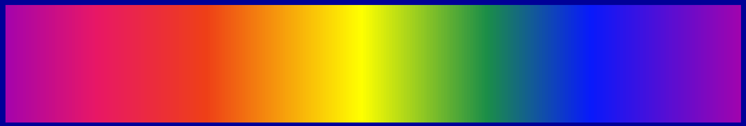


"Nano-infused solar cells: quantum dot/polymer and block copolymer approaches

Prof. Michael S. Wong (mswong@rice.edu)
Prof. Rafael Verduzco, Prof. Lisa Biswal

Department of Chemical and Biomolecular Engineering
Rice University, Houston, TX

Rice Technology Showcase
Power Generation, Storage and Transmission
Nassau Bay, TX
July 29, 2014

RICE

The first generation: Silicon-based solar cells

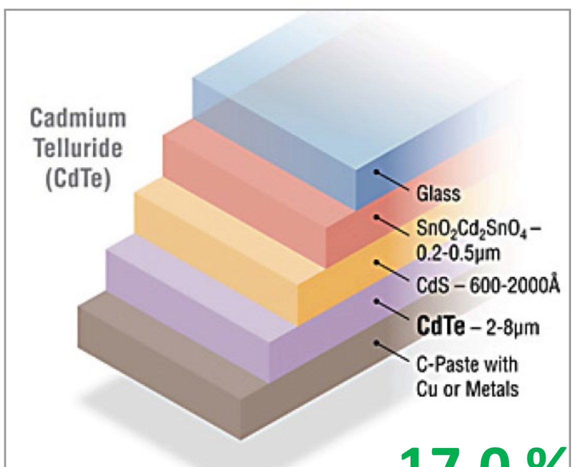
Theoretical power conversion efficiency (PCE) limit = ~33 %

MRS Bulletin, 2008, **33**, 355-364

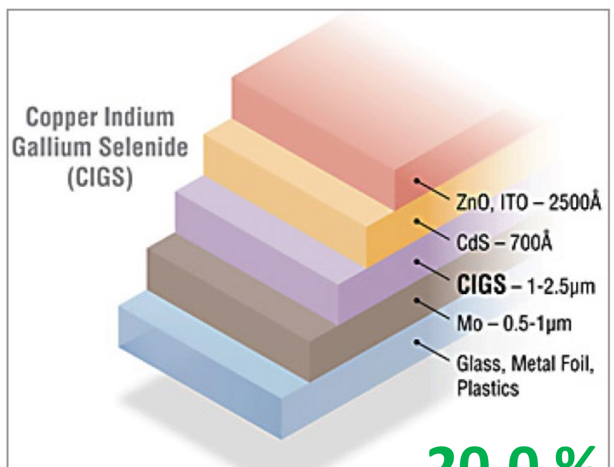
Pros: Good PCE

Cons: High cost

The second generation: Advanced thin film solar cells



17.0 %



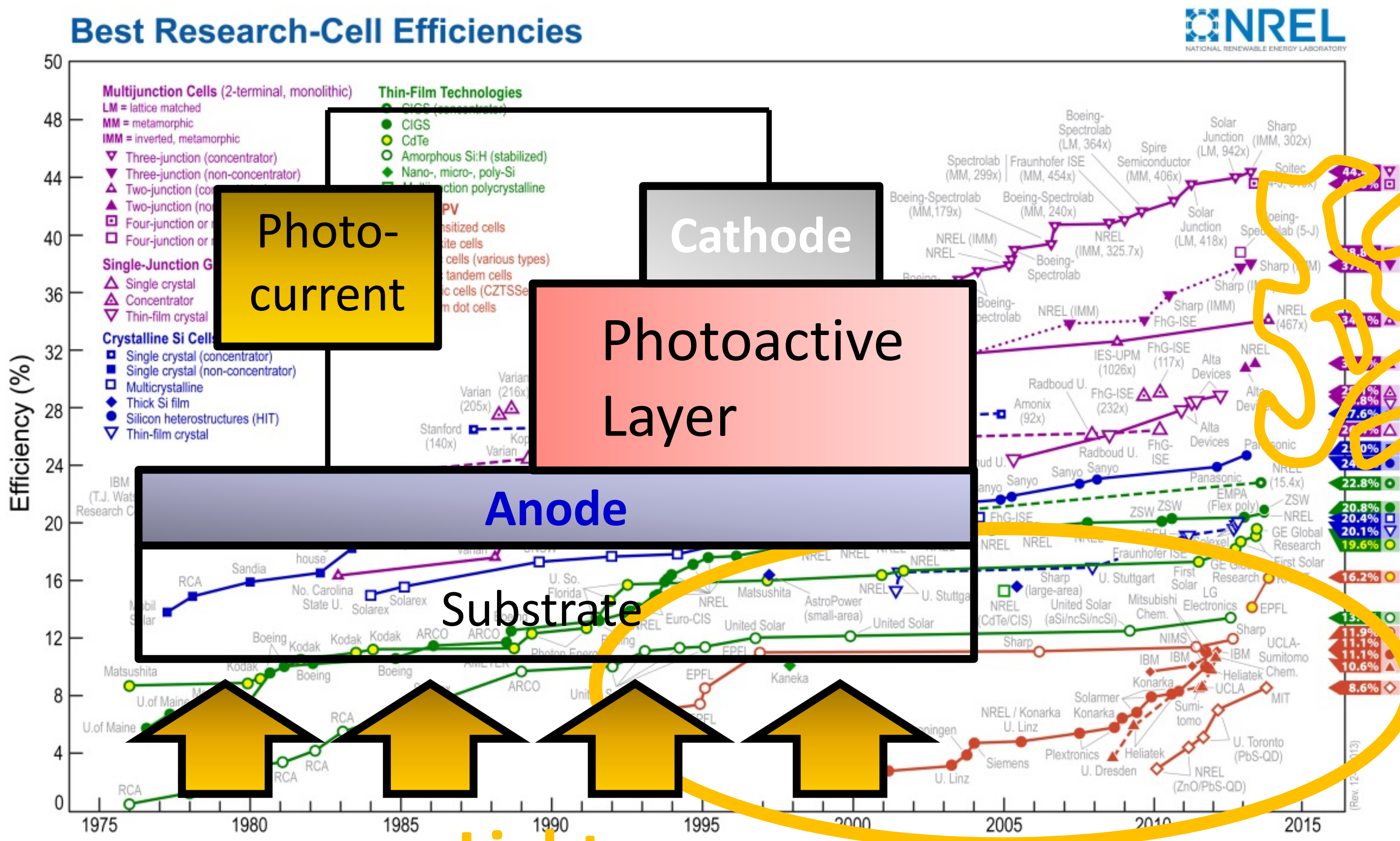
20.0 %

Pros: Lower cost

Cons: Market share

National Renewable Energy Laboratory (NREL)

The basic facts about the third generation solar cells



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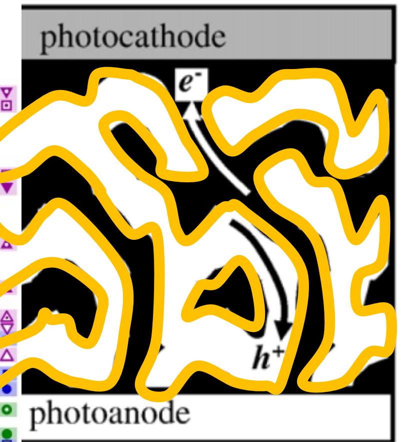


nge:

rphology inside
ive layer is difficult
trol

Advantage:

