

# Going Slow to Go Far: A Scientific Journey To Power the World

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Prof. Emilio Palomares



Barcelona Institute of  
Science and Technology

# AKNOWLEDGMENTS



Barcelona Institute of  
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<https://www.facebook.com/alwayspalomares/>  
<https://twitter.com/palomaresgroup>

# The biggest challenge...



# The biggest challenge...

A screenshot of a Twitter timeline. The tweet is from **Magdalena Skipper** (@Magda\_Skipper). The text of the tweet is: "Can we imagine a solution to climate change without economics? - social science is key to global solution; Calhoun #ISCLaunch". The tweet was posted at 1:44 - 5 de jul. de 2018. It has 3 retuits and 8 agradaments. Below the tweet, there is a reply from **Seamus McCelt** (@1ineq) who says: "Humans are screwing up so bad - problems are going to solve themselves (force upon them by the earth)". The bottom right corner of the screen shows the date and time as 11:43 05/07/2018.

# The biggest challenge...



“

**Renewables should be like the Manhattan Project and the Apollo Project — the government should put tens of billions of dollars into R&D**

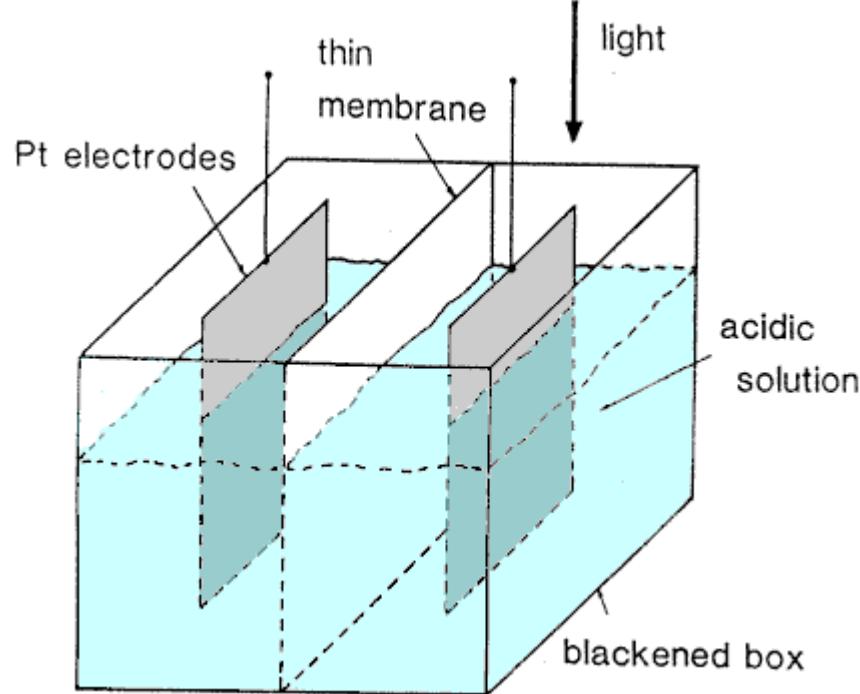
”

# What occurs when light strikes on a material?



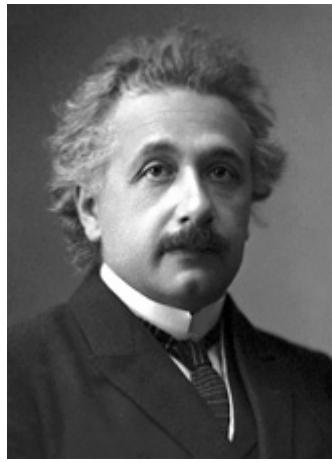
1839 ( 19 years old)

Photoelectric Effect



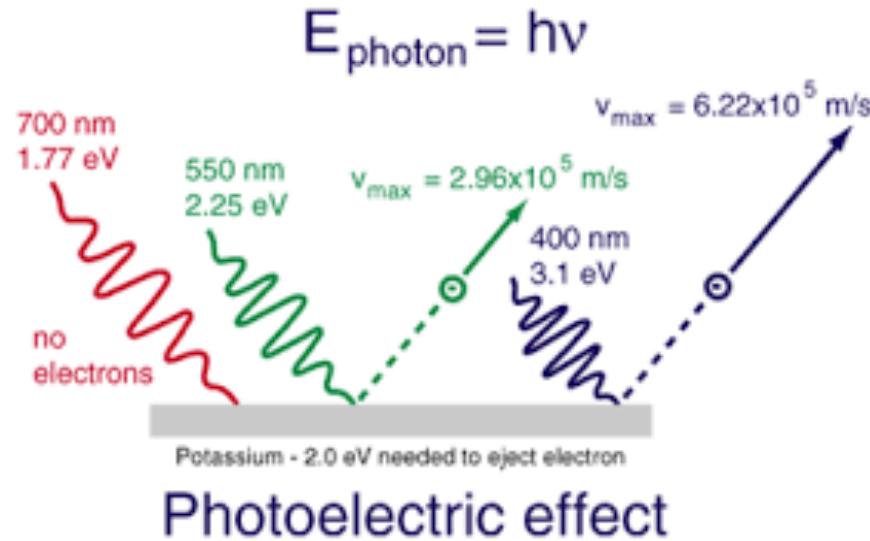
First photoelectrochemical cell with silver chloride in acidic media and illuminated while connected to Pt electrodes

