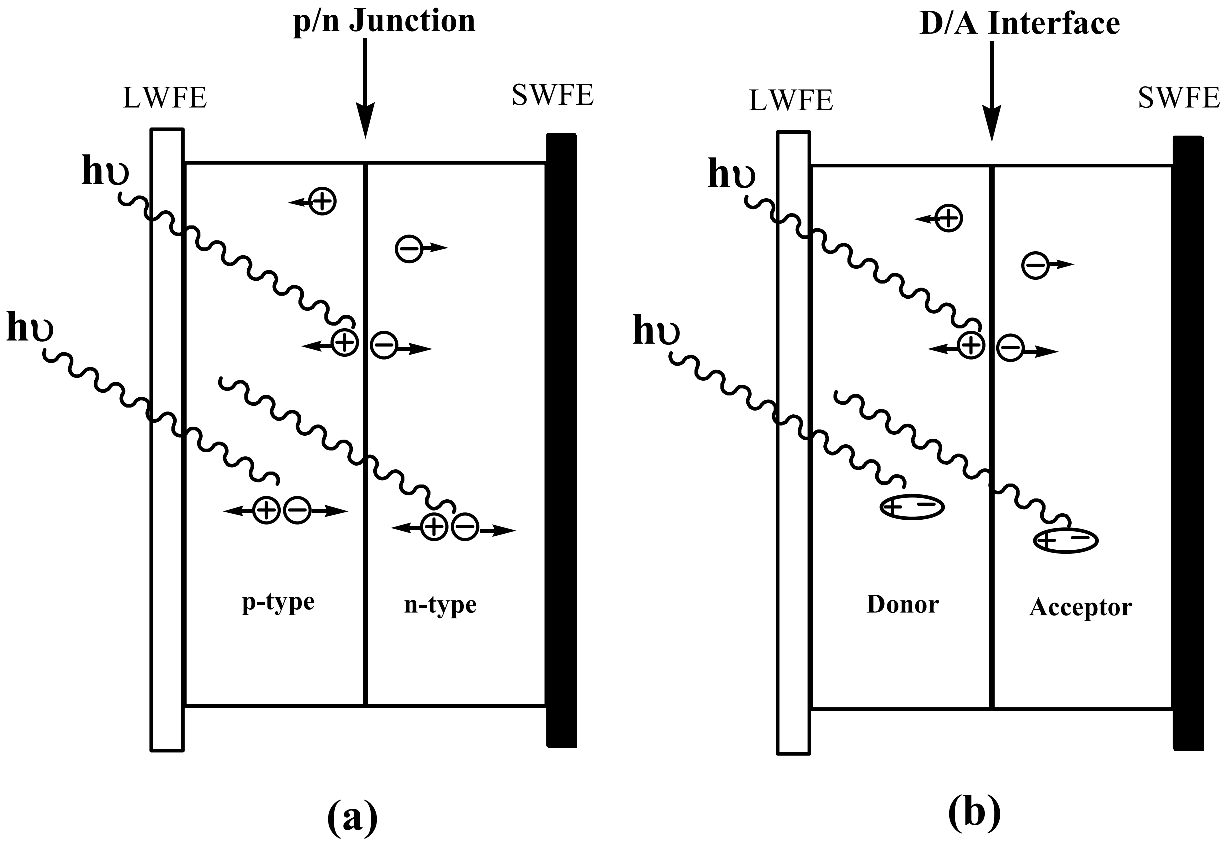
(Sun, S. "Organic and Polymeric Solar Cells", in *Handbook of Organic Electronics and Photonics*, edited by S. H. Nalva, American Scientific Publishers, Los Angeles, California, **2008,** Vol. 3, Chapter 7) .

D/A Interface



Double Layer Solar Cell Device Structures

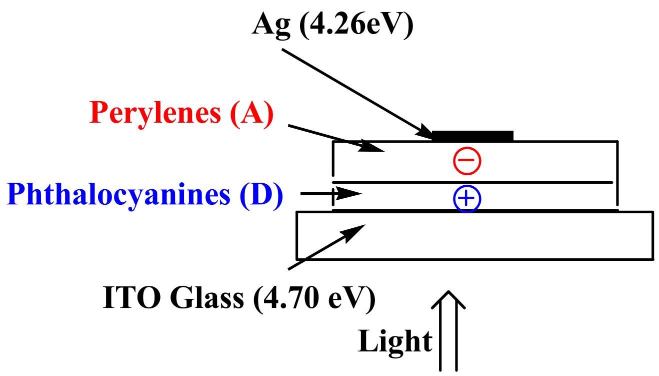
(Sun, S. "Organic and Polymeric Solar Cells", in *Handbook of Organic Electronics and Photonics*, edited by S. H. Nalva, American Scientific Publishers, Los Angeles, California, **2008**, Vol. 3, Chapter 7) .



"Bell Lab Cell" 1954 **"Tang Cell" 1986**

Organic D/A Bilayer Solar Cell 'Tang Cell'

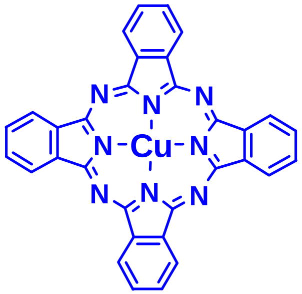
First Organic D-A Type Solar Cell



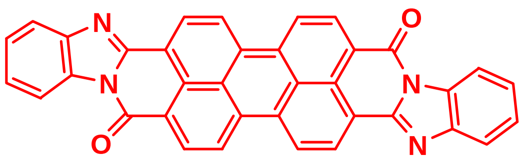
C. W. Tang

Eastman Kodak Co.
Appl. Phys. Lett., 48(2), 183(1986)

Efficiency 1%
0.75 Sun @ AM 2
Voc = 0.45 V
Isc = 2.3 mA/cm^2

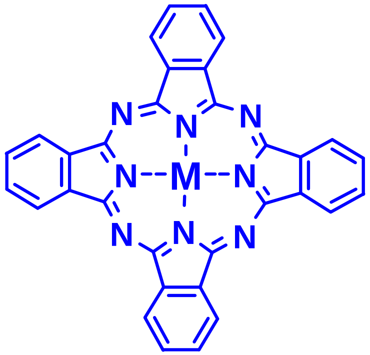


Phthalocyanines (Donor)

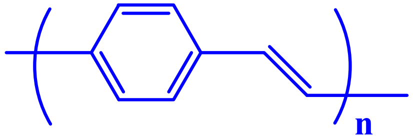


Perylenes (Acceptor)

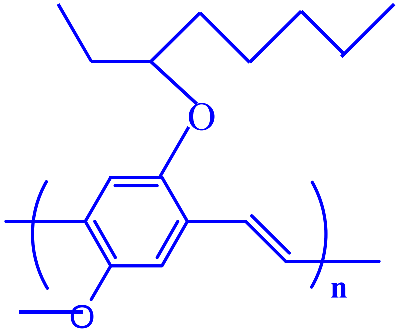
Representative Organic Donors



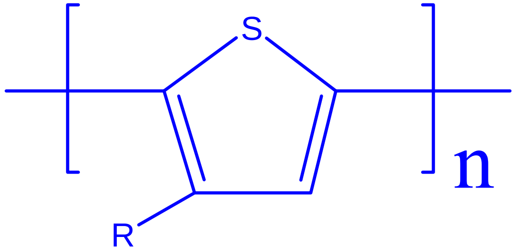
Phthalocyanines (MPc)
***e.g.*, H_2Pc when $M=H_2$**