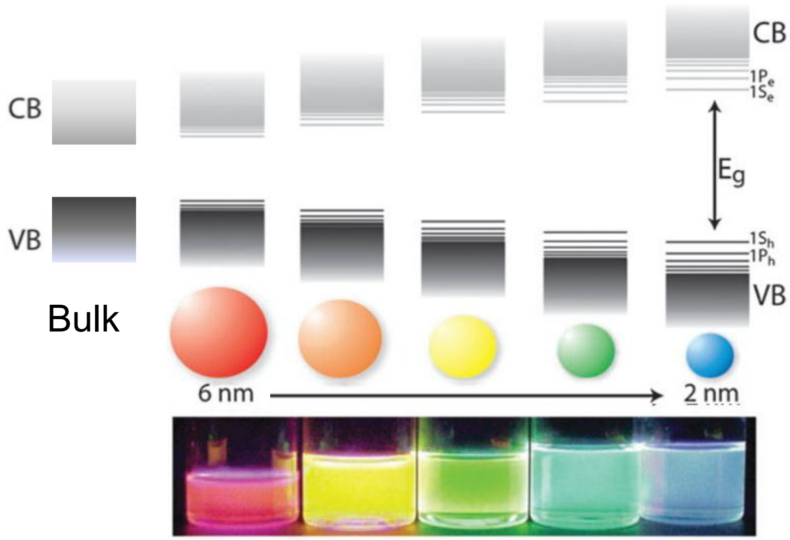
low cost, light weight, easy to process, strong optical absorption

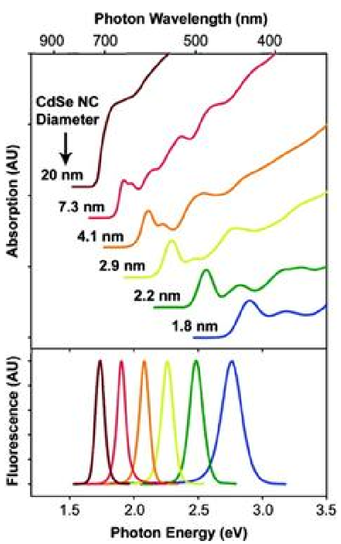
Adv. Coll. Interface Sci., 2008, **138**, 1-23
National Renewable Energy Laboratory (NREL)

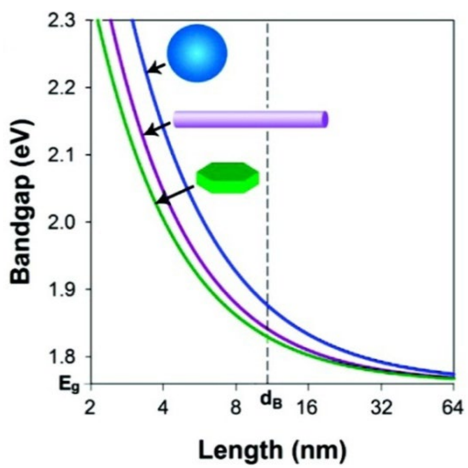
Semiconductor Nanomaterials

At least one feature in 1-100 nanometer (nm; 10^{-9} m) range

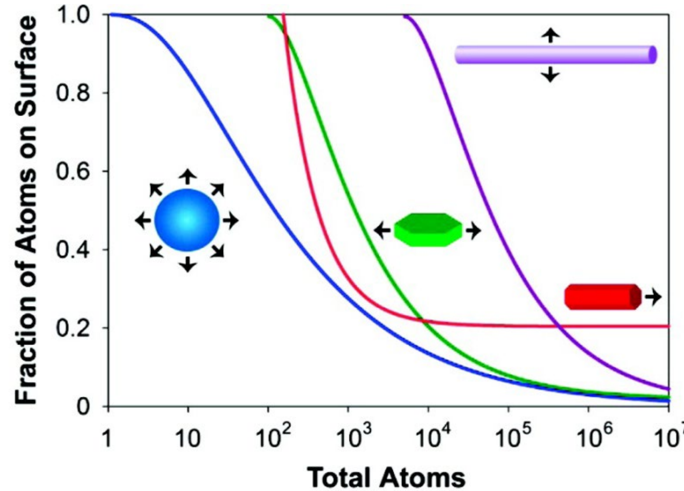
Electronic Structure

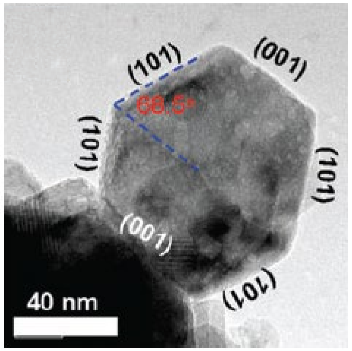






Surface Properties

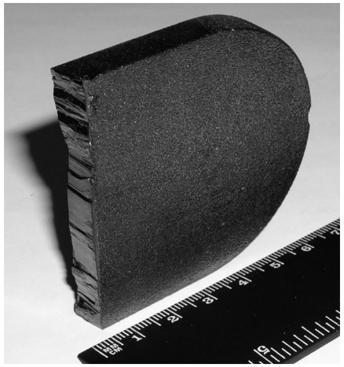




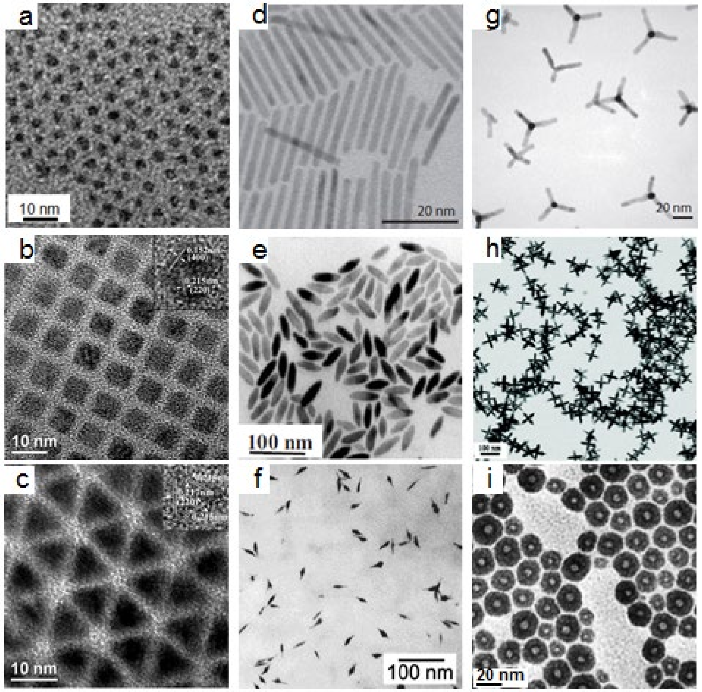
Donega, C. M.; *Chem. Soc. Rev*. **2011**, 40, 1512-1546.
Smith, A. M. *et al.*; *Acc. Chem. Res.* **2010**, 43, 190-200
Liu, G. *et al.*; *Chem. Commun.* **2010**, 46, 755-757.

Cadmium Selenide (CdSe)

- Bulk CdSe
  - Semiconductor
  - Fixed Band gap – 1.74 eV
  - High electron mobility (600 cm^2/Vs)



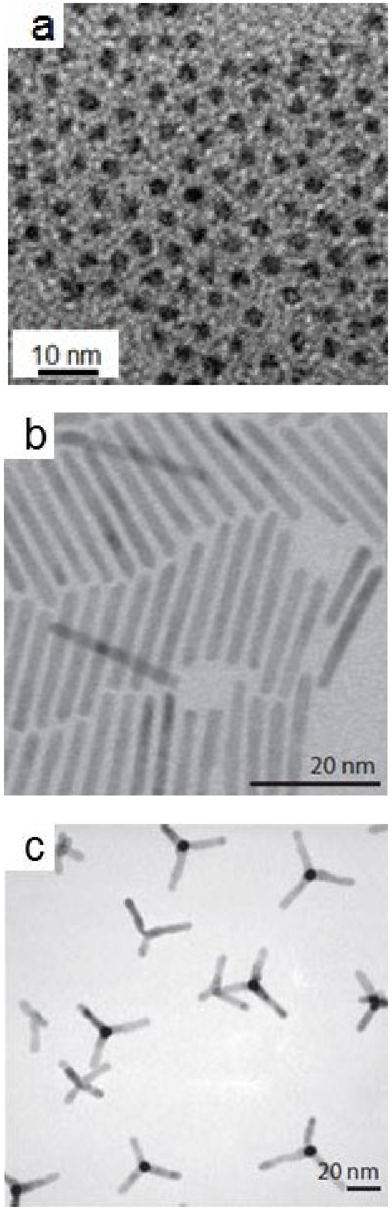
- CdSe nanoparticles (NPs) < 10 nm
  - Size dependent variable band gap
  - 1.74 eV to 2.75 eV; Visible spectrum
  - Discrete absorption spectrum
  - Wide variety of shapes



Madelung O., *Crystal and Solid State Physics*, Vol. 17, **1982**,Springer-Verlag, Berlin.
Saunders B.R. *et al.*, *Adv. Coll. Interface Sci.*, **2008**, 138, 1-23.
Peng X., *Adv. Mater*. **2003**, 14, 459-463.
Manna L. et al., *J. Am. Chem. Soc.*, **2000**, 122, 12700-12706.

