ELEC-E9210 Organic Electronics: Materials, Devices & Applications

Organic Photovoltaics I

Aalto University
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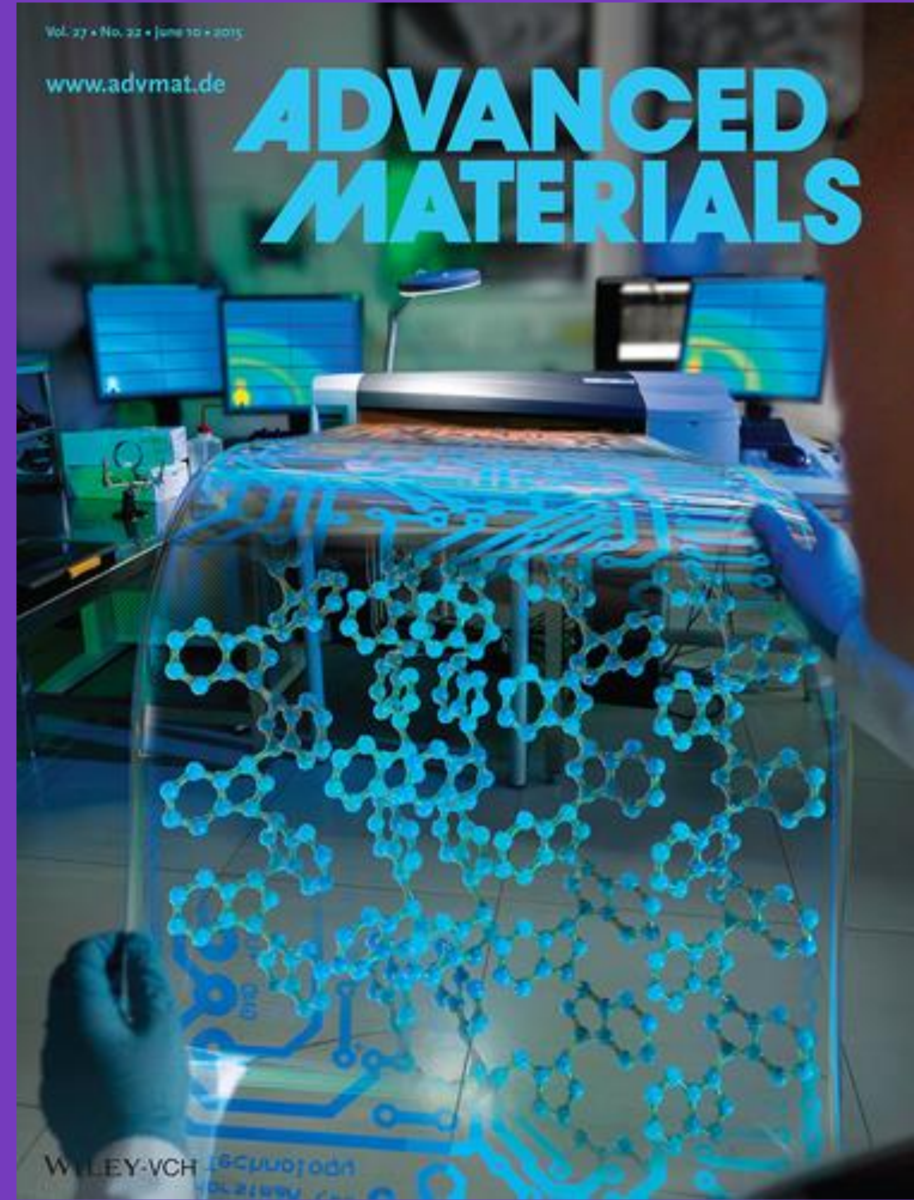
Engineering

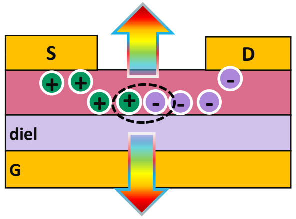
organicelectronics.aalto.fi



Organic Photovoltaics (OPV)

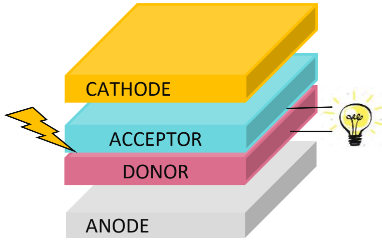
Last Class

- organic light emitting transistors: organic transistors capable of emitting light
- basic working principles
- applications and potentials of OLETs

