Functional Materials for Energy Conversion and Storage

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https://lppi.cyu.fr www.cyu.fr/thanh-tuan-bui

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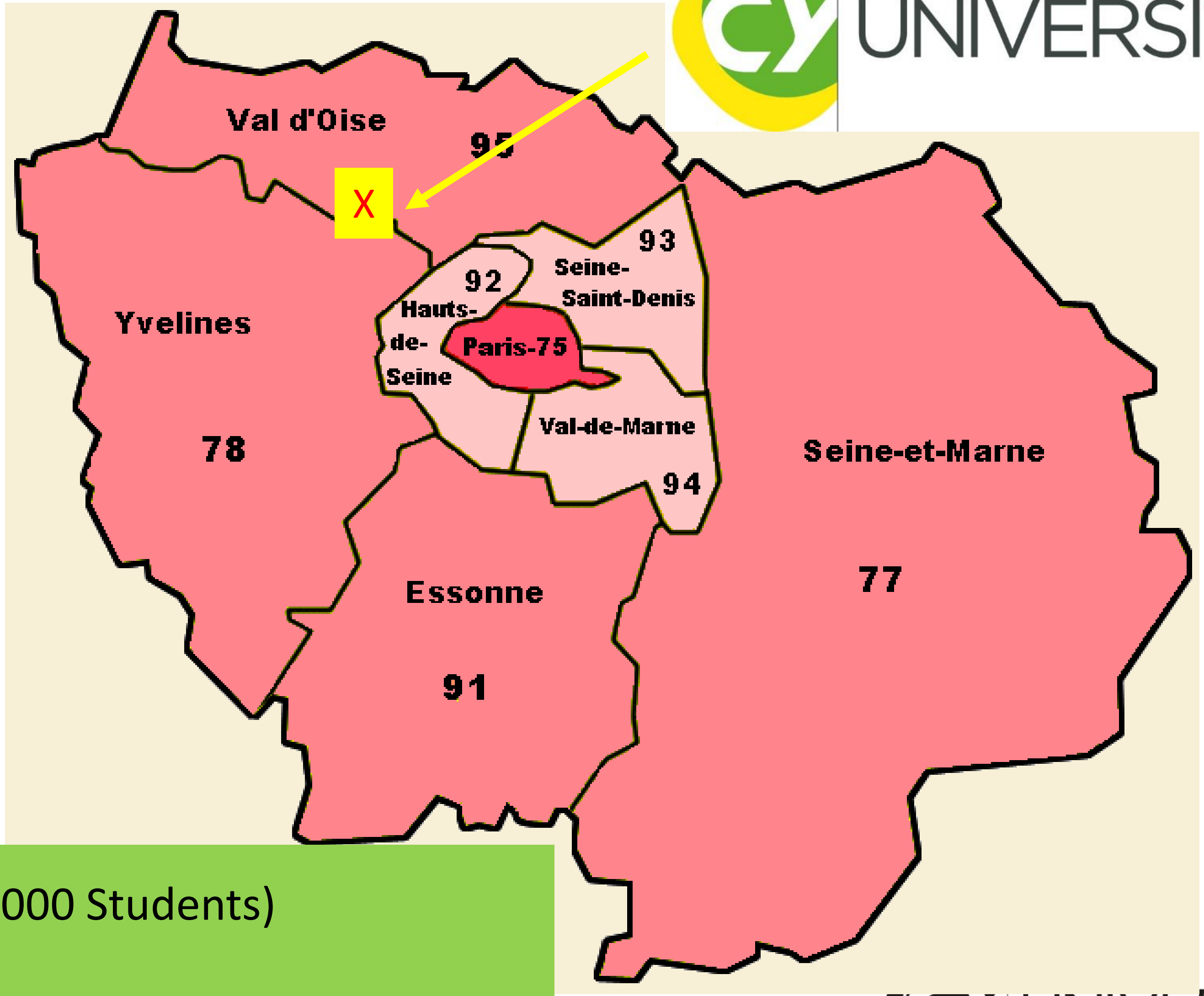
About our university

France

Paris area



Public national university in Paris area (≈ 25 000 Students)

West of Paris, ~ 30 km from Paris center

About our university

23 research units: 2 chemistry institutes

(i) biochemistry

(ii) <u>polymer chemistry</u>

Laboratory of Physicochemistry of Polymers and Interfaces (LPPI)

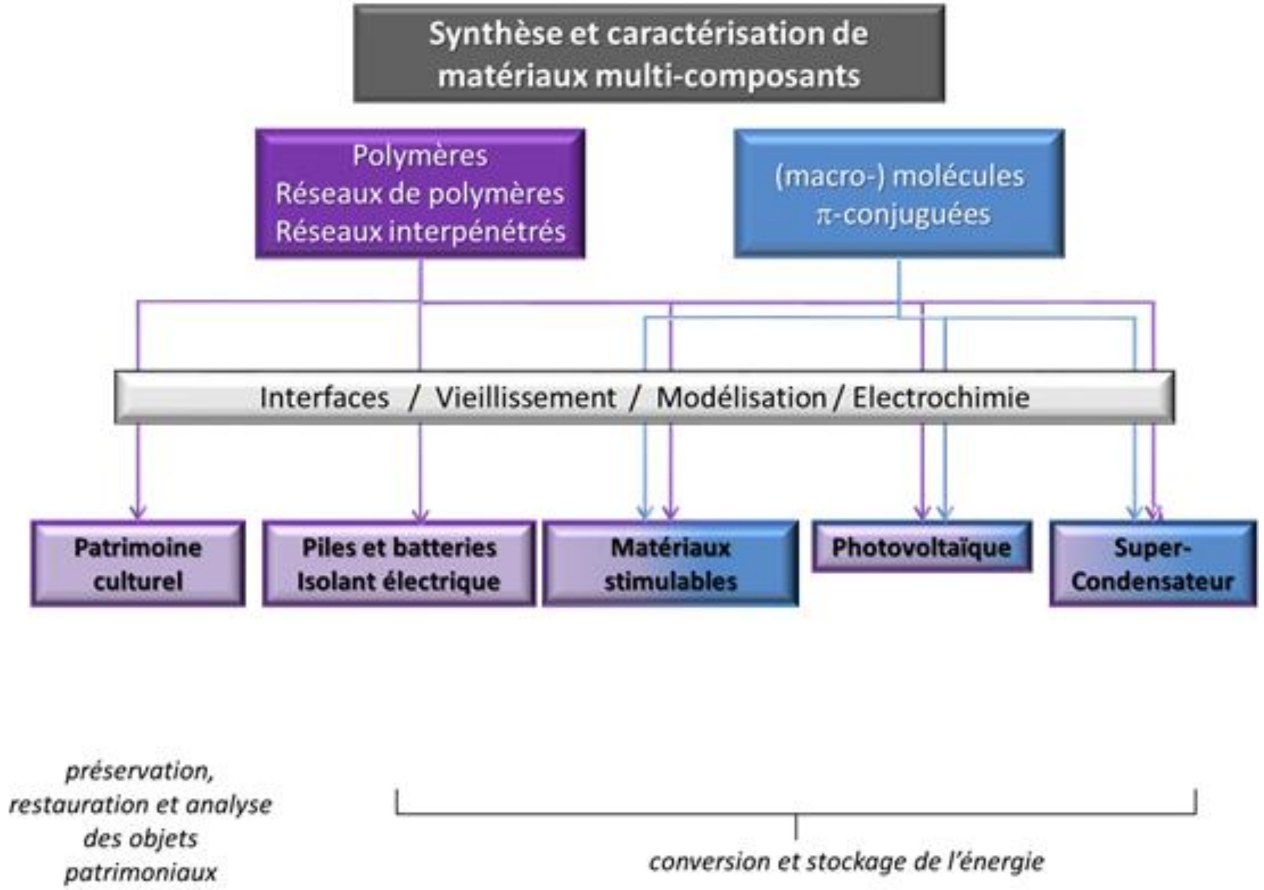
https://lppi.cyu.fr

Permanent staff: 20
(5 Full Prof, 11 Assoc. Prof,
2 Lecturer + 4 Technical staffs)

