Research and Development Issues for Organic Photovoltaics

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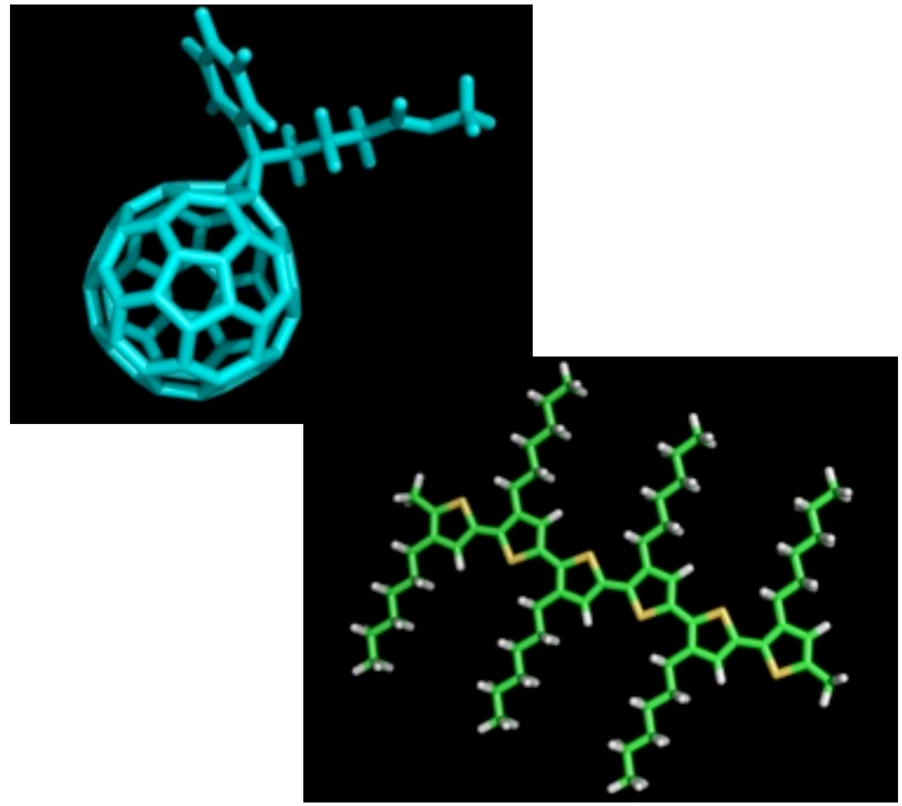
NREL

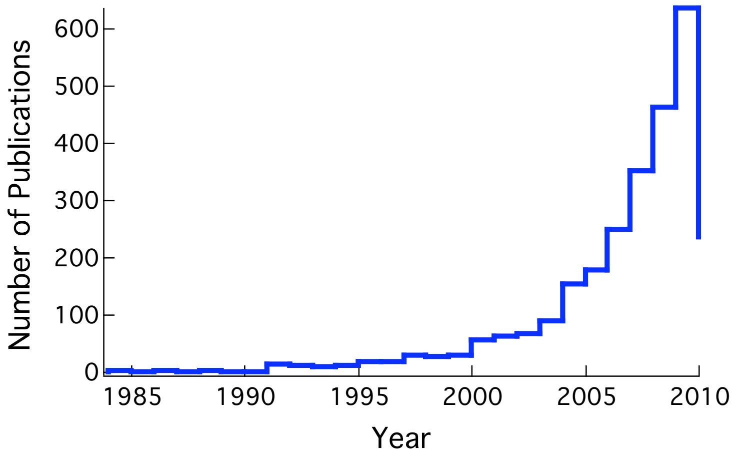


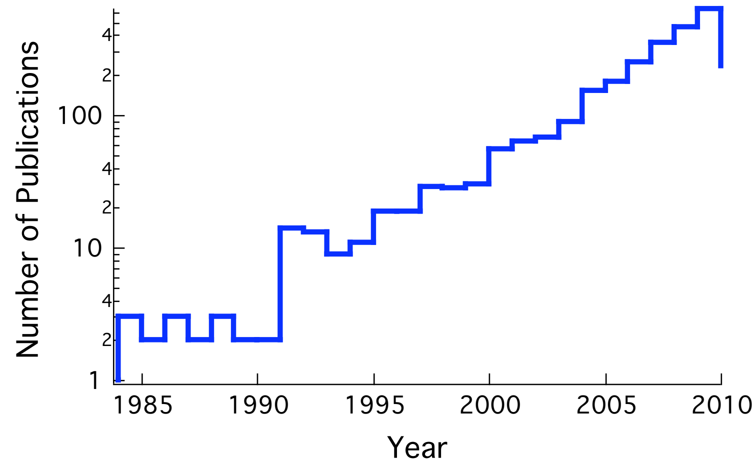
NSF Workshop on Catalyzing Innovation in PV Manufacturing
May 6, 2010

The growth of the OPV field

- The research output in OPV continues to grow:

  ISI search of "organic photovoltaic" returns 2,747 hits





- U.S. government agencies investing in OPV

DOE Energy Frontier Research Centers (EFRC's)
  - 7 of 46 EFRC's are devoted to some aspect of OPV (~$116 M / 5 yr.)

NSF SOLAR program is underway

Upcoming **NIST** workshop covering all aspects of solar energy technologies

Compelling results from industry and national labs

- New efficiency records being set on a regular basis
  - multiple groups reporting >7%.
- Impressive lifetimes being reported
  - thousands to 10’s of thousands of hours
- Initial efforts at large scale production are underway
- Materials (inks) and devices available commercially
- Many new material systems (active layer and electrodes) being investigated

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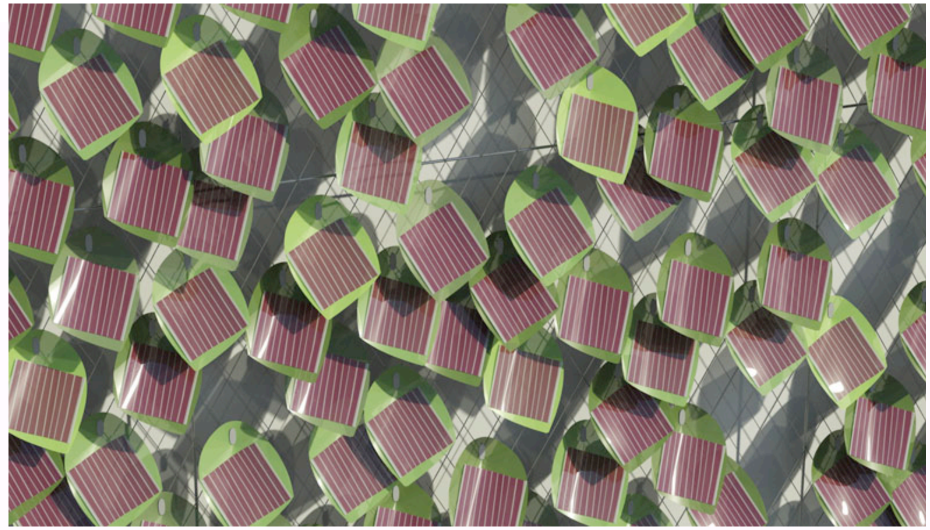
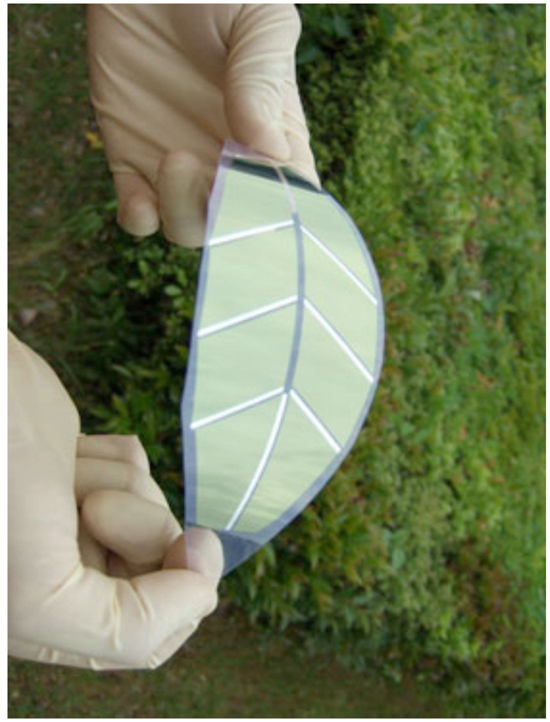
OPV products: prototype and on the market!