# What occurs when light strikes on a material?



Physics Nobel Prize 1921

Photoelectric Effect



Light can interact with matter and transfer its Energy as discrete wave packets (photons)

# What is a semiconductor?



Shockley

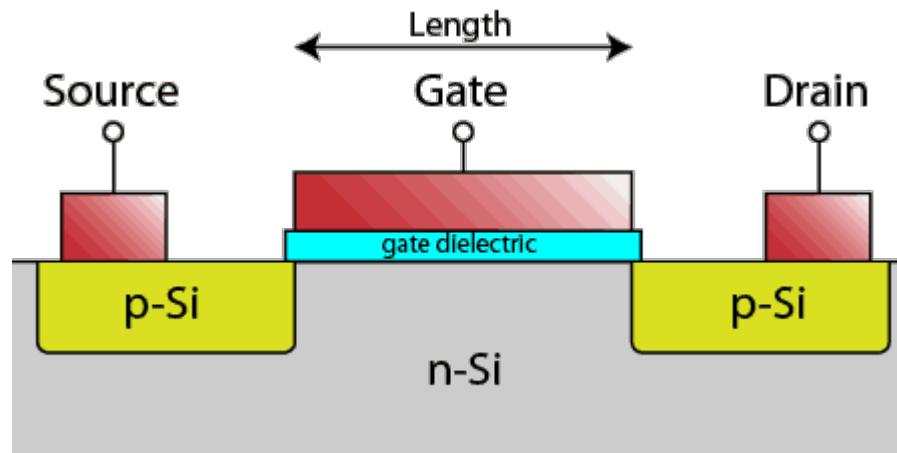