Total : ≈ 50

PhD Students & Post-docs: 20-30
Undergrad: 10-20

Research in our institute



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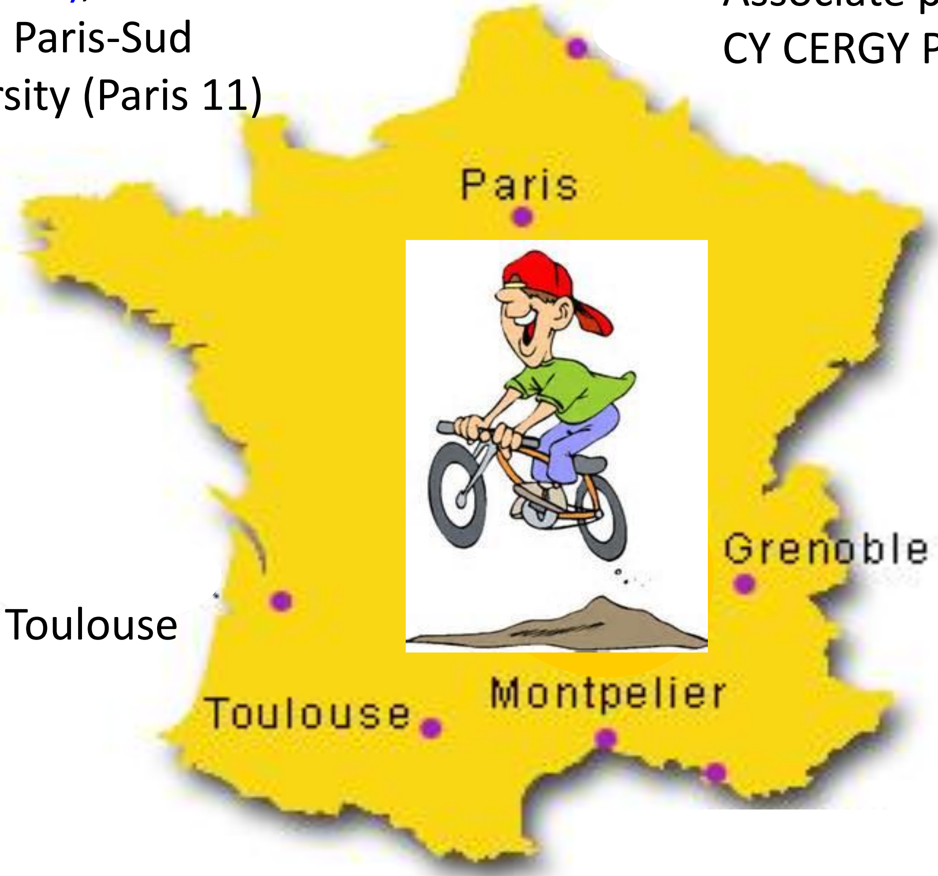
About me

1983: Born (1983) and grown up in Phu Tho, Vietnam

Education

BSc (2004), **MSc** (2005) Paris-Sud University (Paris 11)

PhD (2010)
University of Toulouse



MS (2007)
ENSCM Montpellier

Professional Career

Since 09/2013:
Maître de conférences
Associate professor
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Postdoc + Lecturer (2011-2013)
University of Cergy Pontoisr

Postdoc (2011)
University of Grenoble

Research stays: Germany, Poland, Japan, China, Korea (from 1 – 4 months)

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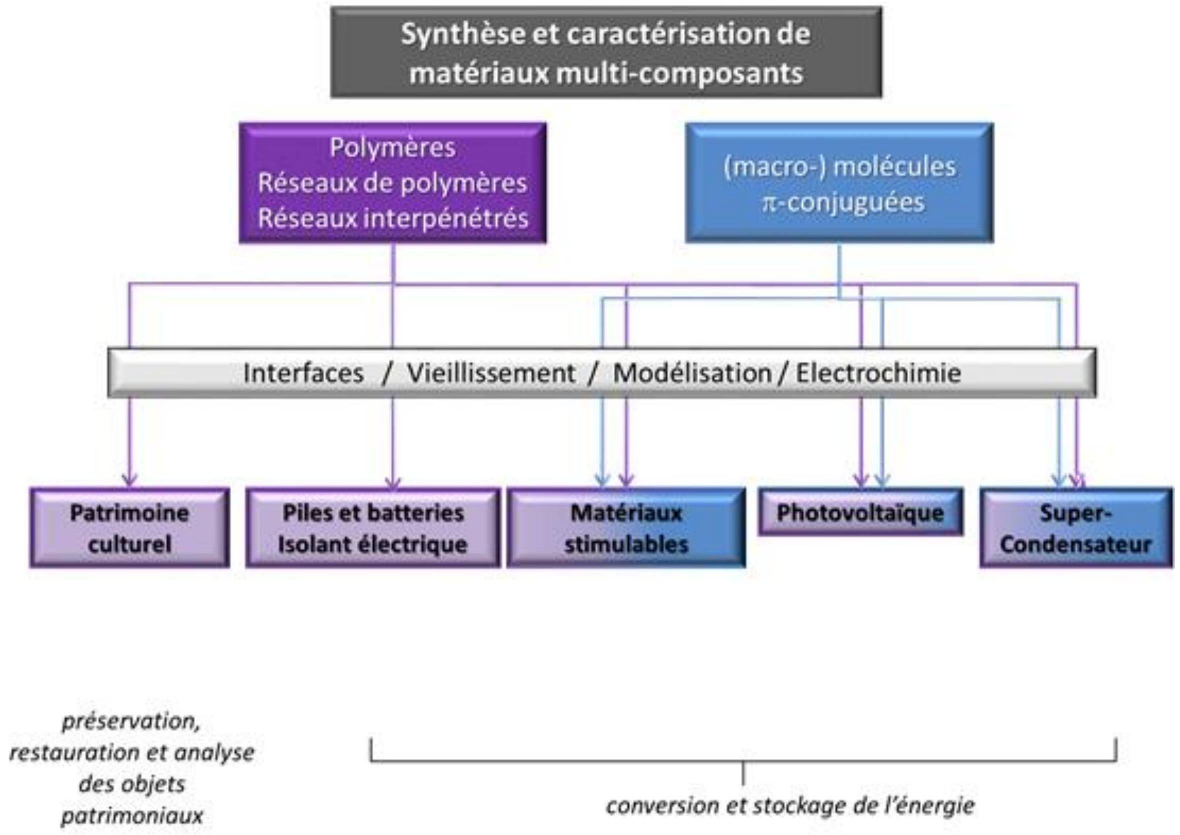
About my research