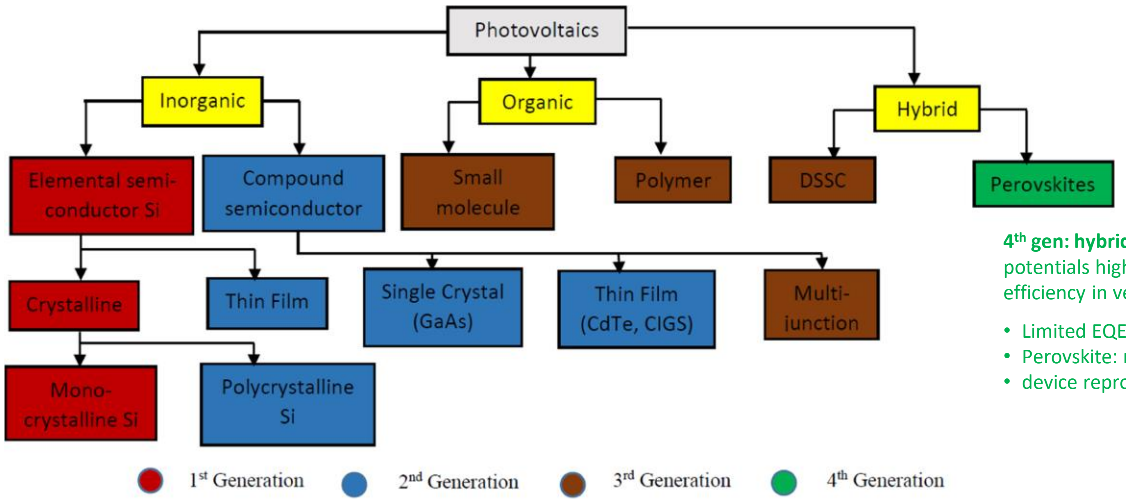


Today´s Class

- organic photovoltaics (OPV): basic mechanisms and device structure
- OPV field of applications



Solar Cell Technology



1st gen: based on **crystalline Si**, and have dominated the PV market for the past half a century

- high processing cost of crystalline Si-based solar cells (not affordable worldwide)
- environmental impact from Si wafer processing

2nd gen: thin film inorganic compounds (*i.e.* a-Si:H, CdTe, CIGS)

- expensive manufacturing equipment (CVD for thin film fabrication)

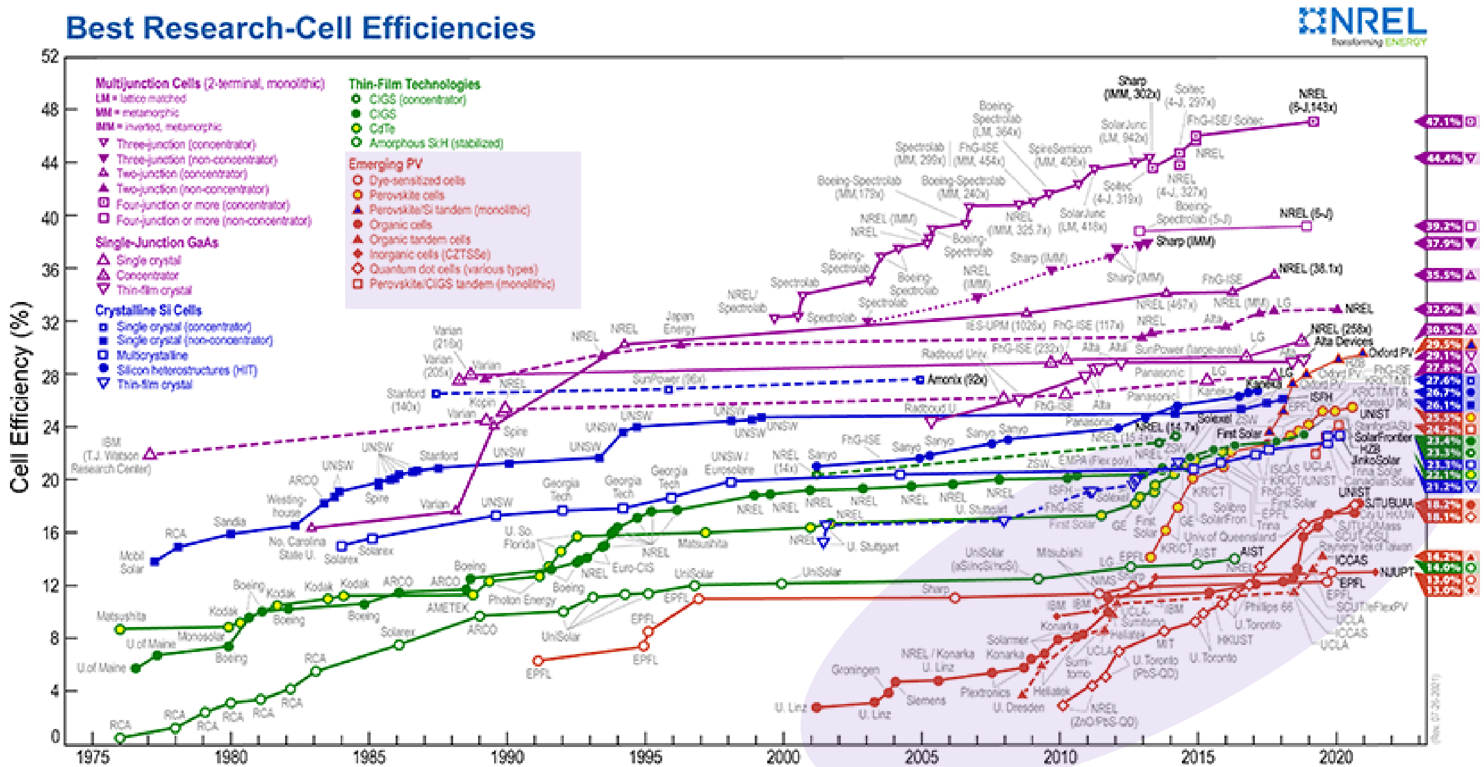
3rd gen: solution-processable thin film solar cells, capable of generating high power conversion efficiency at low fabrication cost