Bardeen

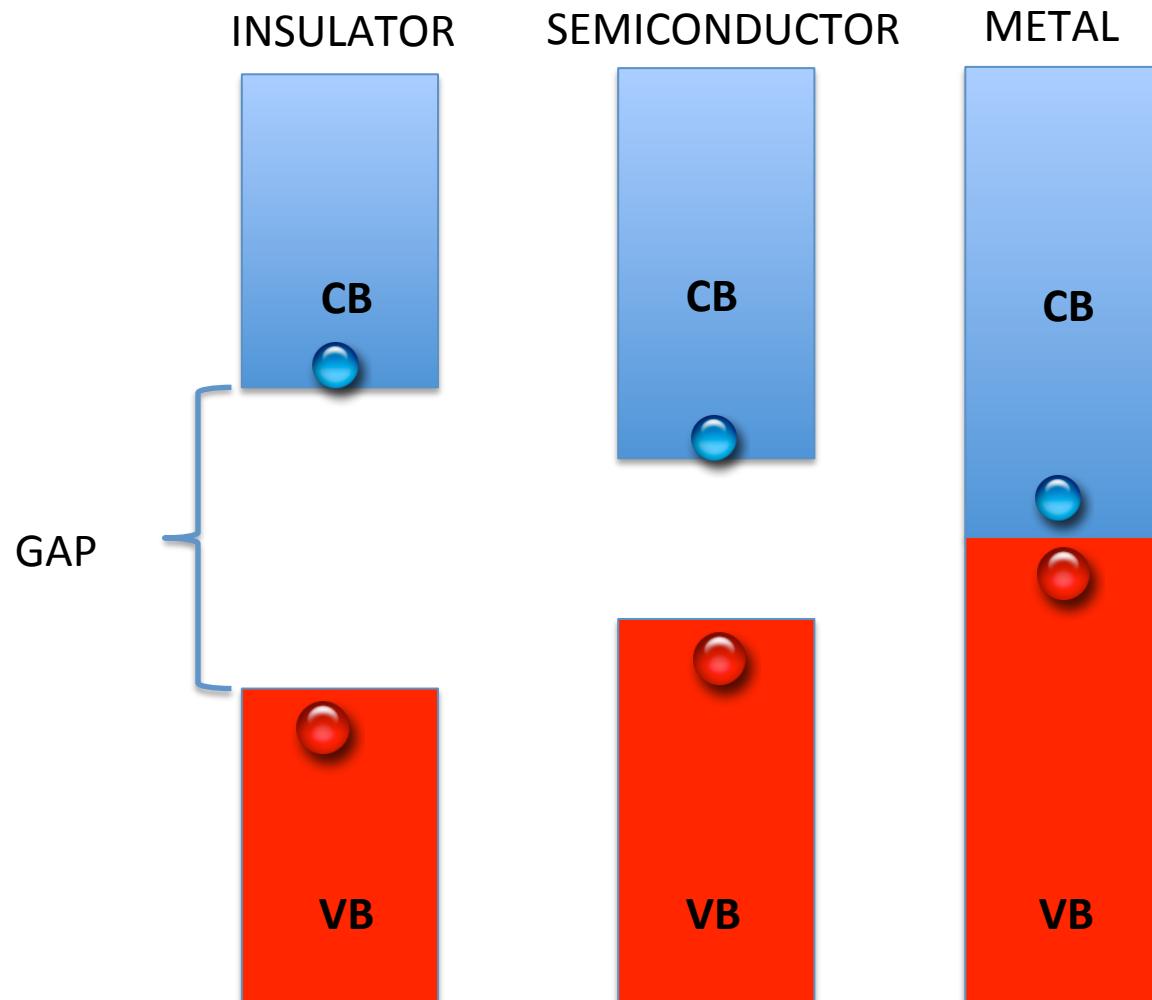


Brattain

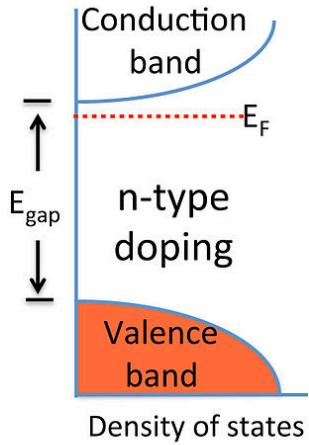
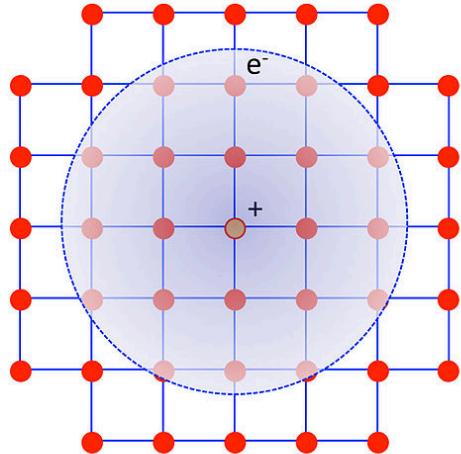
Physics Nobel Prize 1956



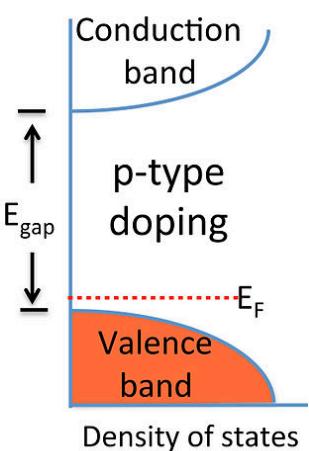
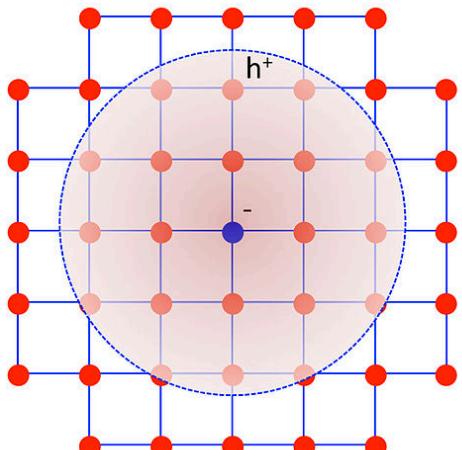
# What is a semiconductor?