Leekumjorn S., **Gullapalli S.** and Wong M.S. et al., *J. Phys. Chem. B*, **2012**, 116, 13063-13070.
Gullapalli S. *et al.*, *Nanotechnology*, **2012**, 23, 495606 (1-10).

Shapes of CdSe NPs Used for Solar Cells



The Effect of Nanoparticle Shape on the Photocarrier Dynamics and Photovoltaic Device Performance of Poly(3-hexylthiophene):CdSe Nanoparticle Bulk Heterojunction Solar Cells

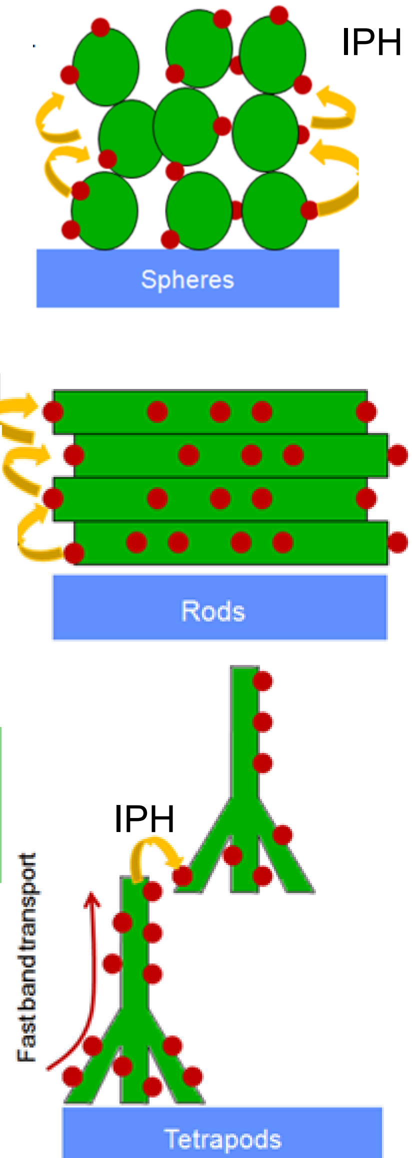
By *Smita Dayal,* Matthew O. Reese, Andrew J. Ferguson, David S. Ginley, Garry Rumbles,* and *Nikos Kopidakis**

Adv. Funct. Mater. **2010**, *20*, 2629–2635

Table 1. Open circuit voltage (V_{OC}), short-circuit current (J_{SC}, corrected for spectral mismatch), fill factor (*FF*), and power conversion efficiency (η) for nanoparticle:P3HT devices under simulated AM 1.5G light illumination. The errors represent the variation between 6 devices on the same substrate.

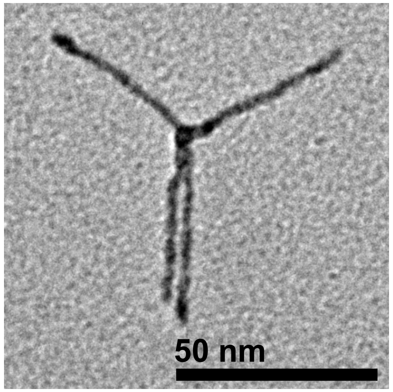
	V_{OC} [mV]	J_{SC} [mA cm^{-2}]	*FF*	η [%]
CdSe QD:P3HT	700 ± 50	0.24 ± 0.02	40 ± 2	0.066 ± 0.005
CdSe NR:P3HT	680 ± 15	4.15 ± 0.17	38 ± 3	1.1 ± 0.1
CdSe TP:P3HT	633 ± 2	4.83 ± 0.03	52 ± 1	1.49 ± 0.03
CdSe TP only	415	0.34	26	0.03
P3HT only	870	0.035	30	0.009

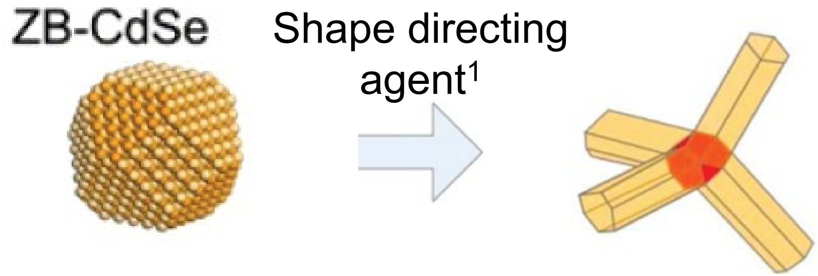
IPH: Inter particle hopping



Leekumjorn S., **Gullapalli S.** *et al.*, *J. Phys. Chem. B*, **2012**, 116, 13063-13070.
Choi C.L. *et al.*, *Annu. Rev. Phys. Chem.* **2010**, 61, 369-389.
Saunders B.R. *et al.*, *Adv. Coll. Interface Sci.*, **2008**, 138, 1-23.

CdSe Tetrapod (TP) Solar Cell Applications





CdSe TPs demonstrate the highest power conversion efficiencies in hybrid solar cells[2]

APPLIED PHYSICS LETTERS **99**, 223515 (2011)

Enhanced performance of hybrid solar cells using longer arms of quantum cadmium selenide tetrapods

Kyu-Sung Lee,[1] Inho Kim,[2] Sravani Gullapalli,[3] Michael S. Wong,[3,4] and Ghassan E. Jabbour[1,5,a)]

	V_{OC} [mV]	J_{SC} [mA cm^{-2}]	*FF*	η [%]
Long TP: P3HT	730	3.36	46	1.12
Short TP: P3HT	860	2.33	40	0.8

1. Huang J. *et al.*, *J. Am. Chem. Soc.*, **2010**, 132, 15866-15868.
2. Saunders B.R. *et al.*, *Adv. Coll. Interface Sci.*, **2008**, 138, 1-23.

New Method to CdSe HNPs

1. **Cd precursor**
   $Cd(NO_3)_2 \cdot 4H_2O$
   (Melting Point: 59.5 °C)
2. **Selenium Precursor**
   Se powder in
   Octadecene (ODE)
3. **Surfactant**
   Cetyltrimethylammonium
   bromide (CTAB)
4. **Solvent**
   Octadecene