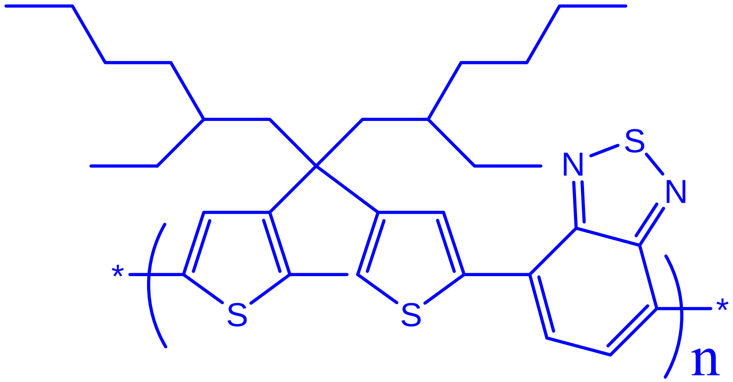
PPV



MEH-PPV

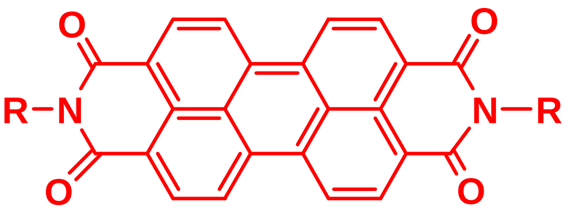


PT, *e.g.*, P3HT when $R=C_6H_{13}$

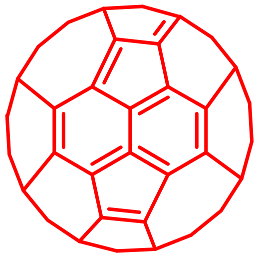


PCPDTBT

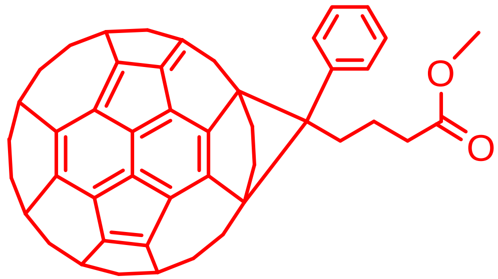
Representative Organic Acceptors



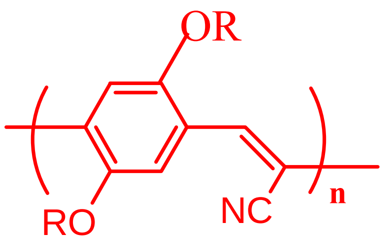
Perylenes
***e.g.*, Me-PTC when R=Me**



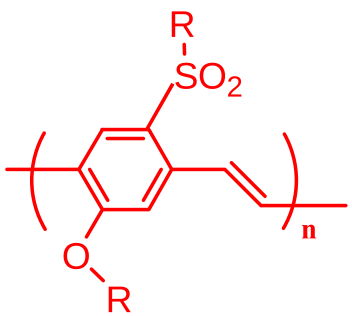
C_{60}



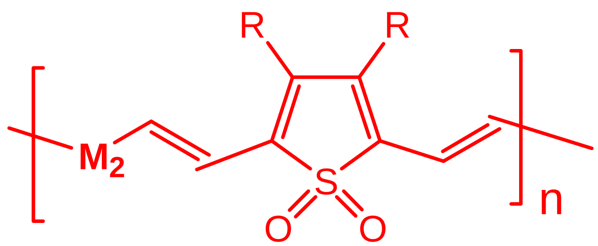
PCBM



CN-PPV



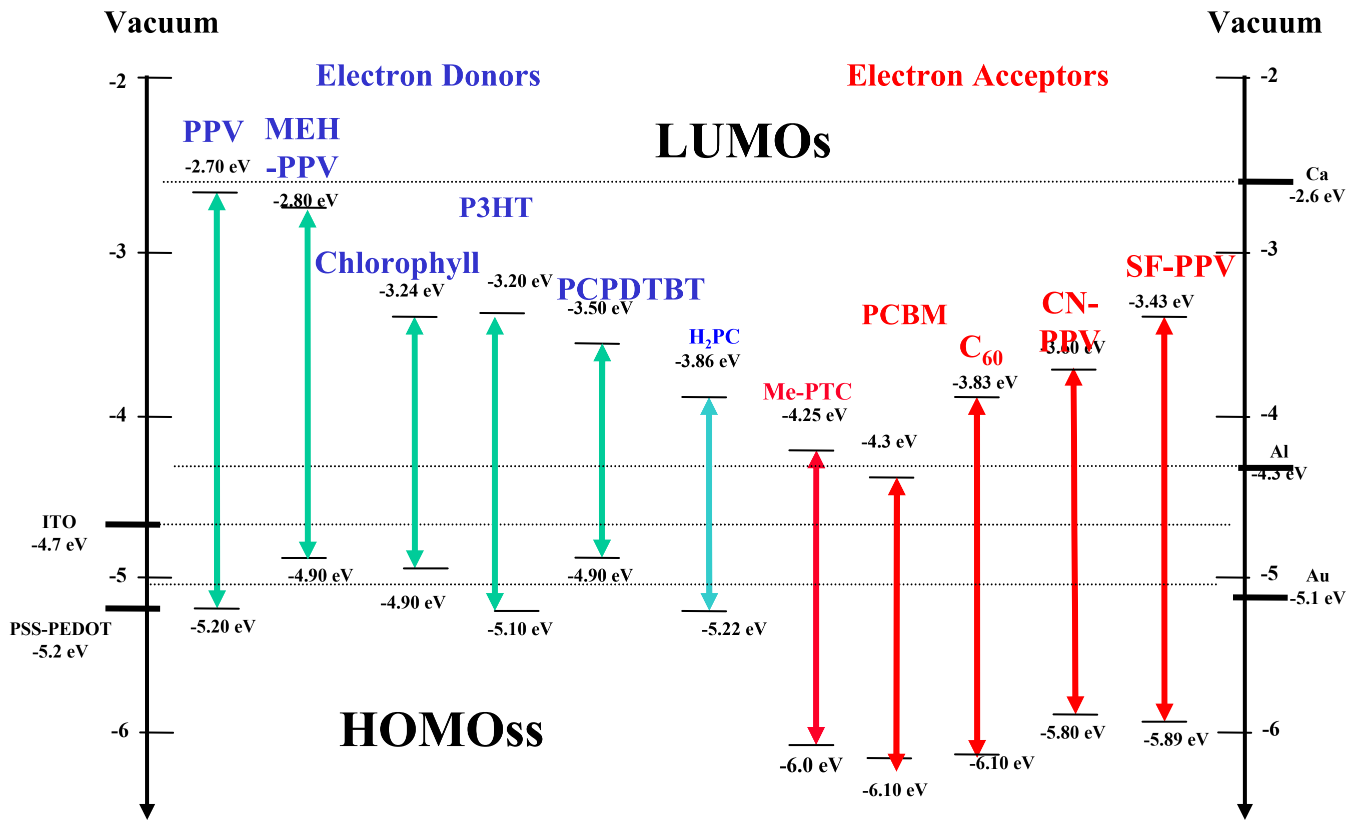
SF-PPV



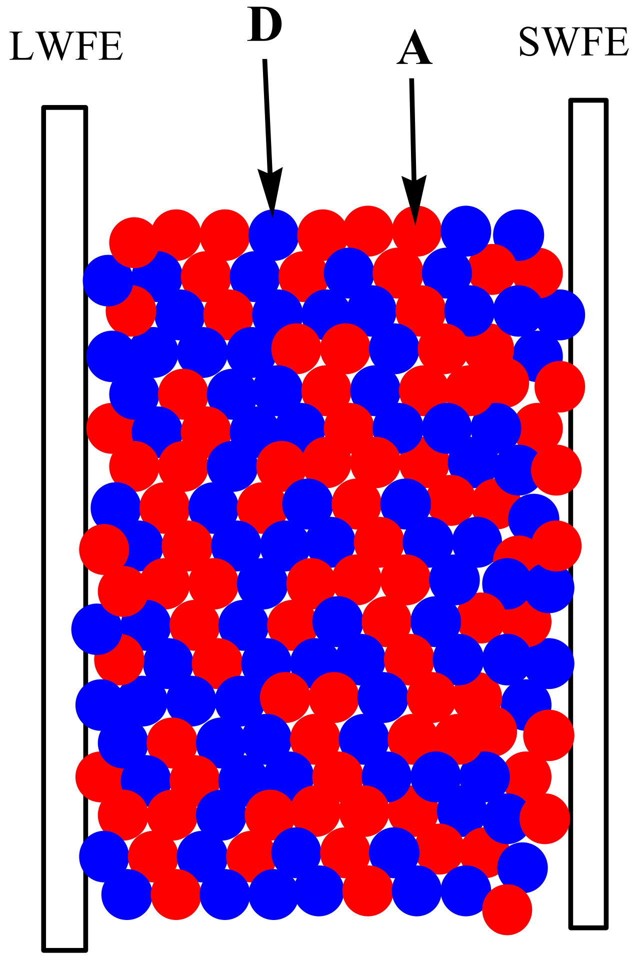
SF-PTV

HOMO/LUMO Levels

(Sun, S. et al. "Sunlight Energy Conversion via Organics", an invited review article in *Handbook of Photovoltaic Science and Engineering*, Luque, A and Hegedus, S., eds., Wiley, the Atrium, England, **2009** .