# What is a semiconductor?



**Negative** charged materials are  
Called **n-type**



**Positive** charged materials are  
Called **p-type**

# What is a semiconductor?



Shockley



Bardeen



Brattain

Physics Nobel Prize 1956

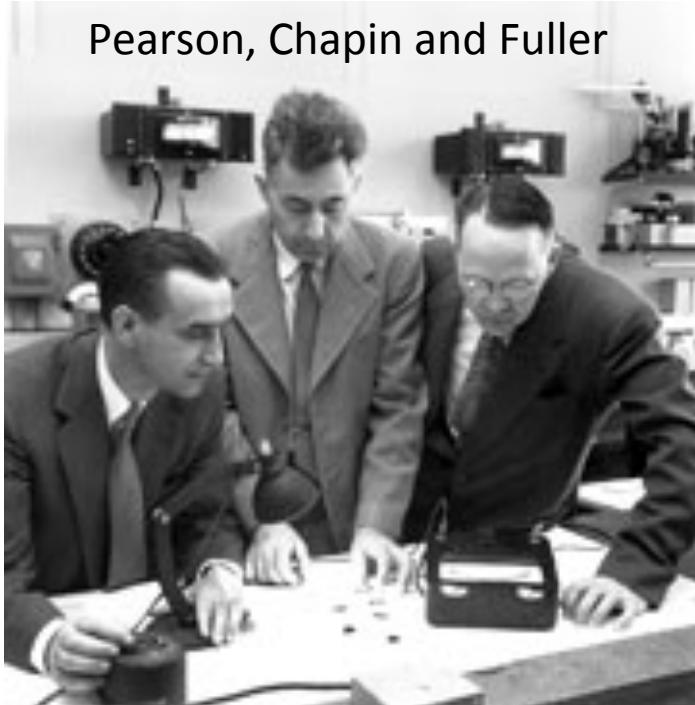
Basic electronic device that was the open door to integrated electronic circuits.

## The P-N junction

# What is a semiconductor?



Pearson, Chapin and Fuller

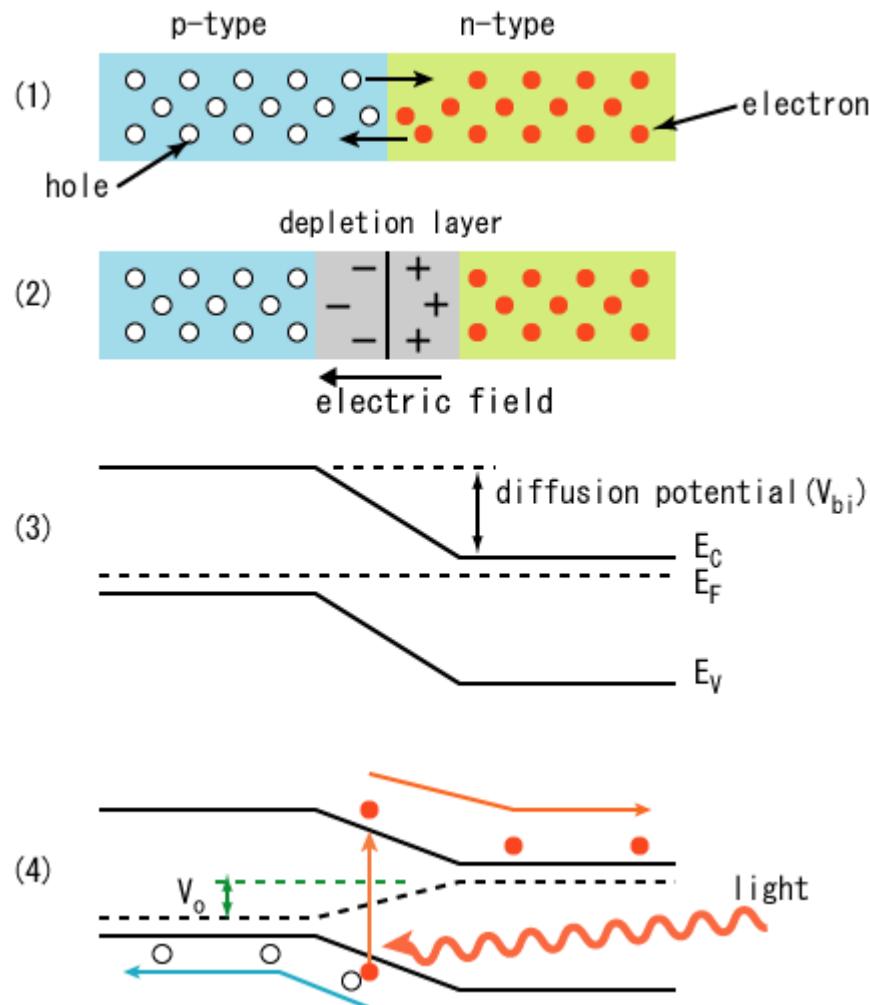


1954-First Practical Solar Cell with efficiency of 6%

FIRST SOLAR CELL.

## The P-N junction

# What is a semiconductor?



## What is a semiconductor?



Heeger



MacDiarmid



Shirakawa

Chemistry Nobel Prize 2000

New game, new rules,  
new science



ICIQ



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# What is a semiconductor?