Functional Materials for Energy Conversion and Storage

Main Topics

1. **Organic materials for Organic and Hybrid Photovoltaics:** dye sensitized solar cells, perovskite solar cells, organic photovoltaics, charge transporting materials (hole, electron), interfacial materials, dopant
2. **Organic photoinitiator for polymerization**
3. **Conjugated materials for organic thermoelectrics**
4. **Organic materials for rechargeable organic batteries**



Other Topics

Flexible conductive polymer electrodes for flexible, Flexible and Wearable Electronics

Perovskite based composites for humidity sensing

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Do it yourself, but don't do it alone

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LPPI laboratoire de physicochimie des polymères et des interfaces

- Design, Synthesis, Structural characterization
- DFT calculation
- Characterization: Thermal, Morphological, Optical, Electrochemical properties (AFM, SEM, Raman, SEM/RAMAN, CLMS)…..
- Basic solar cells device making/characterization

Main active collaborations

Swansea University Prifysgol Abertawe

Prof. T. Watson,
Prof. M. Carnie
et al.

大阪大学 OSAKA UNIVERSITY

Prof. A. Fujii,
Prof. M. Ozaki, et al.

成均館大學校 SUNG KYUN KWAN UNIVERSITY

Prof. N. G. Park
et al.

Institut de Recherche de Chimie Paris (IRCP)

Prof. T. Pauporté, et al.

University of California Santa Barbara

Prof. Thuc-Quyen Nguyen

UNIVERSITÉ HAUTE-ALSACE

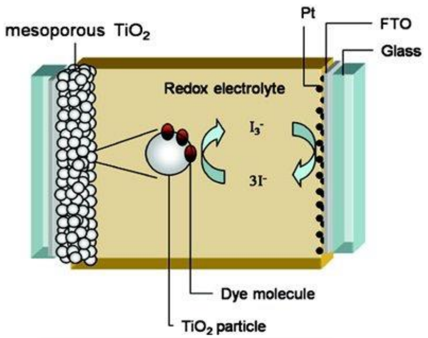
Prof. J. Lalevée, et al

CHIANG MAI UNIVERSITY

Dr. N. Kungwan, et al.

Hybrid solar cells: from DSSCs to perovskite solar cells

Dye-sensitized solar cells (DSSC)

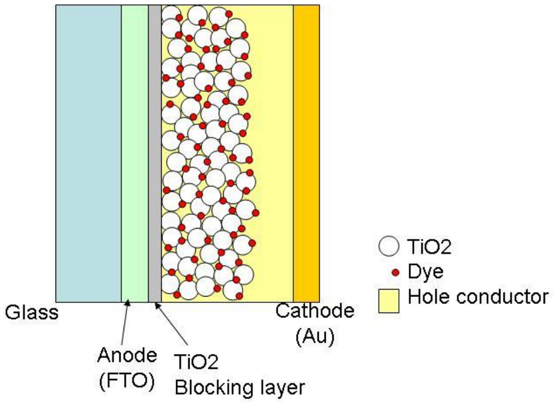


Gratzel, Nature 1991

Replace liquid electrolyte by a organic solid hole conductor

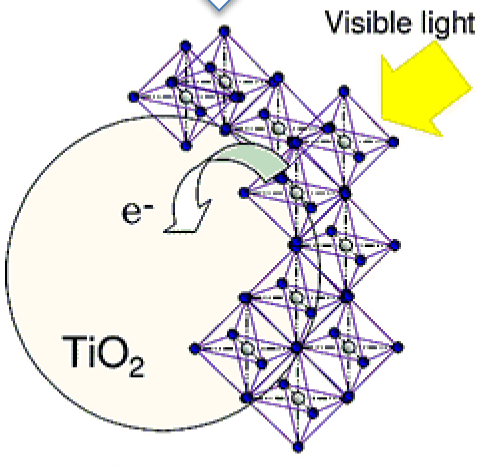
Gratzel et. Nature 1998

Solid state DSSC



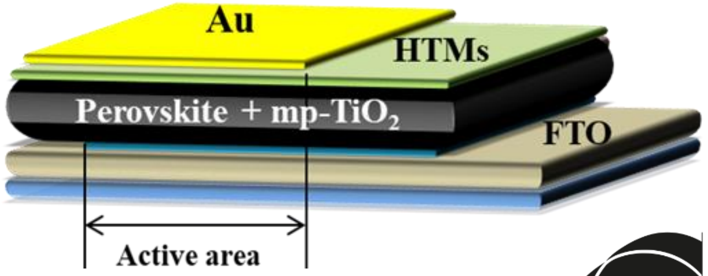
Miyasaka, et al. JACS 2009

Replace molecular dyes by hybrid perovskites



Perovskite nanocrystalline sensitizers

Halide Perovskite Solar Cells (HPSC)



Park, Gratzel, et al. Sci. Rep. 2012
Snaith et al., Science 2012

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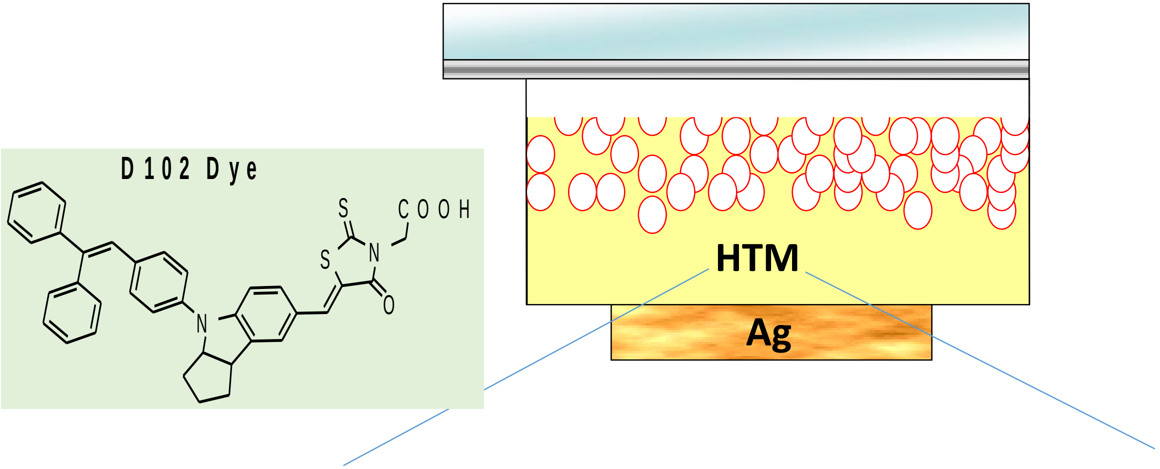
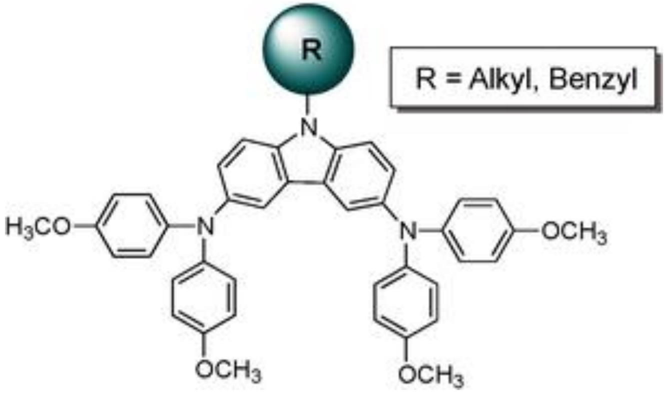
Organic Charge Transport Materials for Hybrid Solar Cells