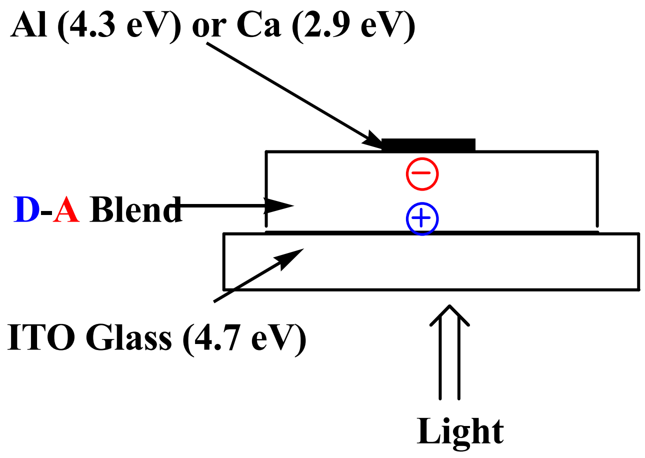
D/A Blend Solar Cells: "Bulk Heterojunction"



G. Yu, J. Gao, J. Hummelen, F. Wudl, and A. Heeger, Science, **270**, 1789 (1995).

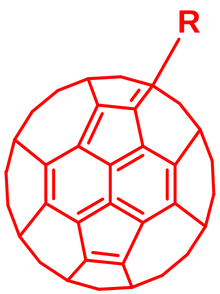
Current State-of-the-Art Polymer Solar Cells

"Bulk D-A Heterojunctions" Single Layer Organic Solar Cell

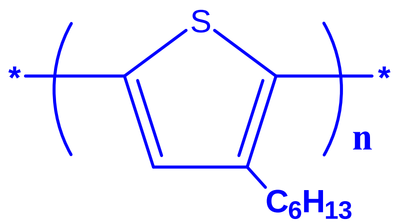


Y. Yang, *et. al.* at UCLA
***Nature Materials*, 4, 864 (2005)**
η ~ 5%

A. Heeger, *et. al.* at UCSB
***Science*, 317, 222 (2007)**
η = ~6%

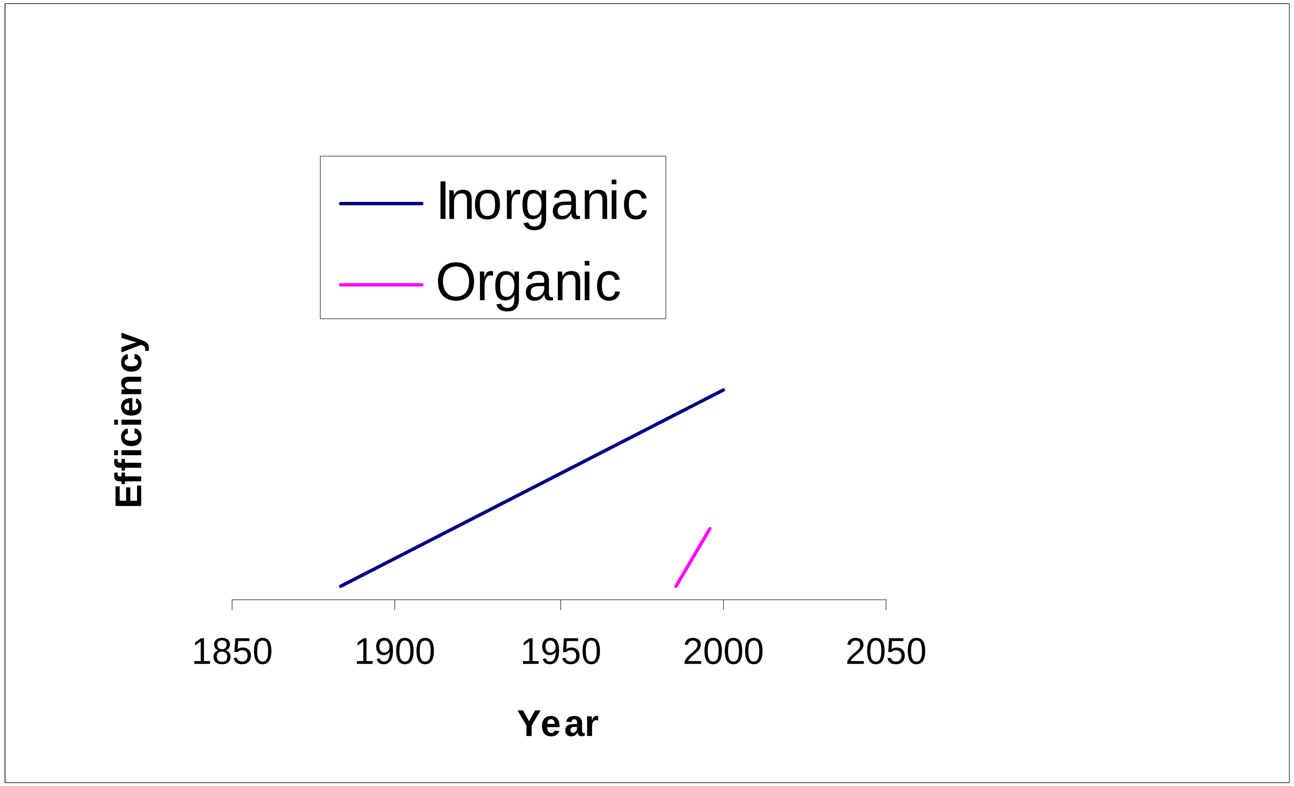


PCBM (Acceptor)



P3HT (Donor)

PV Efficiencies of Inorganic vs. Organic Cells



Five Critical Steps in Organic Photovoltaic

1. **Photon Capture (Solar radiation: 1.0-2.0 eV on surface of the earth, 2.0-3.0 eV in space, Materials Engineering at Energy Domain).**
2. **Exciton Diffusion (D/A interface within 5-50 nm region, Materials Engineering at Spatial Domain).**
3. **Charge Separation (Orbital Couplings, Offsets, Materials Engineering at Spatial Domain and Energy Domain).**
4. **Charge Transportation (Morphology, Materials Engineering at Spatial Domain)**
5. **Charge Collection at Electrodes (Engineering at Energy Domain)**

Three Key 'Losses' of Organic Photovoltaics

(Sun, S., *Sol. Energy Mater. Sol. Cells*, 2003, *79(2)*, 257-264)

- **1. Photon Loss**

(Materials Excitation Energy Gaps vs. Sunlight Spectrum)

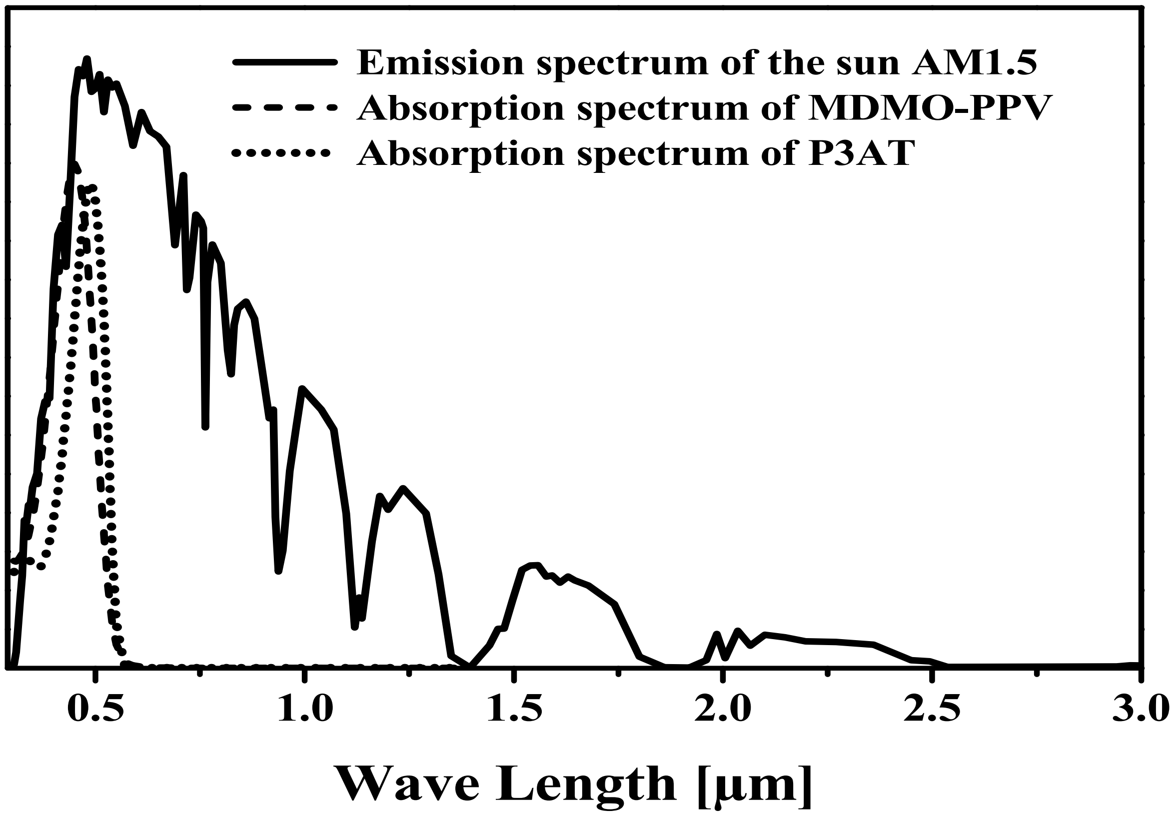
- **2. Exciton Loss**

(D/A Domain Size, Morphology, D/A Orbital Coupling and Energy Offsets)

