

Conjugated Polymers for Optoelectronic Applications

Polymer Electronics is expected to become one of the key technologies in the 21st century. Semiconducting polymers are predicted to become the semiconducting material of this century, gaining a comparable share on the market as Si based technology gained during the previous century.

Conjugated polymers exhibit a great variety of technologically relevant properties as for example absorption and emission of light or electrical and photoconductivity, thus making them useful materials for the application in electronic devices (Figure 1).^[1]

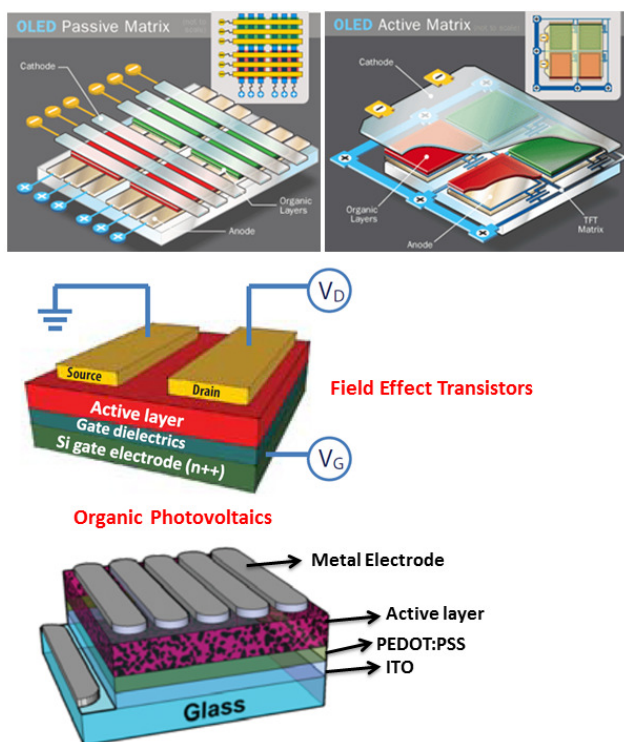


Figure 1. Organic light emitting diodes, organic photovoltaics and field effect transistor device architectures

Organic polymers typically offer the advantage that they are light-weight and flexible materials which can be processed from solution by spin coating or inkjet printing at room temperature. Especially, low band gap (LBG) donor-acceptor polymers are of interest owing to the possibility of attaining multiple redox states (*p*-type or *n*-type doping) in a small potential window.^[2] This is due to the placement of the valence band relative to the conduction band. By using strong donors with high HOMO energy levels, and strong acceptors with low LUMOs, one can control the magnitude of the polymer band gap.^[3] This makes them promising for the production at low cost and for large-area employments in supercapacitors, ambipolar field-effect transistors, solar cells, light-emitting devices and electrochromic devices.

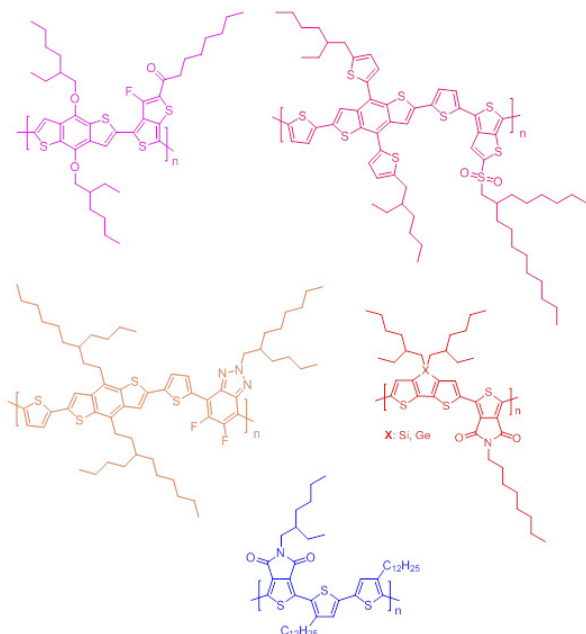
Significant revolution in the chemistry and molecular engineering of conjugated polymers has been witnessed by the increased demand for novel electron donor conjugated polymers in the area of organic photovoltaics (OPVs).^[4] New electron donor conjugated polymers were developed, based on the design rules presented below:

- low band gap of 1.4 – 1.8 eV,
- deep HOMO level of around 5.4 – 5.6 eV,
- LUMO level of 3.4 – 3.6 eV,
- high molecular weight for high quality thin films
- charge carrier mobility of 10^{-3} cm²/Vs

that when blended with [6,6]-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) fullerene derivative, significant improvements in device performance has been observed.^[5]

For example, power conversion efficiencies (PCEs) of ~8%, based on blends of conjugated polymers as electron donors and soluble fullerene derivatives, especially PC₆₁BM or [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) as electron acceptors, have been presented.^[6] Some of the state-of-the-art

electron donor conjugated polymers are presented on Scheme 1.



