UMONS
Université de Mons

CIRMAP
Center of Innovation and Research in Materials and Polymers

Research activities on organic photovoltaics

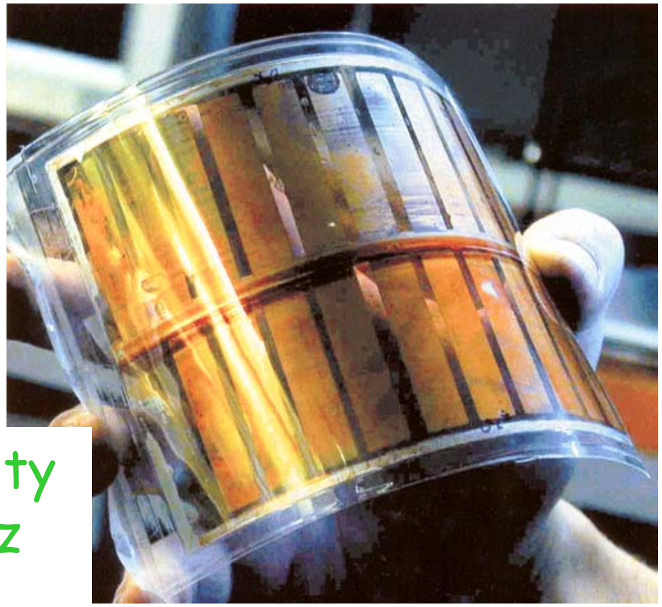
at the Center of Innovation and Research in MAterials and Polymers – CIRMAP

University of Mons

Roberto Lazzaroni

Journée scientifique des comices 'Energie solaire' – Namur 23/04/2012

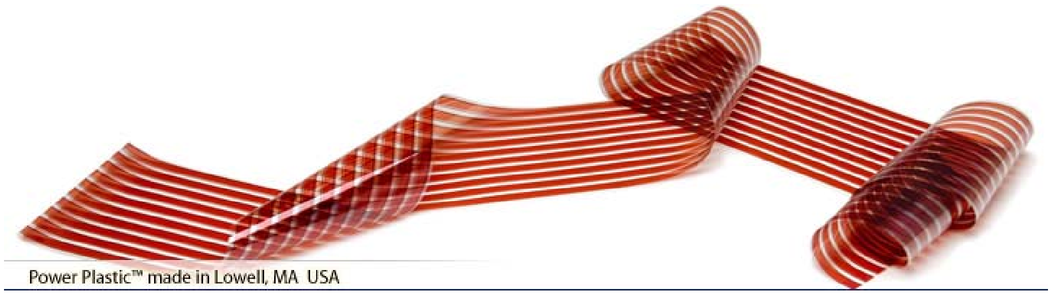
Organic Solar Cells



University of Linz 2004

Active material is much cheaper to produce than Si

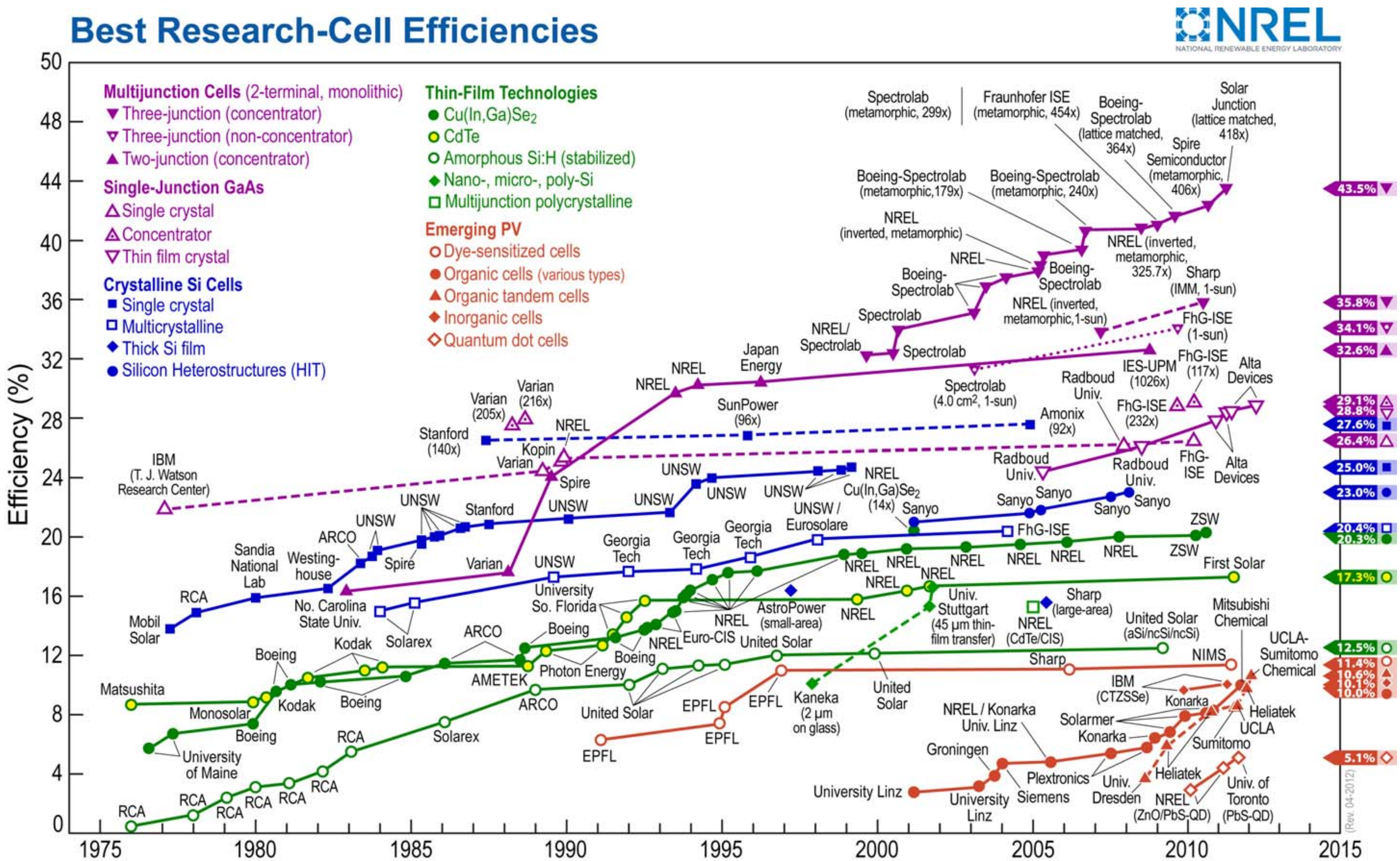
Easily deposited as thin films over large (flexible) areas



Power Plastic, Konarka, 2007

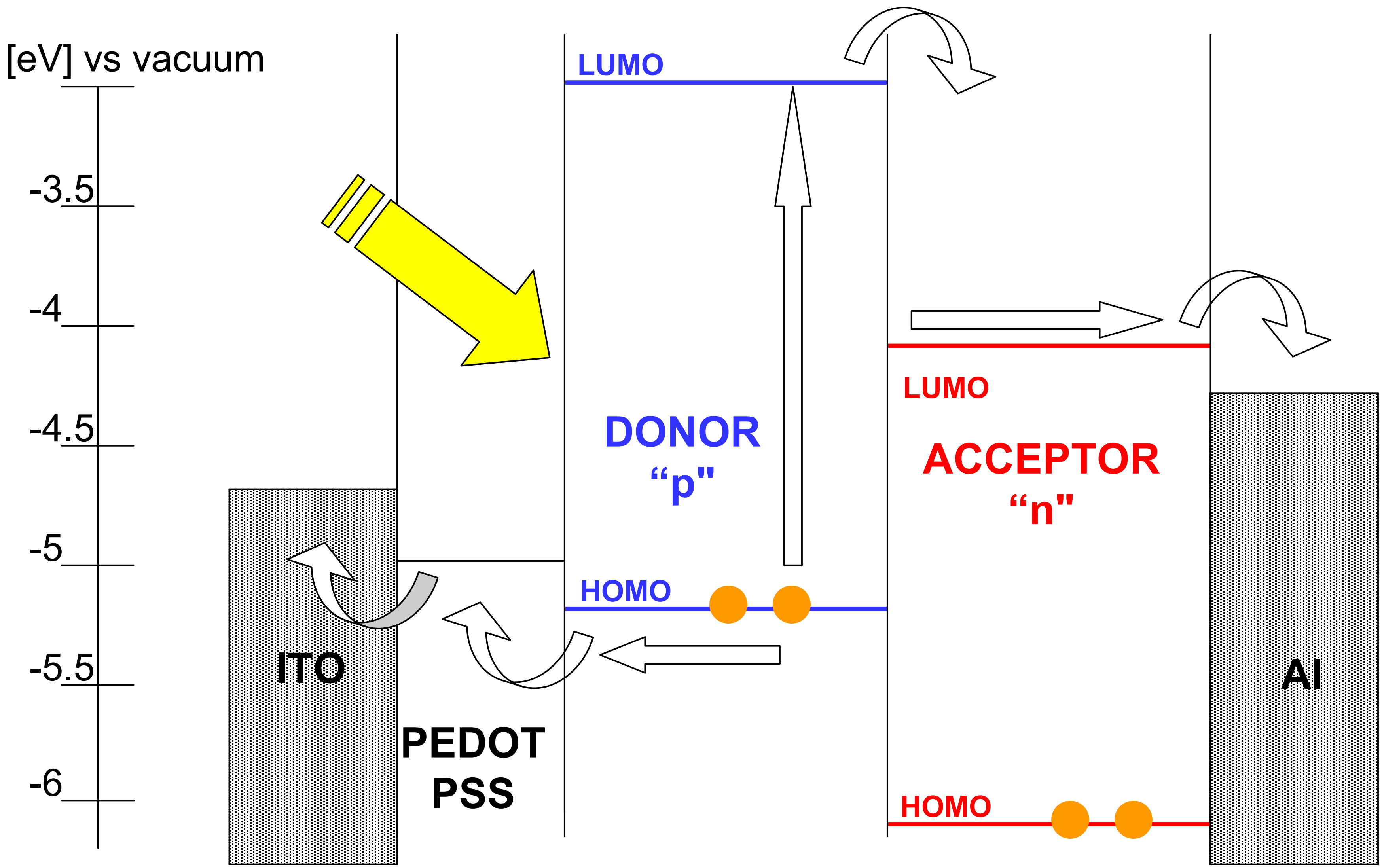
Power Conversion Efficiency

April 2012



Organic solar cell structure

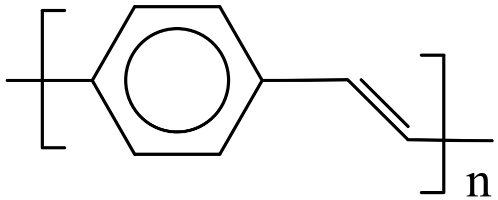
Gilles Dennler, KONARKA



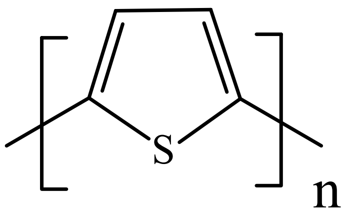
V_{oc} is set by LUMO(acc) - HOMO(don)

Materials for organic photovoltaics

Conjugated polymers



Poly(p-phenylenevinylene), PPV

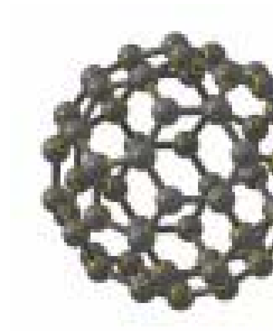


Polythiophene, PT

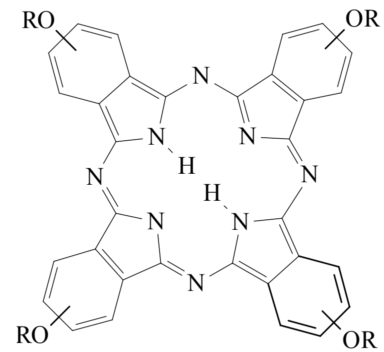
* Thin film deposition from solution
(spin coating, inkjet printing,Dr.Blading,...)