- **3. Carrier Loss**

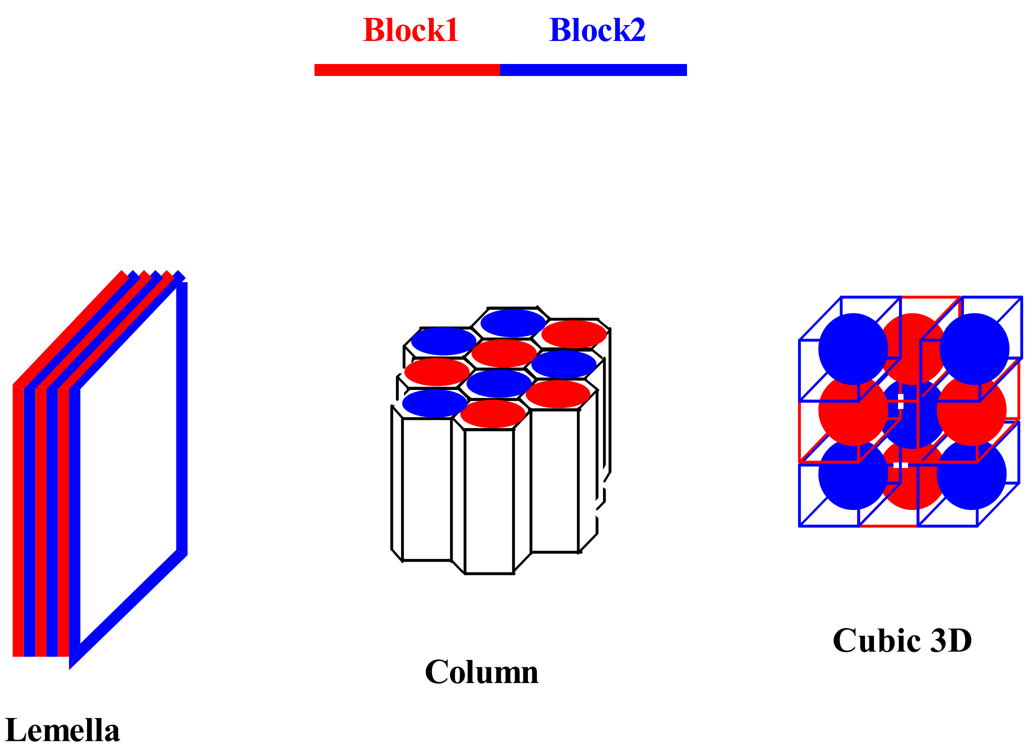
Carrier Transport Pathways, Morphology, Electrodes

Solar Spectrum on Earth Surface (AM 1.5)



Optimizations at Spatial Domain

AB Diblock Copolymer Morphologies

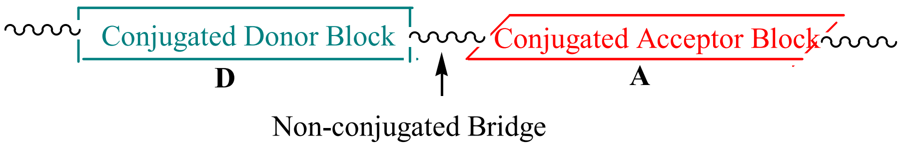


Representative Block Copolymer Morphologies

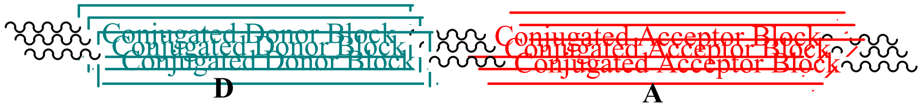
A ‘Tertiary’ Nano Structured Polymer Solar Cell

(Sun, S., *Sol. Energy Mater. Sol. Cells*, 2003, *79(2)*, 257-264)

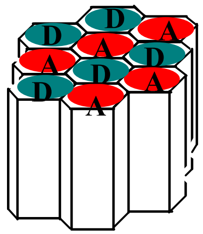
i) "Primary Structure"

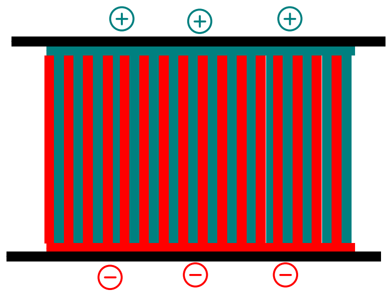


ii) "Secondary Structure"



iii) "Tertiary Structure"