Heeger

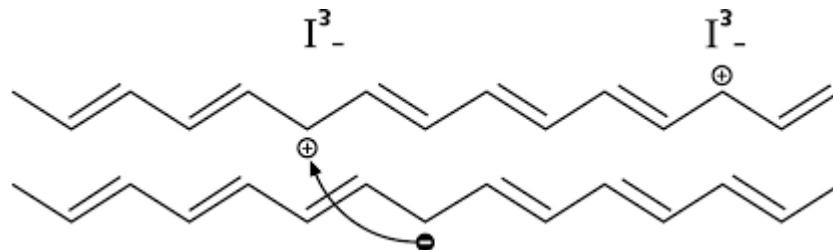


MacDiarmid



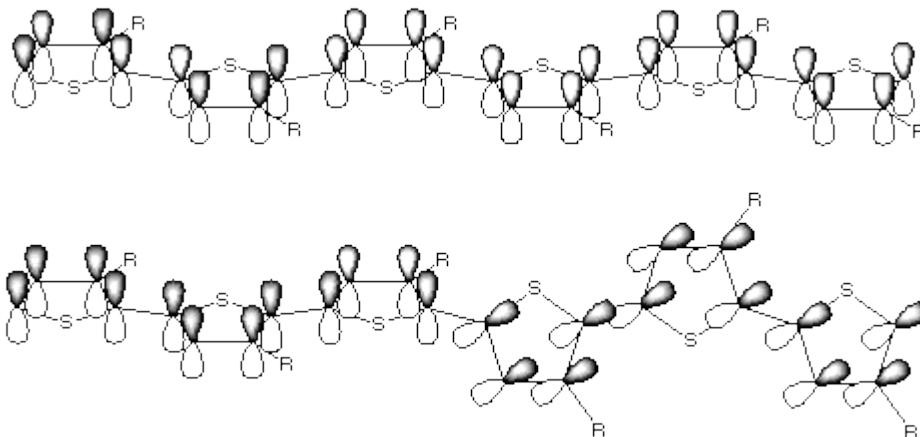
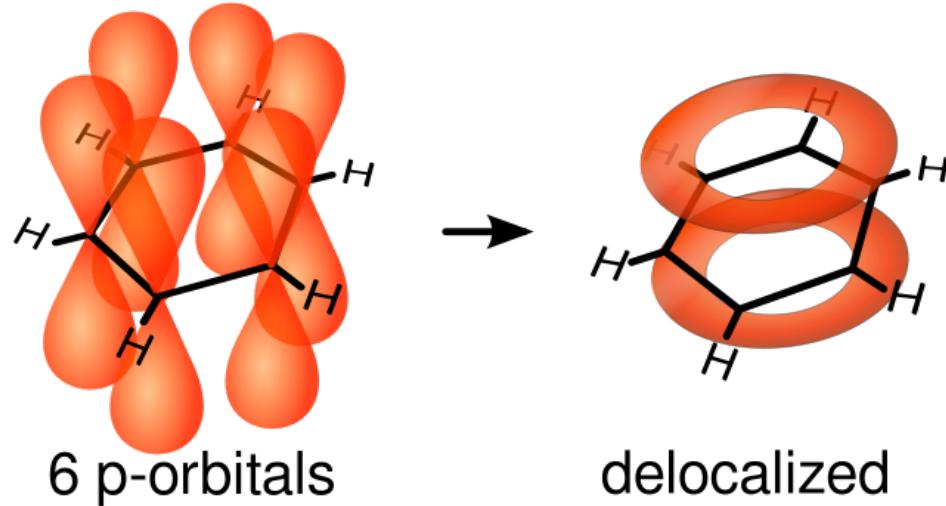
Shirakawa