* Wide range of chemical substitution
⇨ 'Molecular engineering'

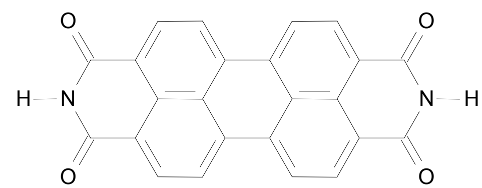
'Small' molecules



C_{60}



phthalocyanine



perylene

* Deposition by vacuum sublim. into highly-ordered thin films

* Chemical purity

Research activities on organic photovoltaics at CIRMAP - UMONS

CIRMAP: Center of Innovation and Research in MAterials and Polymers

Four research groups : ~ 100 research staff

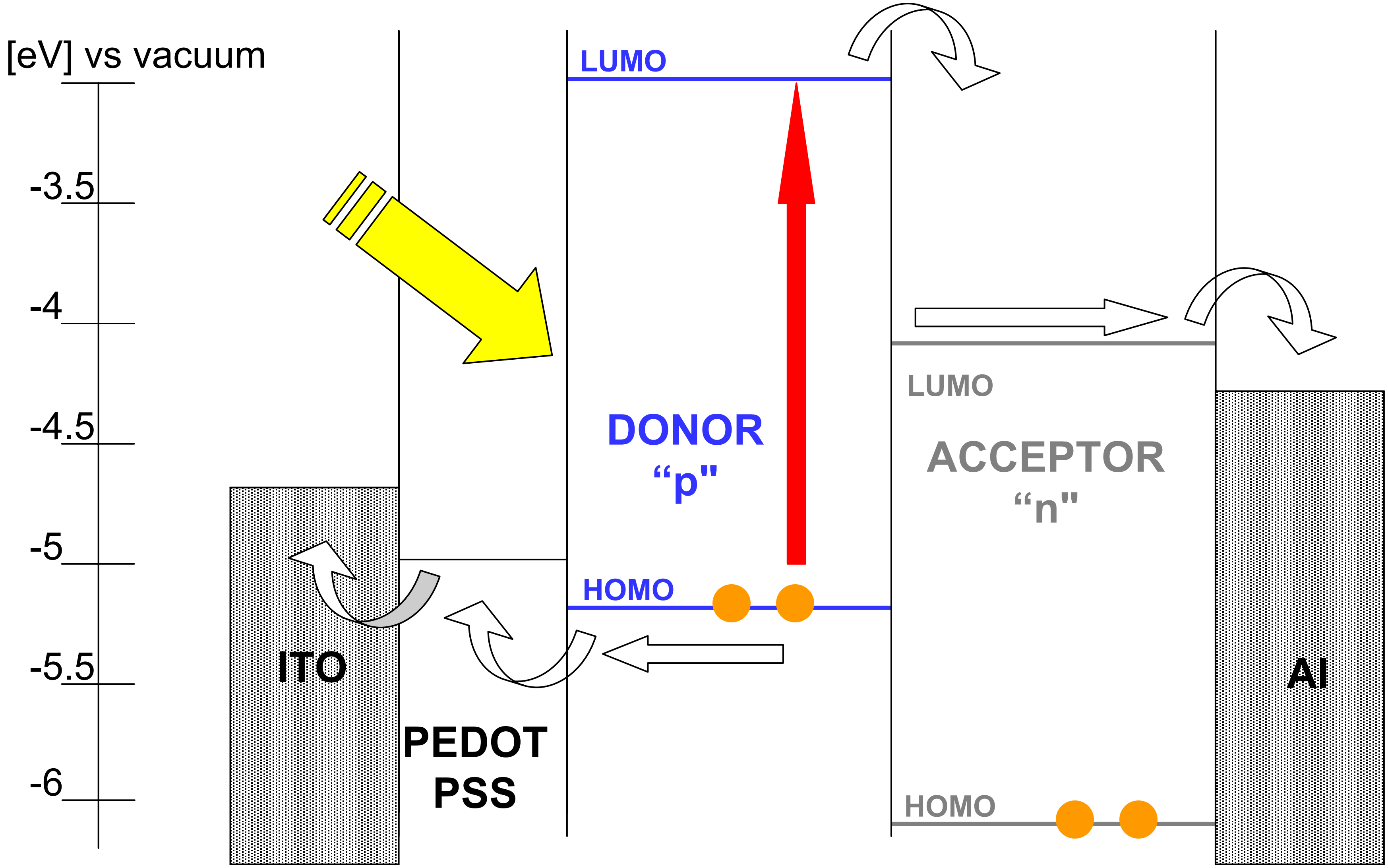
Service de Chimie des Matériaux Nouveaux – SCMN: R. Lazzaroni
Service des Matériaux Polymères et Composites – SMPC : Ph. Dubois
Laboratoire Interfaces et Fluides Complexes – Influx: P. Damman
CHimie des Interactions Plasma-Surfaces – ChIPS: R. Snyders

Design and modeling of materials and photophysical processes: SCMN
Tailored synthesis of polymer semiconductors: SMPC
Thin film morphology and electrical properties : SCMN
Microstructured layers for light management: Influx
Novel materials for electrodes: ChIPS

In close collaboration with
- Materia Nova (P. Viville et al) : device fabrication and testing
- ULB (Y. Geerts), UCL (S. Melinte), ULg (C. Jérôme),…