OPV products: prototype and on the market!

Solarivy.com



OPV products: prototype and on the market!



Some common materials for solution-processable OPV:

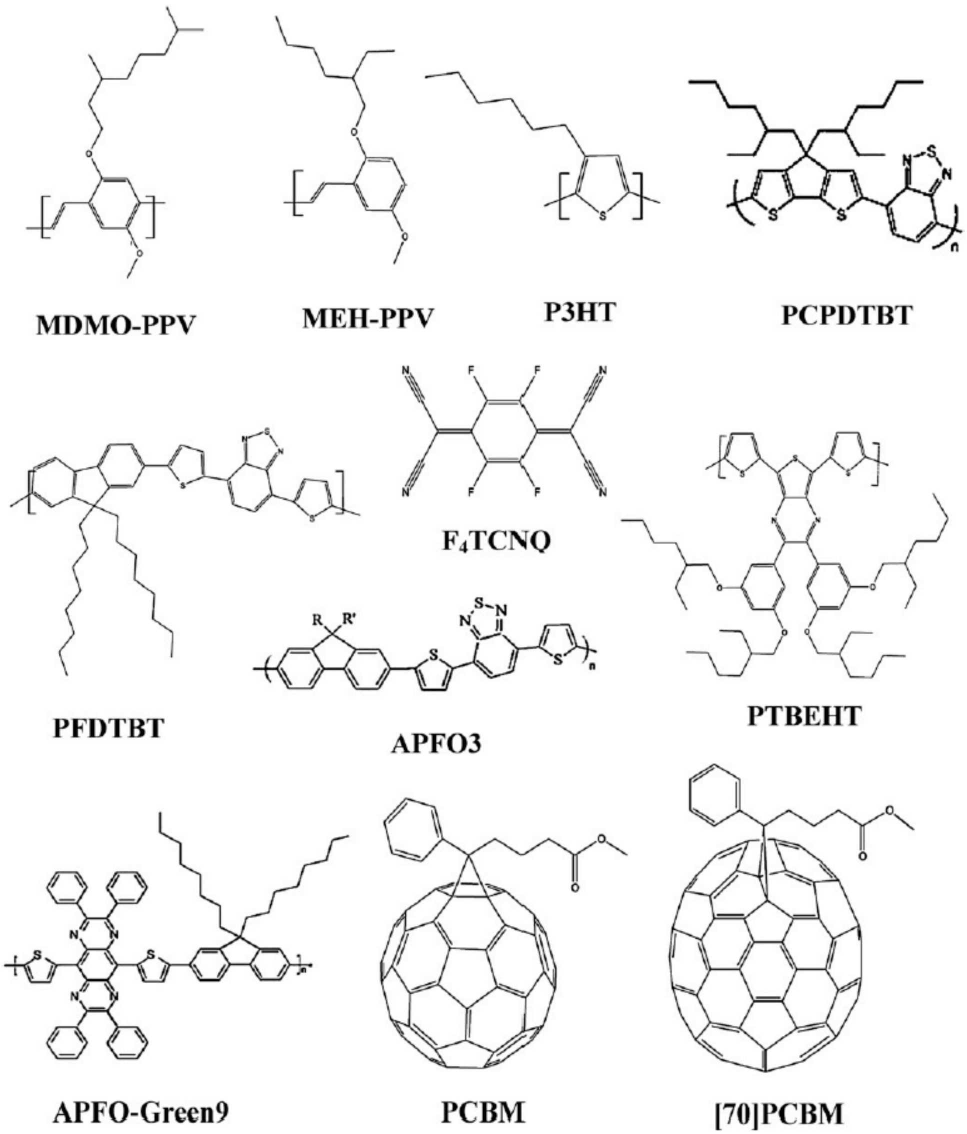


Fig. 20 The chemical structure of all the most used materials in partially or fully solution-processed tandem organic solar cells.

Ameri et al., *Energy & Environmental Science*, **2** 347 (2009).

Some common materials for small-molecule OPV:

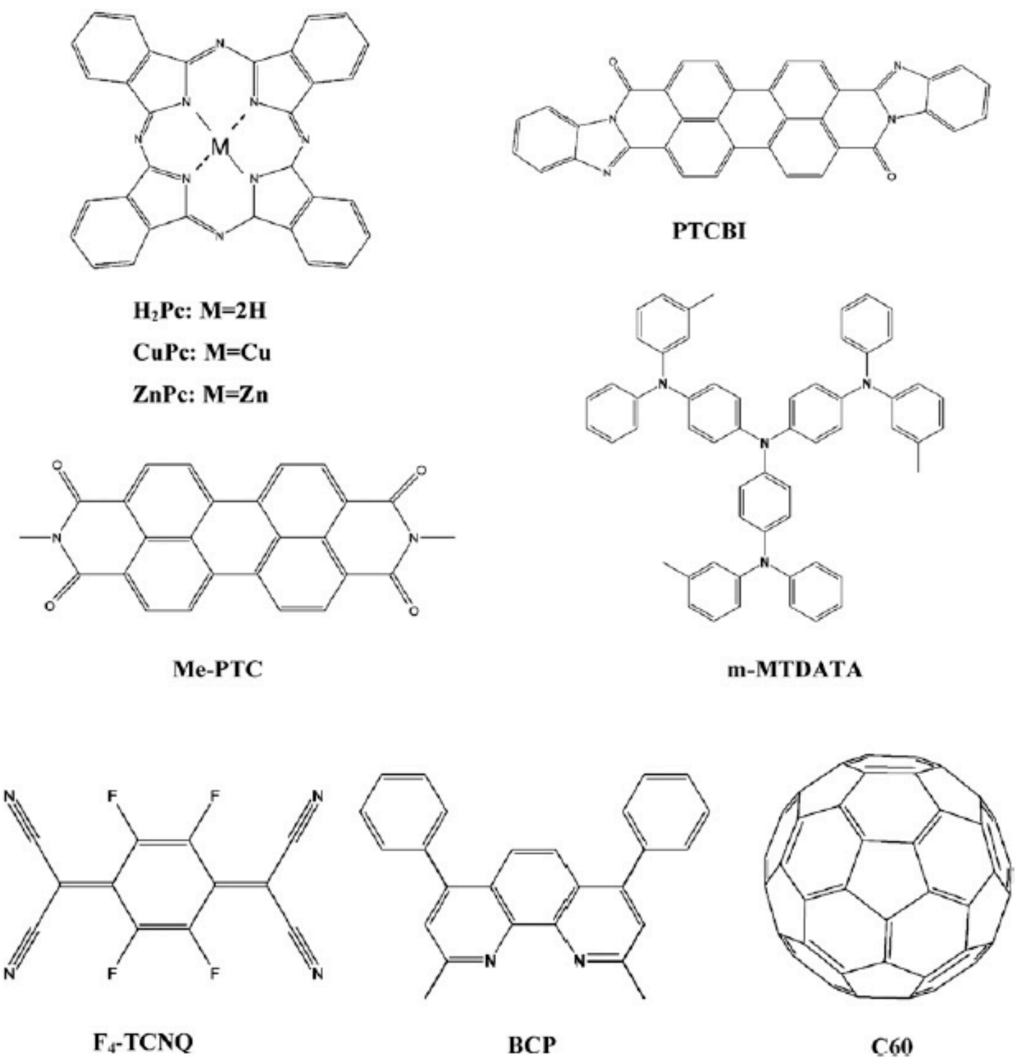


Fig. 14 The chemical structure of the most utilized materials in evaporated small molecule based tandem organic solar cells.