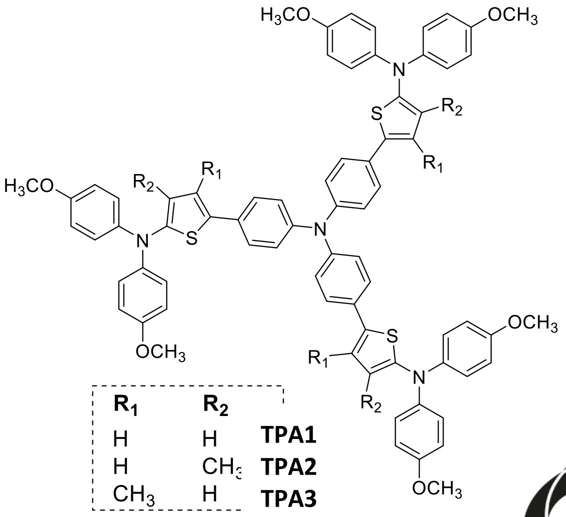
From Solid State DSSCs … to Peroskite solar cells



Triphenylamine based HTM

Carbazole based HTM





ChemNanoMat **2015,** 1, 203 – 210

RSC Adv. **2015,** *5*, 49590

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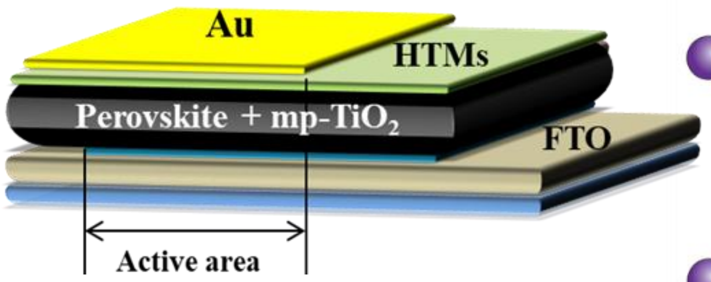
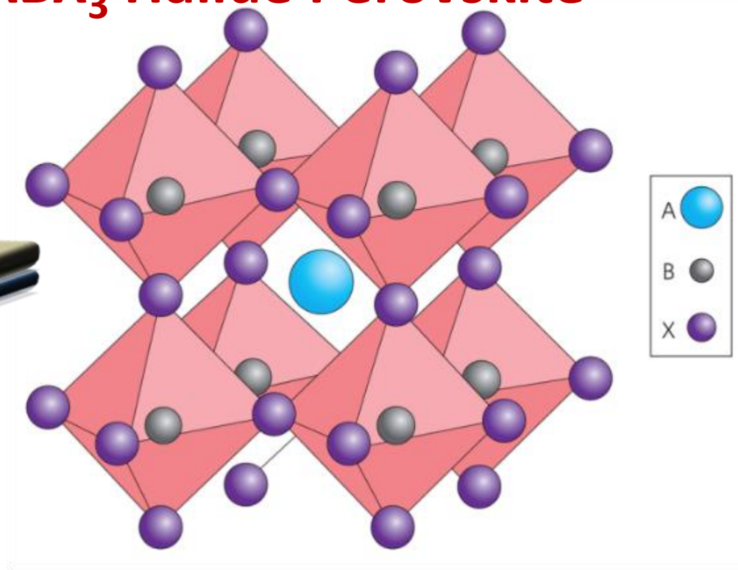
The halide perovskite materials



3D ABX_3 Halide Perovskite



A^+ cation:
MA^+: Methylammonium ($CH_3NH_3^+$)
FA^+ : Formamidinium, ($H_2N\text{-}CH\text{=}NH_2^+$)
Cs^+

B^{2+} cation
Pb^{2+},Sn^{2+},Ge^{2+}

X^- halide anion:
Cl^-,Br^-,I^-

Goldschmidt tolerance factor of ABX_3 structure

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$

Result at 0.8 ～1.0 range, it will be formed black photoactive and stable phase.

- Direct bandgap
- Tunable ($I^- \rightarrow$ 1.5-1.6 eV)
- CBM/VBM position

- Low exciton E_b <10 meV
- High charge mobility/ Diff. Length (1 μm)
- Preparation at low T°C (~ 100°C)/ solutions

New halide perovskite materials (2D, lead-free, earth-abundant element, etc.)

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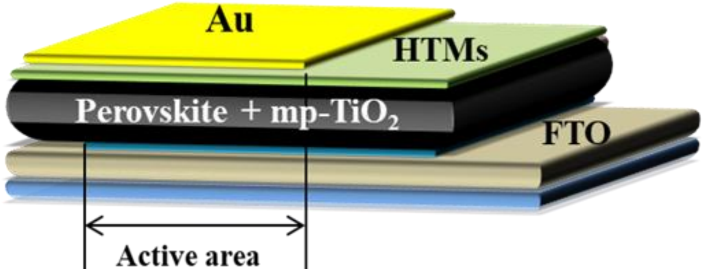
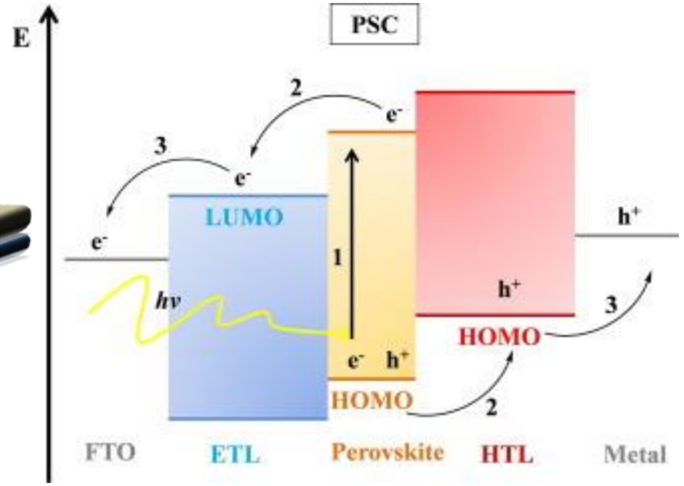
PSC's components