Organic solar cell : light absorption

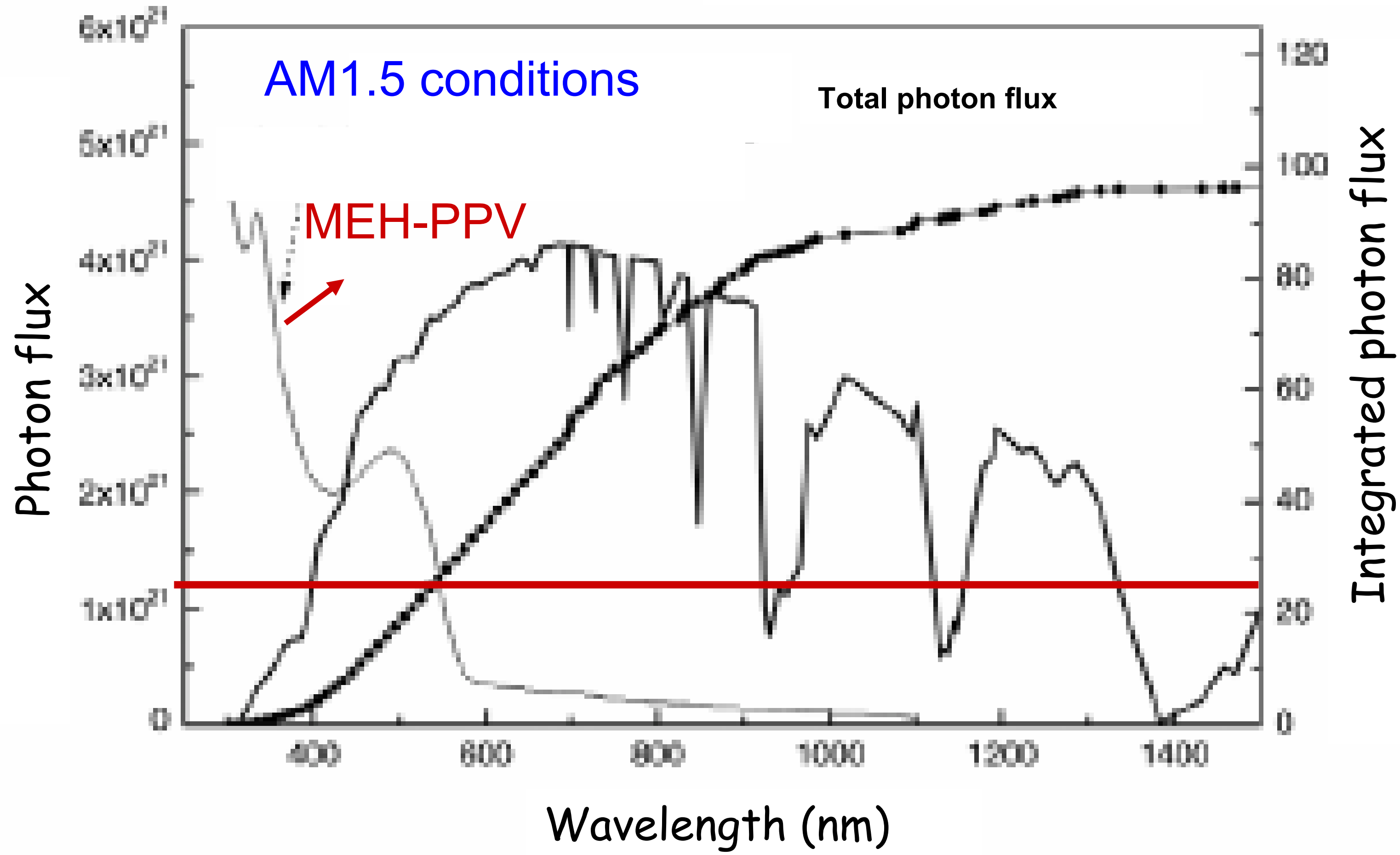
Gilles Dennler, KONARKA



Efficiency of light conversion

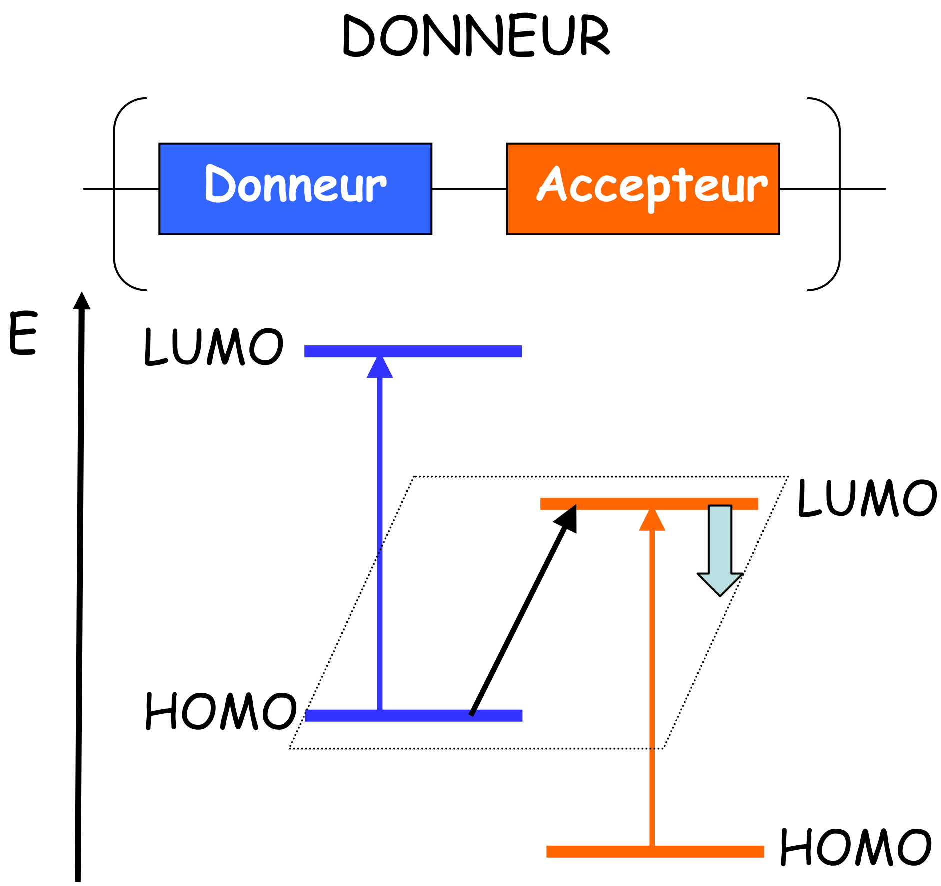
25% of the incoming solar light is harvested for a gap of 2.1 eV

N.S. Sariciftci, Materialstoday, September 2004

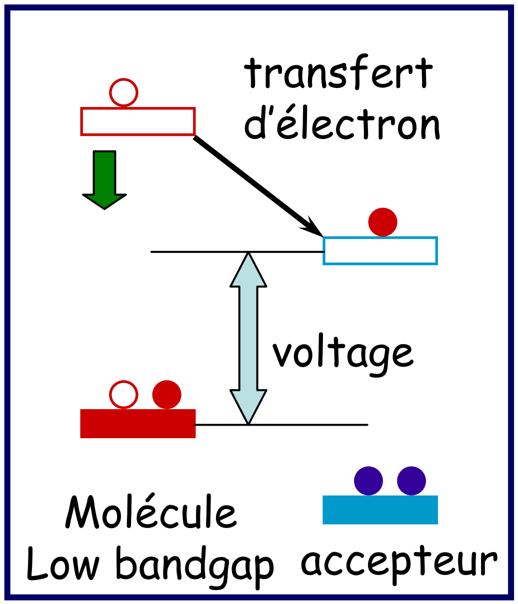


Light harvesting at higher wavelengths is essential

Design de molécules low bandgap : 2e génération



Mélange donneur-accepteur

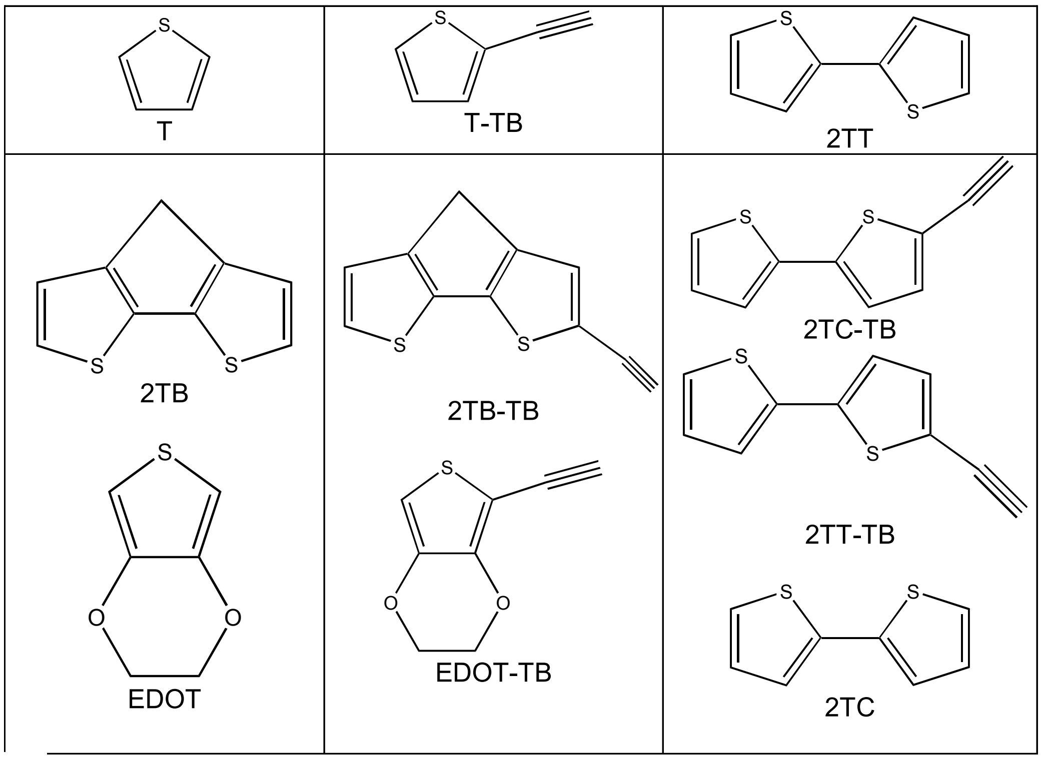


Calcul des propriétés électroniques et optiques
par les méthodes de chimie quantique

Couples donneur-accepteur

Donneurs

Donneurs

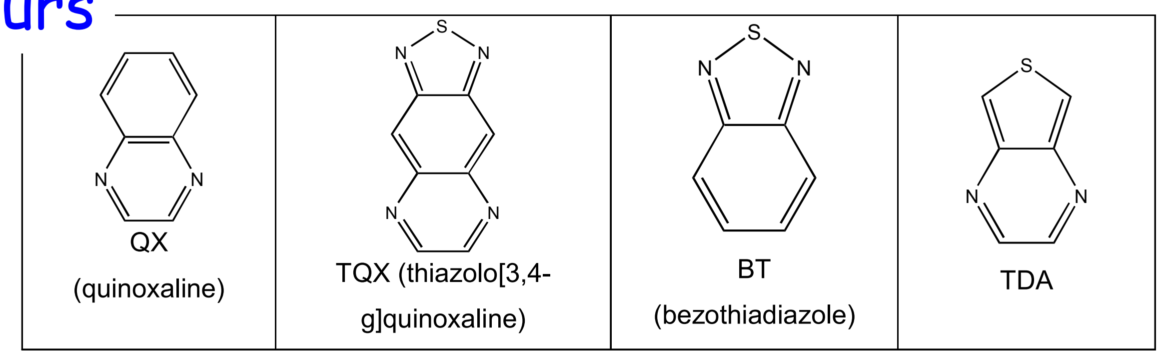


Influence de la structure ?

Influence du pont ethynylene ?

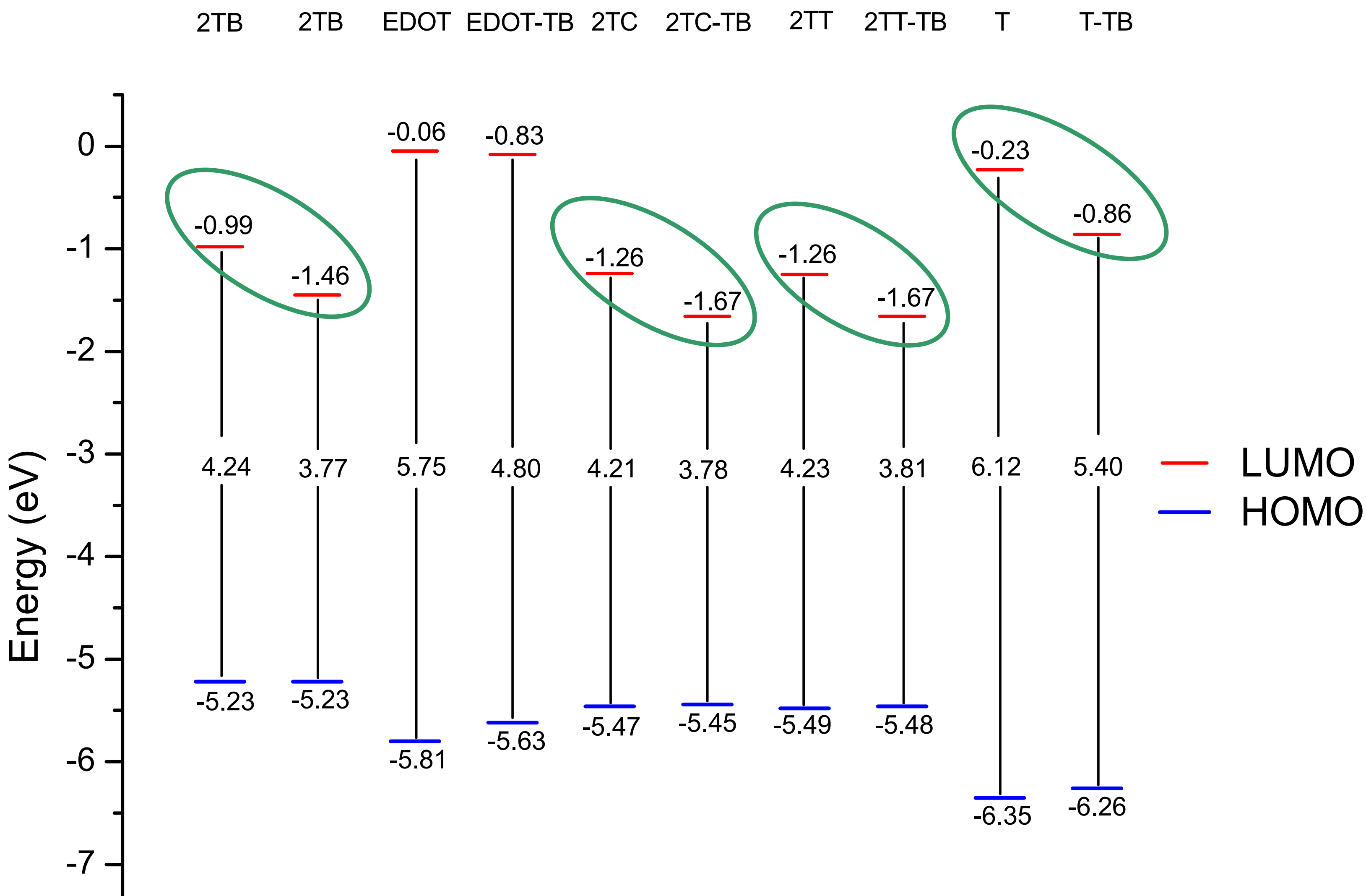
Accepteurs

Accepteurs



Influence de la structure ?