Heat

@ 10 ℃ /min

@ 190 °C

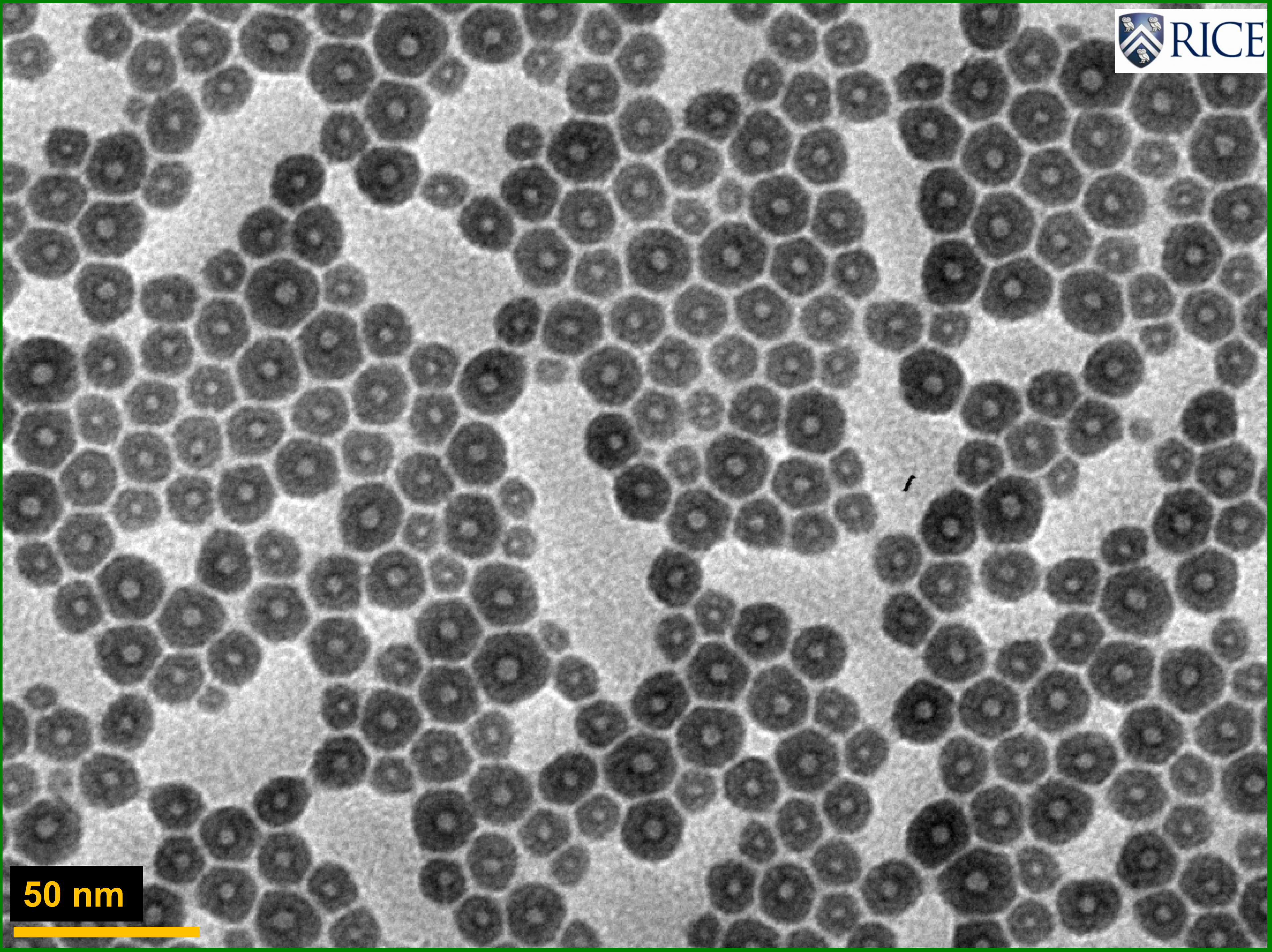
5 min

Reddish brown
cloudy solution

1. Centrifuge
2. Remove solids
3. Ethanol wash
4. Collect cleaned particles
5. Redisperse in chloroform (CF)

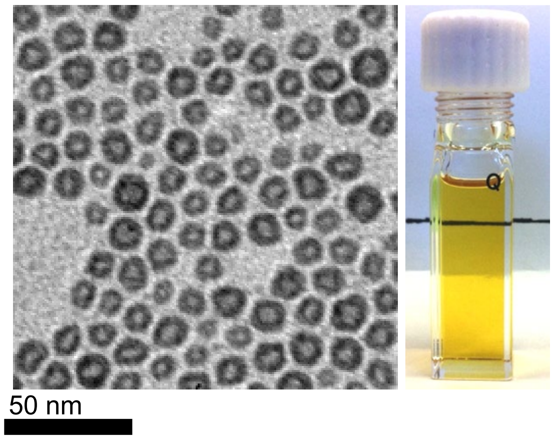
Reddish brown
clear suspension
in CF

Colloidally stable for >24 months

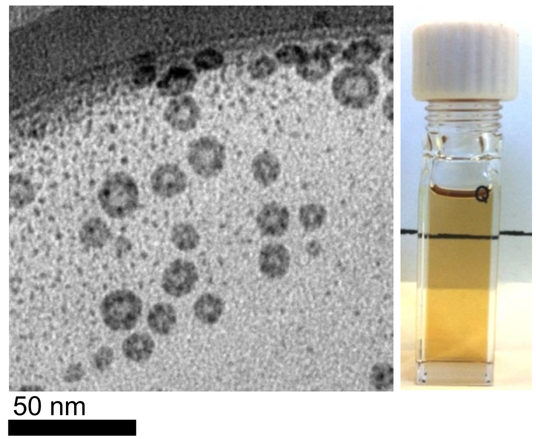

50 nm

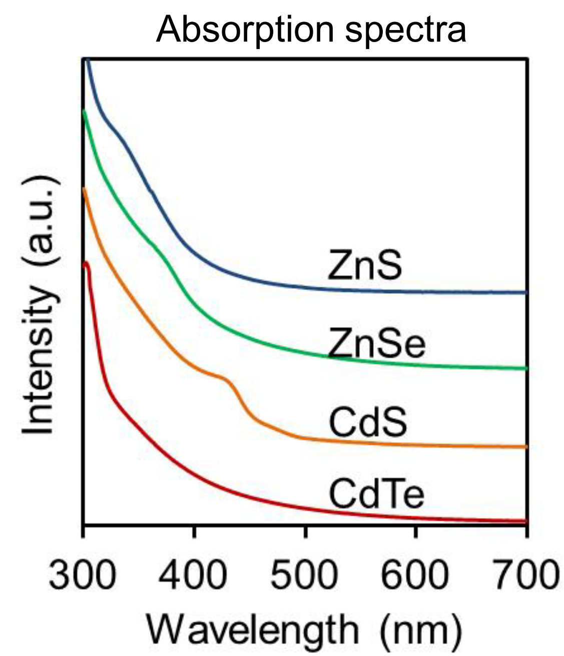
General Synthesis Route for Chalcogenides

CdS

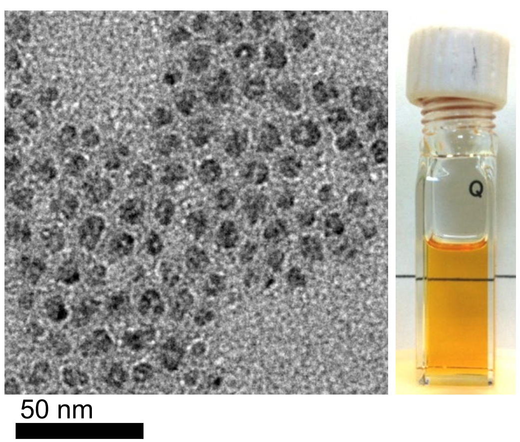


CdTe

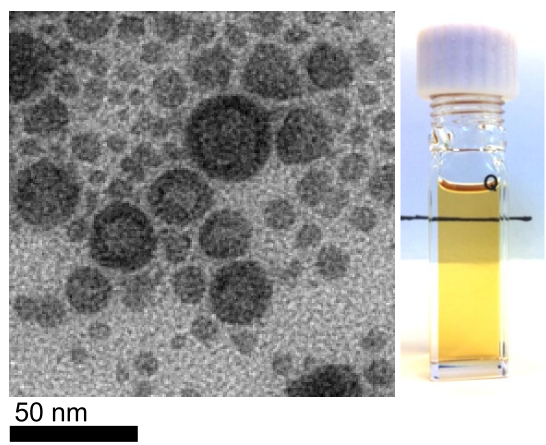




ZnSe

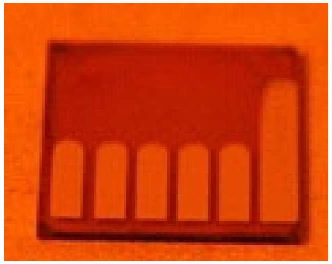


ZnS

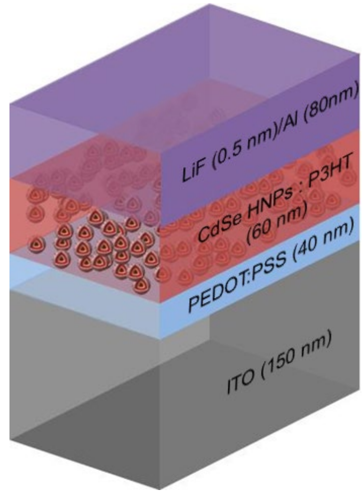


- Synthesis strategy can be applied to other compositions
- Requires optimization