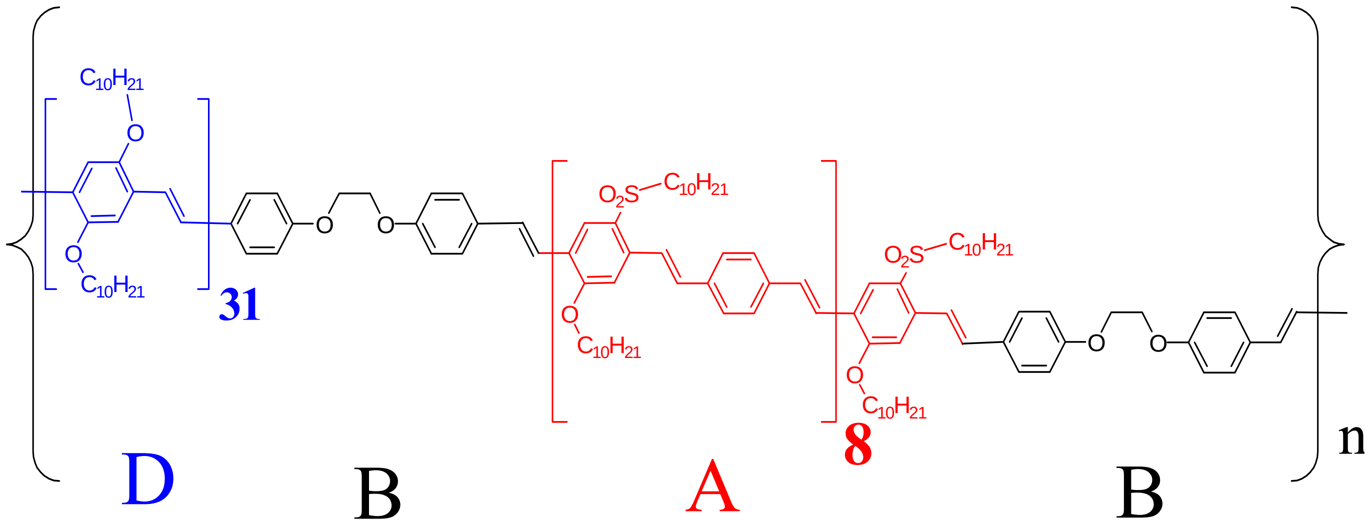




iii-a) Columnar 'HEX' Morphology **iii-b) PV Device Architecture**

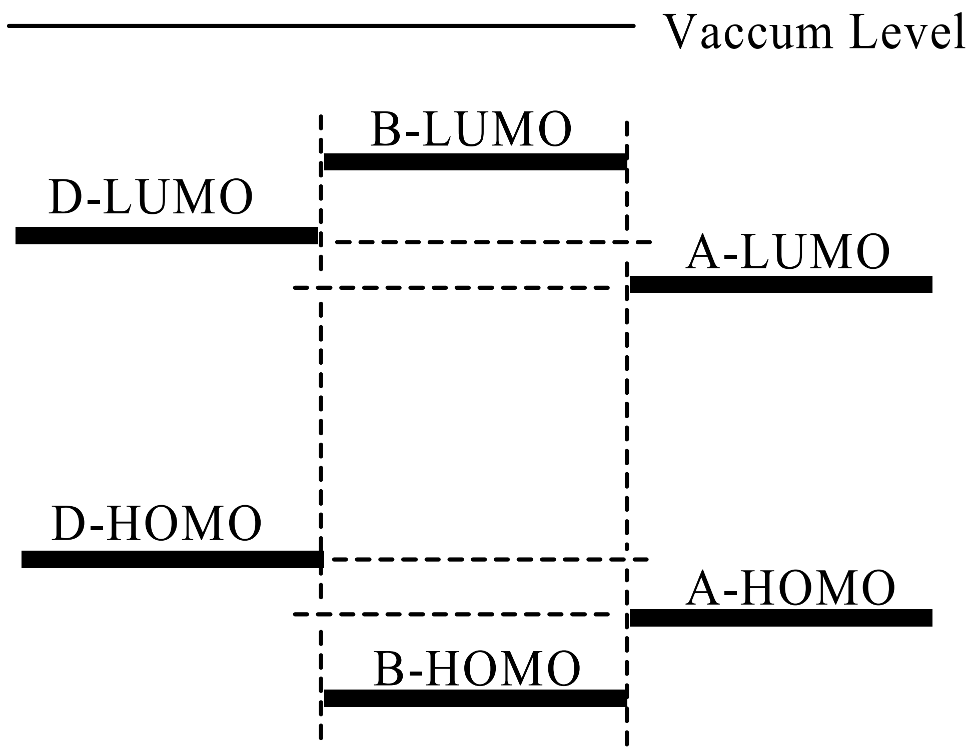
Most Recent Block Copolymers Developed at NSU

Zhang, C., *et al*. *Macromolecules*, **2006**, *39*, 4317-4326.



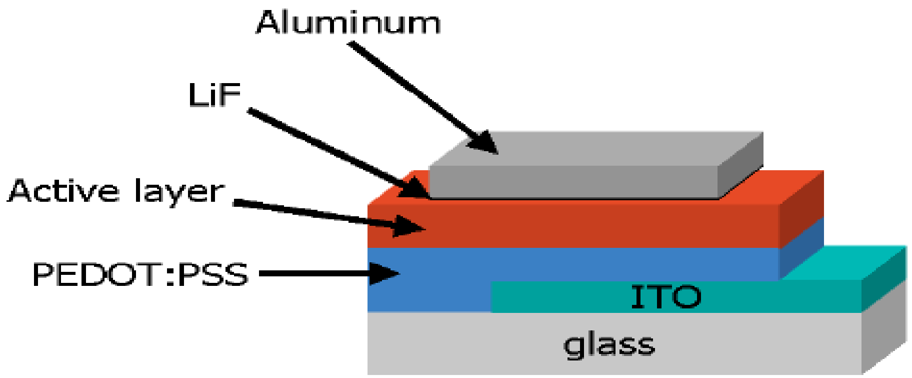
Energy Levels of -DBAB- Block Copolymer

(Sun, S.; et al., *J. Mater. Sci.*, 2005, *40*, 1429-1443.)



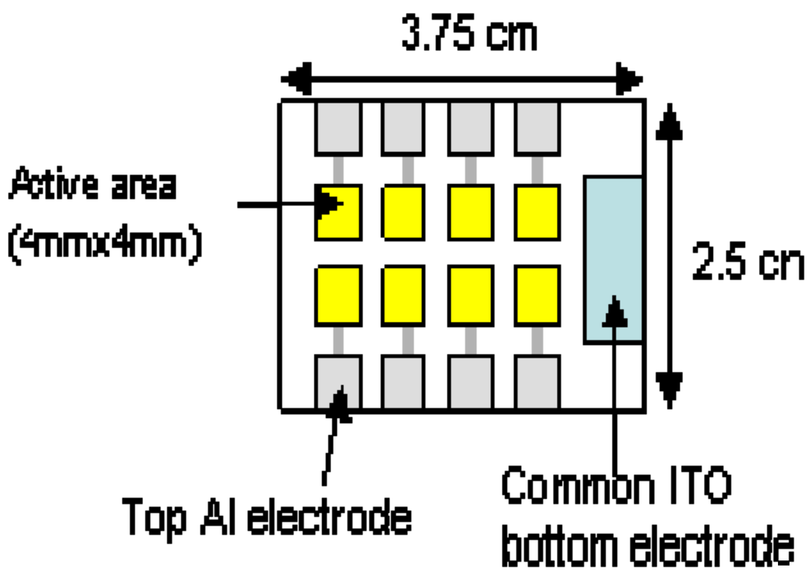
Intra-chain energy level schematic diagram of -DBAB- type block copolymer

Device Fabrication



- **ITO/Glass substrate**
- **Etched ITO (top 1/3)**
- **PSS:PEDOT spin coated**
- **PSS:PEDOT wiped (bottom1/3)**
- **Active layer spin coated**
- **LiF deposited (0.6 nm)**
- **Aluminum deposited (~100 nm)**

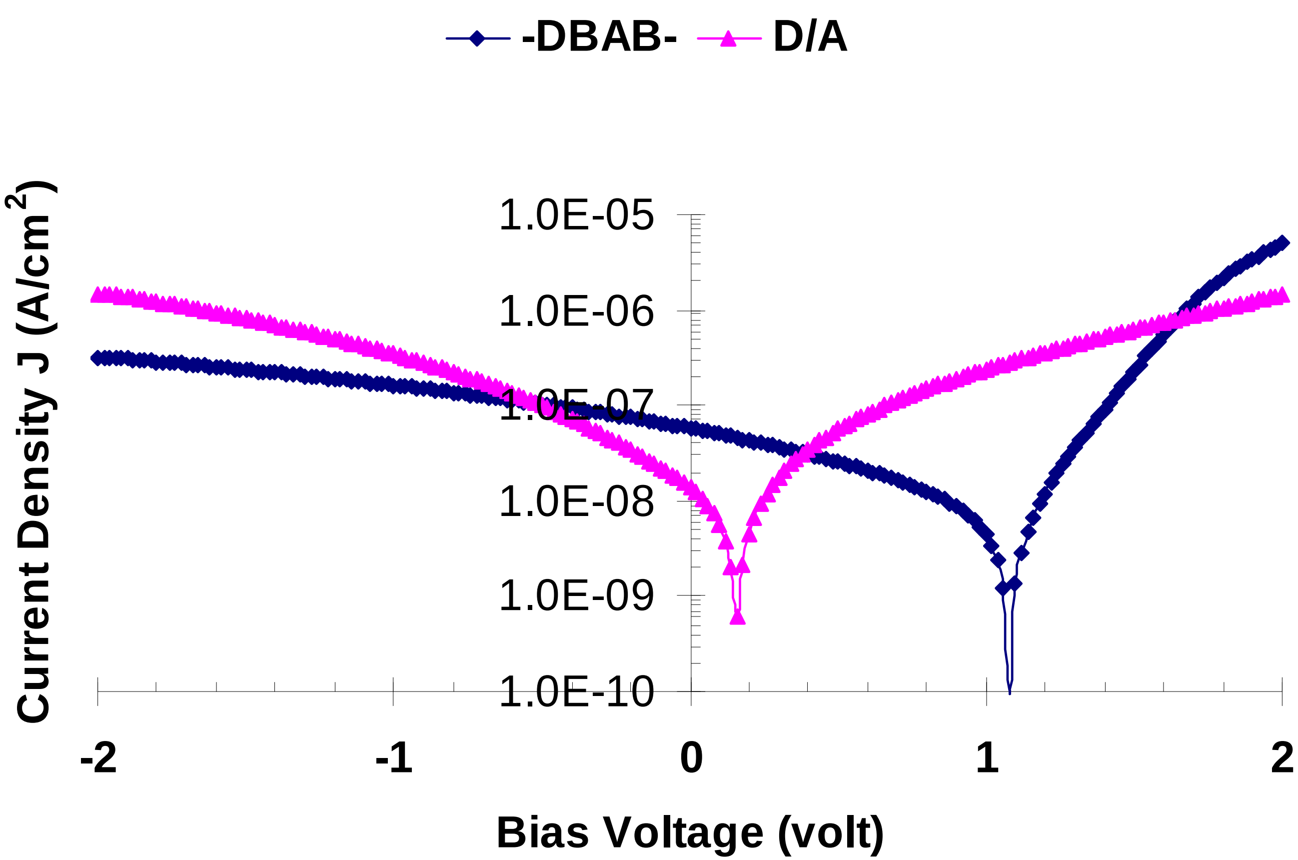
Representative Polymer Solar Cells Fabricated at NSU