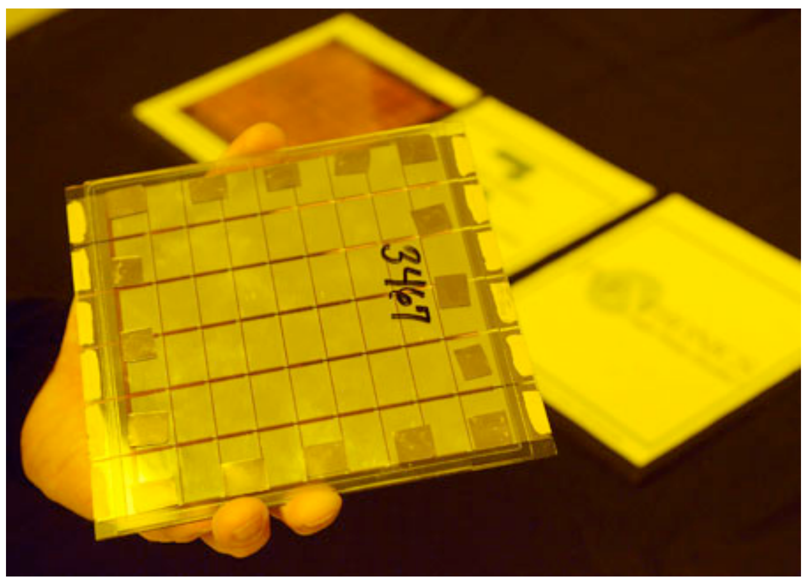
Ameri et al., *Energy & Environmental Science*, **2** 347 (2009).

Improved standardization in measurement

• *The state of the field in accuracy in reported efficiencies is much better than it was a few years ago*

- Issues of spectral mismatch and device active area have been largely resolved

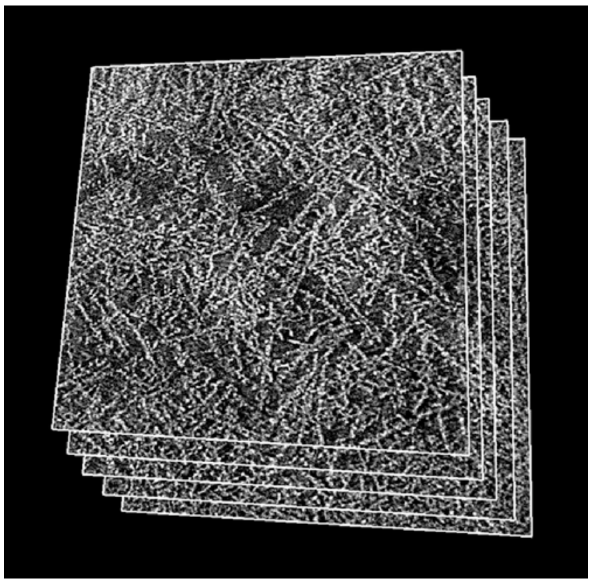
Next steps for field:
- standardize device geometry for certified measurement?
- scale-up high efficiencies to mini-modules and modules

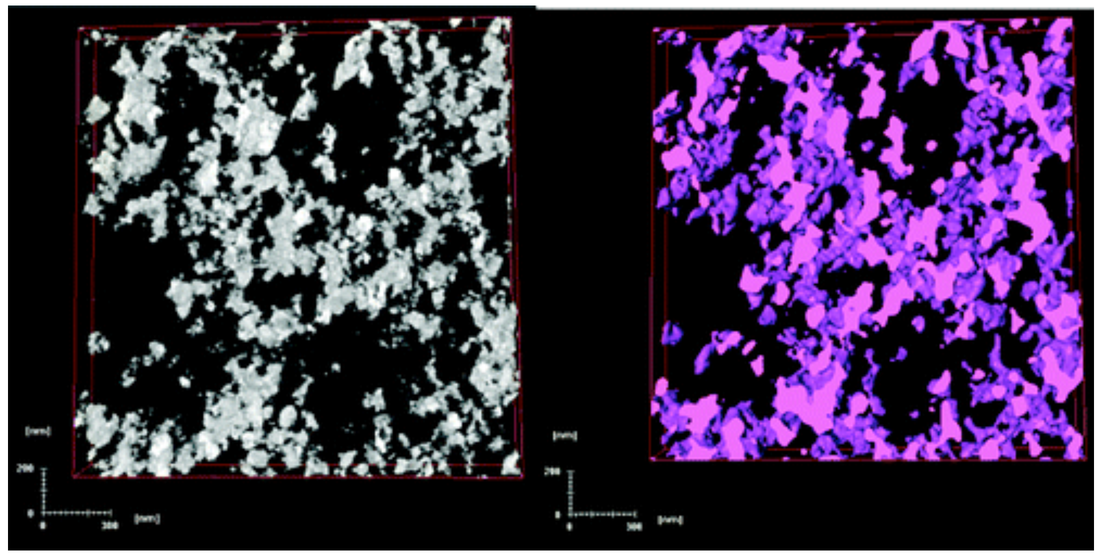


Improved characterization of structural and electronic properties

• *The tools available for resolving the nanoscale donor-acceptor structure have gotten much more powerful*