Scheme 1. State-of-the-art electron donor polymers for organic photovoltaics

In order to further increase the PCE, one approach is to stack, in series, multiple photoactive layers with complementary absorption spectra to construct a tandem OPV.^[7] In a typical double-junction cell, such a tandem structure consists of a bottom cell with a high-bandgap material, an interconnecting layer (ICL), and a top cell comprising a low-bandgap material. When compared to a single-junction device made using low-bandgap materials, this tandem structure has a reduced photovoltage loss during the photon-to-electron conversion process (Figure 2).

Because the two cells are connected in series, the total current will be limited by the bottom sub-cell with the lower current. Obtaining a high current in the bottom cell is a great challenge, because most of the high-energy portion of the incident light will have already been absorbed by the bottom device. Therefore, a carefully designed semiconducting

polymer will perform well in tandem cells only if it can achieve high current by efficiently using the low-energy portion of the solar spectrum.^[8]

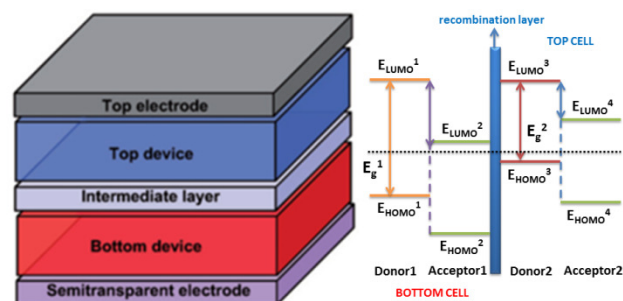


Figure 2. Schematic representation and a simplified band diagram of an organic tandem device comprised of two sub-cells connected via a recombination layer

The most representative high-bandgap polymer donor is regioregular poly(3-hexylthiophene) (rrP3HT). rrP3HT:PC₆₁BM OPV devices have reached PCEs over 4% by device optimization.^[9] However, the further improvement of the photovoltaic performance of the rrP3HT:PC₆₁BM system is mainly limited by the high LUMO offset between rrP3HT and PC₆₁BM. By careful molecular engineering, a new indacene bisadduct fullerene derivative (ICBA) was synthesized that presented up-shifted LUMO level, as compared to PCBM (Figure 3).^[10]

OPV devices based on rrP3HT:ICBA exhibited higher PCE (5.5-6.5%) with simultaneously enhanced short-circuit current (J_{sc}), open-circuit voltage (V_{oc}) and fill factor (FF) as compared to rrP3HT:PC₆₁BM.^[11] Therefore, rrP3HT:ICBA represents today the system of choice as bottom sub-cell for high performance tandem solar cells. This breakthrough in the increase of the PCE of rrP3HT:ICBA paves the way for the development of other high bandgap conjugated polymers with enhanced photovoltaic performances as compared to those of rrP3HT:ICBA.

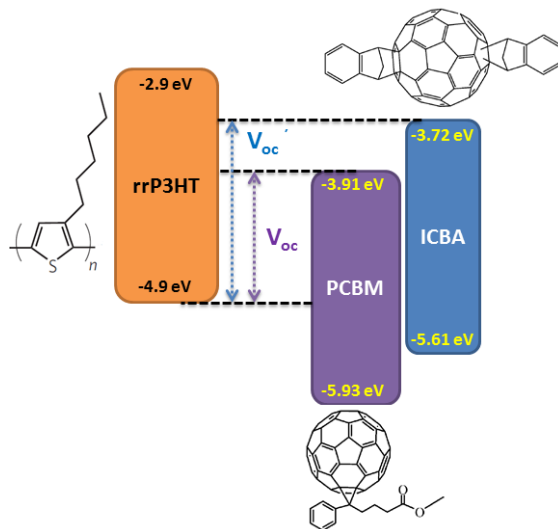


Figure 3. Energy band diagram of the rrP3HT, PCBM and ICBA.