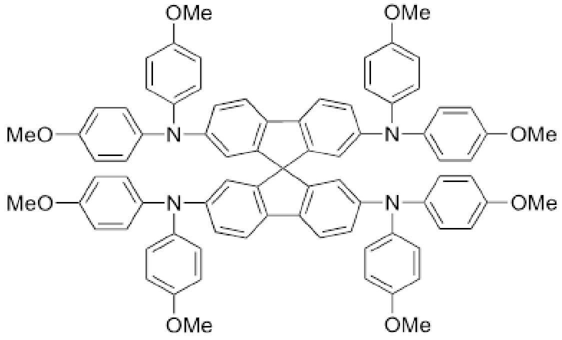




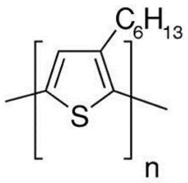
Organic HTM

- HOMO/LUMO Energy levels / Perovskite
- Mobility
- Morphology
- Processability
- Stability

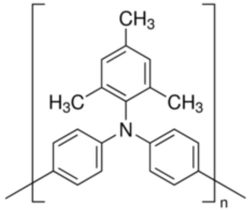
Molecular *vs* polymeric HTM for perovskite solar cell application



Spiro-OMeTAD



P3HT



PTAA

Molecular HTMs :
good reproducibility; well-defined molecular weight and structure.

Polymeric HTMs :
processability, thermal and mechanical stability, and higher intrinsic hole mobility.

Organic HTM

⇩

- Improving the stability
- Lowering the fabrication cost
- Understanding the electrical response

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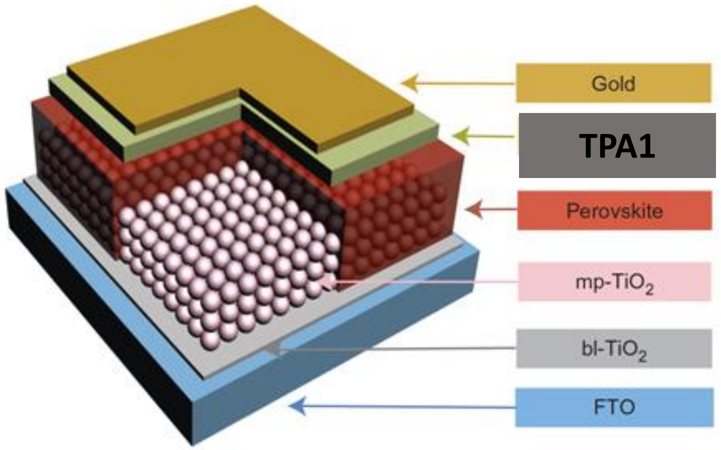
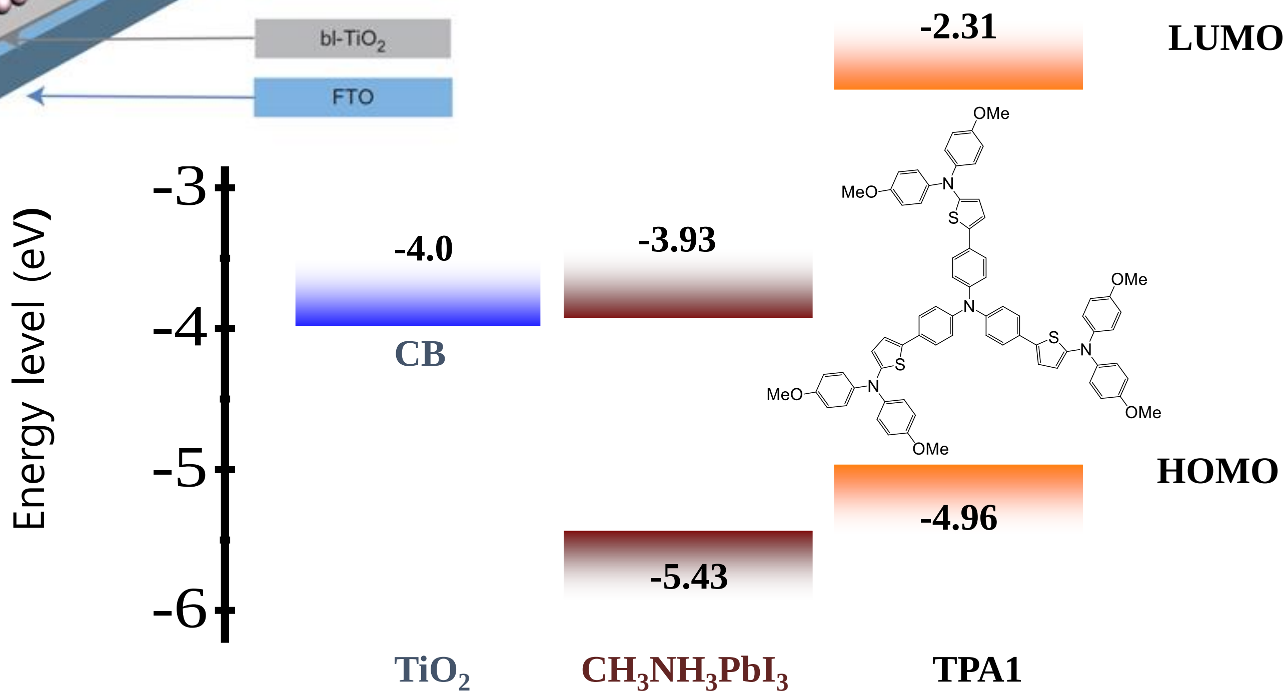
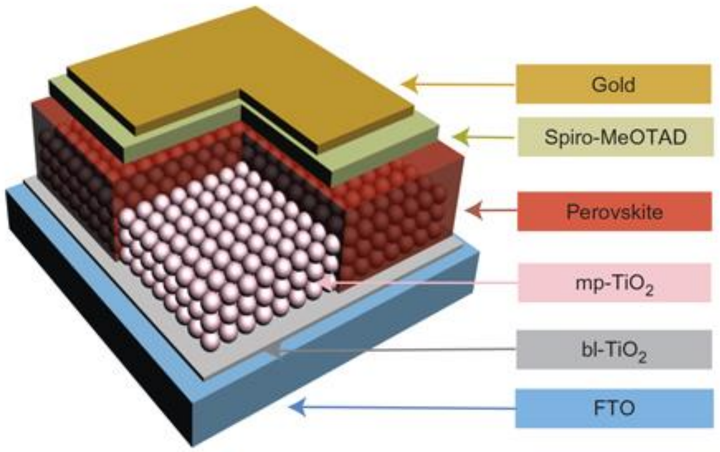
TPA as HTM on Perovskite Solar cell