<u>3-D TEM tomography</u>



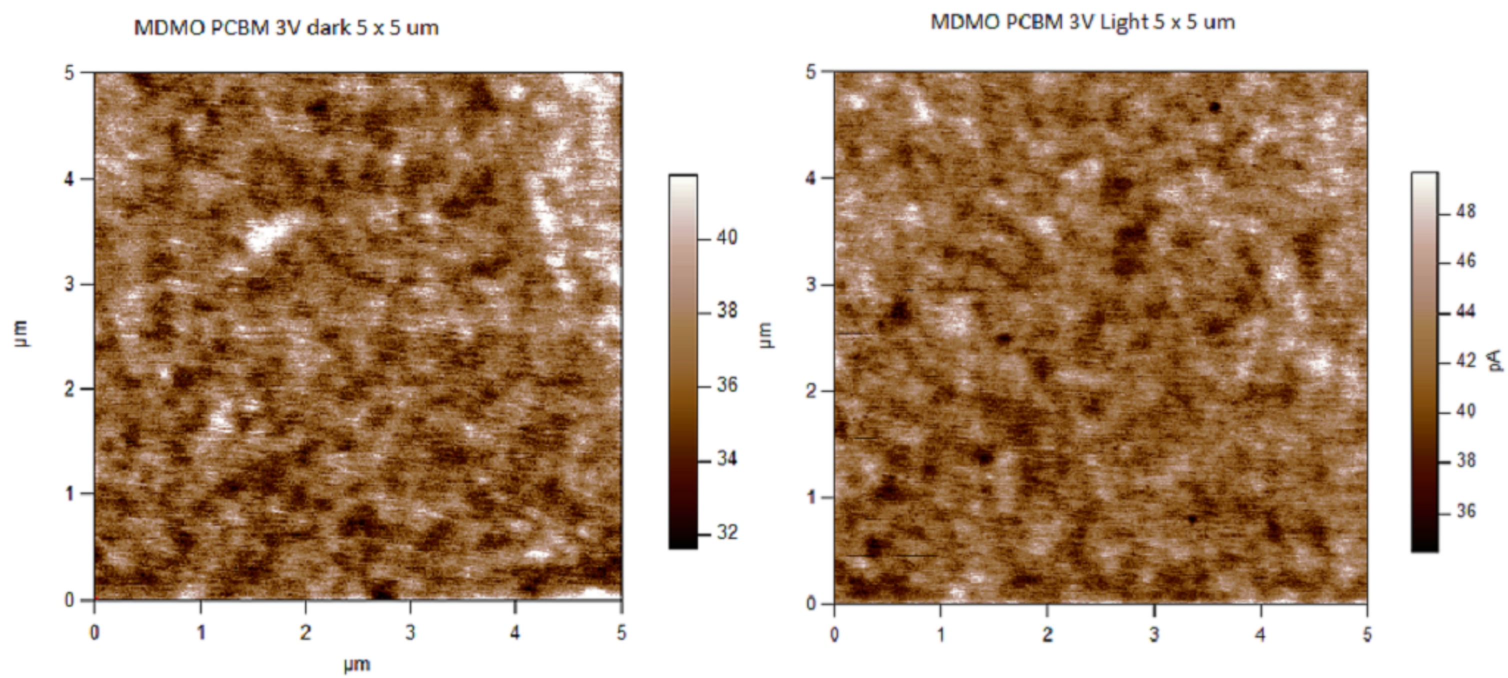


(See for example publications by J. Loos and R.A.J. Janssen groups)

Improved characterization of structural and electronic properties

• *The tools available for resolving the nanoscale donor-acceptor structure have gotten much more powerful*

<u>Scanning Conductive Tip Photocurrent Mapping</u>



(Measurements courtesy Alex Dixon, University of Denver graduate student)

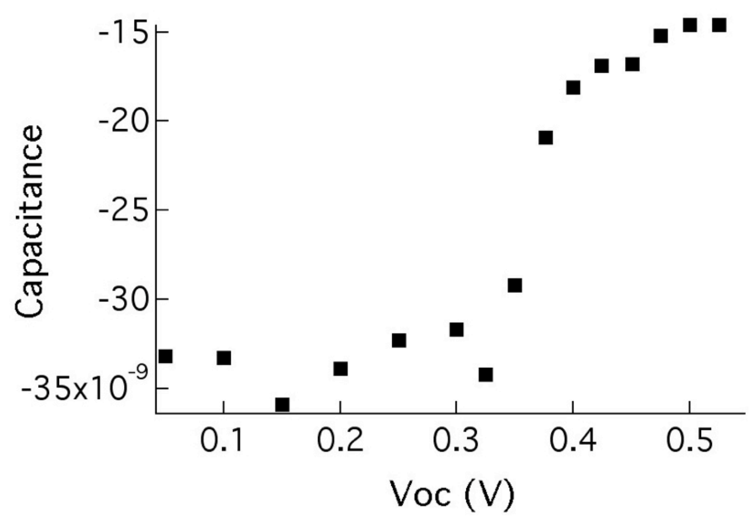
(See for example publications and Asylum Research application note by group of David Ginger)

There is no consensus in the OPV community as to what is the "optimal" morphology!

Improved characterization of structural and electronic properties

- *Electronic characterization techniques have become more refined and powerful*
  - transient photovoltage, photocurrent
  - transient conductivity and microwave conductivity
  - impedance spectroscopy being used to characterize a wide range of phenomenon
    - i) Schottky barriers
    - ii) built-in field
    - iii) intrinsic carrier density
    - iv) carrier mobility
    - v) defect levels
    - vi) density-of-states

Impedance spectroscopy as a direct measure of the Density-of-State (DOS) of a material*



$$C_\mu = d\ q^2 g(E_F)$$

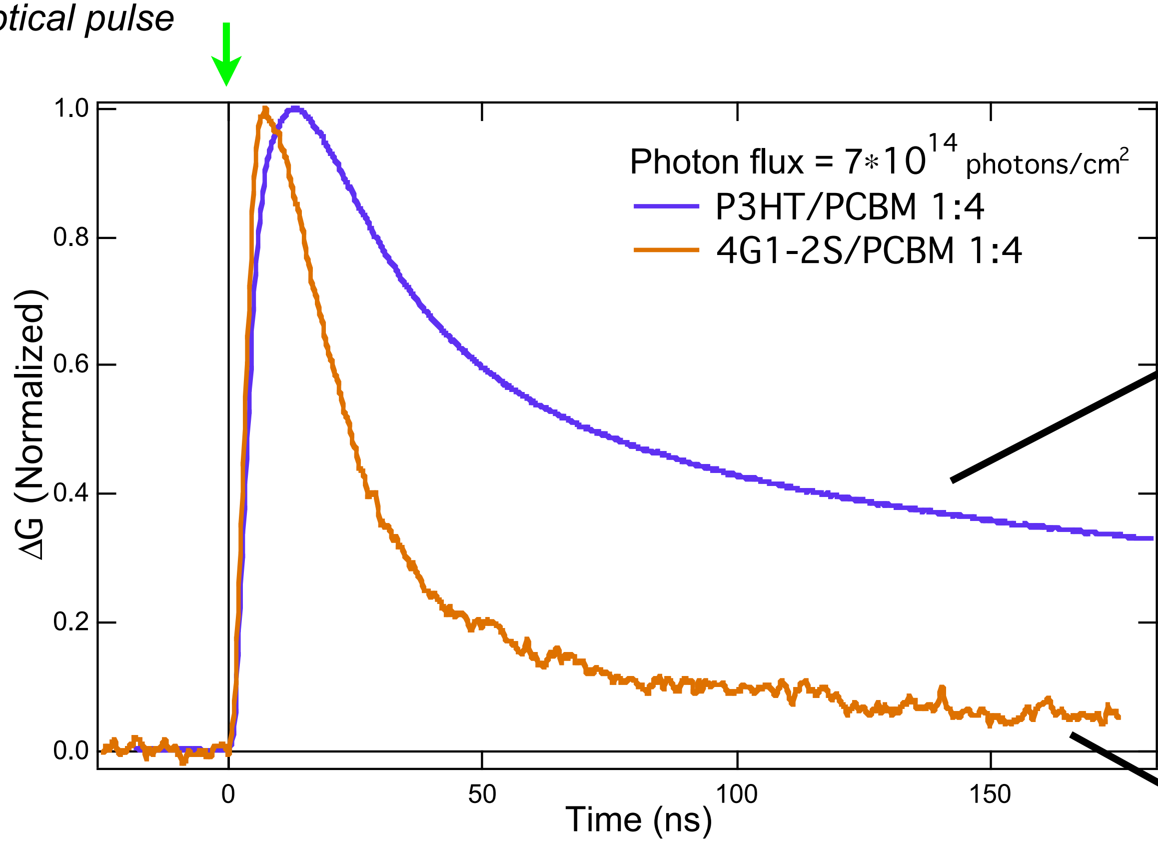
*G. Garcia-Belmonte, P. P. Boix, J. Bisquert, M. Sessolo, H. J. Bolink, *Sol. Energy. Mater. and Sol. Cells* (2009).