Photovoltaic Performance of CdSe HNPs



Actual hybrid solar cell device



Device schematic

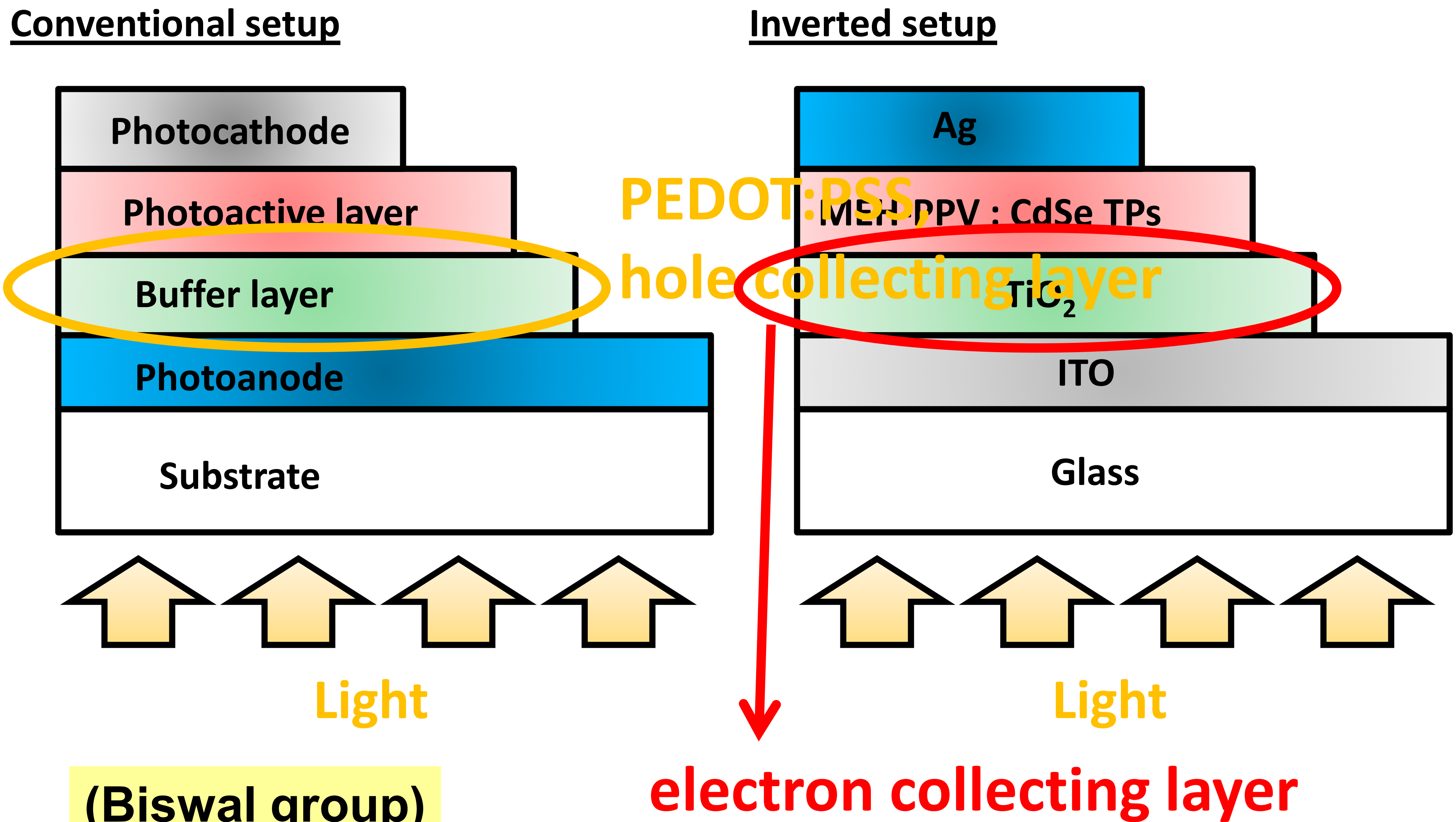
List of abbreviations

$P_{incident}$ – Incident Power
Open circuit voltage – V_{oc}
Short circuit current – J_{sc} or I_{sc}
Fill Factor - FF
Power conversion efficiency – PCE
Series Resistance – R_s

$$PCE = \frac{I_{sc} \times V_{oc} \times FF}{P_{incident}}$$

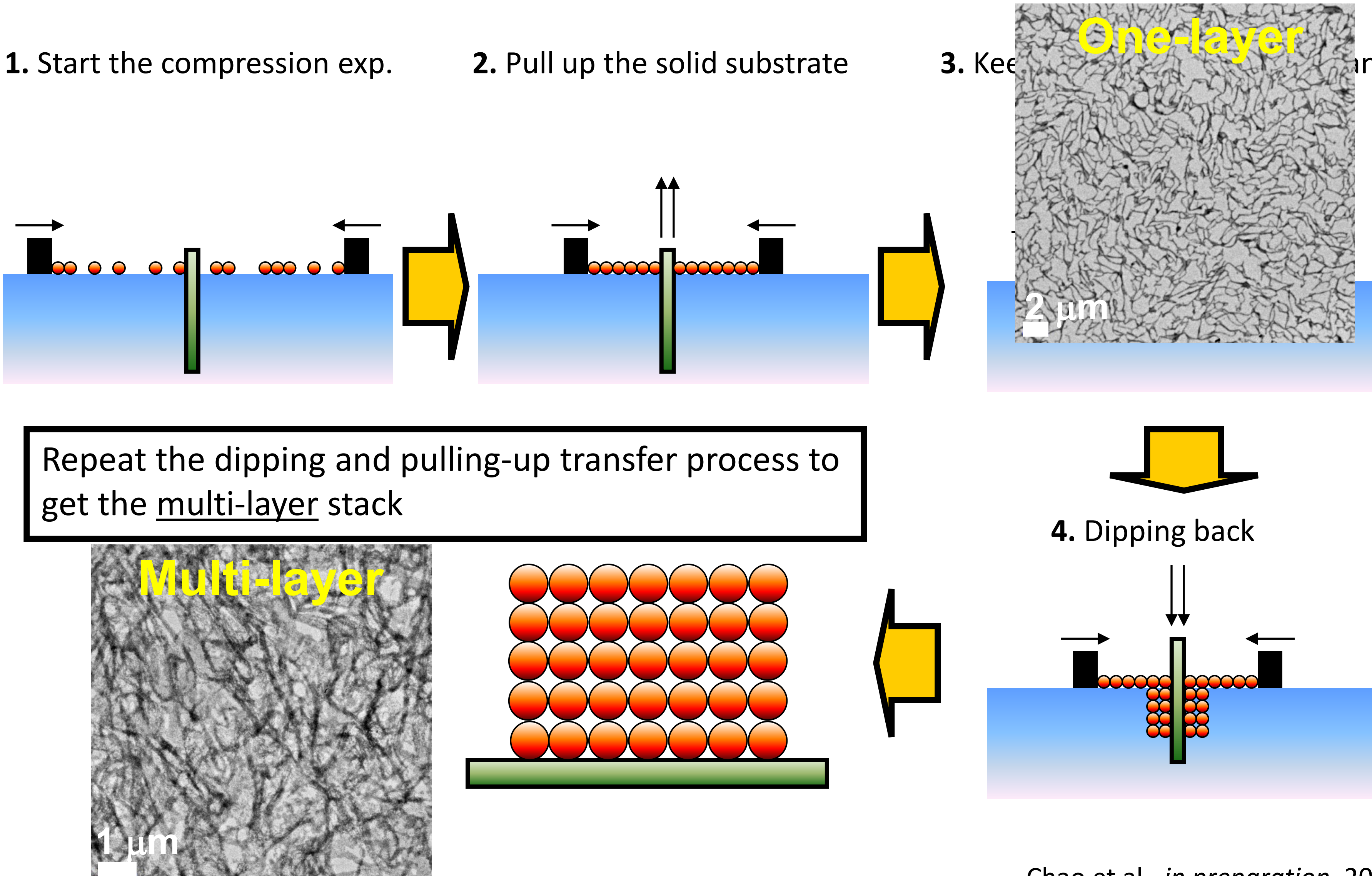
Sample	Photoactive Layer	PCE (%)	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	R_s(Ωcm^2)
Standard	QD(90 wt%):P3HT(10 wt%)	0.16±0.09	0.86±0.18	0.48±0.14	38.1±4.5	27.5±11.5
HNP S1	HNP(90 wt%):P3HT(10 wt%)	0.08±0.02	1.36±0.09	0.18±0.02	31.6±1.0	10.7±3.2
HNP S2	HNP(80 wt%):P3HT(20 wt%)	0.10±0.02	1.34±0.07	0.23±0.03	33.6±1.3	10.9±3.4