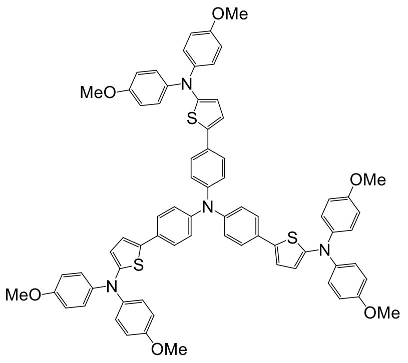


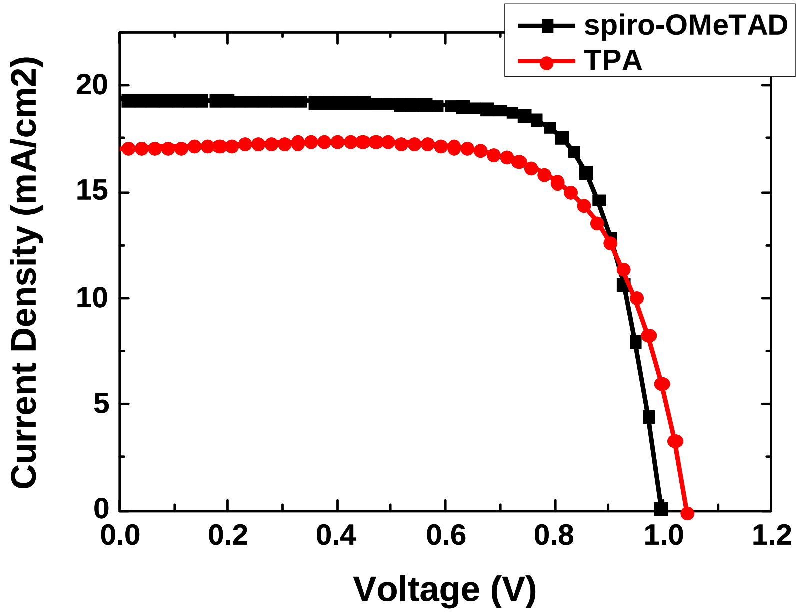
Coll. N.-G. Park, Sungkyunkwan Univ (Suwon, Korea)
RSC Adv 2016,

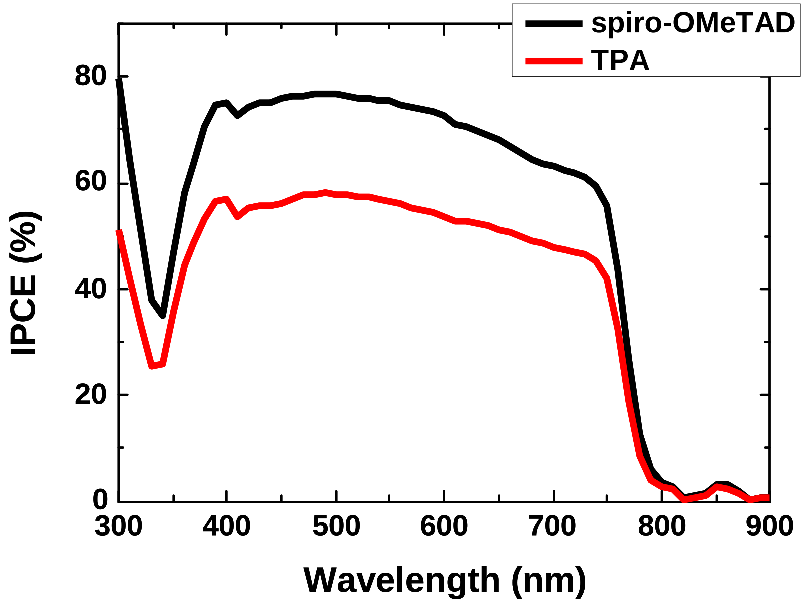
TPA as HTM on Perovskite Solar cell



$FTO/TiO_2/CH_3NH_3PbI_{3-x}Cl_x/HTM/Ag$







Coll. N.-G. Park,
Sungkyunkwan Univ (Suwon, Korea)
RSC Adv 2016,

	Jsc	Voc	FF	η
Spiro-OMeTAD	19.384	0.9945	0.7405	14.28
TPA	17.037	1.0432	0.7012	12.46

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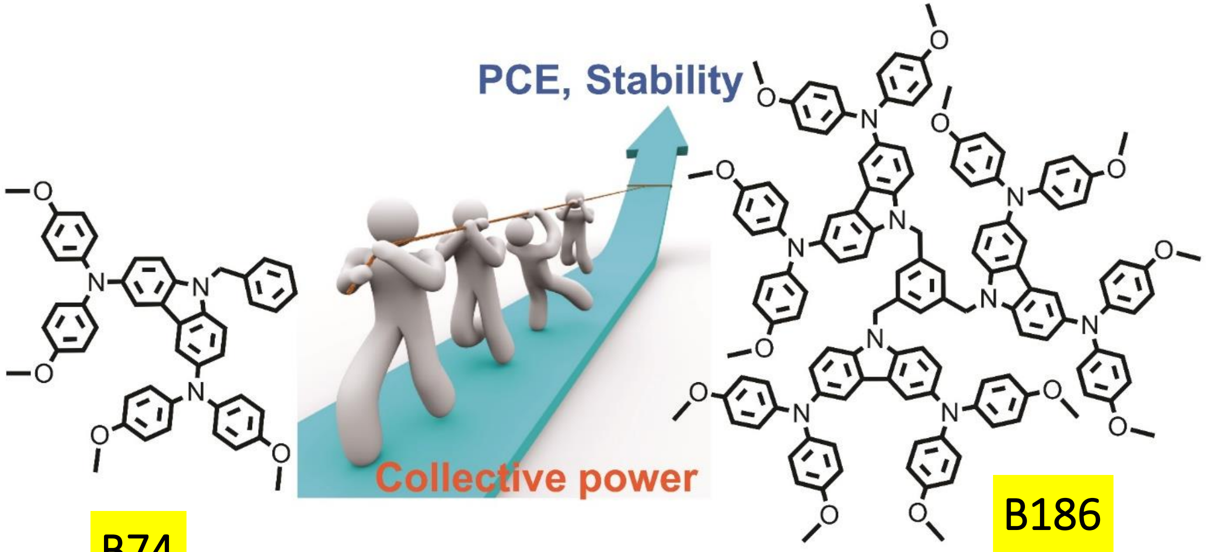
Carbazole-based HTMs



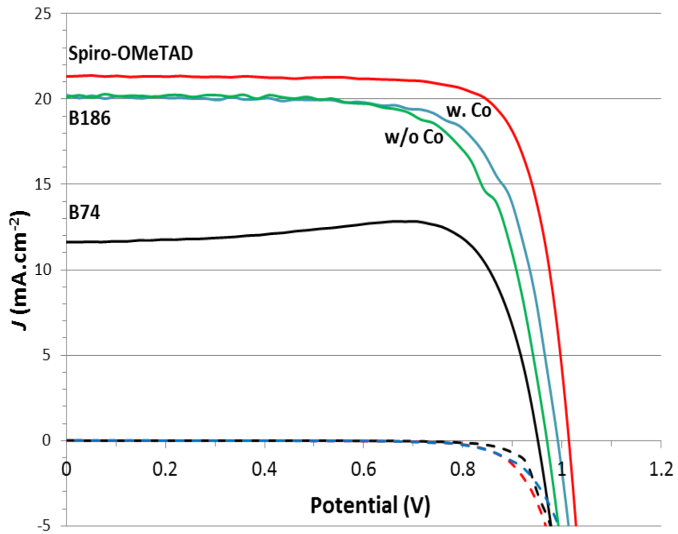
B74

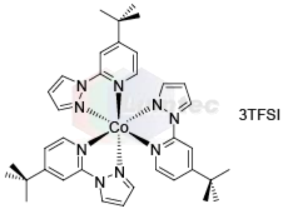
B186

(a)