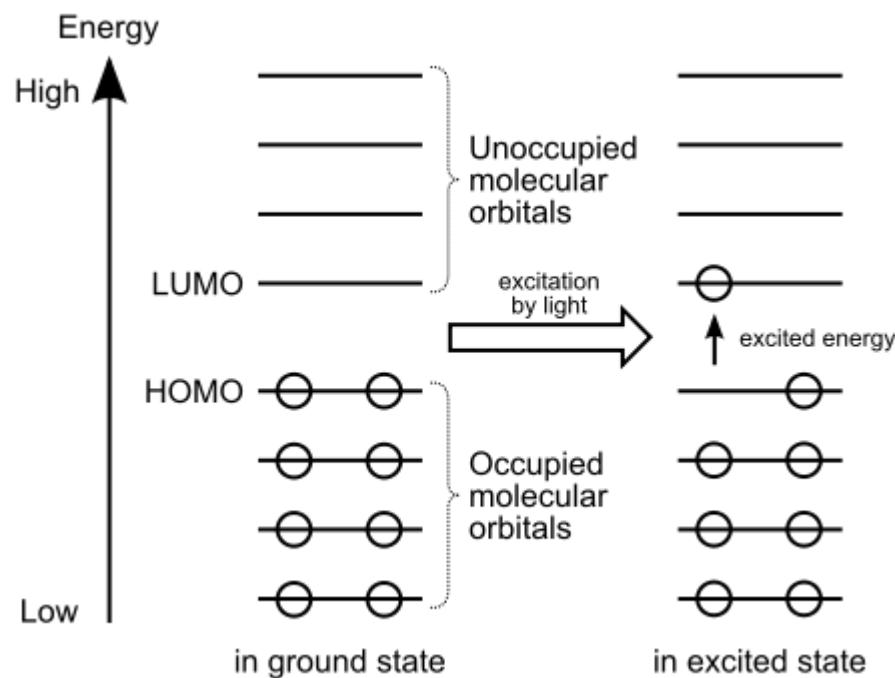
Chemistry Nobel Prize 2000



Polaron

# What is a semiconductor?



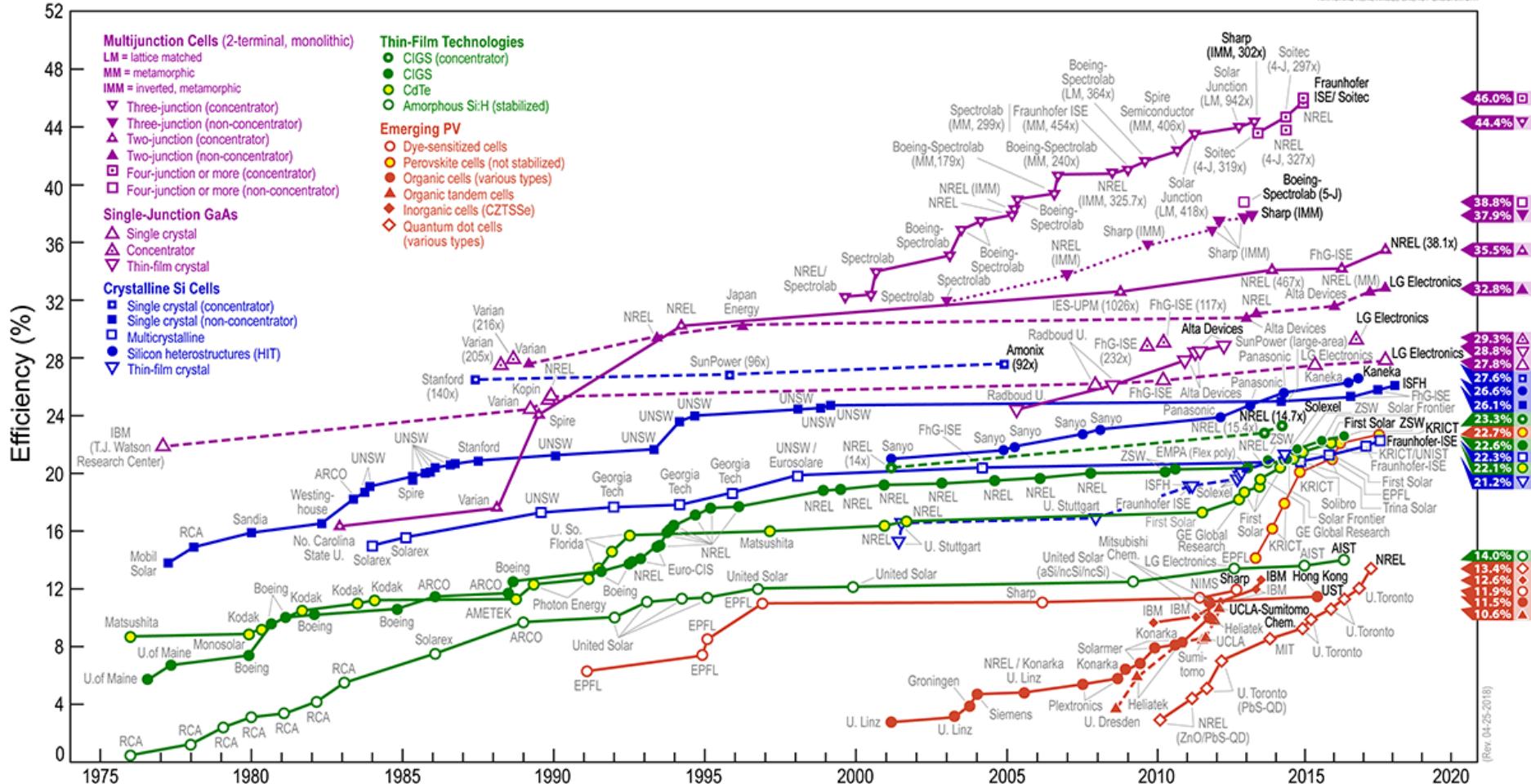


# Solar Power.



## Best Research-Cell Efficiencies