Block copolymer solar cells on one ITO slide substrate	V_{oc} (V)	I_{sc} (μA)	J_{sc} (μA/cm^2)
#1	0.88	0.942	5.9
#2	1.05	1.154	7.2
#3	**1.15**	**1.235**	**7.7**
#4	0.90	0.783	4.9
#5	1.00	1.138	7.1
#6	0.67	0.76	4.8
#7	1.06	0.75	4.7
#8	1.10	0.353	2.2

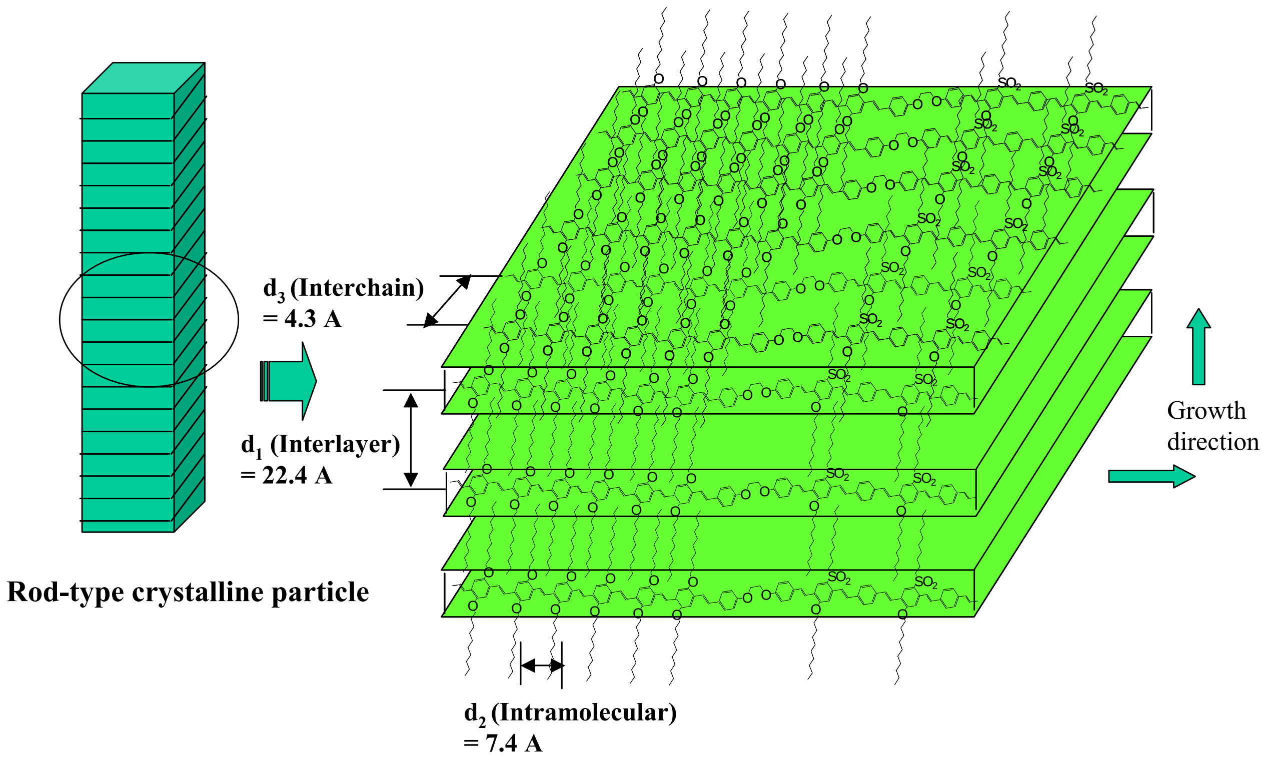
Photo J-V Data of a –BDBA- vs. D/A PV Device

(Sun, S., *et al*., *Appl. Phys. Lett.*, 2007, *90,* 043117)



Block Copolymer Self Assembly

(Sun, S., *et al.*, *Appl. Phys. Lett.*, 2007, *90*, 043117)



Stacking scheme of –DBAB- block copolymer film after annealing at 140^{o}C for 5 hr.

Optimizations at Energy Domain

Scheme of Photo Induced Electron Transfer Processes of a D/A Pair
Frontier Orbital Level Diagram

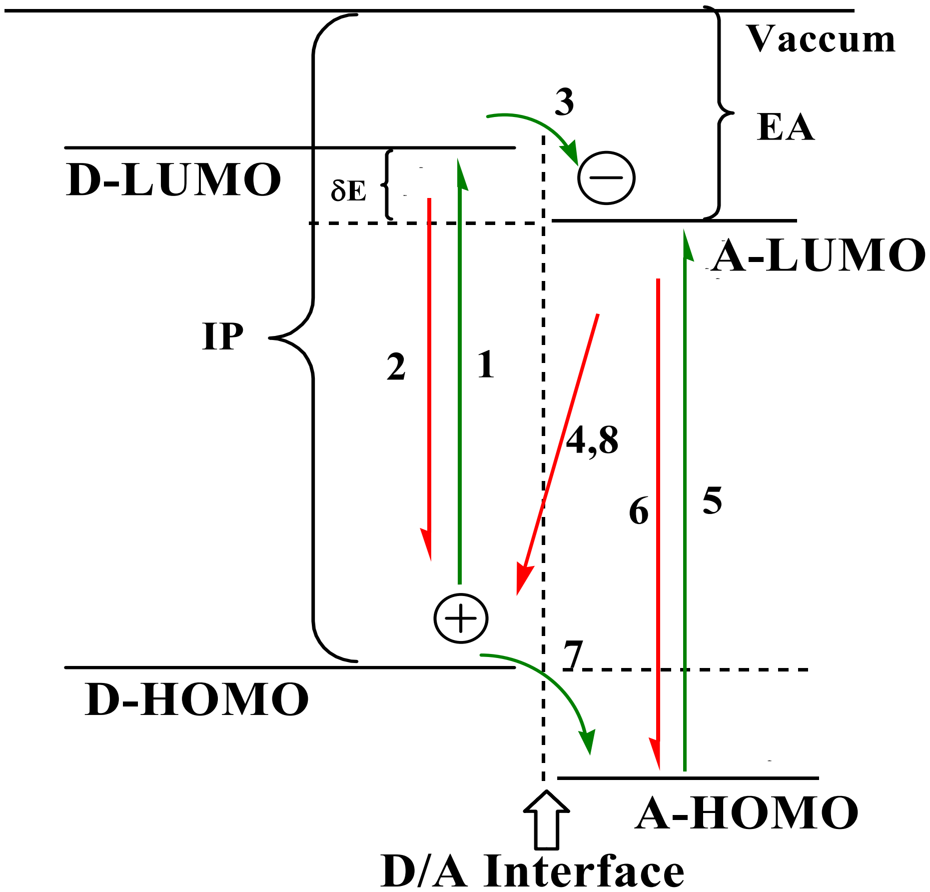
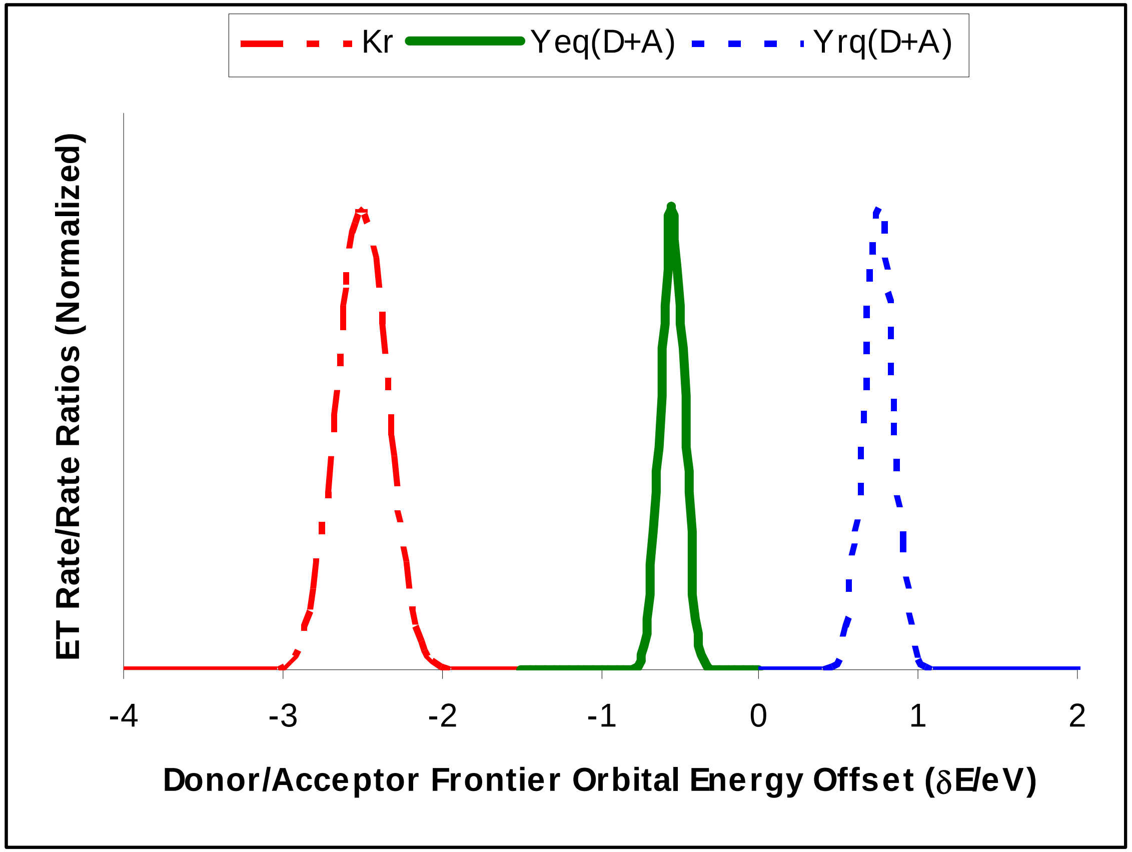