ADVENT Technologies (<http://www.advent-energy.com>) is involved in the production of innovative materials and systems for their application in renewable energy sources and has commercial activity related to fuel cells^[12-14] and organic photovoltaics.^[15-17]

ADVENT Technologies provides:

High and Low-bandgap conjugated polymers which are available for laboratory evaluation and research proposal via Custom Synthesis

The conjugated polymers or blends thereof with ICBA or PCBM as electron acceptors can be applied in:

- Field Effect Transistors
- Single solar cells
- Tandem solar cells
- Dye-sensitized solar cells

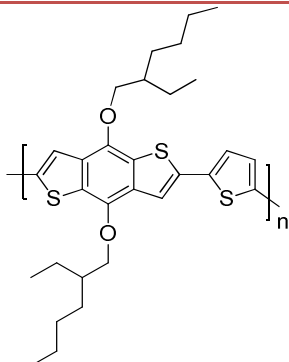


Name	Structure	Quantity	Optoelectronic Data
ADVPOL001a ADVPOL001b (rrP3HT)		500mg 1g	$E_g^{opt} = 2.00\text{eV}$ [18] LUMO= -2.90eV HOMO= -4.90eV Hole mobility (TOF)= 5.1×10^{-5} cm^2/Vs PCE = 4.4%
ADVPOL002a ADVPOL002b (APFO)		500mg 1g	$E_g^{opt} = 1.90\text{eV}$ [19] LUMO= -3.40eV HOMO= -5.50eV Hole mobility (SCLC)= 6.0×10^{-6} cm^2/Vs PCE = 3.5%
ADVPOL003a ADVPOL003b		500mg 1g	$E_g^{opt} = 1.82\text{eV}$ [20] HOMO= -5.39eV Hole mobility (FET)= 1.0×10^{-3} cm^2/Vs PCE = 5.45%
ADVPOL004a ADVPOL004b (PCDTBT)		500mg 1g	$E_g^{opt} = 1.88\text{eV}$ [21] LUMO= -3.60eV HOMO= -5.45eV Hole mobility (FET)= 1.0×10^{-3} cm^2/Vs PCE = 6.1%
ADVPOL005a ADVPOL005b		500mg 1g	[22] $E_g^{opt} = 1.57\text{eV}$ Hole mobility (FET)= 2.0×10^{-4} cm^2/Vs PCE = 2.10%
ADVPOL006a ADVPOL006b		500mg 1g	[23] $E_g^{opt} = 1.53\text{eV}$ LUMO= -3.17eV HOMO= -4.99eV Hole mobility (SCLC)= 3.0×10^{-6} cm^2/Vs PCE = 2.95%
ADVPOL007a ADVPOL007b		500mg 1g	[24] $E_g^{opt} = 1.46\text{eV}$ LUMO= -3.43eV HOMO= -5.00eV PCE = 2.18%



[25]

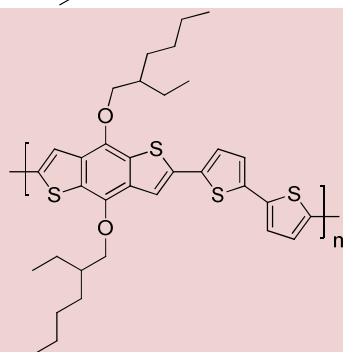
ADV POL008a
ADV POL008b



500mg
1g

$E_g^{opt} = 2.06\text{eV}$
LUMO = -2.69eV
HOMO = -5.05eV
PCE = 1.6%

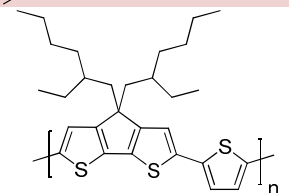
ADV POL009a
ADV POL009b



500mg
1g

-

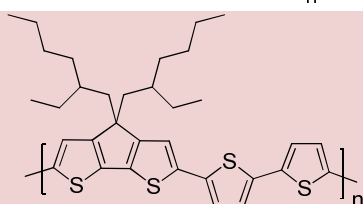
ADV POL010a
ADV POL010b



500mg
1g

-

ADV POL011a
ADV POL011b

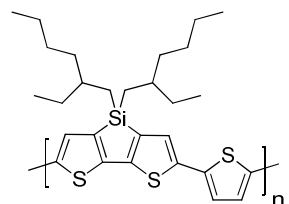


500mg
1g

$E_g^{opt} = 1.88\text{eV}$
LUMO = -2.89eV
HOMO = -5.38eV
Hole mobility (FET) = 1.9×10^{-3}
 cm^2/Vs
PCE = 2.22%

[26]