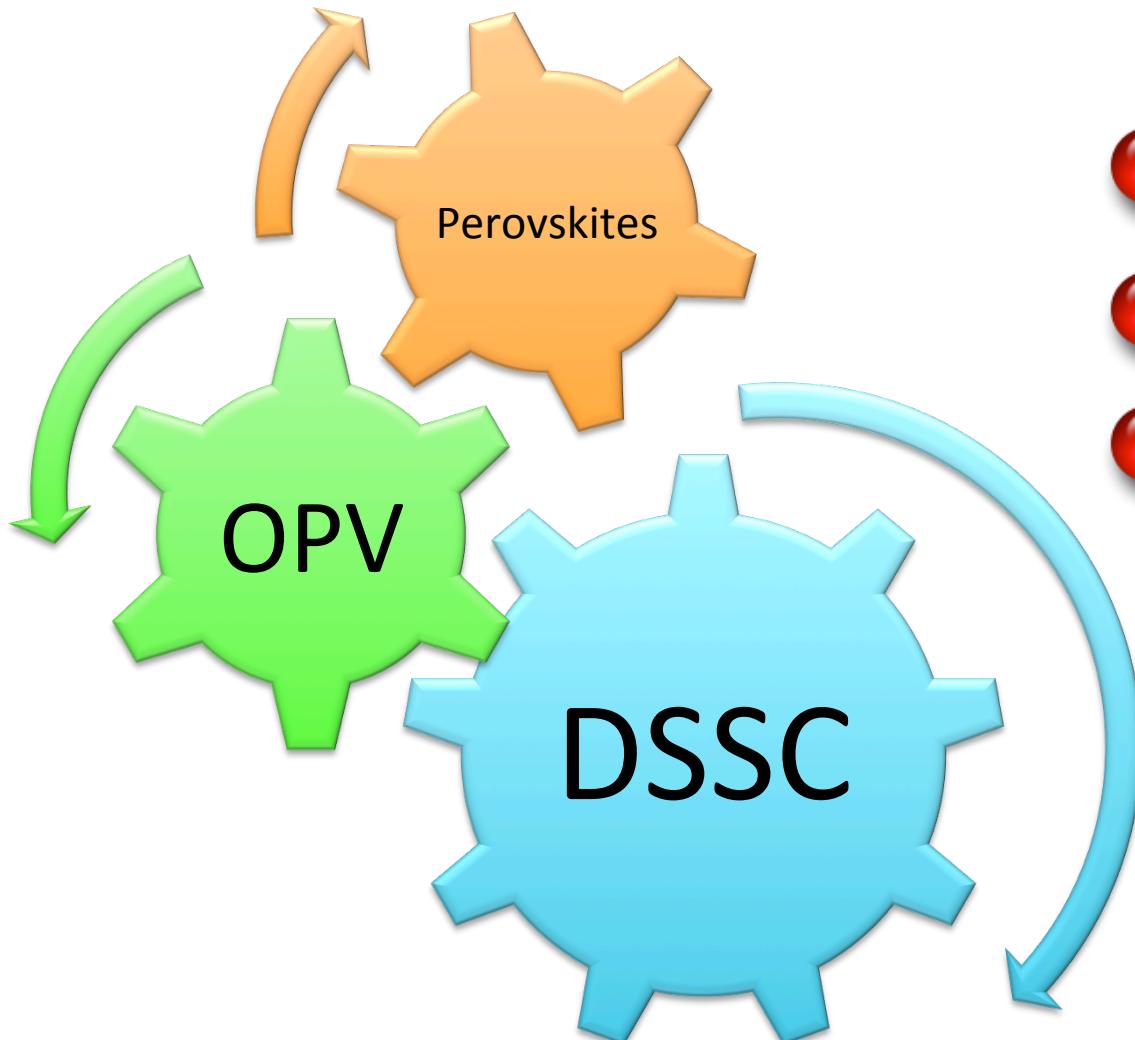
**NREL**  
NATIONAL RENEWABLE ENERGY LABORATORY



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# Third generation PV. Powering the World with Solar Energy