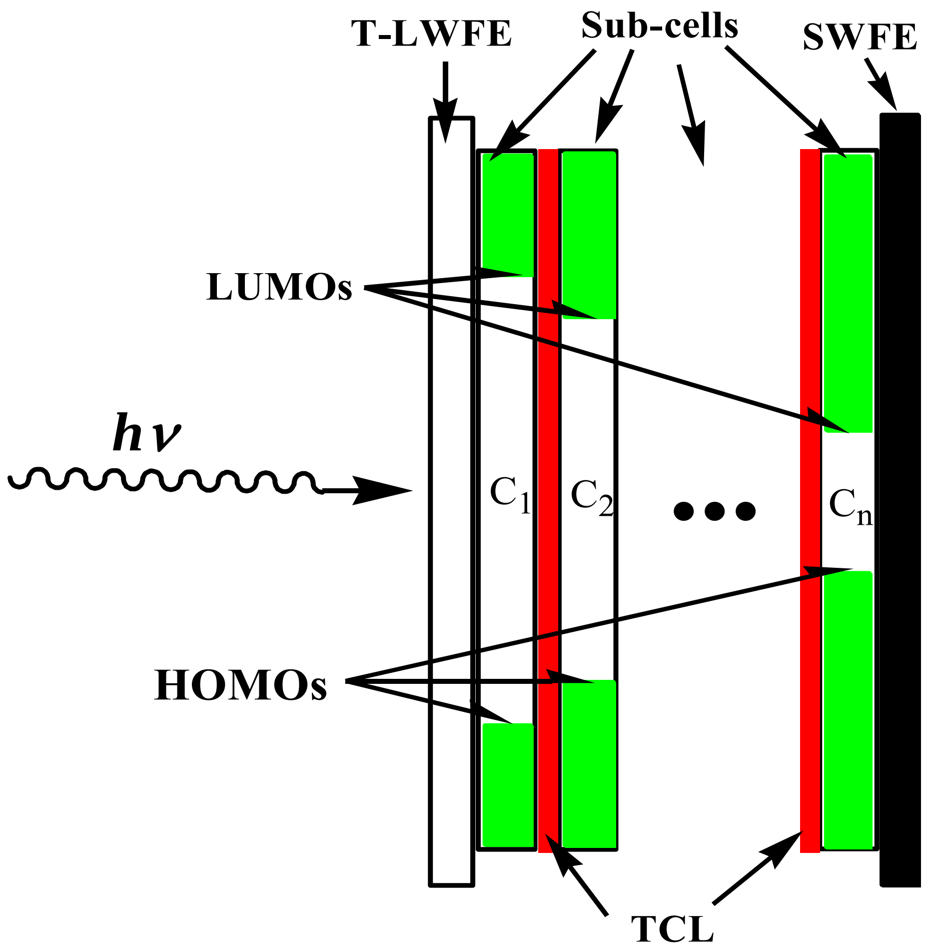
Photo Induced Electron Transfer Rates/Rate Ratios vs. LUMO offsets

(Sun, S., *Mater. Sci. & Eng., B*, 2005, *116 (3)*, 251-256.)

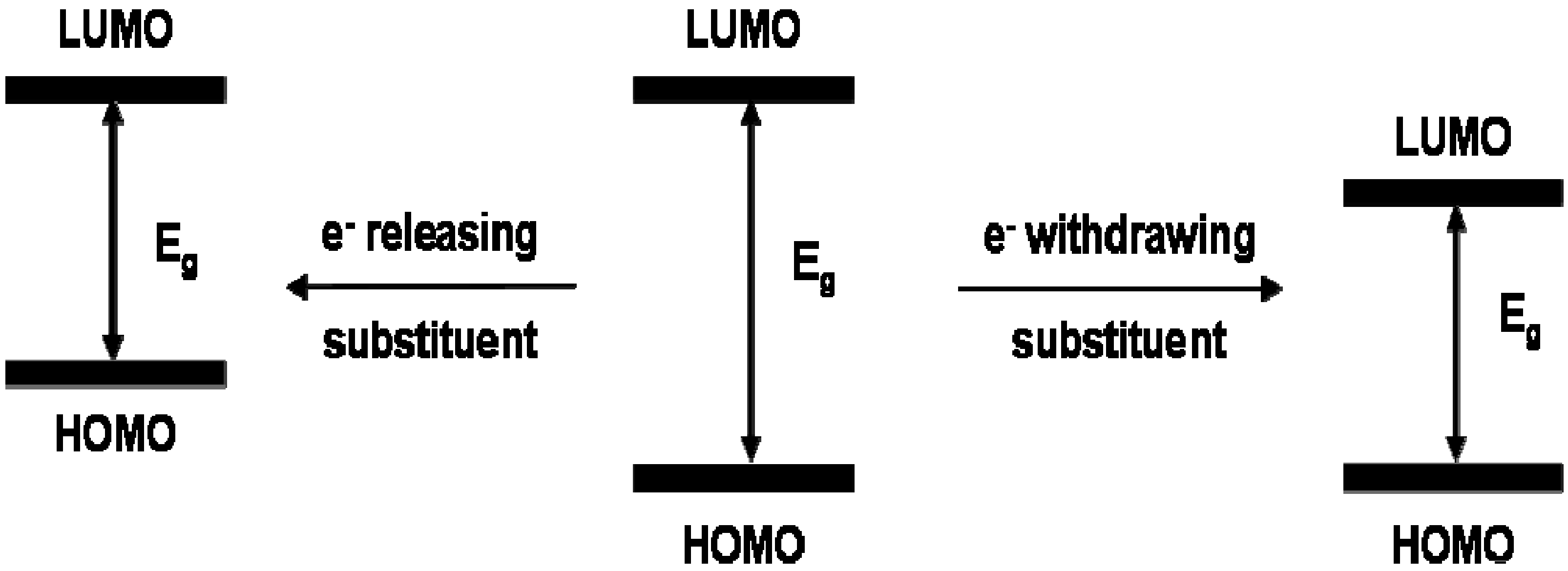


Tandem Energy Gap Graded Solar Cell Structure

(Sun, S. "A Tandem Style Photovoltaic Device With Nano Structured Sub-Cells", 2005 US patent pending)



Effect of electron donating or electron withdrawing substituents on Eg of CPs

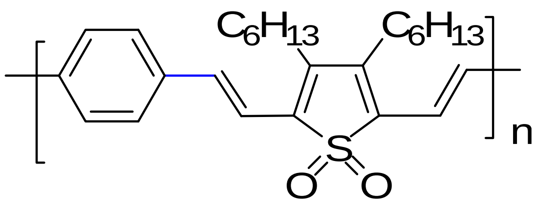


PTV Series Synthesized

Zhang, C., *et al*. *Macromolecules*, **2009**, *42*, 663-670.