- light condensed cells
- organic photovoltaic cell (OPV)
- dye-sensitized solar cells (DSSCs)

4th gen: hybrid organic/inorganic with potentials high power conversion efficiency in very short period of time

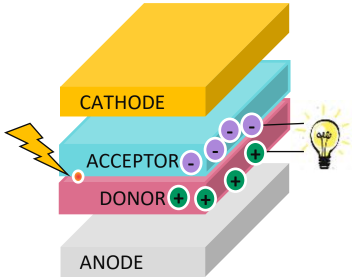
- Limited EQE (few >22%)
- Perovskite: materials instability
- device reproducibility

Current Efficiency in PV Technology



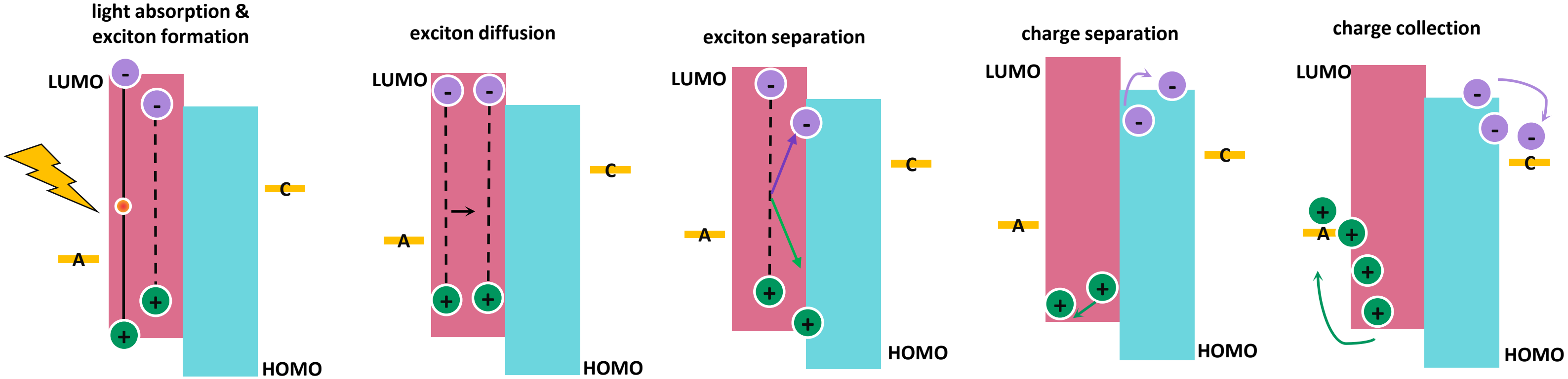
https://www.nrel.gov/pv/cell-efficiency.html (13.09.2021)

Organic Photovoltaics (OPV)

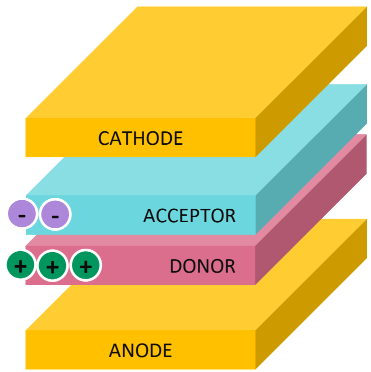


Organic photovoltaic devices ***convert light (sunlight)*** to *electrical energy,* with the active region is based on organic materials (donor donates electrons and mainly transports holes, while acceptor withdraws electrons and mainly transports electrons)