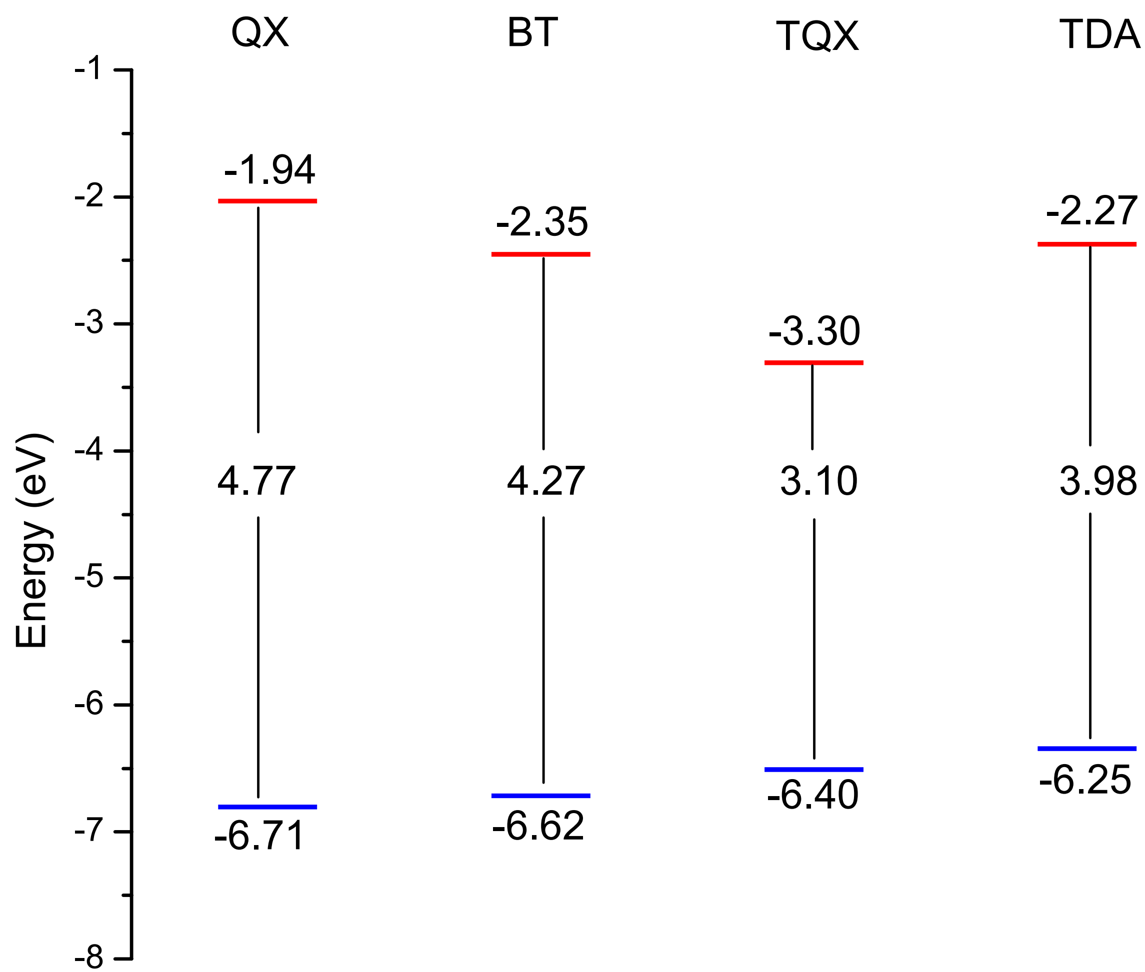
Niveaux énergétiques: Donneurs

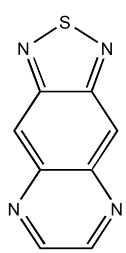


La triple liaison abaisse la LUMO sans toucher à la HOMO

→ Pas de diminution du voltage final

Niveaux énergétiques: Accepteurs

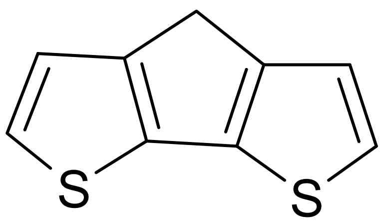




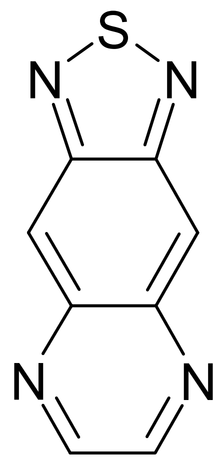
L'accepteur TQX présente la LUMO la plus basse

Conclusions

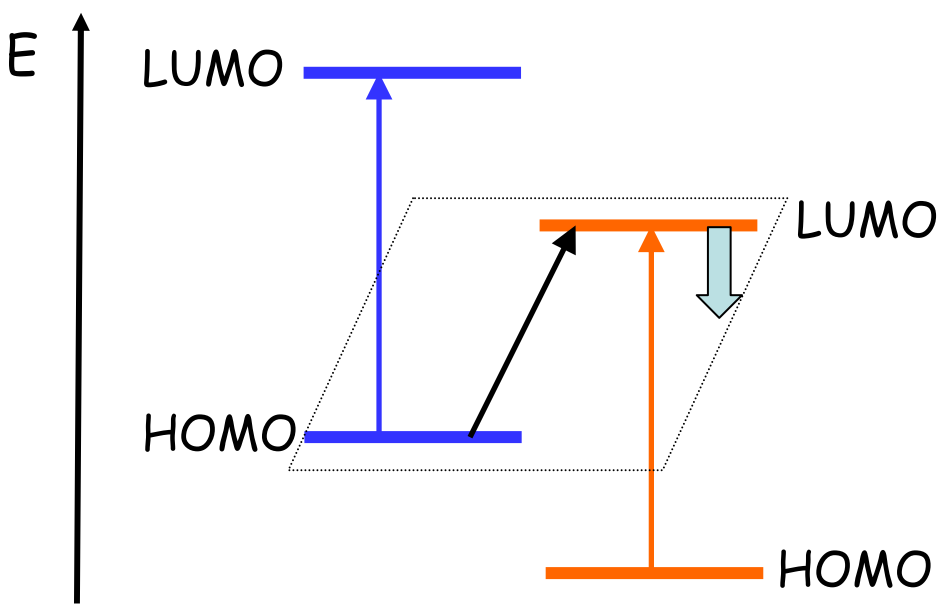
Sélection des meilleurs couples donneur-accepteur