Structures of hybrid solar cells



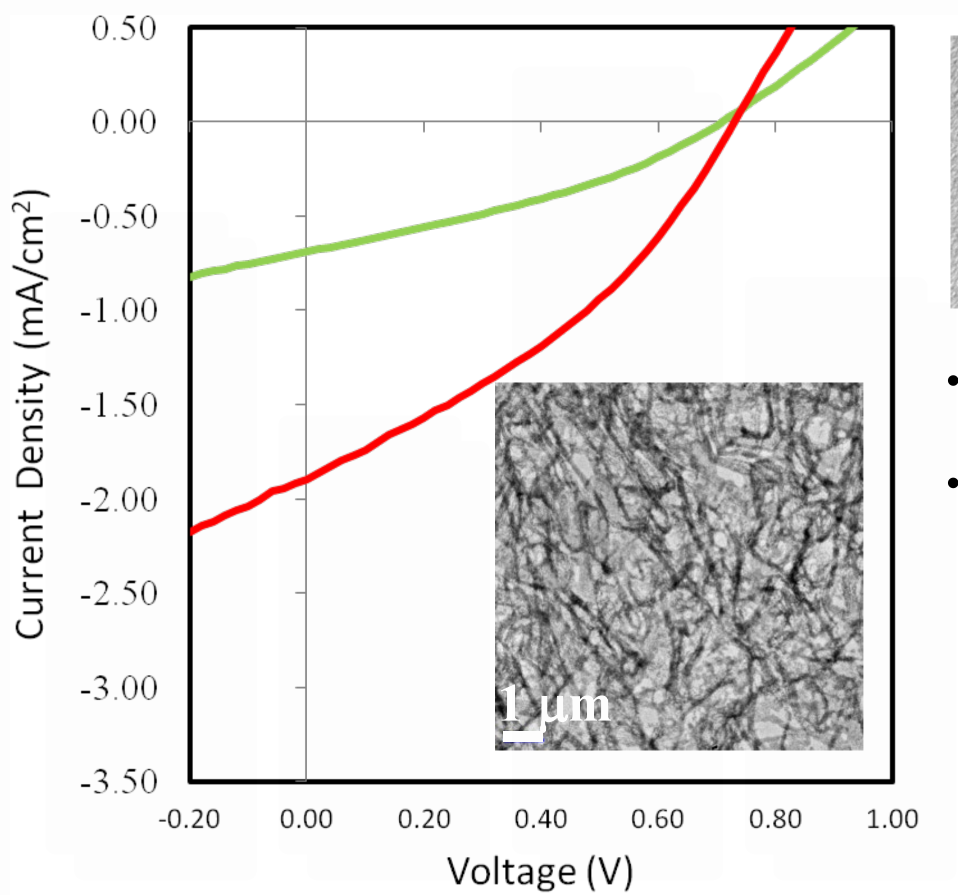
(Biswal group)

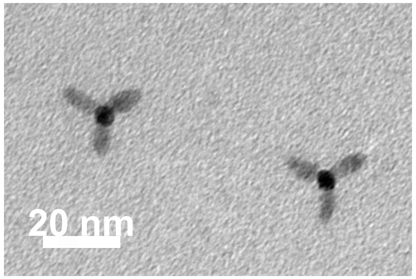
Multilayer deposition by LB technique



Chao et al., *in preparation*, 2014

New fabrication with short TPs





- MEH-PPV: short TPs = **1:3**, [MEH-PPV] = 2.5 mg/mL
- **LB-SC**:
  → LB for 5-layer
  → **Spin-coating MEH-PPV**
  → LB for 5-layer

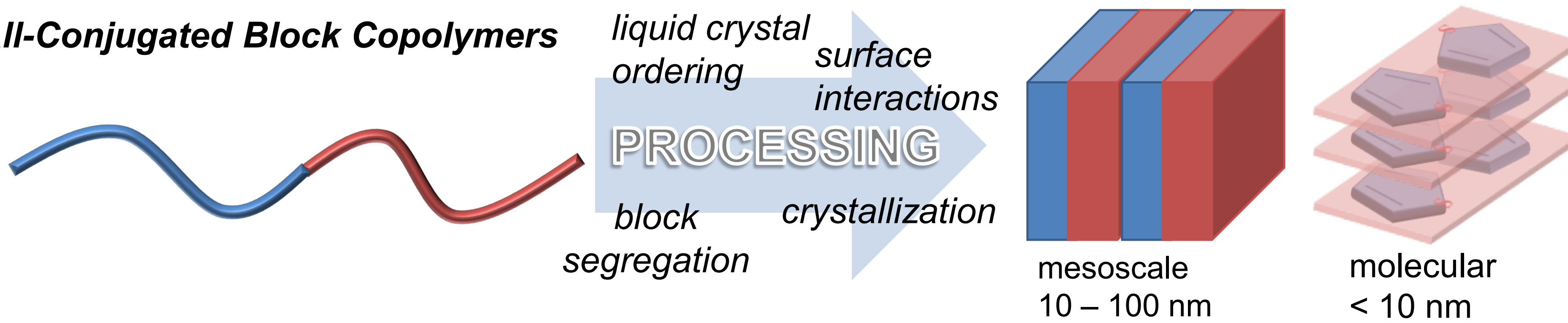
Method	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
SC	**0.70**	**0.690**	**34.1**	**0.165**
LB-SCmix	**0.74**	**1.895**	**34.4**	**0.482**

Chao et al., *in preparation*, 2014

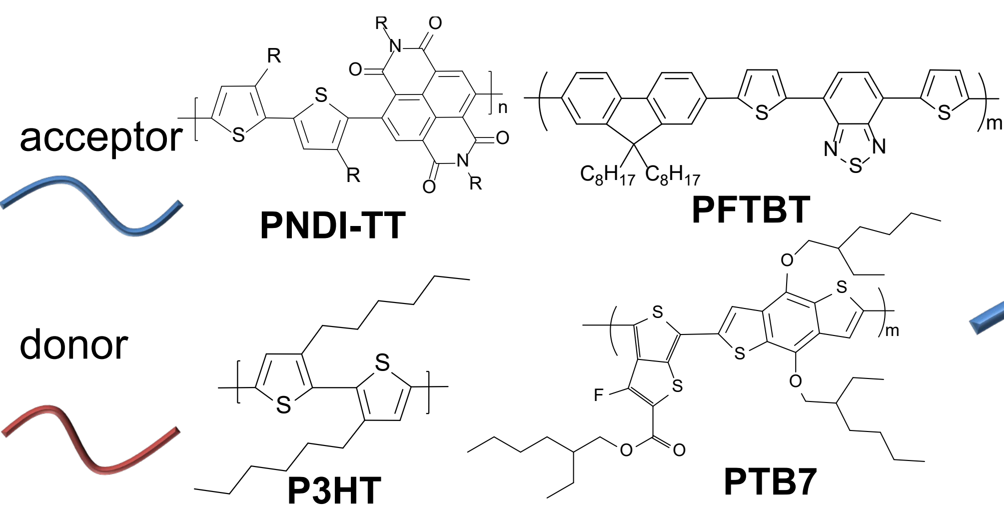
All-conjugated block copolymers provide molecular control over organic semiconductor interfaces