Sunlight is absorbed in the photoactive layers and generate currents. Photoactive materials harvest photons from sunlight to form excitons from which charges are collected



OPV: Favouring Exciton Formation

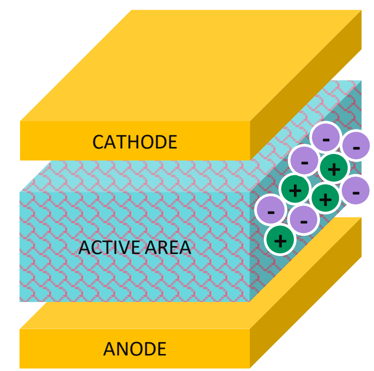


(Planar) Bilayer cells (1986)

- excitons can only dissociate at the interface D/A and can only diffuse few nm before decaying to ground state
- thicker active layers (>100nm) are usually required to absorb light efficiently
- very low efficiency

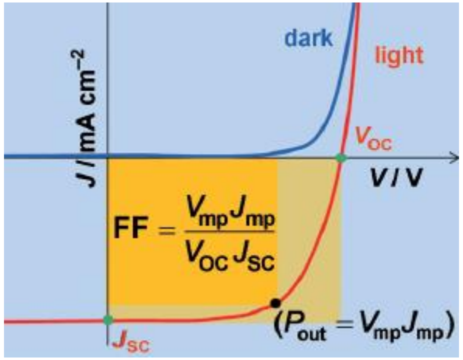
Bulk Hetero-Junction, BHJ (1995)

- donor/acceptor are mixed at the nanoscale level
- diffusion length is consistent with A/D separation whilst maintaining thickness for absorption
- higher efficiency (>13%)



Organic Photovoltaics: Key Parameters

characteristic **J-V curve** for an (organic) solar cells and functional parameters



$$\eta = \frac{P_{out}}{P_{in}} = \frac{V_{mp}J_{mp}}{P_{in}} = \frac{V_{oc}J_{sc}FF}{P_{in}}$$

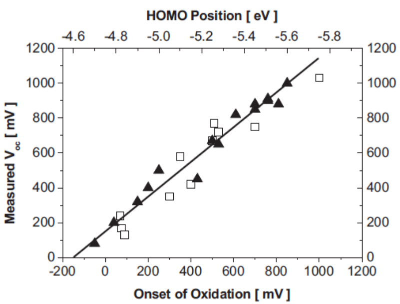
Device Parameter	Materials Optimization
Open Circuit voltage, V_{OC} [V]	molecular energies HOMO (donor)/LUMO (acceptor)
Short-circuit Current Density J_{SC} [mA/cm^2]	**E_{gap}** (band gap) **α** (absorption coefficient) charge transport & extraction
Fill factor, FF [%]	morphology charge mobility & recombination
Power Conversion Efficiency (PCE), η [%]	all above parameters (P_{in} = 100mW/cm^2 or 1Sun)

Organic Photovoltaics: Key Parameters (II)

Open Circuit Voltage

in a *p-n* junction, maximum available voltage is determined by the difference of the quasi-Fermi levels of the two carriers

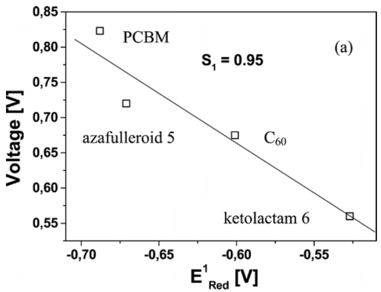
V_{OC} linearly dependent on donor HOMO (*p*-type)



Adv. Mat. **18**, 789 (2006)

different donor polymers

V_{OC} linearly dependent on acceptor LUMO (*n*-type)



Adv. Func. Mat. **11**, 374 (2001)

acceptor fullerene derivative

Short Circuit Current

$$I_{SC} = ne\mu E \ (ideal\ case - no\ losses)$$

in the limit of 100% efficiency:
→ *n:* number of absorbed photons/unit volume

for a given absorption profile, charge mobility is the limiting factor:

- OSC nanoscale morphology
- fabrication process (solvent, solvent evaporation time, substrate temperature, deposition method)

Organic Photovoltaics: Key Parameters (III)