Improved characterization of structural and electronic properties

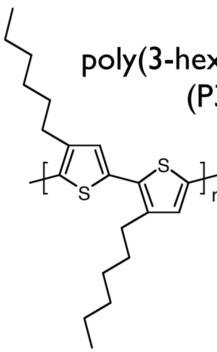
Time Resolved Microwave Conductivity (TRMC) measurements

Comparing carrier lifetimes in different donor-acceptor blends

optical pulse

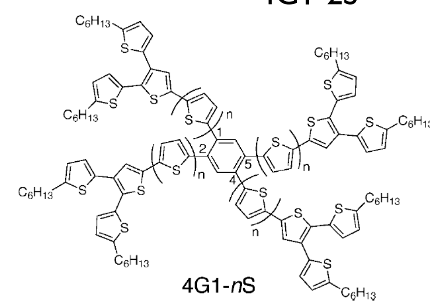


poly(3-hexylthiophene) (P3HT)



Device efficiency ~4%

4G1-2S



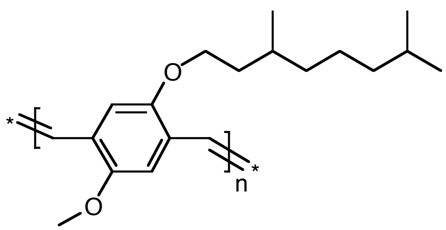
Device efficiency ~1.5%

TRMC measurements courtesy William Rance and Dr. Nikos Kopidakis

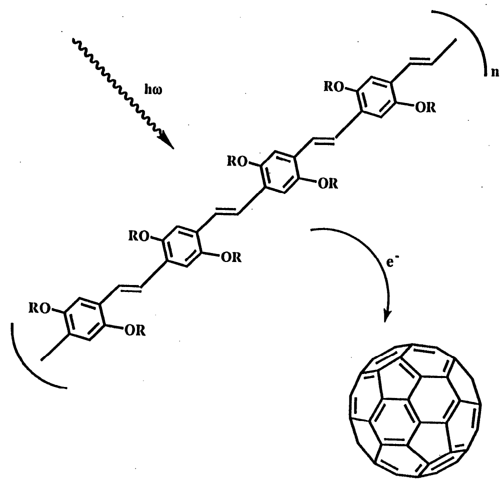
Exciton quenching by C_{60}

Ultrafast photoinduced electron transfer between a conjugated polymer and a fullerene was discovered in 1992*.

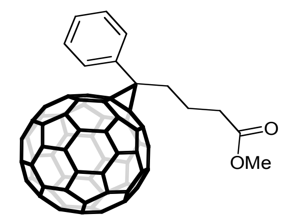
Donor



OC_1C_{10}-PPV
3,7 - dimethyloctyloxy methyloxy PPV



Acceptor



PCBM
1-(3-methoxycarbonyl) propyl-1-phenyl $[6,6]C_{61}$

Forward electron transfer rate: 45 fs†

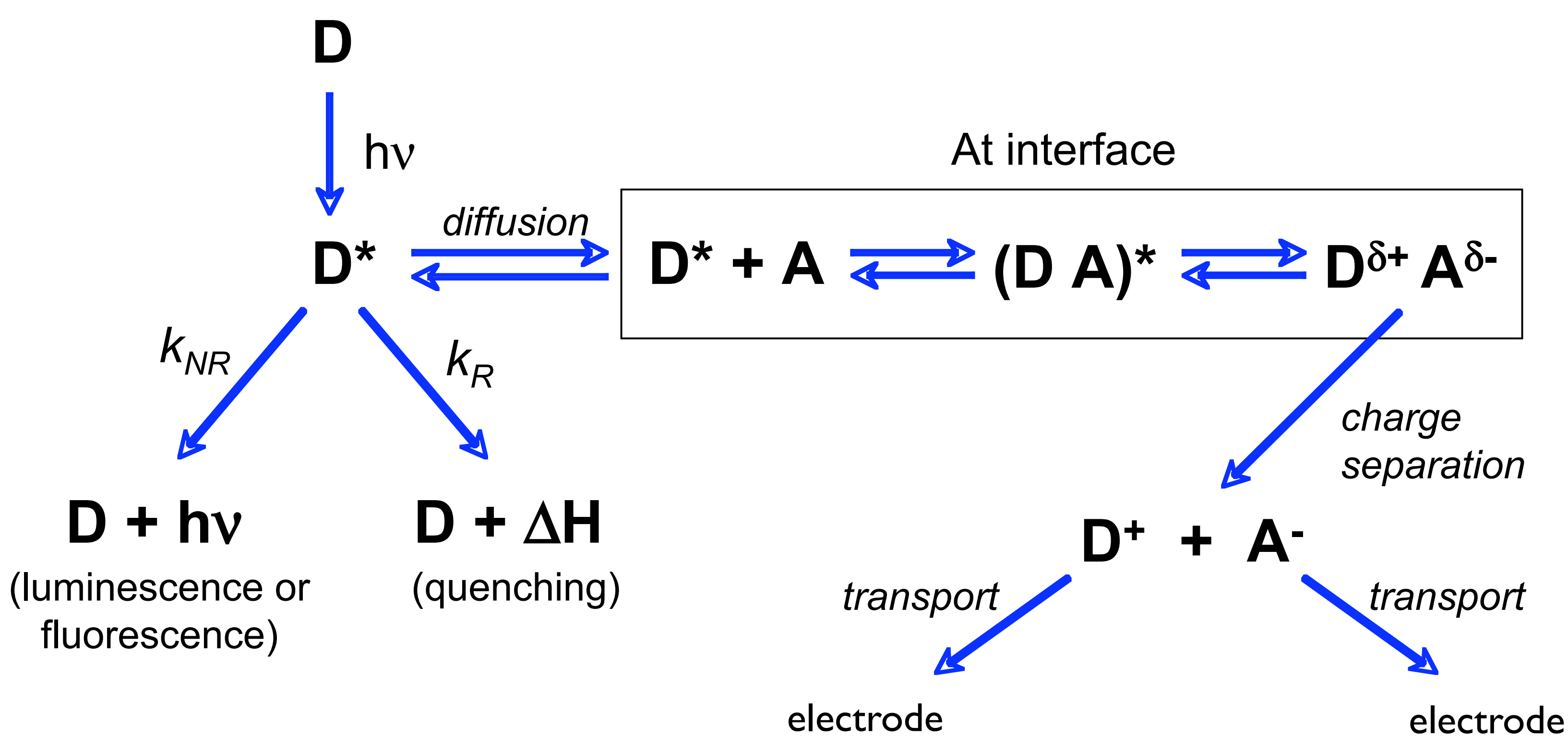
Backward electron transfer rate: ~1 μs

*N. S. Sariciftci, L. Smilowitz, A. J. Heeger, and F. Wudl, *Science* **258**, 1474 (1992).
†C. J. Brabec, G. Zerza *et al*., *Chem. Phys. Lett.* **340**, 232 (2001).

Kinetic pathways for OPV devices

• Many kinetic pathways are available to an exciton.

• For a working solar cell, we need charge transfer at D-A interface to yield free carriers.