(Verduczo group)

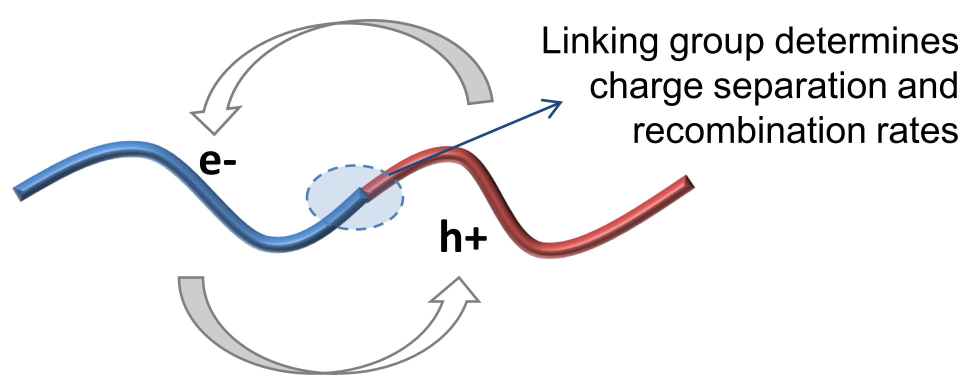
All-Conjugated Block Copolymers



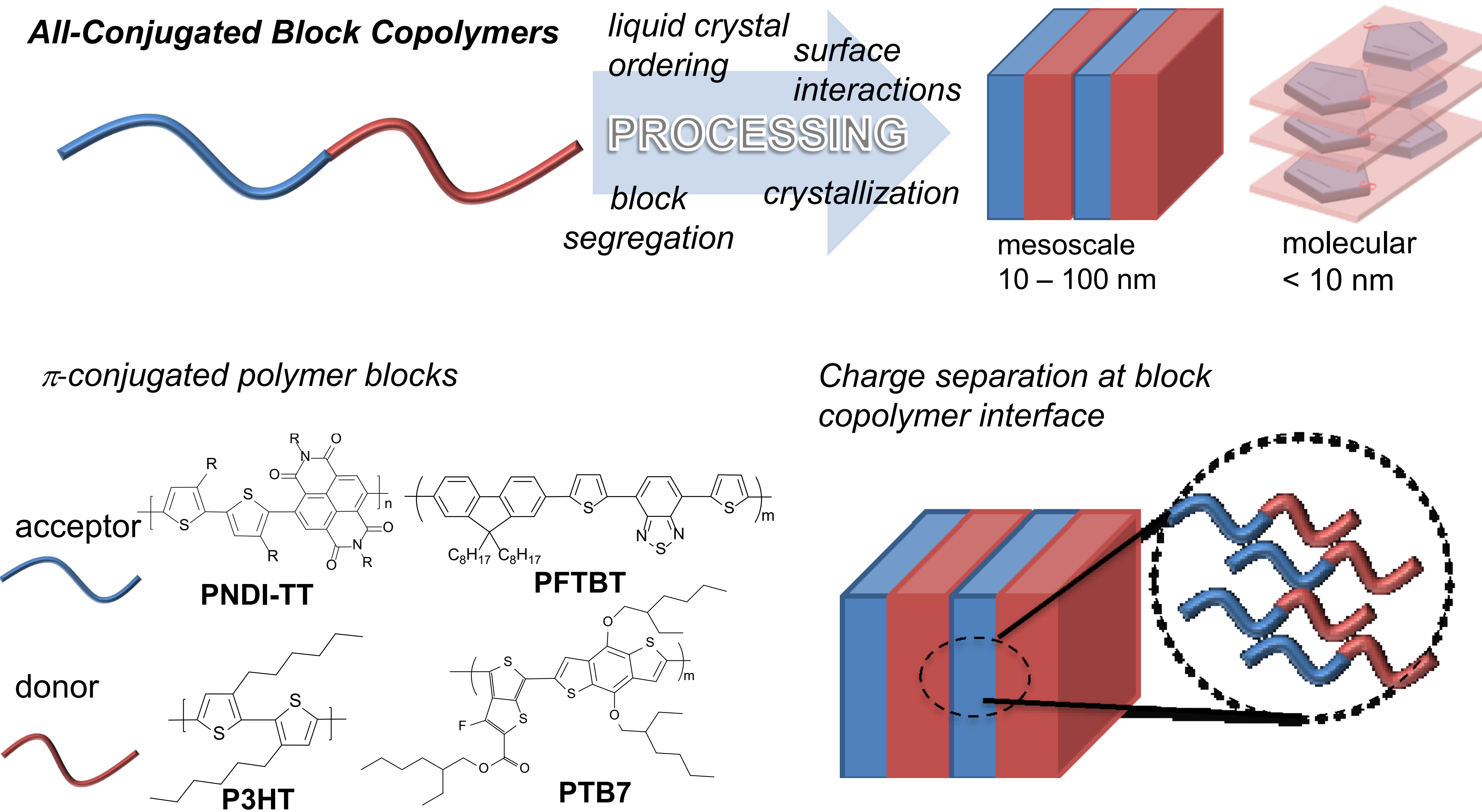
π-conjugated polymer blocks



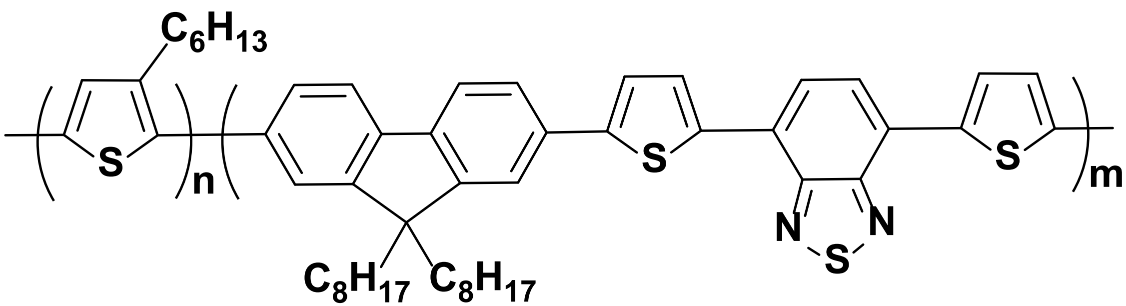
Charge separation at block copolymer interface



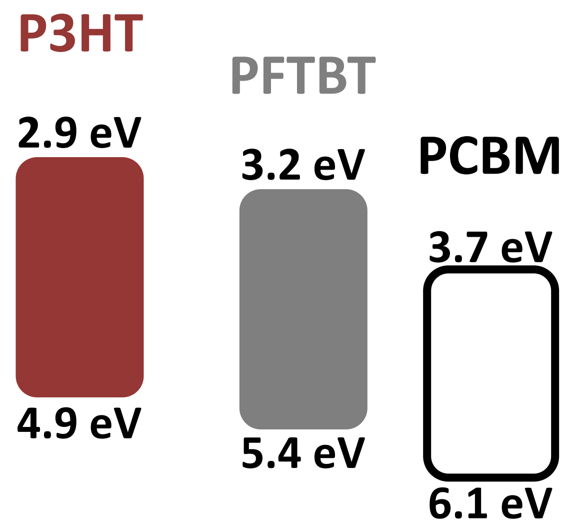
All-conjugated block copolymers provide molecular control over organic semiconductor interfaces