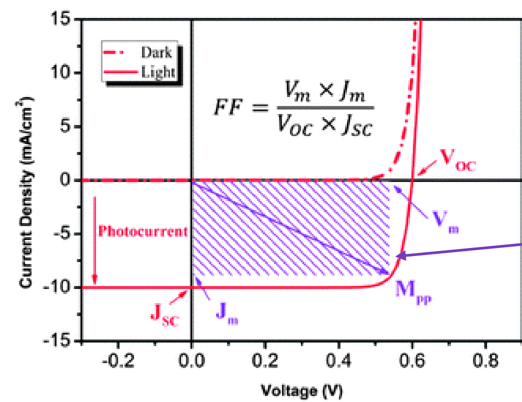
Internal Photon-to-Current Efficiency

$$\text{IPCE} = \frac{\text{\# of electrons collected under short circuit conditions}}{\text{\# of incident photons}} = \frac{(\mathbf{1240} * I_{SC})}{\boldsymbol{wavelenght} * P_{in}}$$

Fill Factor represents how “difficult” or “easy” is the extraction of the photo-generated carriers from the device, where recombination and transport are competing phenomena

FF limitations:

- series resistances (should be minimized).
- ITO finite conductivity (on large area solar cells)
- “shorts” between electrodes

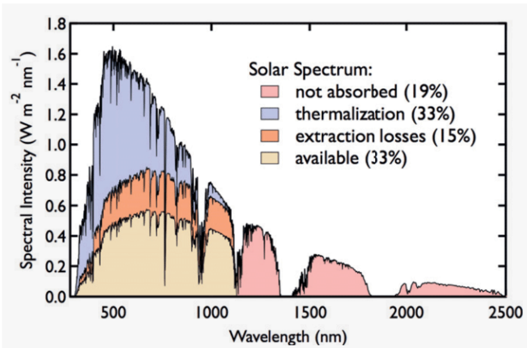


how *square* is this part of the curve

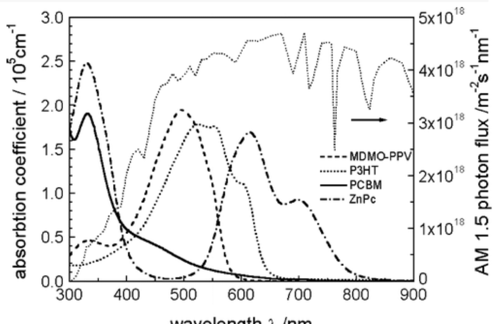
FF100% (perfect square)→ small voltage deviating from the V_{OC} (<V_{OC}) leads to current density rise perpendicularly to the maximum value (J_{SC}), and keep constant while the applied voltage changes from V_{OC} to zero and even a large reversed bias

Shockley-Queisser Limit

Shockley-Queisser limit: solar cells with only one single layer suffers efficiency limitations, since they are unable to fully absorb solar



- Yellow: maximum available theoretical energy (single junction cell)
- Orange: charge extraction losses (technological/material imperfection losses)
- Blue: part of absorbed radiation is converted into heat (for energy higher than bandgap, all part of energy transforms into heat)
- Pink: not enough energy to create charges ($E<E_g$)

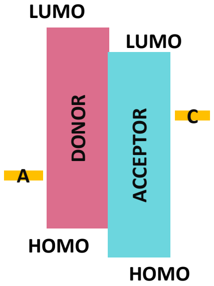


E_g of 1.1eV (1100 nm) will absorb 77% of the solar irradiation on earth. most SC polymers have E_g>2eV (620 nm) → max harvesting of ~30%

high absorption coefficients ($10^5 cm^{-1}$), 100 nm thickness is enough to absorb most of the photons

better “spectral” harvesting of solar photons via lower band gap polymers

(Electron) Donor Materials

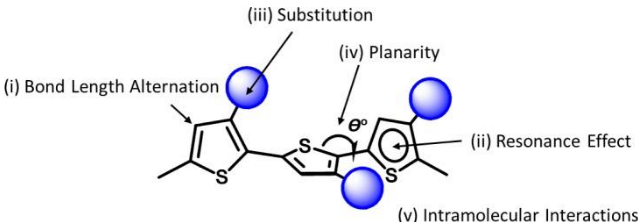


organic solar cells materials are the same used for OLED (both CVD or solution-processed)

conjugated polymers are efficient electron donor materials, leading to high efficiency

Polythiophene (PT) derivatives

Polythiophenes are a widely used class of polymer donors due to ***their excellent thermal*** and ***chemical stability*** as well as ***good light-harvesting*** and ***charge-transporting properties***

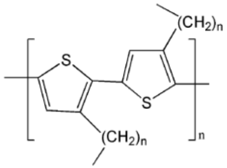


Band gap depends on:
- bond length alternation
- resonance effect
- introduction of *e*-deficient or *e*-sufficient substituent
- dihedral angle θ between consecutive units
- intermolecular interactions

absorption & energy levels can be modulated by introducing conjugated substituents into the side/main chains

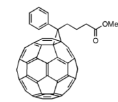
Materials **7**, 2411 (2014)