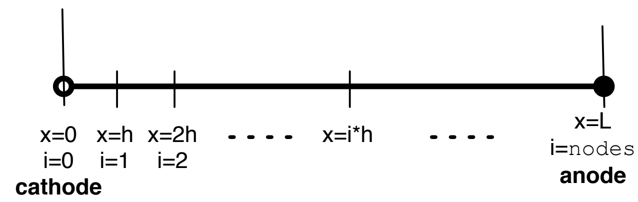


One dimensional steady-state drift-diffusion equations:

Poisson Equation:

$$\frac{\partial^2}{\partial x^2}\psi(x) = \frac{e}{\varepsilon}(n(x) - p(x) - C(x))$$

C = net positive fixed charge



Continuity Equations:

$$\frac{\partial}{\partial x}J_n(x) = eU(x)$$

$$\frac{\partial}{\partial x}J_p(x) = -eU(x)$$

$$J_n = enE + D_n \frac{\partial}{\partial x} n$$

$$D_n = \mu_n k_B T / e$$

$$J_p = epE - D_p \frac{\partial}{\partial x} p$$

$$D_p = \mu_p k_B T / e$$

$$E = -\frac{\partial}{\partial x}\psi$$

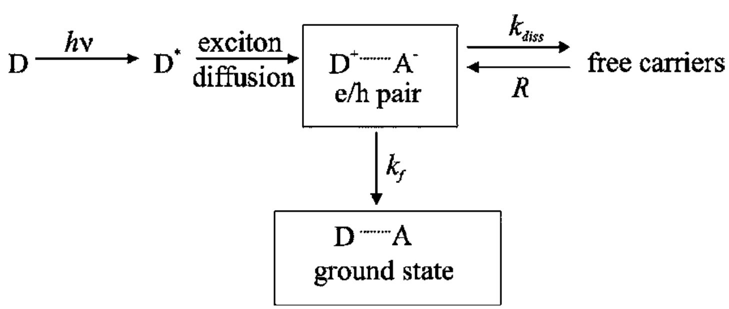
U = net generation rate

- Simple model to start with
  - 1-dimensional treatment
  - BHJ + ideal (Ohmic) contacts, no other layers (e.g. PEDOT:PSS)
- Bulk heterojunction transport parameterized by $\mu_{n,p}$
- Generally following Koster, et al., Phys. Rev. B 72 085205 (2005)

Software (Python) implementation performed by Peter Graf, NREL Scientific Computing Center

Development of an open-source modeling platform for OPV devices

Exciton dynamics are captured in the model



$$U = PG - (1 - P)R$$

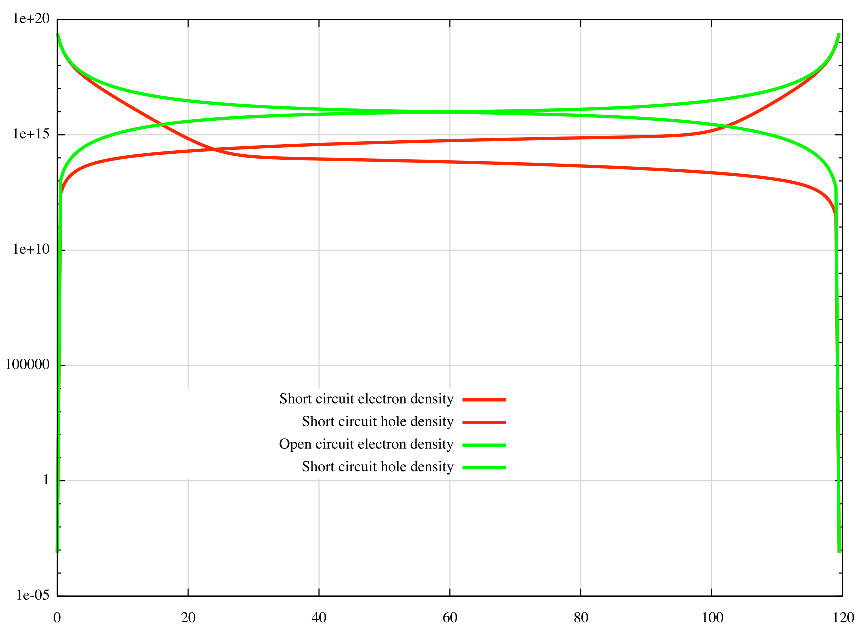
$$R = \gamma(np - n_i^2)$$

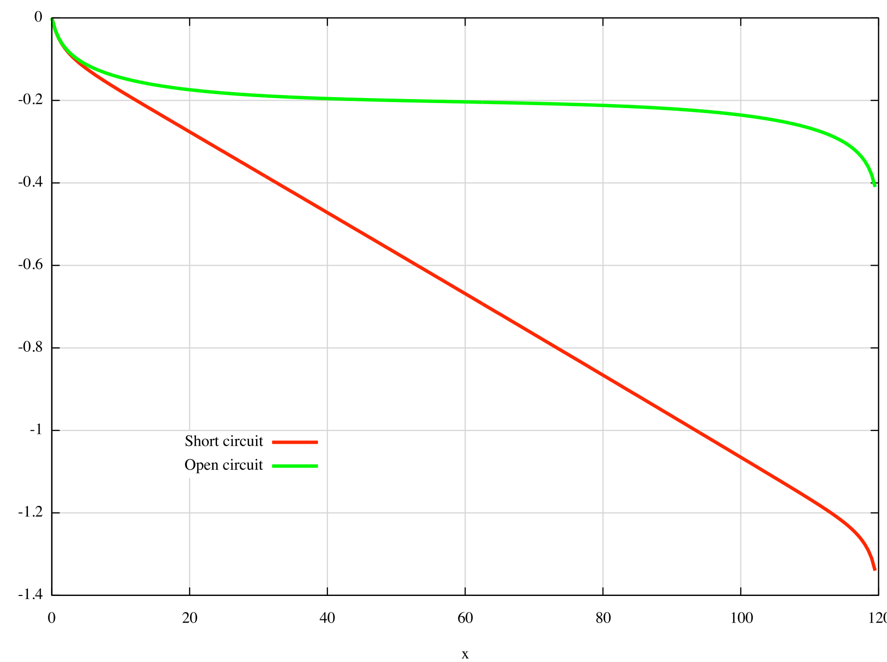
$$P = \frac{k_d}{k_d + k_f}$$

$$k_d = k_d(x, T, E, E_b)$$

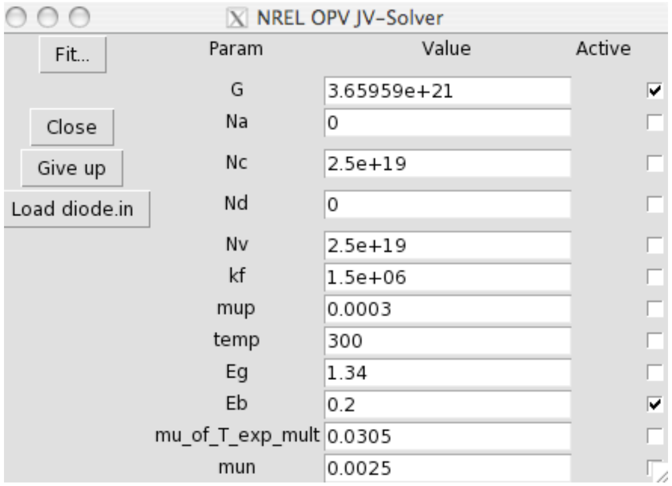
$$k_f = \text{parameter}$$

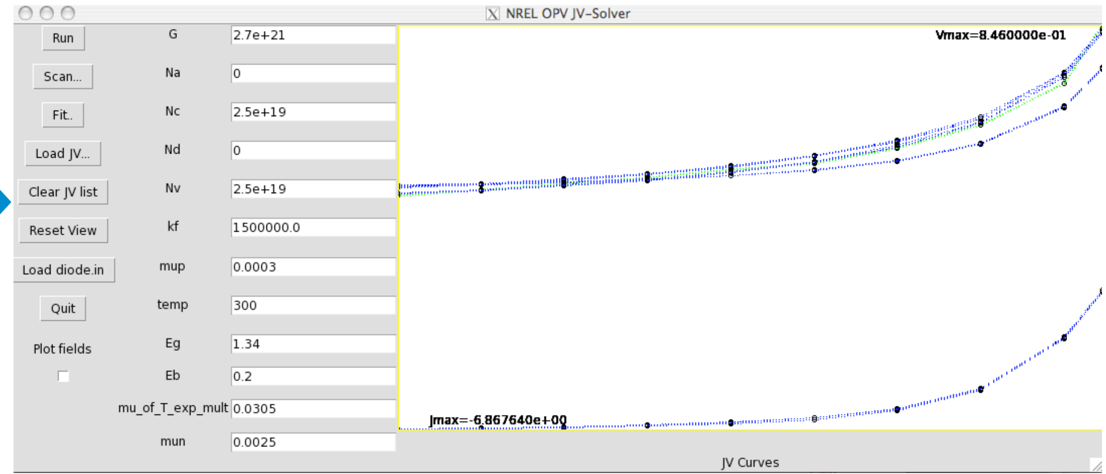
Device parameters such as electric potential and carrier density can be visualized