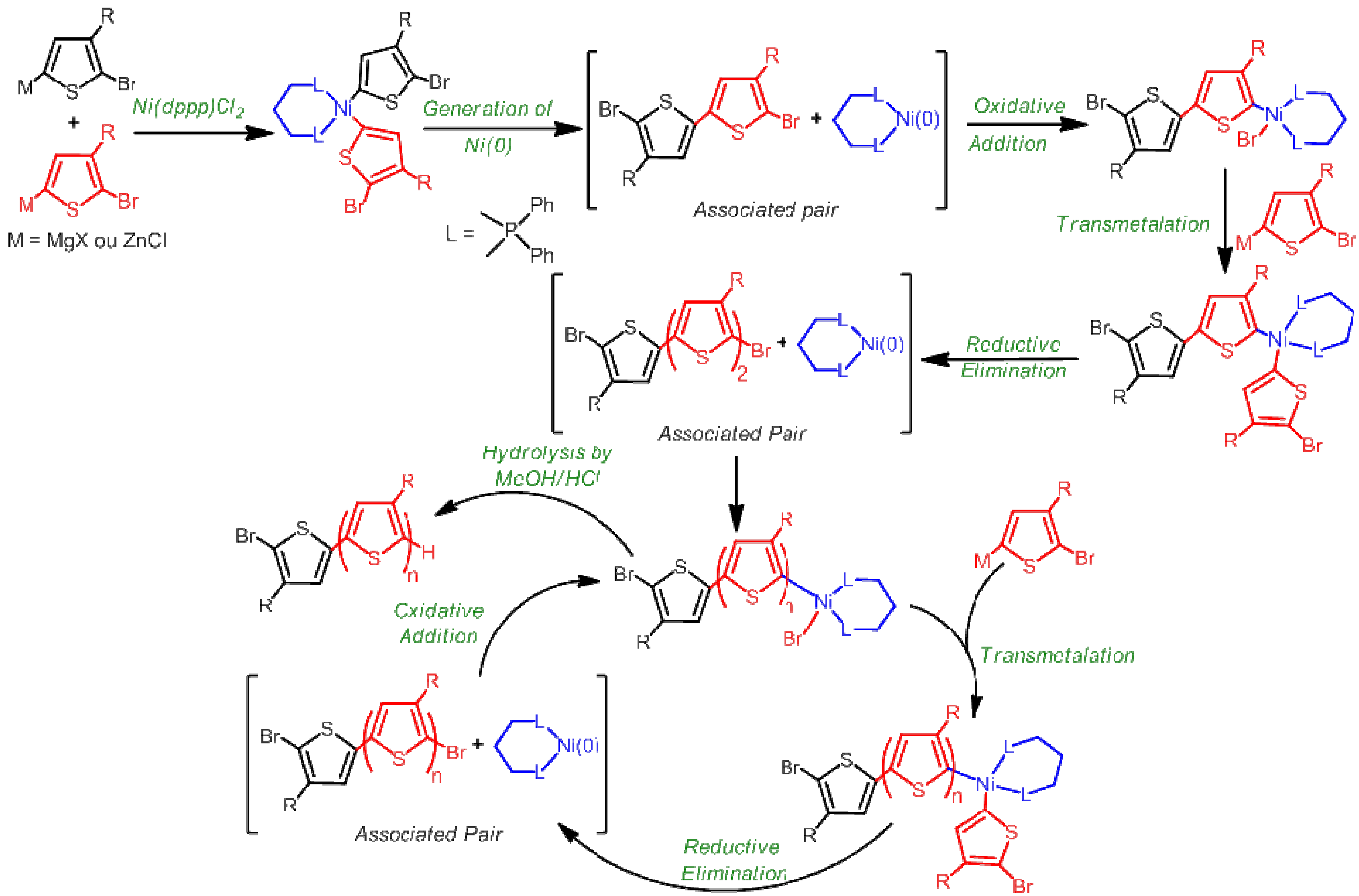
2TB



TQX



Controlled synthesis of P3HT via GRIM mechanism

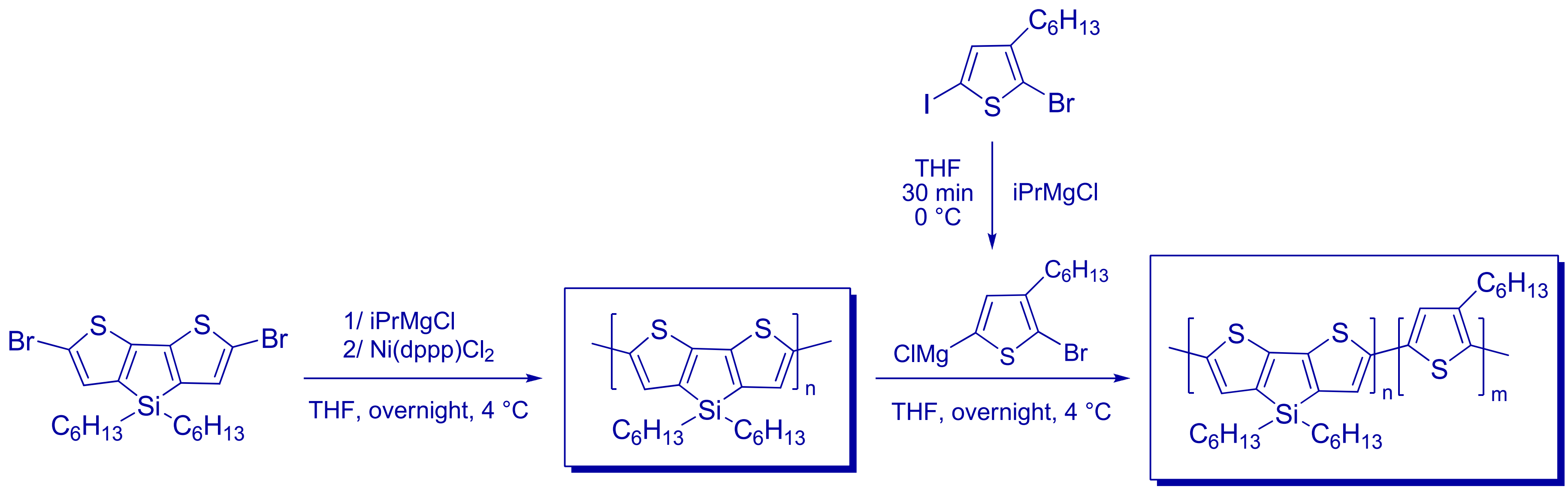


McCullough, R. D. et al. *Acc. Chem. Res.* **2008**, *41*, 1201272-1214.
Yokozawa, T. et al. *J. Am. Chem. Soc.* **2005**,, 17542-17547.

Tuning the optical and electronic properties by the block copolymer approach

Silole-based conjugated block copolymers

Poly(4,4-dihexyl-4*H*-silolo[3,2:b-4,5:b']dithiophene)-*b*-Poly(3-hexylthiophene) **P2**

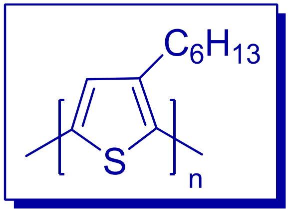


B1 **P2**

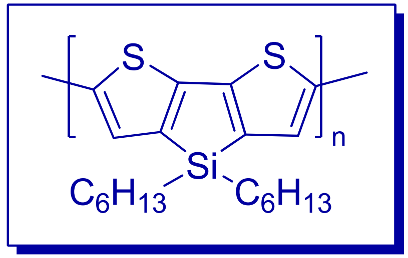
Entry	Si/3HT*	M_nGPC (g/mol)	Đ	λ_{max} (nm)
1	23/77	6000	1,3	507
2	38/62	34.000	2,1	596

(*) as determined by ^{1}H-NMR

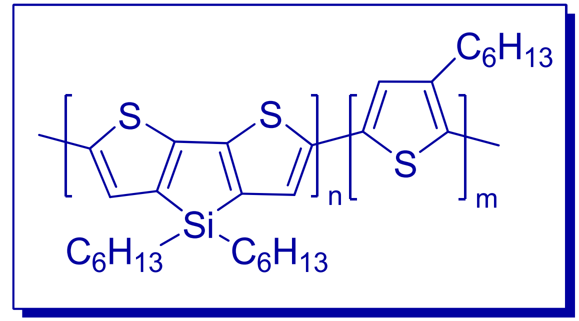
Silole-based (co)polymers : optical absorption properties



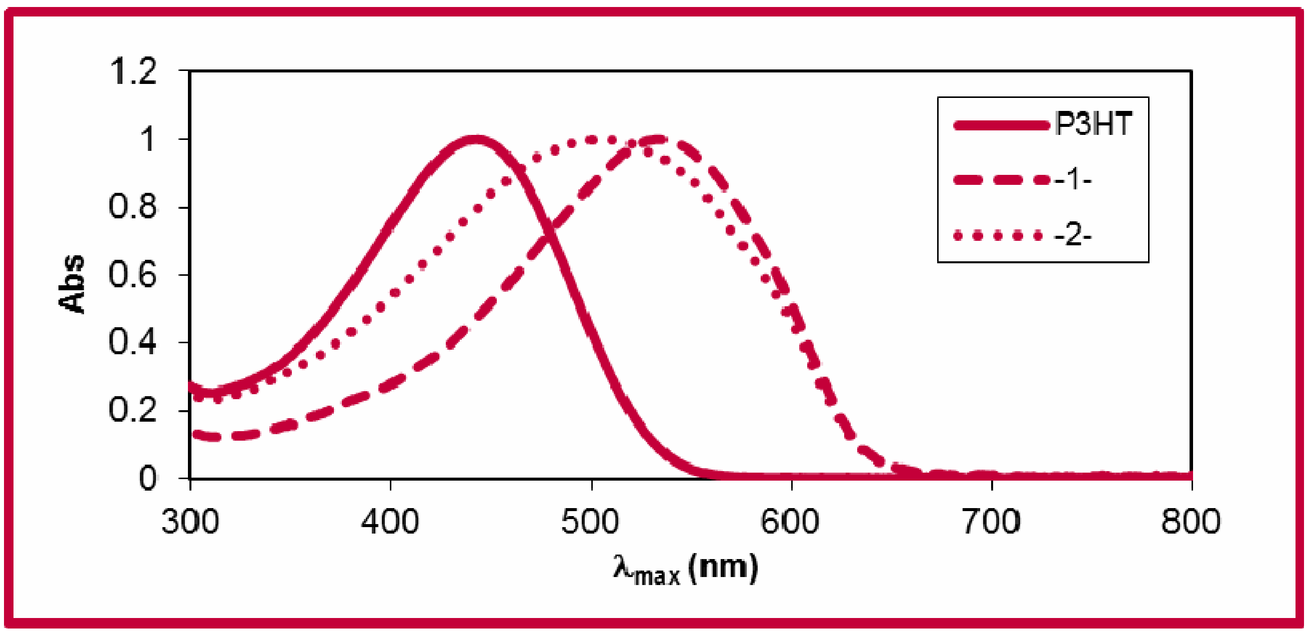
P3HT



P1



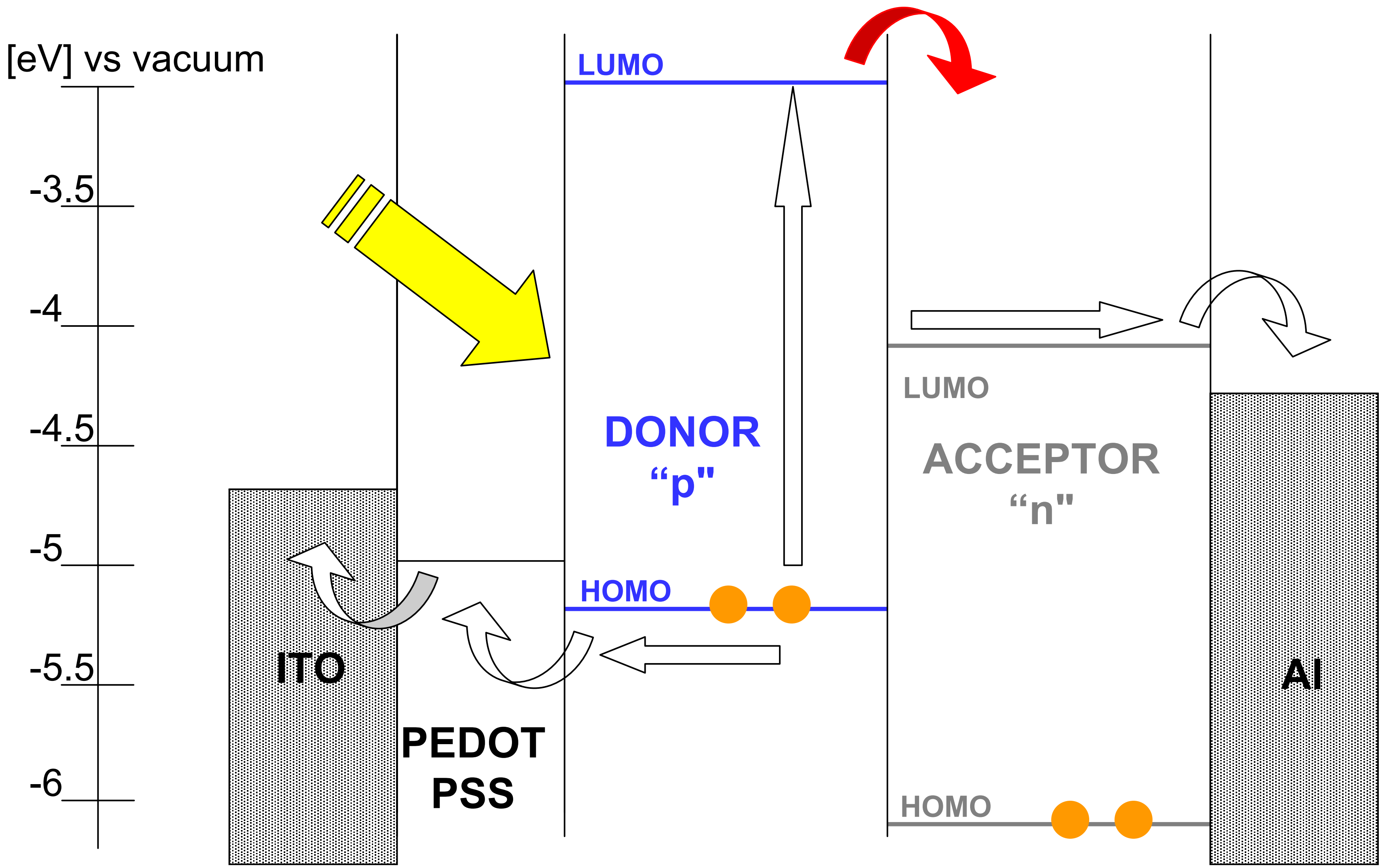
P2



The block copolymer has a broader absorption spectrum

Organic solar cell : charge generation

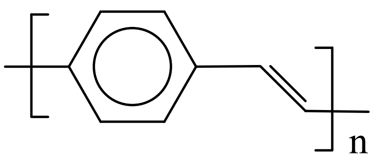
Gilles Dennler, KONARKA

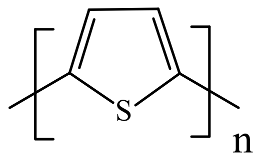


V_{oc} is set by LUMO(acc) - HOMO(don)