(Electron) Donor: P3ATs Family

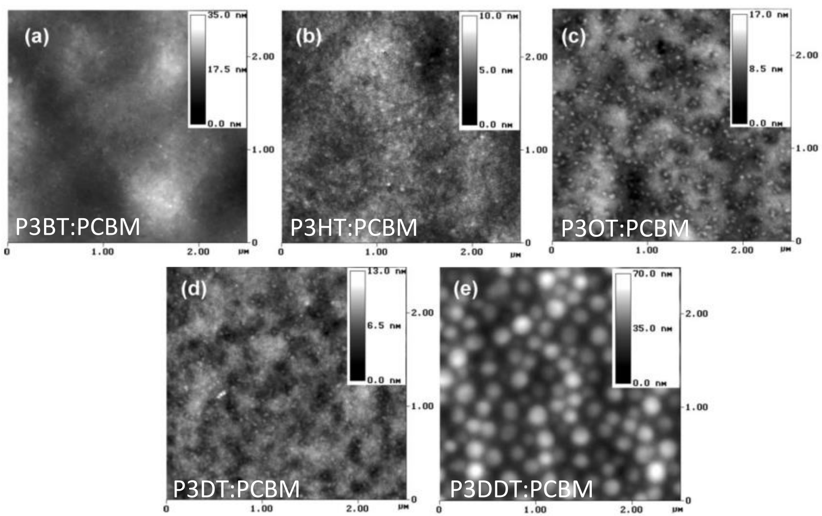


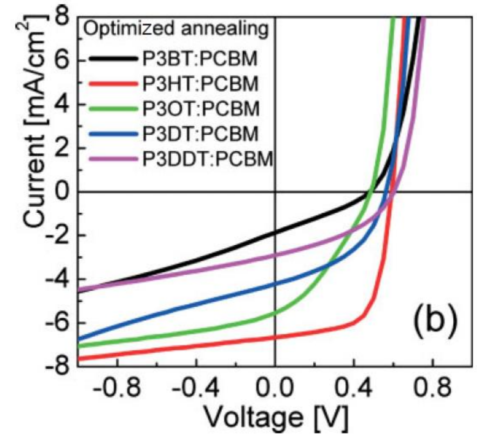
Alkyl group length* plays leads to different materials properties (*i.e.* solubility, crystallinity and morphology)

larger interspace between the rigid conjugated backbones



donor (PCBM) will have less constraints to move within the layer

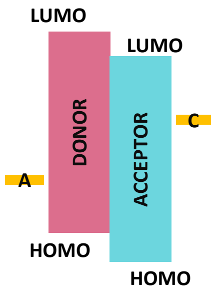




* P3BT(1.28nm), P3HT (2.6nm), P3OT(2.05nm), P3DT(2.35nm), P3DDT (2.6nm)

JV characteristics (AM 1.5, 100mW/cm^2) of P3AT:PCBM blend films upon annealing

(Electron) Acceptor Materials

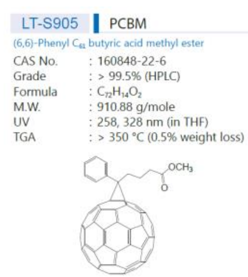


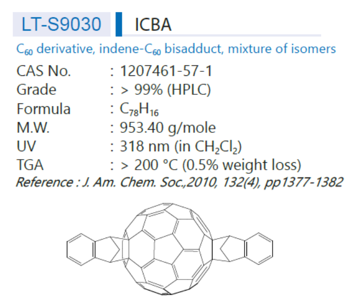
Fullerene (or C60)

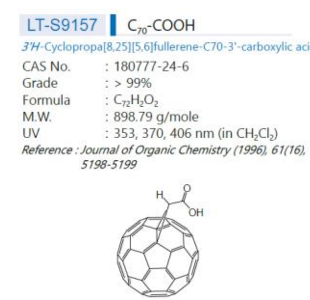
- is naturally *n*-type materials and behaves as good acceptor
- weak optical absorption (VIS) due to high symmetry of the C60 and its derivative

C60 derivatives

- optical absorption can be enhanced by replacing symmetric C60 cage with one of lower symmetry (*i.e.* C70, which leads to strong blue-green absorption)
- enhanced compatibility with the other components