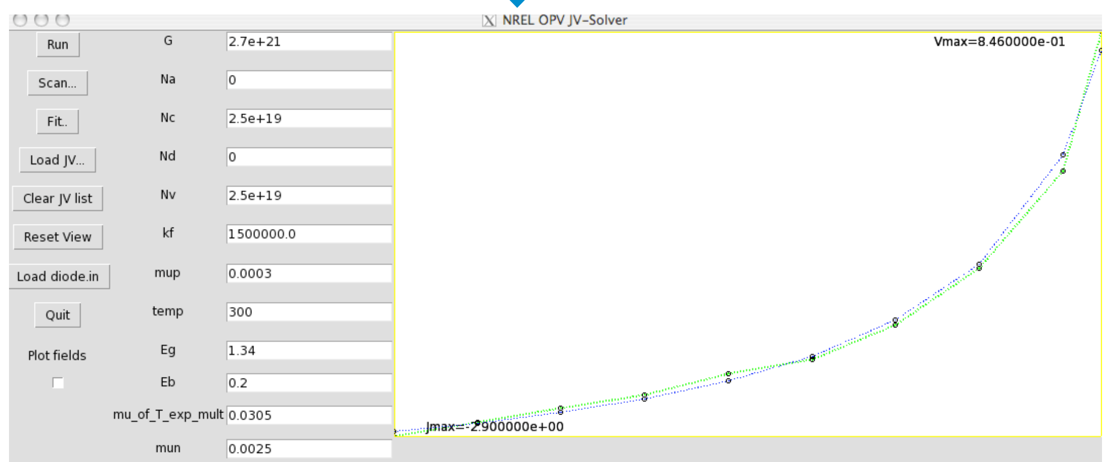




Development of an open-source modeling platform for OPV devices







- Curve fitting to yield extraction of parameters

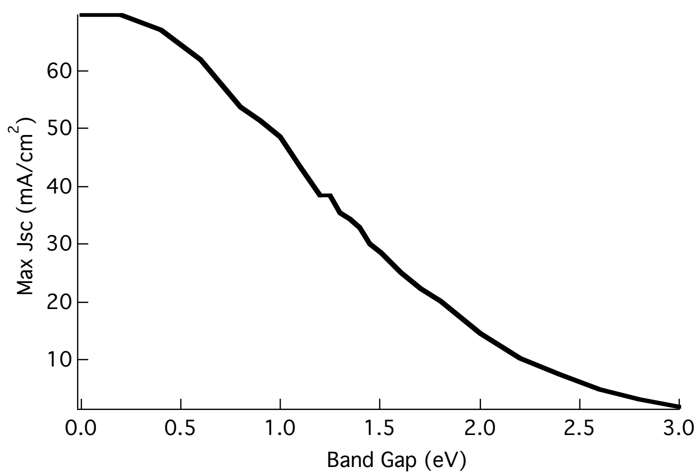
$G = 1.66e+21$
$E_b = 2.82e-01$

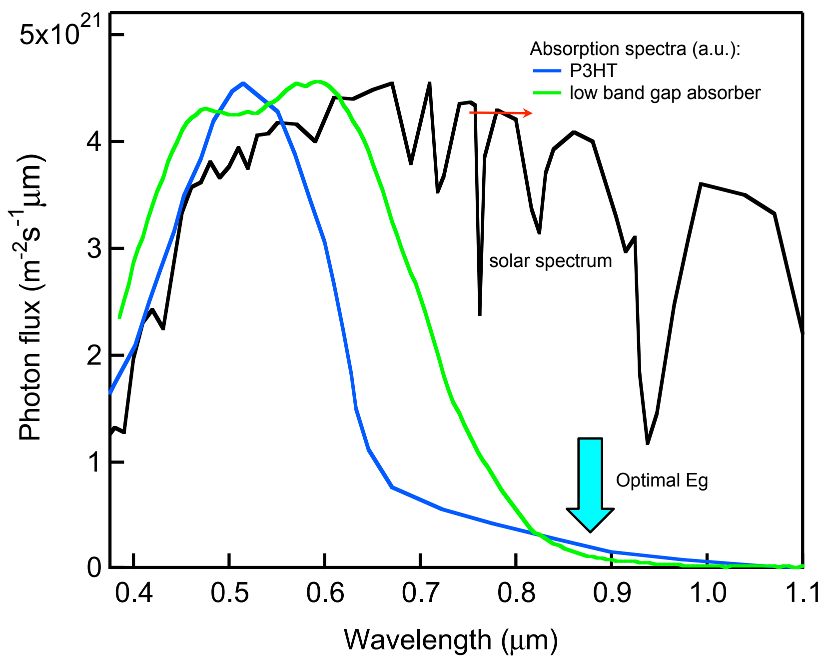
The model will be made available (hosted at NREL) as an open-source, extensible platform for the OPV community

Reaching the near term efficiency target

➡ Low band gap absorbers to increase J_{SC}

Calculated maximum J_{SC} vs. Eg:





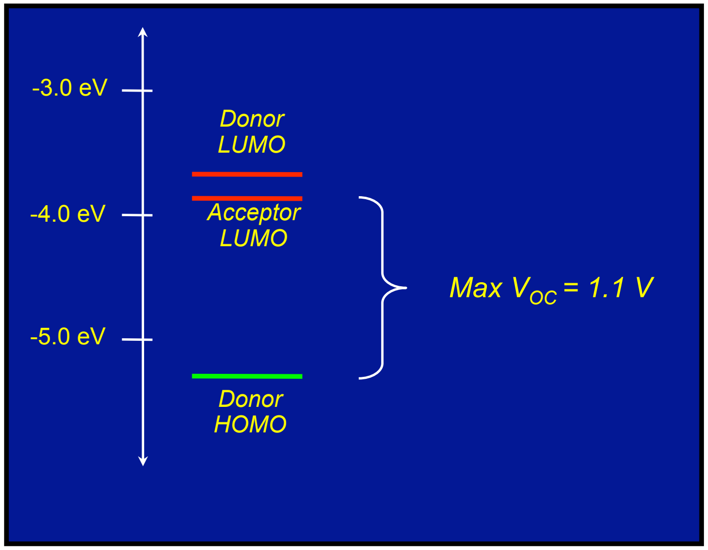
Assume absorber Eg = 1.4 eV (890 nm) ➡ Max J_{SC} = 32.9 mA/cm^2

Assume real J_{SC} = 60% x 33 mA/cm^2 = 20 mA/cm^2

Reaching the near term efficiency target

- Improve band alignment to increase V_{OC}

Idealized band diagram:



Assume band offset of 0.3 eV

C.J.Brabec et al. *Adv. Funct. Mater.* **12**, 709 (2002).

and loss of 0.3 V due to recombination.

M.C. Scharber et al. *Adv. Mater.* **18**, 789 (2006).