P3HT-*b*-PFTBT block copolymer



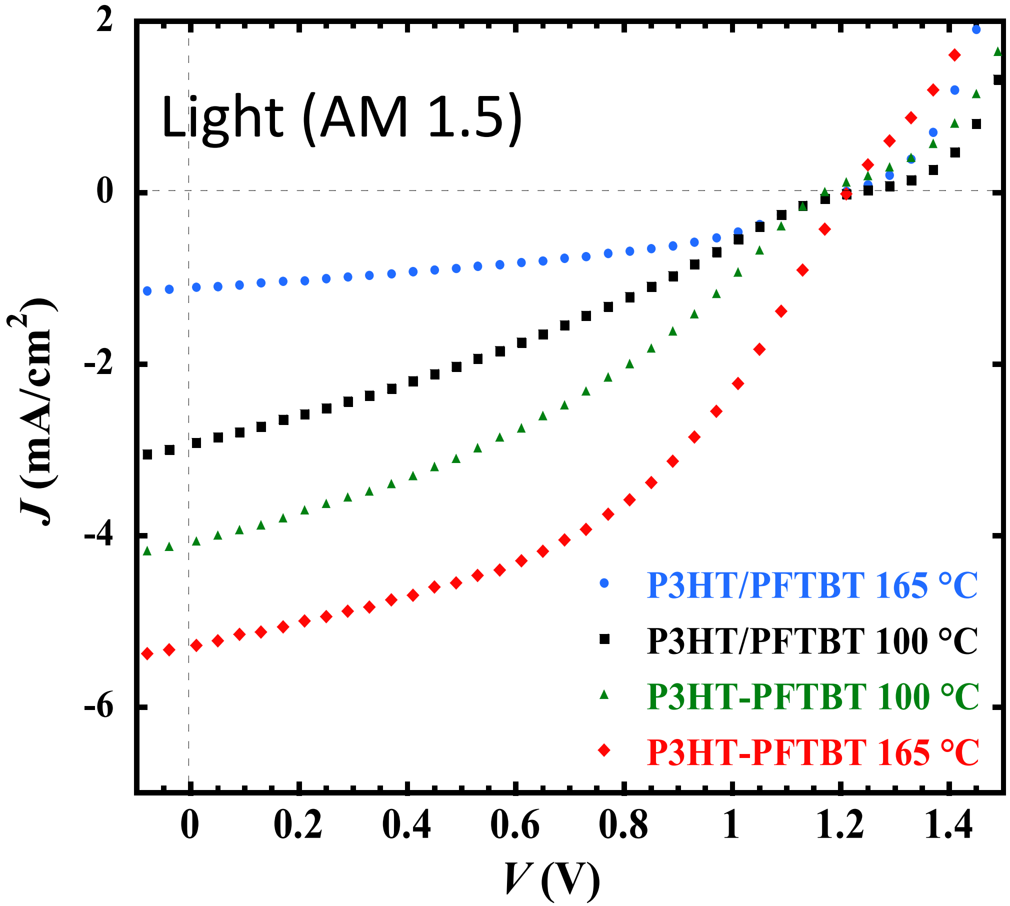
P3HT-*b*-PFTBT



- Majority P3HT (56 wt % P3HT, 44 wt % PFTBT)
- Some homopolymer impurities (17 wt % P3HT homopolymer)
- Conjugation across linker between block copolymer (fluorene linker)
- Large $HOMO_{acceptor}$ $LUMO_{donor}$ offset

Guo, Gomez, Verduzco et al., *Nano Lett.*, **2013**, *13*, 2957.

High-temperature processing leads to Block Copolymer OPVs with near 3% PCE

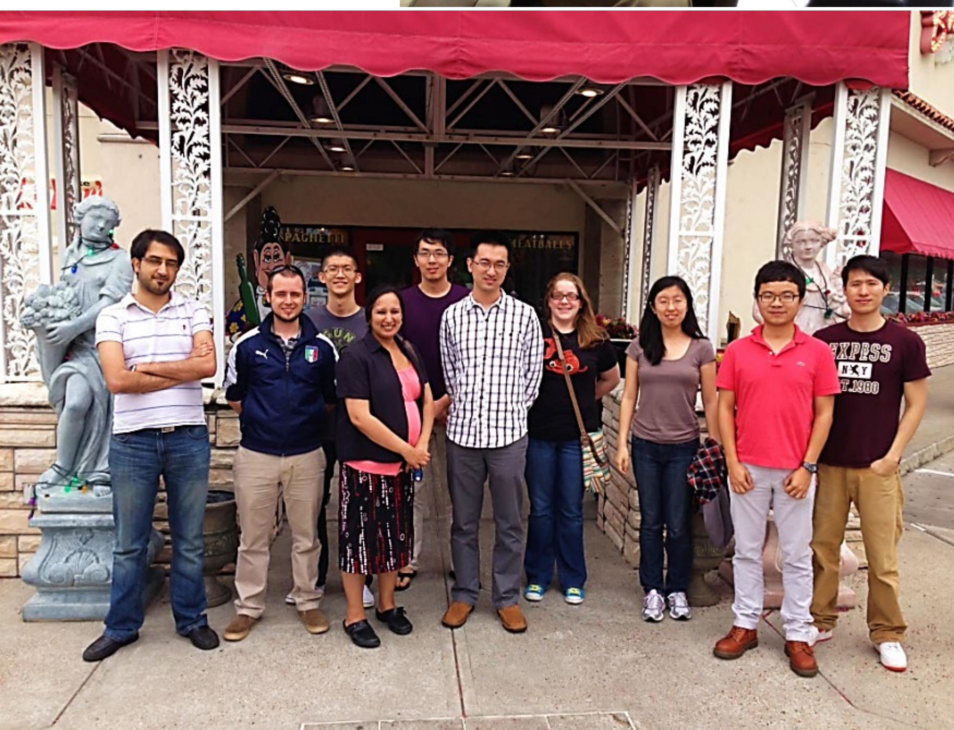


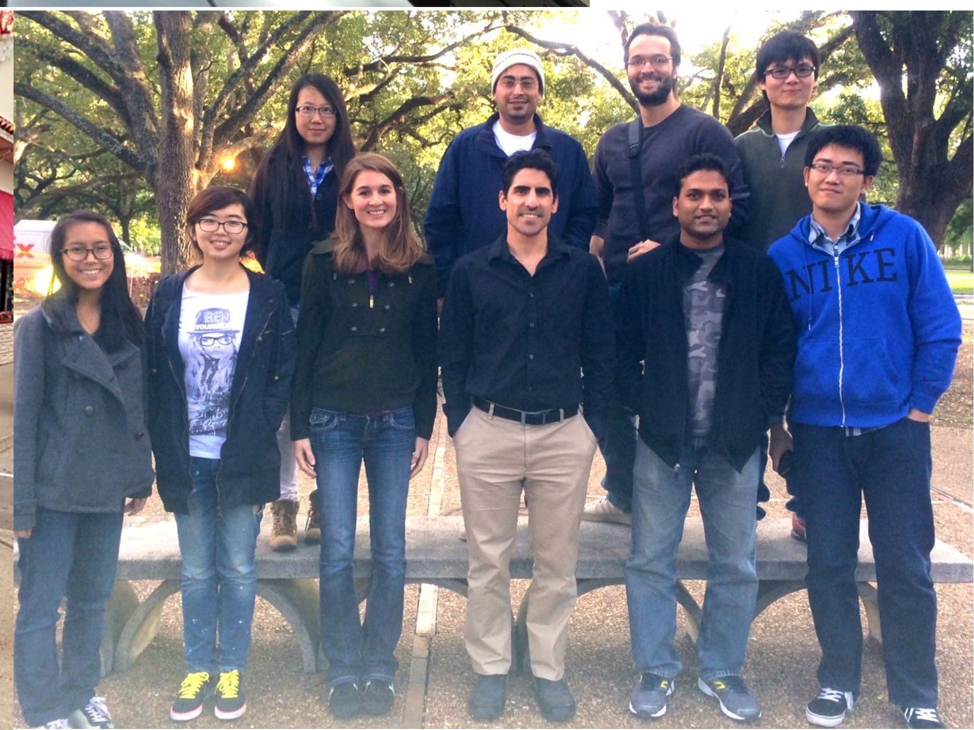
Block Copolymer OPV (annealed at 165 °C):

Efficiency :	3.1 %
Fill Factor:	0.47
V_{OC} :	1.21 V
J_{SC}:	5.28 mA/cm^2

Guo, Gomez, Verduzco et al., *Nano Lett.*, **2013**, *13*, 2957.


VANS
STOP




NIKE