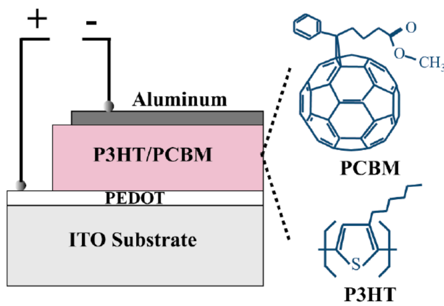


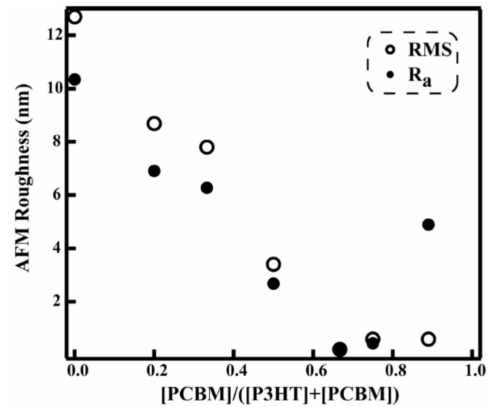




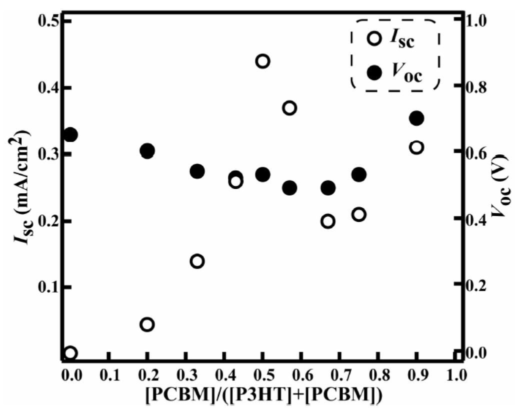
Further reading on fullerenes acceptors: Solar Energy Materials and Solar Cells **161**, 102 (2017)

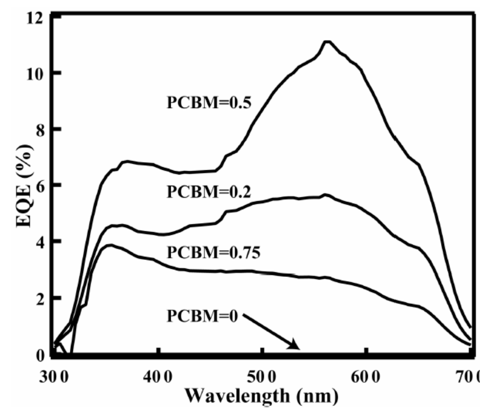
(Electron) Acceptor: PCBM





Typical device structure pf P3HT:PCBM blend organic solar cells, with layer surface properties depending on PCBM concentration



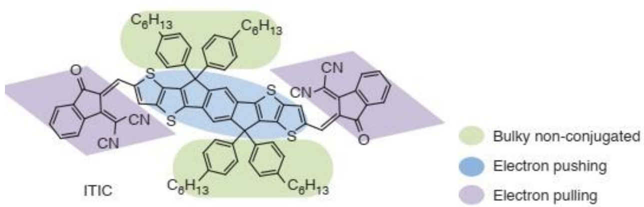


Organic solar cells parameters ad function of the PCBM concentration in the blend

doi: 10.1109/WCPEC.2006.279443

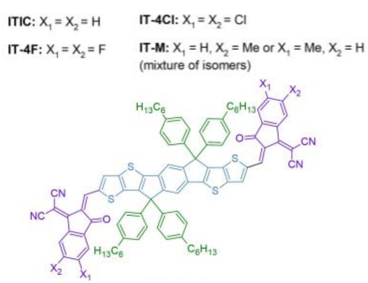
Non-Fullerene Acceptors

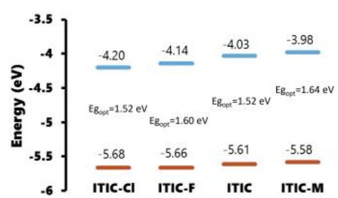
Small molecules and oligomers, have emerged as promising alternative ***non-fullerene acceptors*** in OPV devices

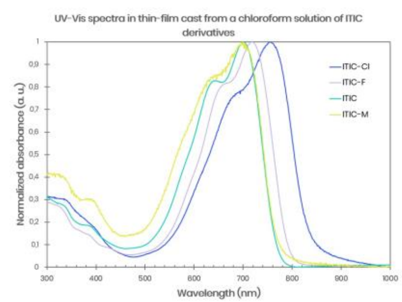


combination of *e*-rich and *e*-poor conjugated moieties (to lower bandgap and achieve a broader absorption):

- *e*-poor side-groups are accessible to interact with the *p*-type material because the *e*-rich core is shielded by bulky side-groups
  → improve driving force to separate charges from the exciton
- higher voltages in OPV devices (compared to fullerene derivatives)
- increased absorption coefficient and photocurrent generation
- easy to synthesize/modify/functionalize