V_{OC} = 0.80 V

- Reduce series resistance (R_S) in device to improve *FF*

FF = 0.70

Combining above idealized J_{SC}, V_{OC}, and *FF* to yield an example efficiency:

20 mA/cm^2 × 0.80V × 0.70 / 100 mW/cm^2 → *11.2% efficiency*

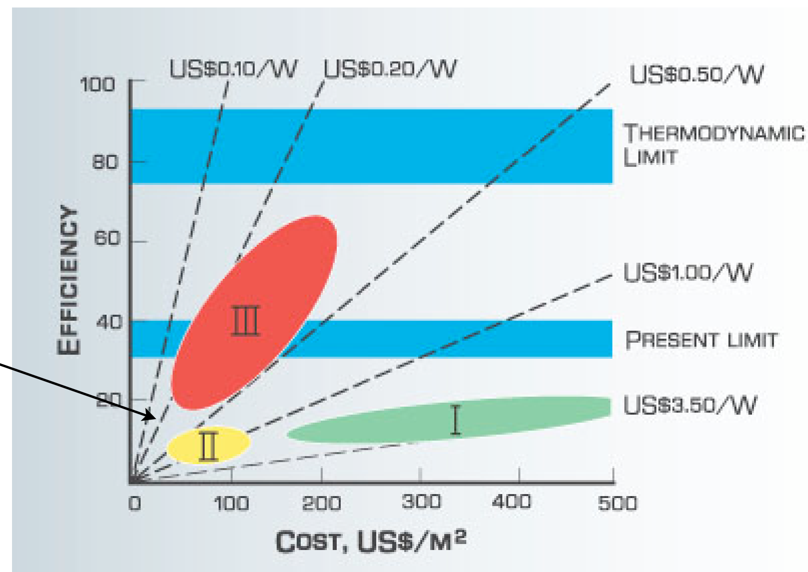
Pathways to higher efficiency

- The pathway to ~11% efficiency is (relatively) clear

- A pathway to 15% efficiency exists, but it is challenging
  - simultaneous optimization of individual components
  - tandem devices

- Reaching efficiencies > 15% may require incorporation of new mechanisms
  - tandem devices
  - more exotic 3rd generation mechanisms
    - Multiple Exciton Generation (MEG)
    - Hot carriers
    - Singlet fusion
    - Optical up-conversion
    - Intermediate band semiconductors
    - ???

OPV



Materials discovery statistics

We are attempting to explore an enormous parameter space:

A (conservative) example calculation for a single junction device:

- 20,000 possible donors
- 2,000 possible acceptors
- 10 solvents
- 10 co-solvents
- 10 possible layer thicknesses
- 10 possible bottom electrodes (TCO or otherwise)
- 10 possible injection layers (either at top or bottom electrode)
- 10 possible top electrodes (metal or otherwise)

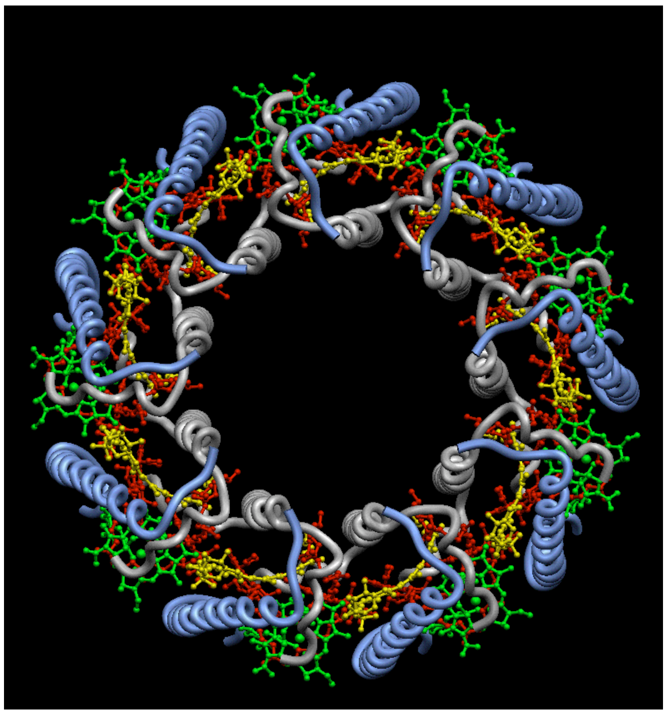
} $>10^{13}$ combinations

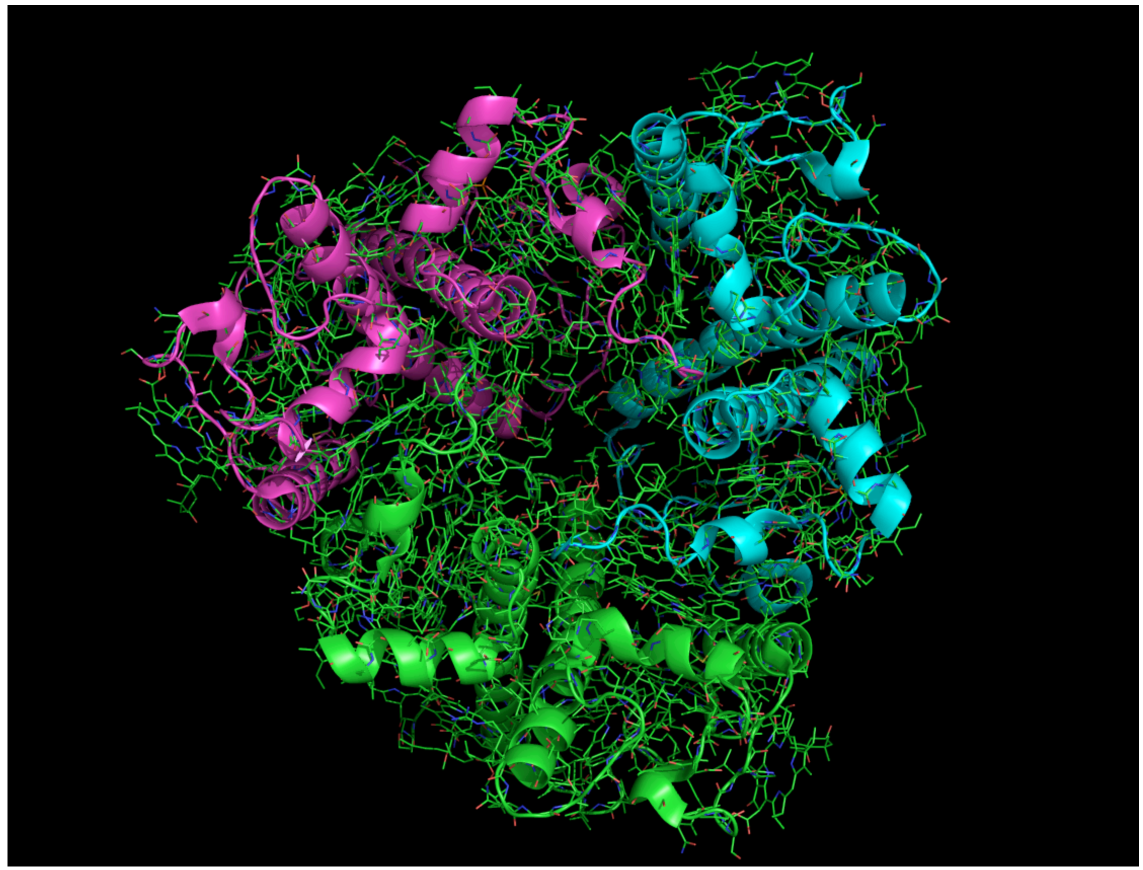
There is a good opportunity for OPV to harness newly emerging tera- and peta-scale computing resources.

OPV can learn a lot from more established technologies.

Closing thought: towards biomimicry?

Our synthetic light harvesting systems are still far simpler than naturally occurring ones, both in *structure* and *function*!





Bacterial Photosynthetic Light Harvesting Complex II
resolved by the group of Neil Isaac, Univ. of Glasgow

Acknowledgements

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