Binary donor-acceptor systems for organic PV

Electron donors





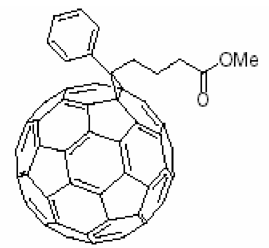
PPV or PT derivatives

Ionization potential is small

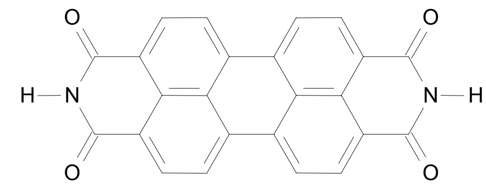
⇨ HOMO energy

(+ hole transport)

Electron acceptors



PCBM



Perylene

Electron affinity is large

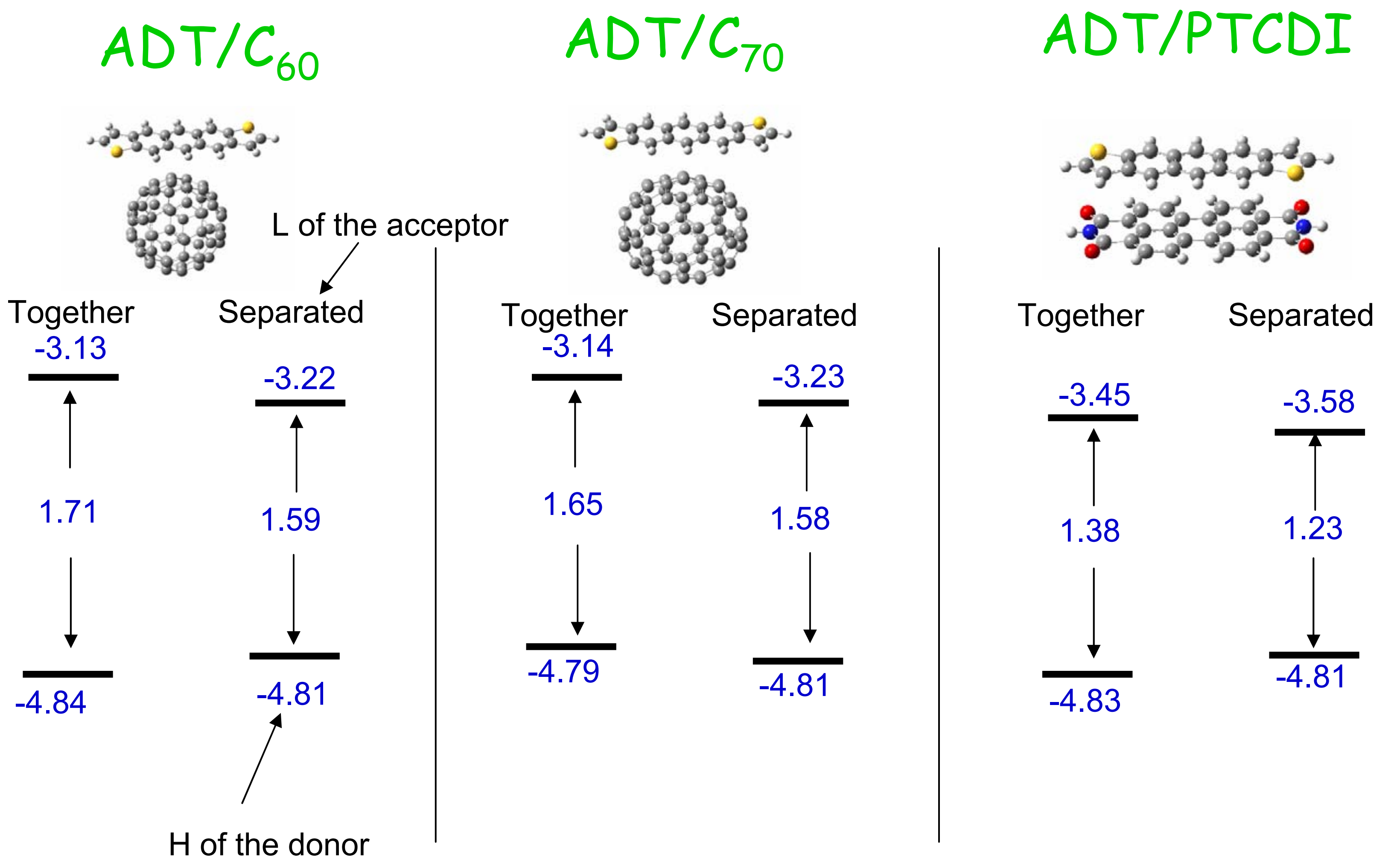
⇨ LUMO energy

(+ electron transport)

All organic PV devices are two-component systems

Charge separation takes place at the D-A interface

Electronic structure at the donor/acceptor interface



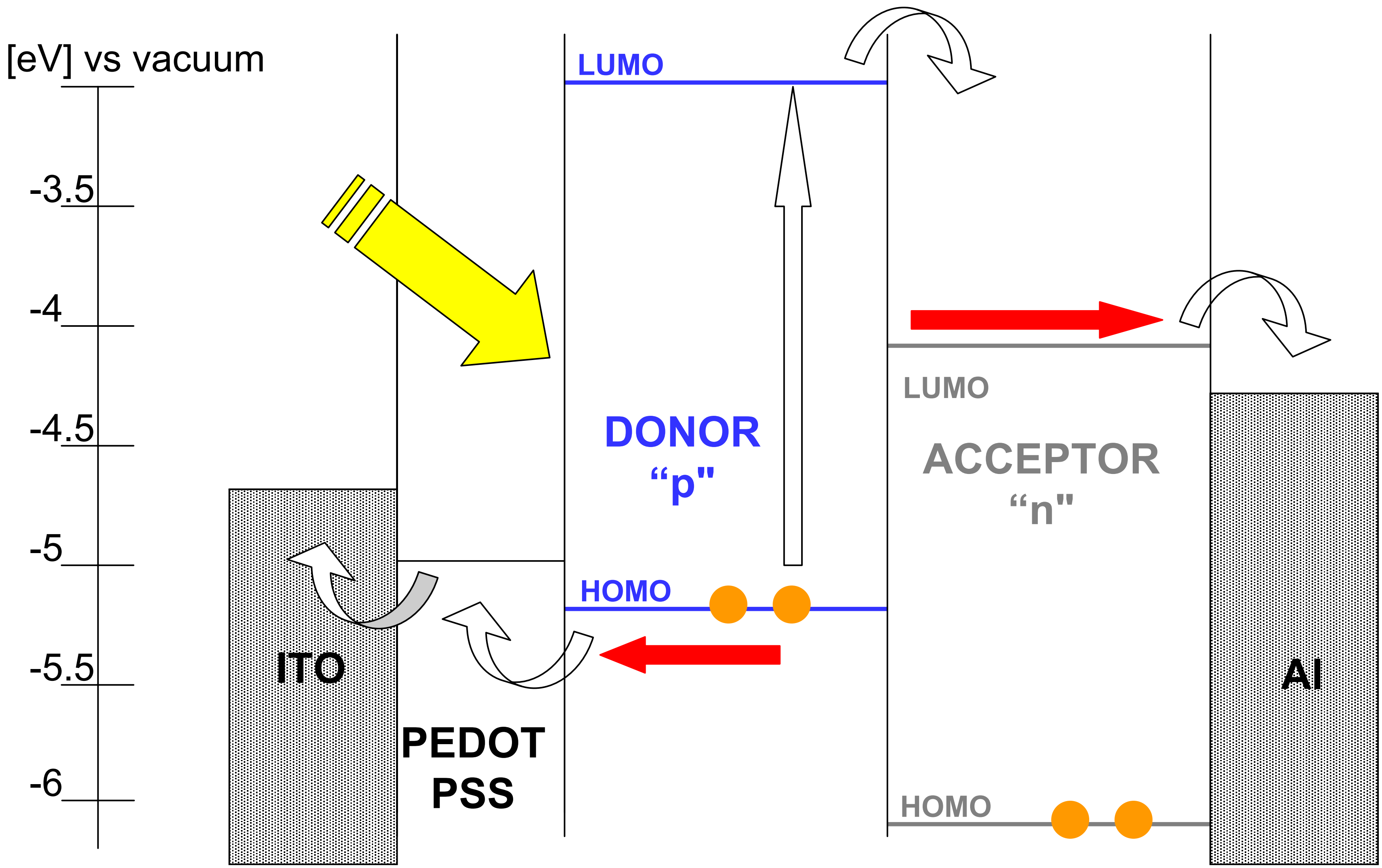
At 4 Å, there is no big shift of the HOMO and LUMO levels of the donor and the acceptor due to the polarization effect.

with Y. Geerts at al.

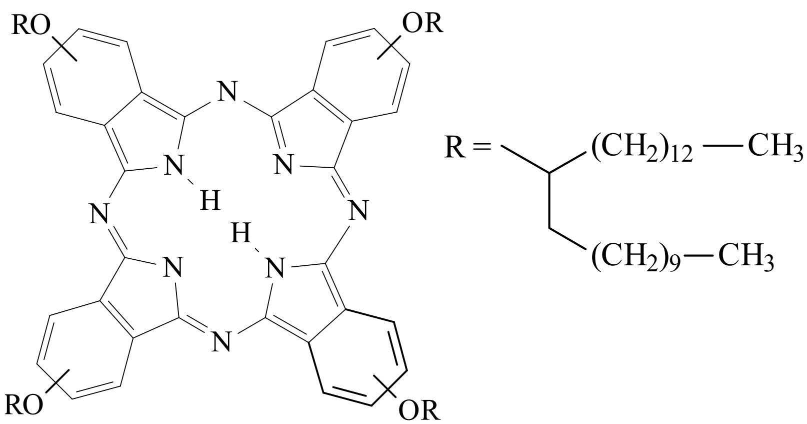
Opt: DFT (B3LYP/6-31G(d,p))