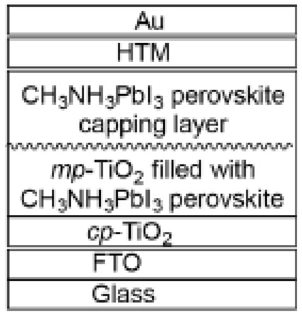
(b)

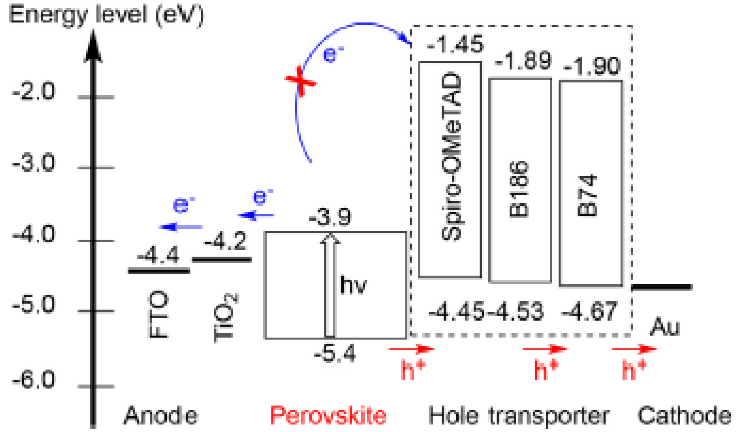
reverse scan direction





FK209 Co(III) TFSI Salt





Chimie Paris ParisTech

IRCP Institut de Recherche de Chimie Paris

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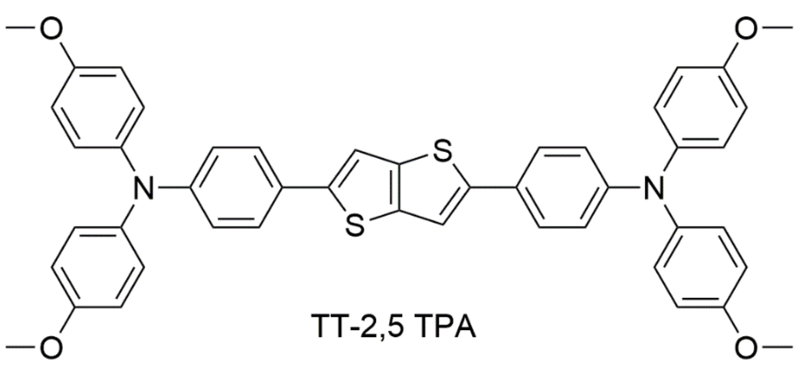
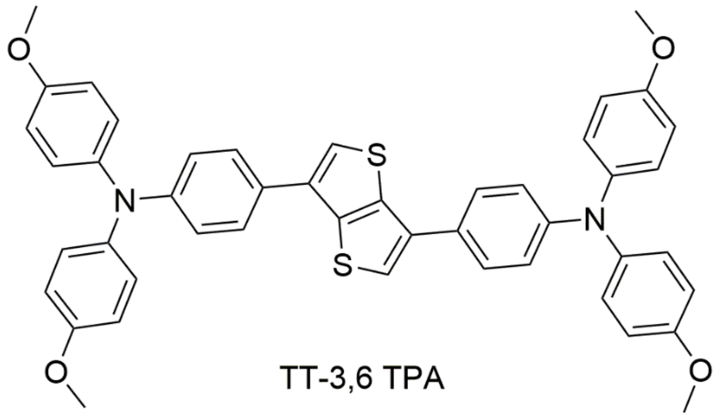
Org. Electron. **2018**, *60*, 22.
J. Phys. Chem. C **2018**, *122*, 11651.

Other Selected Examples

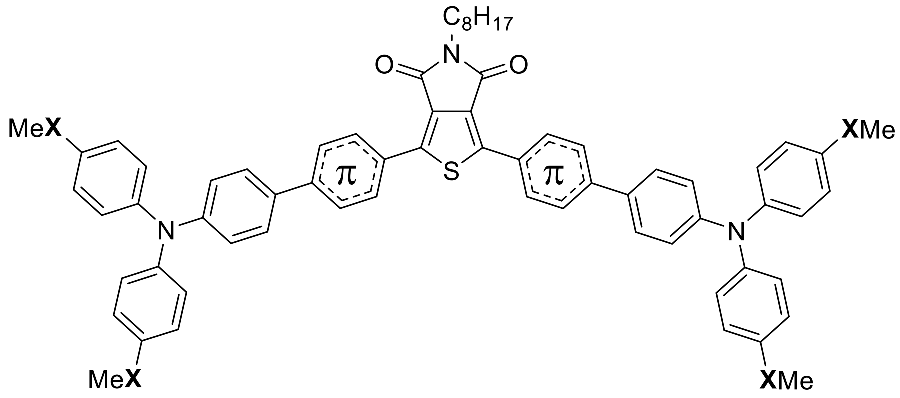
Triphenylamine-Thienothiophene Hole Transporters





Chem. Asian J. 2018, 13, 1302

Triphenylamine/Thieno[3,4-c]pyrrole-4,6-dione based D–π-A–π-D Hole Transporting Materials for Perovskite Solar Cells

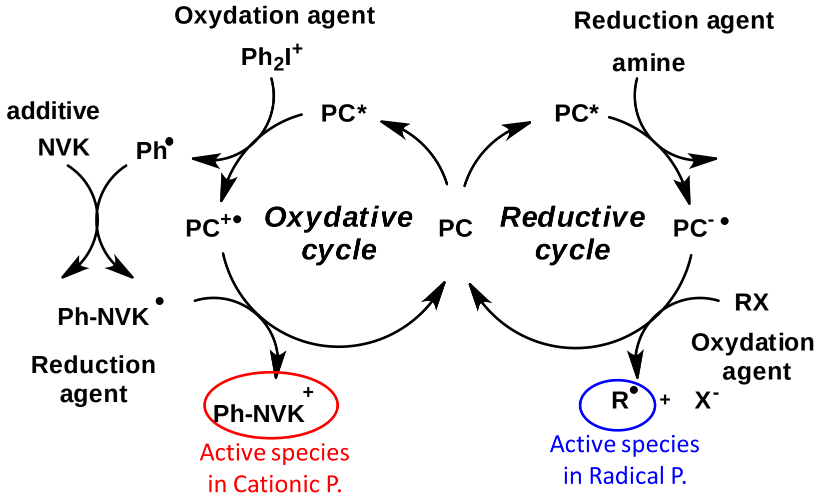


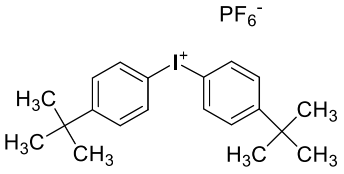
Advanced Materials **2021**, 33 (12), 2007431

Photoinitiators for photopolymerisation process

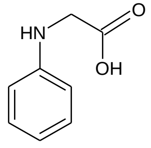
Cationic Photopolymerization (CP) and Free Radical Photopolymerization (FRP)