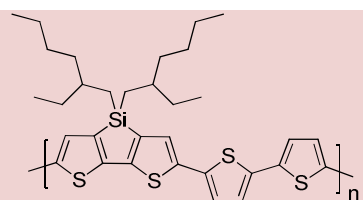
ADV POL012a
ADV POL012b



500mg
1g

-

ADV POL013a
ADV POL013b

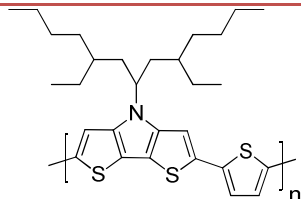


500mg
1g

-



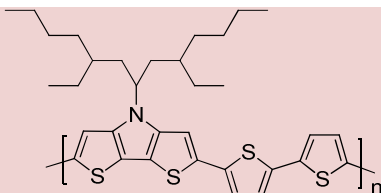
ADVPOL014a
ADVPOL014b



500mg
1g

-

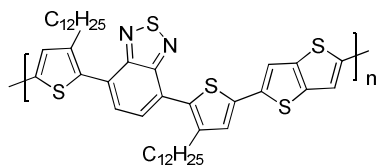
ADVPOL015a
ADVPOL015b



500mg
1g

-

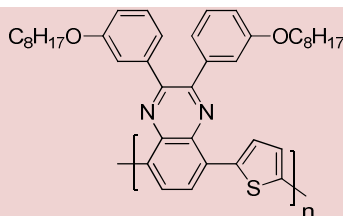
ADVPOL016a
ADVPOL016b



500mg
1g

E_g^{opt} = 1.88eV [27]
LUMO = -3.20eV
HOMO = -5.30eV
Hole mobility (FET) = 5.0x10⁻⁴
cm²/Vs
PCE = 1.0%

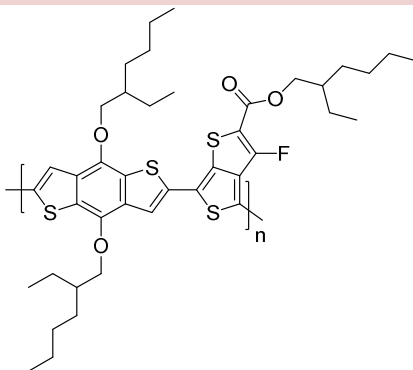
ADVPOL017a
ADVPOL017b



500mg
1g

E_g^{opt} = 1.70eV [28]
LUMO = -3.30eV
HOMO = -5.70eV
PCE = 6.0%

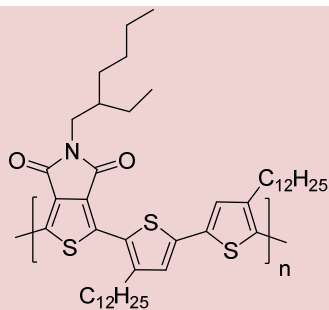
ADVPOL018a
ADVPOL018b



500mg
1g

E_g^{opt} = 1.60eV [29]
LUMO = -3.31eV
HOMO = -5.15eV
Hole mobility (SCLC) = 5.8x10⁻⁴
cm²/Vs
PCE = 9.2%

ADVPOL019a
ADVPOL019b

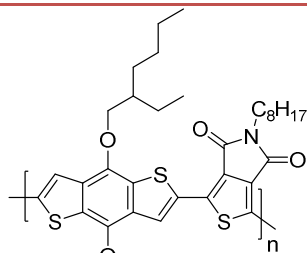


500mg
1g

E_g^{opt} = 1.82eV [30]
LUMO = -3.10eV
HOMO = -5.56eV
Hole mobility (SCLC) = 1.0x10⁻⁴
cm²/Vs
PCE = 7.3%



ADV POL020a
ADV POL020b

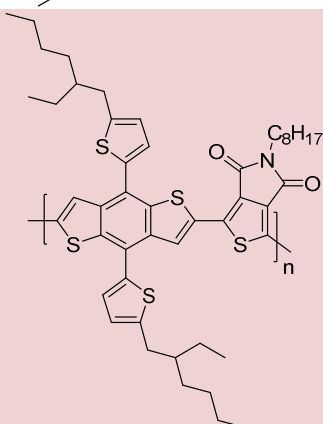


500mg
1g

$E_g^{opt} = 1.82\text{eV}$
HOMO = -5.40eV
PCE = 7.3%

[31]

ADV POL021a
ADV POL021b



500mg
1g

$E_g^{opt} = 1.85\text{eV}$
LUMO = -3.56eV
HOMO = -5.61eV
PCE = 6.17%

[32]

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