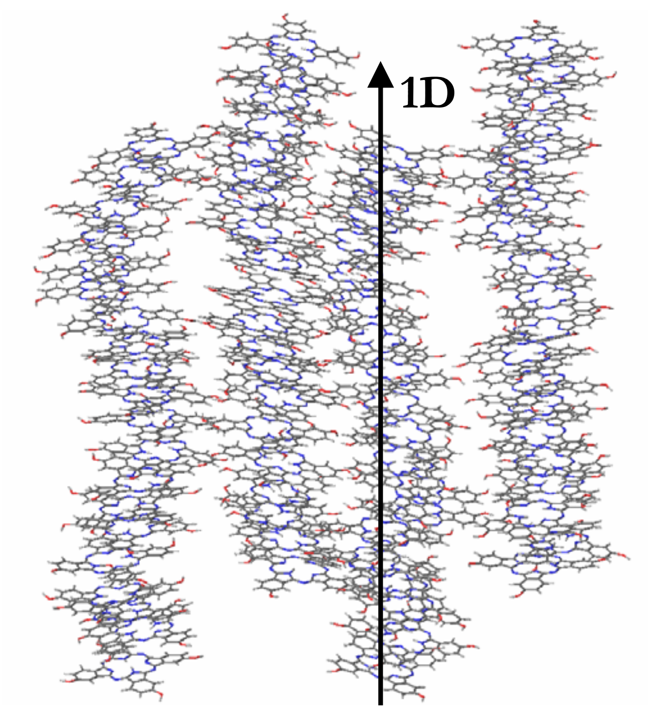
Organic solar cell: charge transport

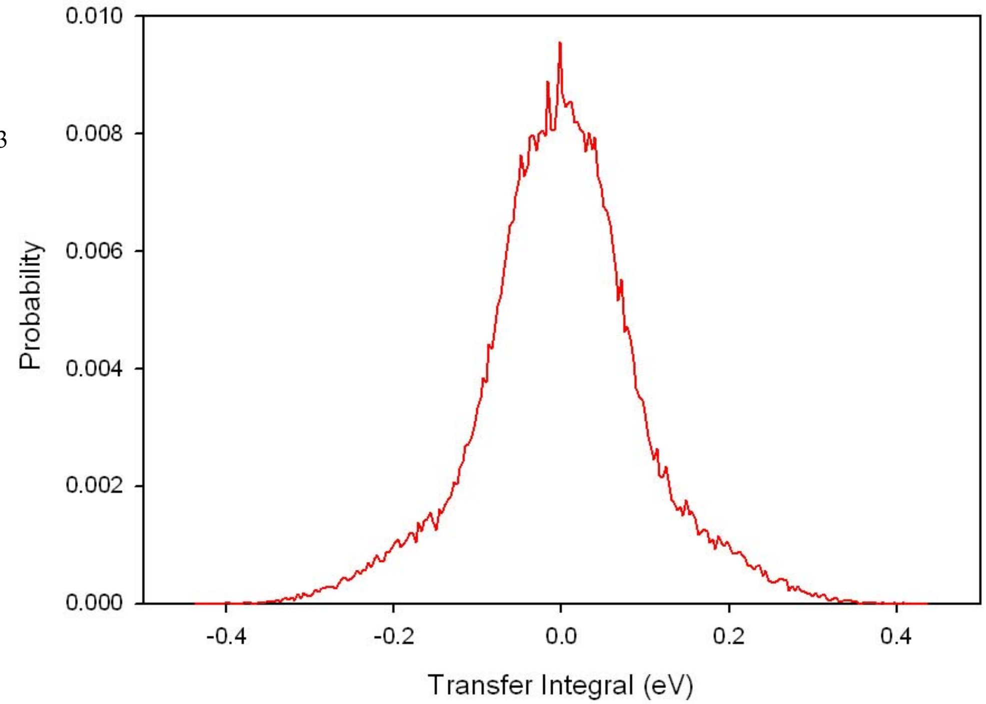
Gilles Dennler, KONARKA



Modeling the supramolecular organisation and charge transport properties







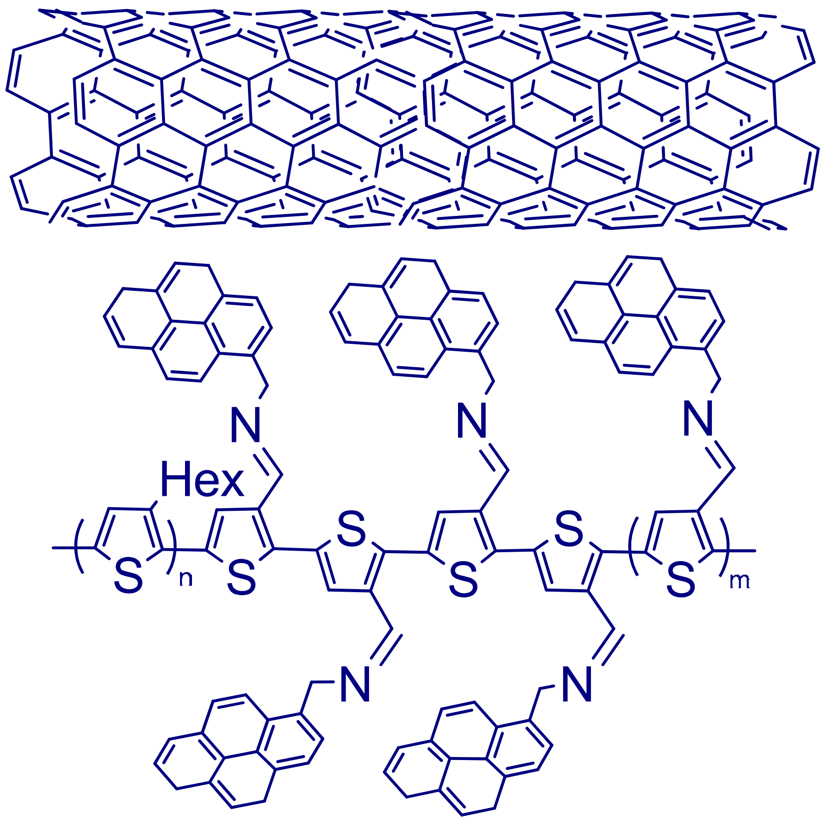
Static stack: μ=0.0135 cm²/ V s

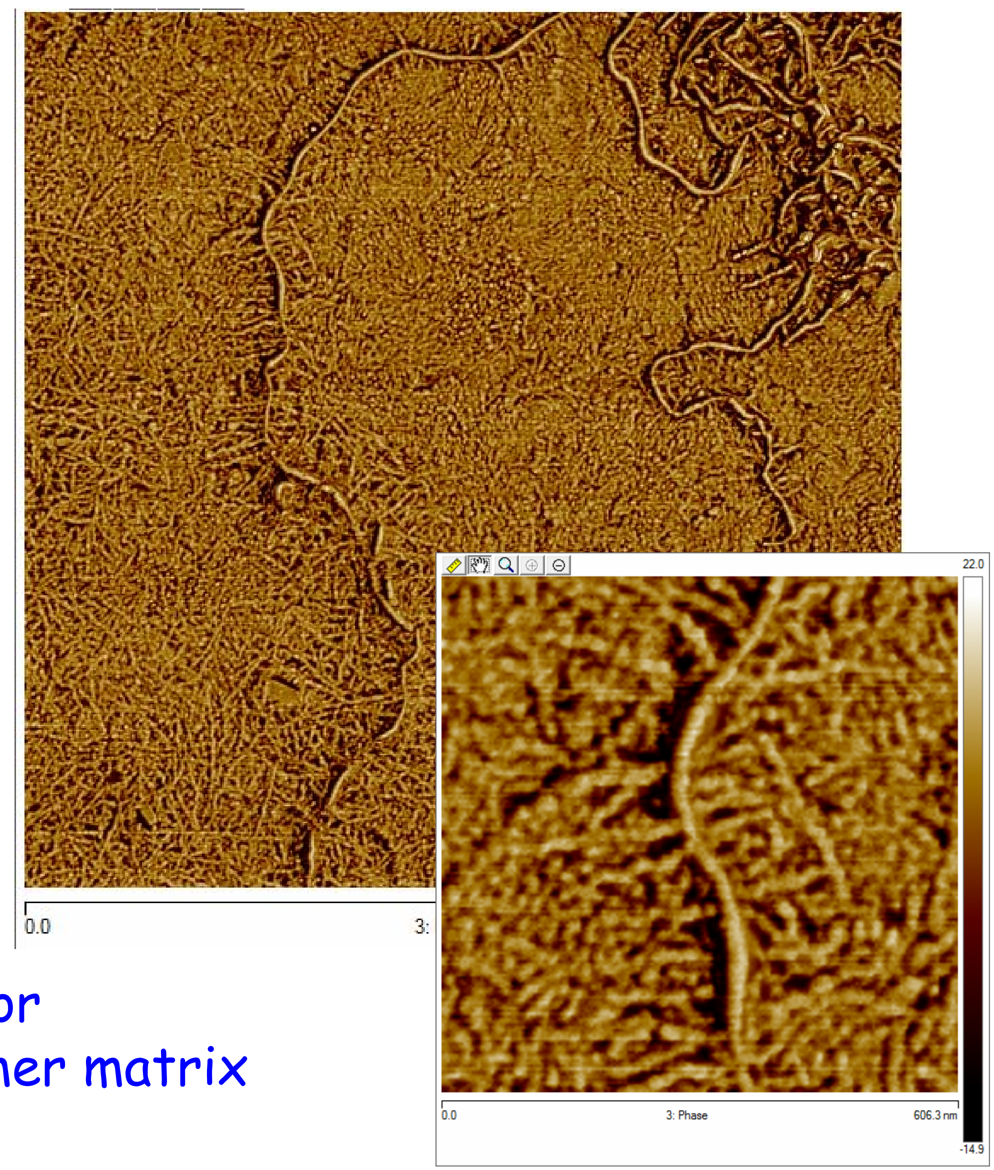
Dynamic stack: μ=0.17 cm²/ V s

Increase in charge carrier mobilities due to dynamical motion

with Y. Geerts at al.