Photoredox catalysis mechanisms

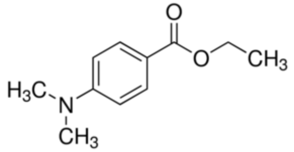




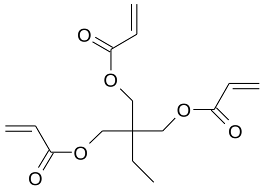
SpeedCure 938 (Iod)



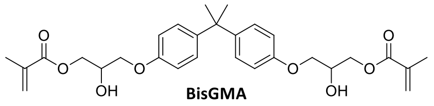
NPG
N-phenyl glycine



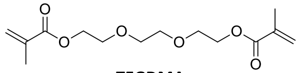
EDB
Ethyl 4-(dimethylamino)benzoate



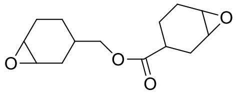
TMPTA



BisGMA



TEGDMA



EPOX

These compounds will be incorporated into different photoinitiating systems (PISs)

2-component (PI/iodonium salt (Iod) or PI/amine (NPG))
3-component (PI/Iod/NPG) photoinitiating systems (PISs)

=> generate reactive species (radicals or cations)
=> initiate both the free radical polymerization of (meth)acrylates and the cationic polymerization (CP) of epoxides upon near-UV or visible light (LED@375 nm, LED@405 nm).

Coll. Prof. J. Lalavée, University of Mulhouse, France

IS2M Institut de Science des Matériaux de Mulhouse

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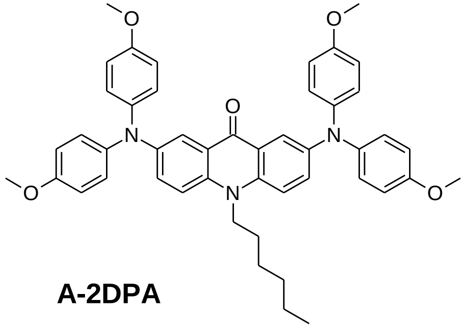
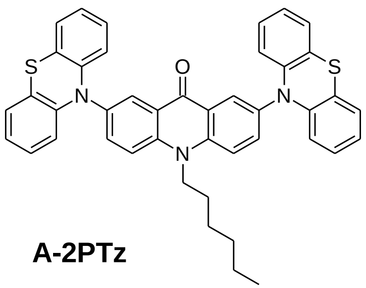
Photoinitiators for photopolymerisation process

Cationic Photopolymerization (CP) and Free Radical Photopolymerization (FRP)



A-2DPA



A-2PTz

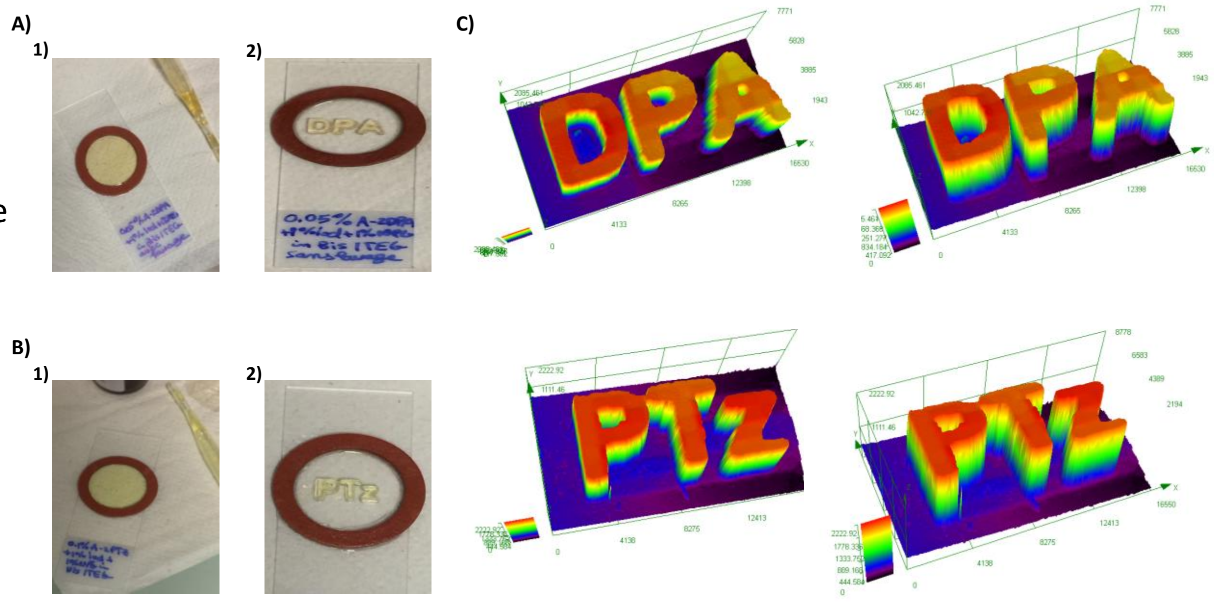
Acridone derivatives as High Performance Visible Light Photoinitiators for Cationic and Radical Photosensitive Resins for 3D Printing Technology and for low Migration Photopolymer Property

FRP experiments for 3D printing:

(A): (1) Photo of the initial formulation of A-2DPA; (2) the pattern obtained after the printing experiment;

(B): (1) Photo of the initial formulation of A-2PTz; (2) the pattern obtained after the printing experiment.

(C): Characterization of the patterns by numerical optical microscopy.



Polymer 2018, 159, 47.
New J. Chem. 2018, 42, 8261.
Molecules 2017, 22, 2143.
Macromolecules 2017, 50, 4913
J. Poly. Sci. Part A: Poly. Chem. 2017, 55, 1189.
Macromol. Chem. Phys. 2015, 216, 218.
ACS Macro Lett. 2013, 2, 736.

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Photoinitiators for photopolymerisation process

Current and Future works: Far Red / Near Infrared absorbing molecules as photocatalysts for polymer synthesis

Advantages of photopolymerization over traditional thermo-processes

- temporal and spatial control of initiation, cost efficiency and eco-friendly (solvent-free)

Some drawbacks

- sensitivity toward oxygen for the radical polymerization
- use of high-energy consumption UV lamp : UV light sources contain toxic mercury and the UV wavelength is known to cause skin and eye damages

It is thus a necessary is to develop new PIS working upon longer (thus safer) wavelength irradiation => FR/NIR photoinitiators

Advantages of FR/NIR photoinitiators

- the NIR light induces a deeper penetration into the bulk material; thus the polymerization of a thick and filled material can be potentially enhanced compared to what UV-visible dyes can do.
- It also offers the possibility to use low-power consumption LEDs and minimize of the risk for the operator by use of a safer irradiation wavelength.

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Acknowledgement

Financial support

French National Research Agency

200 K€

600 K€

Current postdoctoral calls within my university

- CY INEX Talent Junior Chair
- EUTOPIA-SIF Post Doctoral Fellowship
- Paris Region post-doctoral Fellowship
- DIM RESPORE
- Etc.

Need postdoctoral applicant