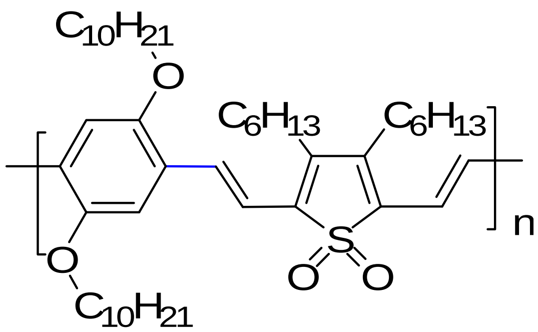
P(PV-SFTV)-1A

2.04 eV



410.61

P(C10OPV-SFTV)-1A

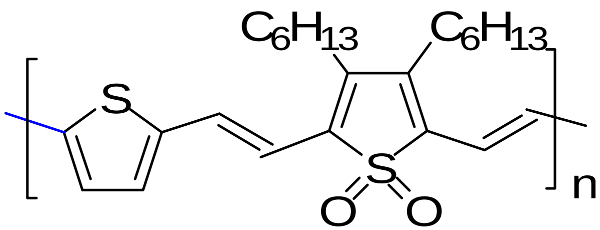


1.85 eV

723.14

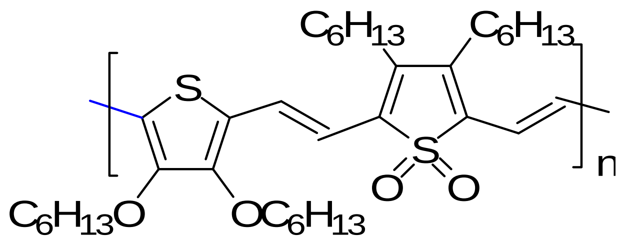
P(TV-SFTV)-1A

1.75 eV



448.72

SF-PTV2



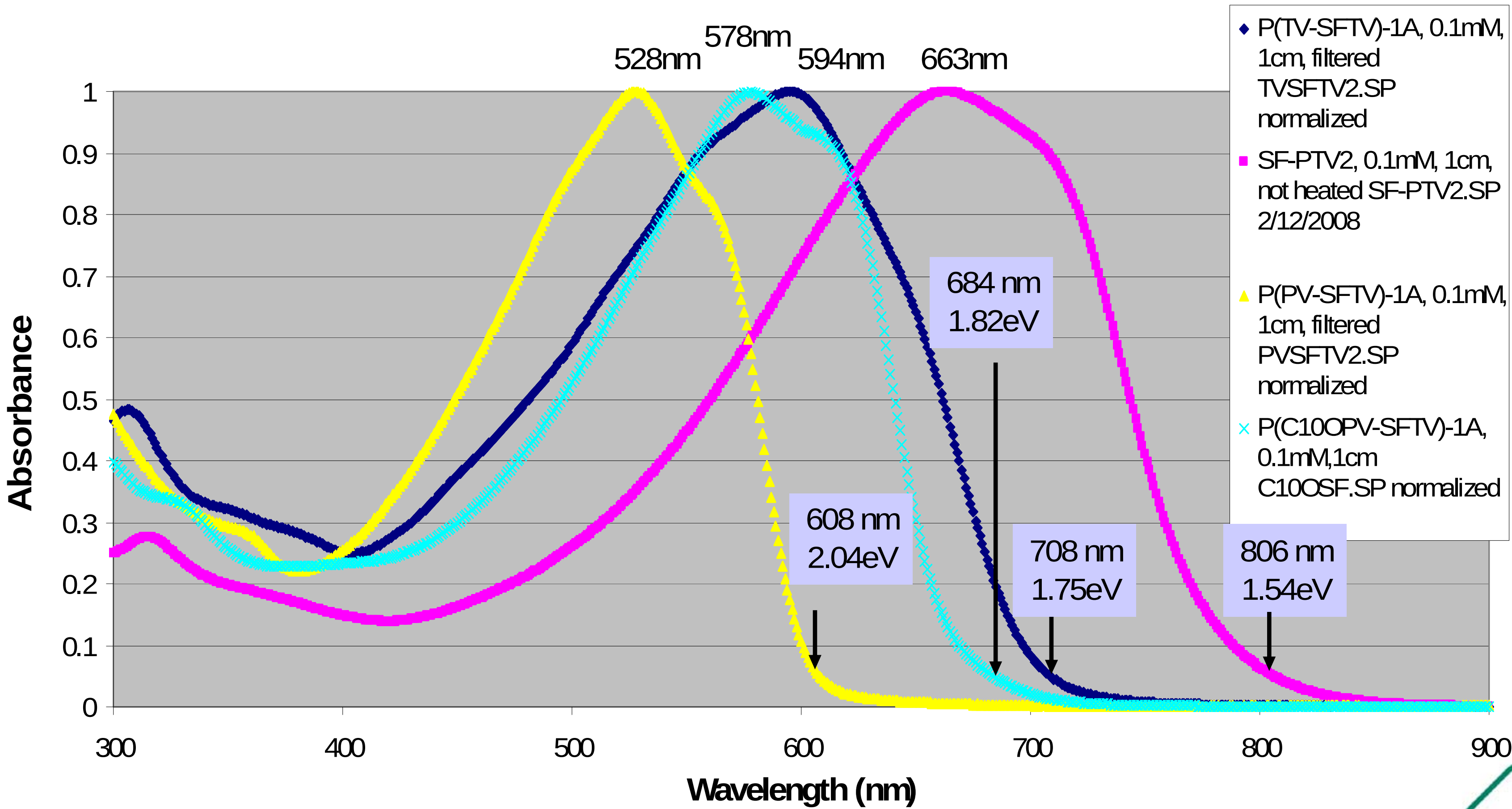
1.54 eV

649.04

n ~ 20

Energy Gap Engineering

Zhang, C., *et al*. *Macromolecules*, **2009**, *42*, 663-670.



Summary

- **1.** Current low efficiency of organic solar cells can be attributed mainly to the three major losses, *i.e.*, the 'photon loss', the 'exciton loss', and the 'carrier loss'. However, high efficiency organic solar cells can be realized via optimization in both space and energy domains to minimize these losses.
- **2.** In spatial domain, a 'D/A nano scale and bicontinuous phase separated morphology' is desired. For instance, a synthesized and not yet optimized –BDBA- type block copolymer exhibits much better photovoltaic properties in comparison to the blends under identical conditions. Orbital coupling between donor and acceptor also needs to be optimized to maximize exciton dissociation and minimize separated charge recombination.
- **3.** In energy domain, materials energy gaps need to be optimized to capture more sunlight. Additionally, donor/acceptor frontier orbital energy levels and offsets need to be optimized to maximize the exciton dissociation and minimize the charge recombination. Multi-layer tandem style structure can be used to further reduce the sunlight photon loss.

Acknowledgement

- Research Associates: Drs. Cheng Zhang, Soobum Choi and Shahin Maaref
  - Graduate Students: Zhen Fan, Charles Taft, Yiqing Wang, James Haliburton,
    - Shanneth Thomas, Zeina Roz, Meina Wang, Shameika Vick, name removed on request
      - Kizzy Winston, Taina Matos, Thuong Nguyen, Eric Anil
        - Simon Sun, Amanda Harding, Tanya David

- Undergraduate Students: Shanneth Thomas, Janelle Saulter, Sheron Waytt, Mitchel Ashanti, Charmaign Harris, Valery Rose, Dena Davis, Jashua Hou, Robert Tew, Taina Cleveland, Tanya David, Mayen Udoetuk, Norman Sturks, Shailise Ross, *etc*.
  - Laser Spectroscopy: Prof. Carl E. Bonner (NSU)
  - ET Theory: Prof. R. Marcus (Cal. Tech., 1992 Chemistry Nobel)
  - $: NASA, DOD (AF, MDA), NSF, OE

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Selected Key Publications relevant to OPV

- Zhang, C.; Nguyen, T.; Sun, J.; Li, R.; Black, S.; Bonner, C.; Sun, S.; "Design, Synthesis, Characterization, and Modeling of A Series of S,S-Dioxo-Thienylenevinylene-Based Conjugated Polymers with Evolving Frontier Orbitals", ***Macromolecules***, **2009**, *42*, 663-670.
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