Carbon nanotubes as additives to favor charge transport in organic photovoltaic cells

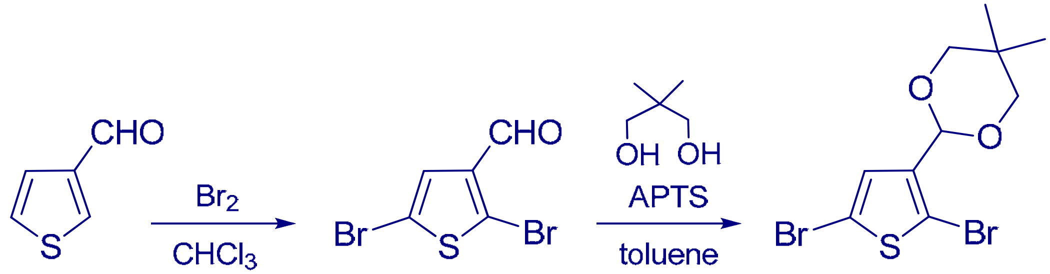




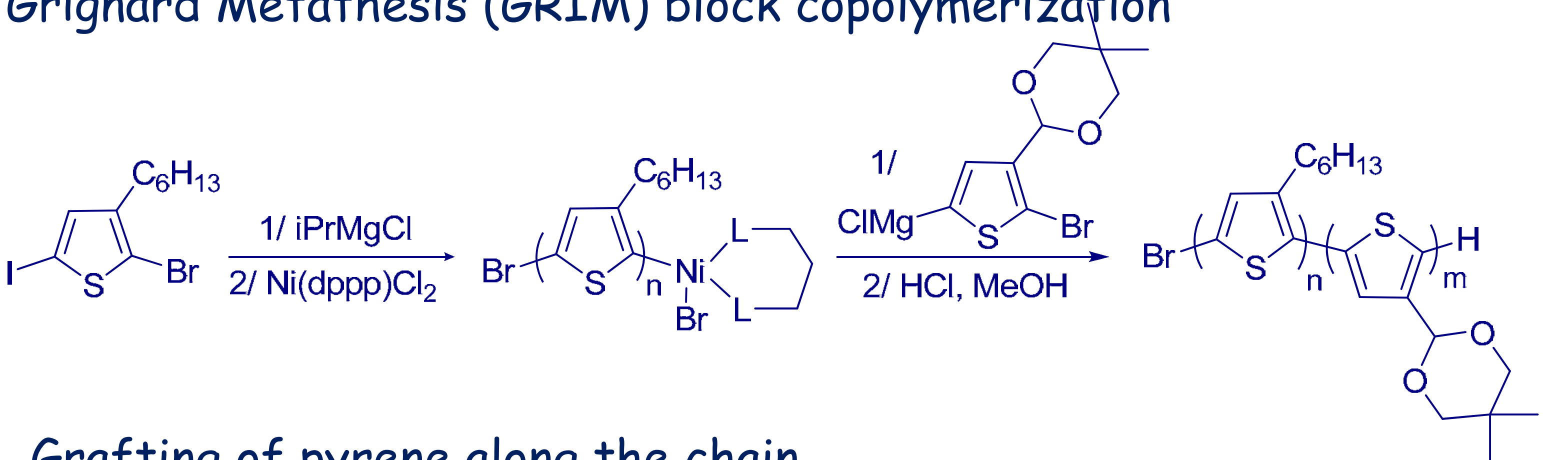
Pyrene-functionalized P3HT to favor
CNT dispersion in conjugated polymer matrix

Synthesis of P3HT-pyrene copolymer

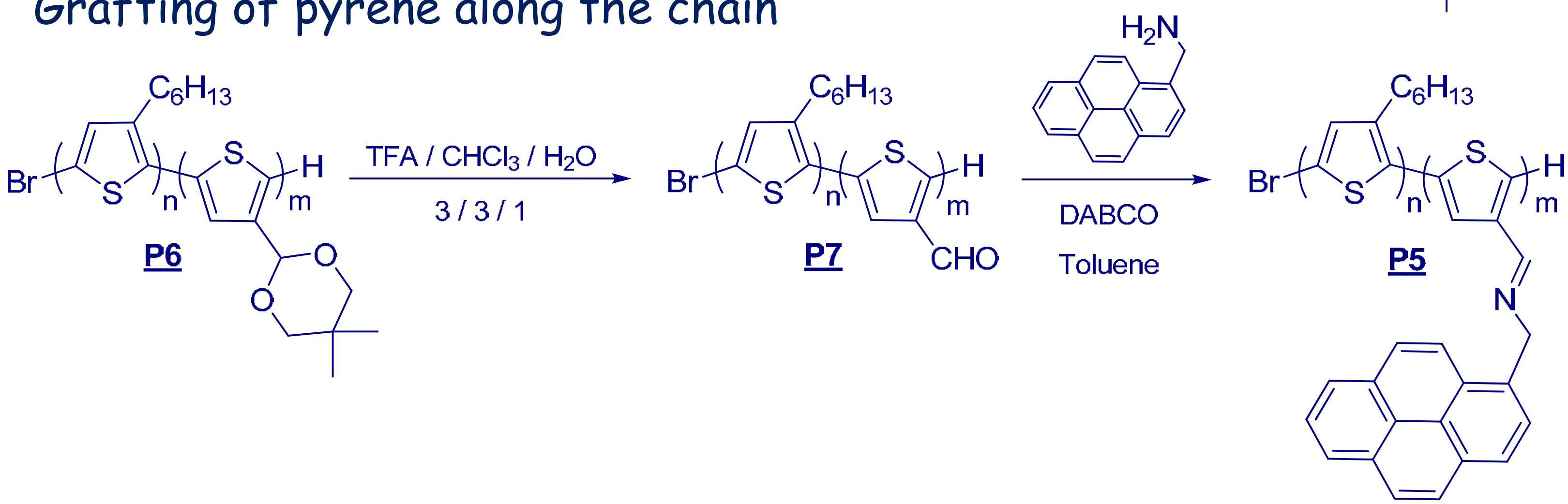
Monomer



Grignard Metathesis (GRIM) block copolymerization

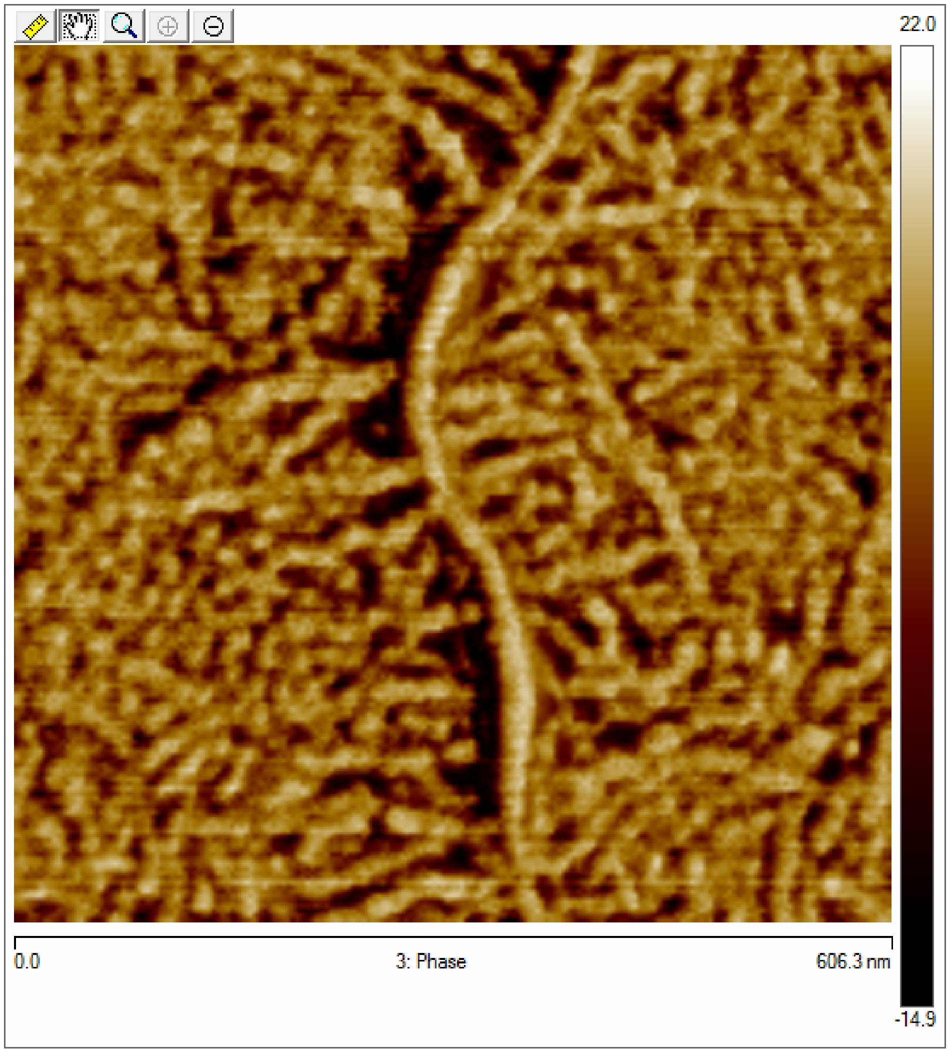


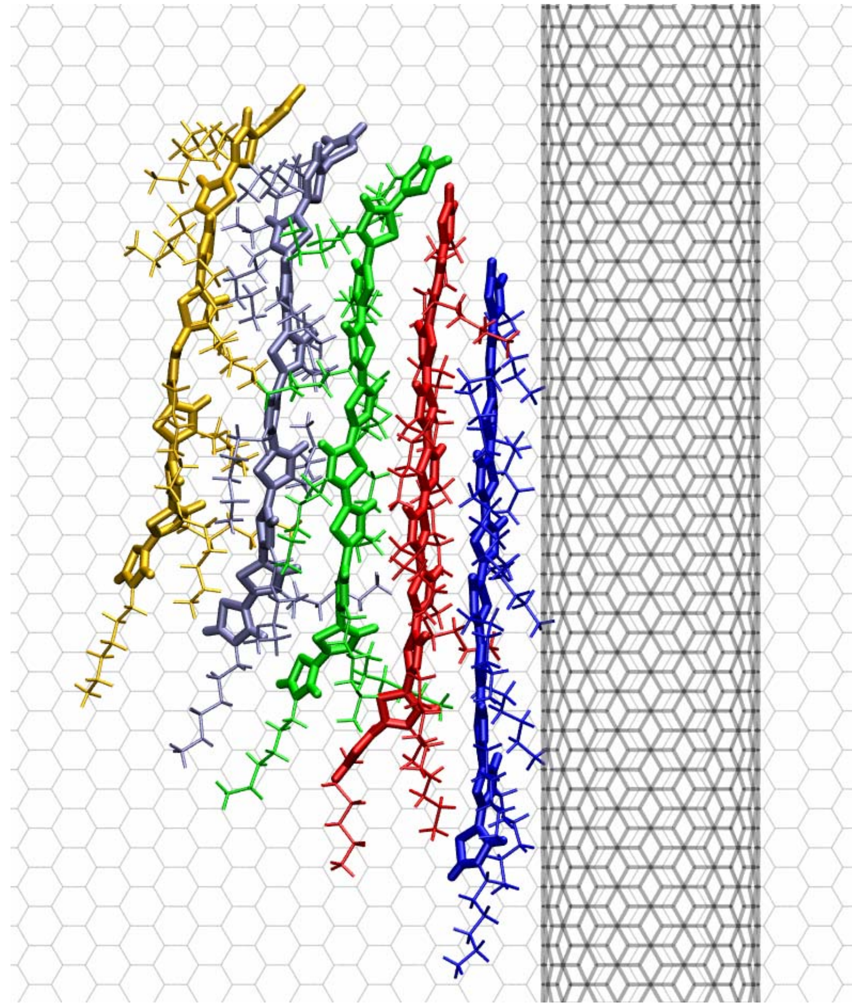
Grafting of pyrene along the chain



Modeling the nanotube/ conjugated polymer interface

P3HT chains interacting with a SWNT





The P3HT fibrils tend to arrange perpendicular to CNT axis

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Tailored synthesis of polymer semiconductors: SMPC
Thin film morphology and electrical properties : SCMN
Microstructured layers for light management: Influx
Novel materials for electrodes: ChIPS

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- ULB (Y. Geerts), UCL (S. Melinte), ULg (C. Jérôme),…