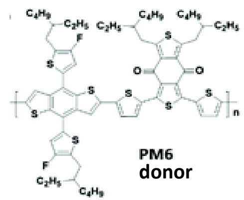


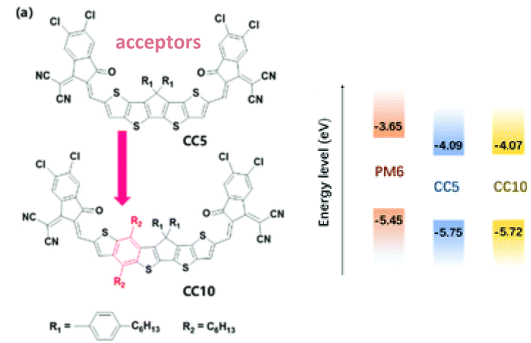
solar cell parameters & lifetime

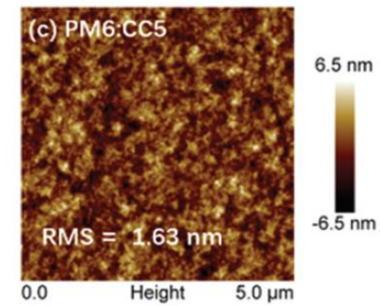
https://www.sigmaaldrich.com/technical-documents/articles/technology-spotlights/non-fullerene-for-opv.html#ref

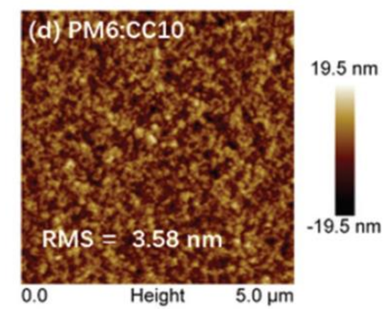
Non-Fullerene Acceptor (II)

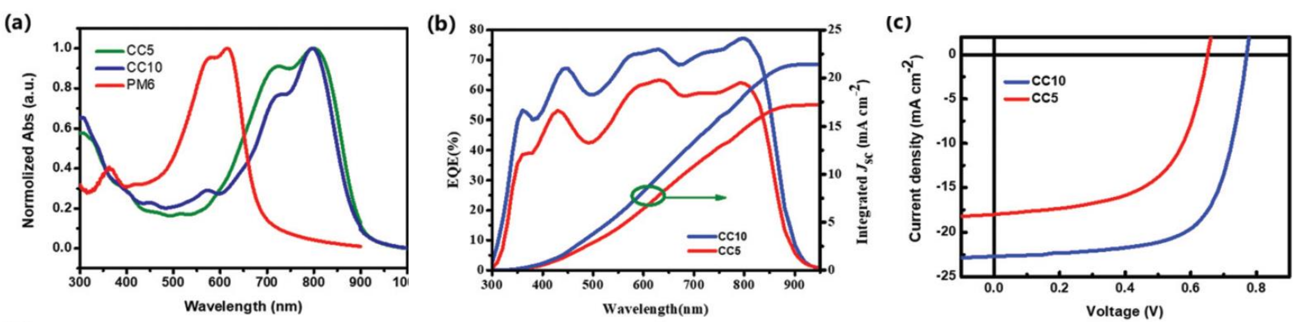
CC5 and CC10 differs in an alkylbenzene unit on the backbone, leading to similar absorption range and energy levels but greatly different molecular packing and blend microscopic morphology (PM6: donor).











J. Mater. Chem. C **8**, 6293 (2020)

(a) Normalized UV-vis absorption spectra of PM6, CC5, and CC10 in thin film; (b) EQE curves, (c) current density–voltage (*J*–*V*) curves for CC5- and CC10-based devices.

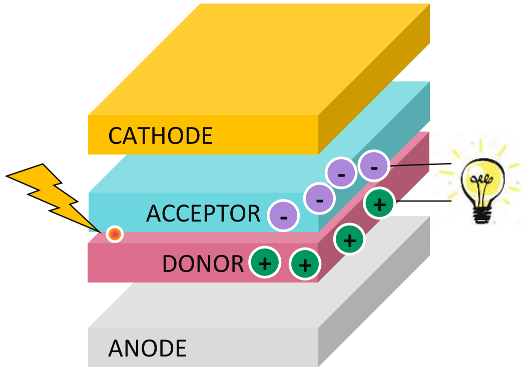
Summary

Today

- organic photovoltaics (OPV): basic mechanisms and device structure
- materials to achieve high efficiency of OPV

Interesting tutorial on perovskite solar cells:
https://www.cei.washington.edu/education/science-of-solar/perovskite-solar-cell/

https://www.ossila.com/pages/perovskites-and-perovskite-solar-cells-an-introduction



Next Class

- Most recent trends in OPV and OPV Applications