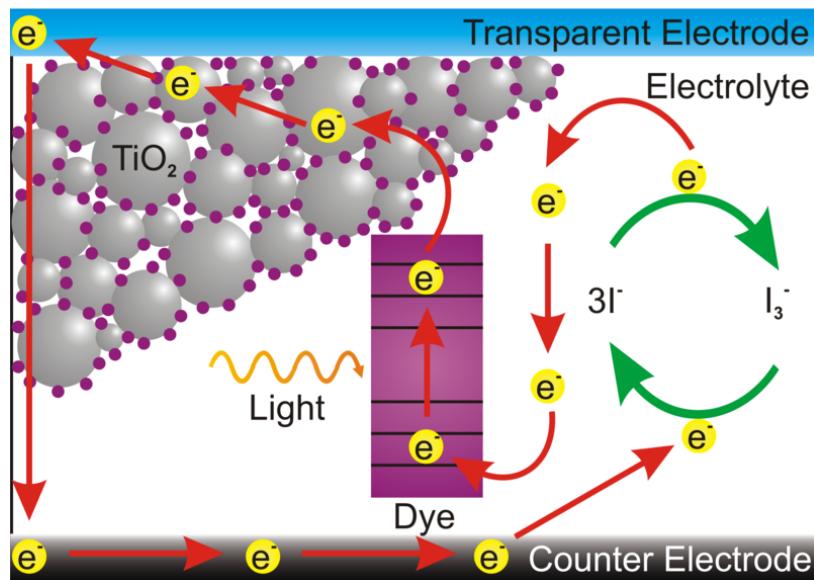
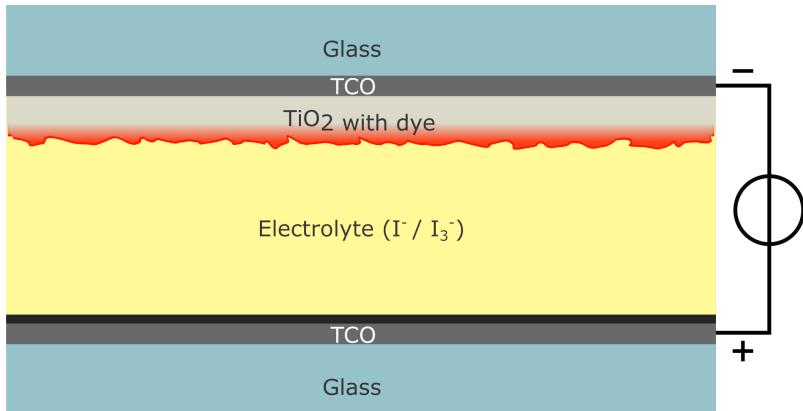
- Low-Cost
- Efficient
- Durable



# Dye Sensitized Solar Cells ( DSSC)



O'Regan & Grätzel



A low-cost, high-efficiency solar cell based on dye-sensitized colloidal  $TiO_2$  films  
B O'Regan, M Grätzel  
Nature 353 (6346), 737-740

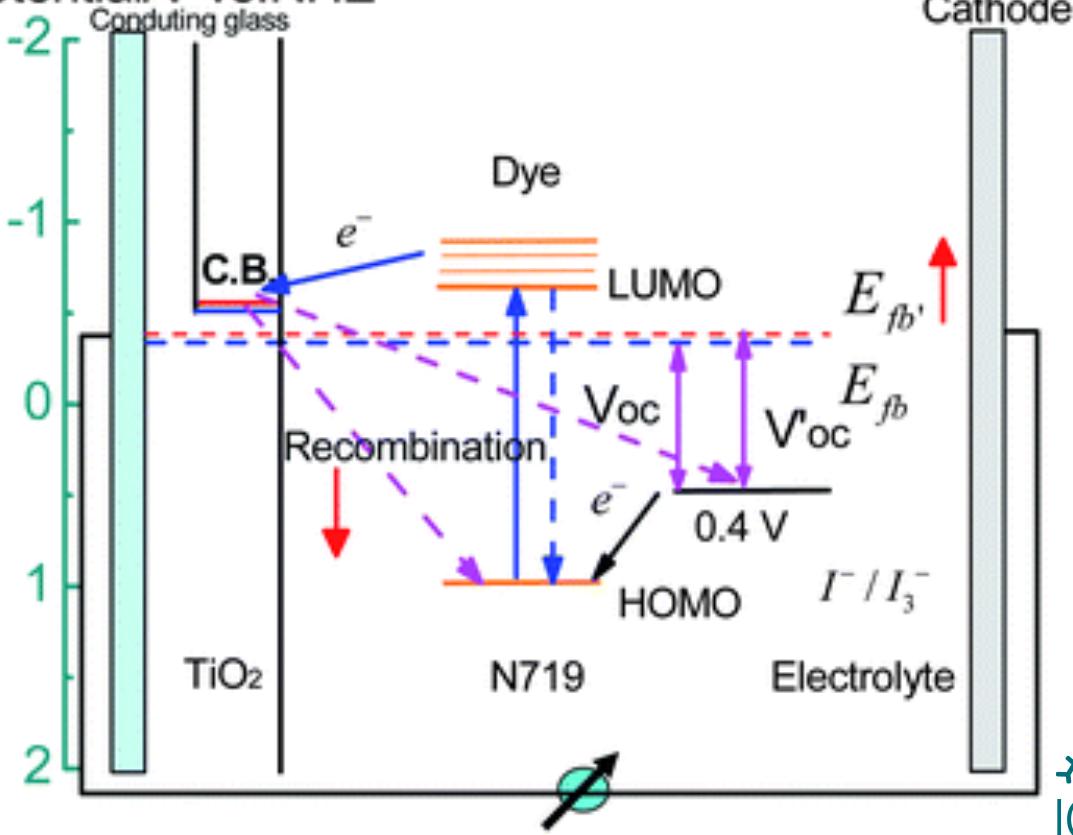
Over 28.000 citations!!!!



# Dye Sensitized Solar Cells ( DSSC)

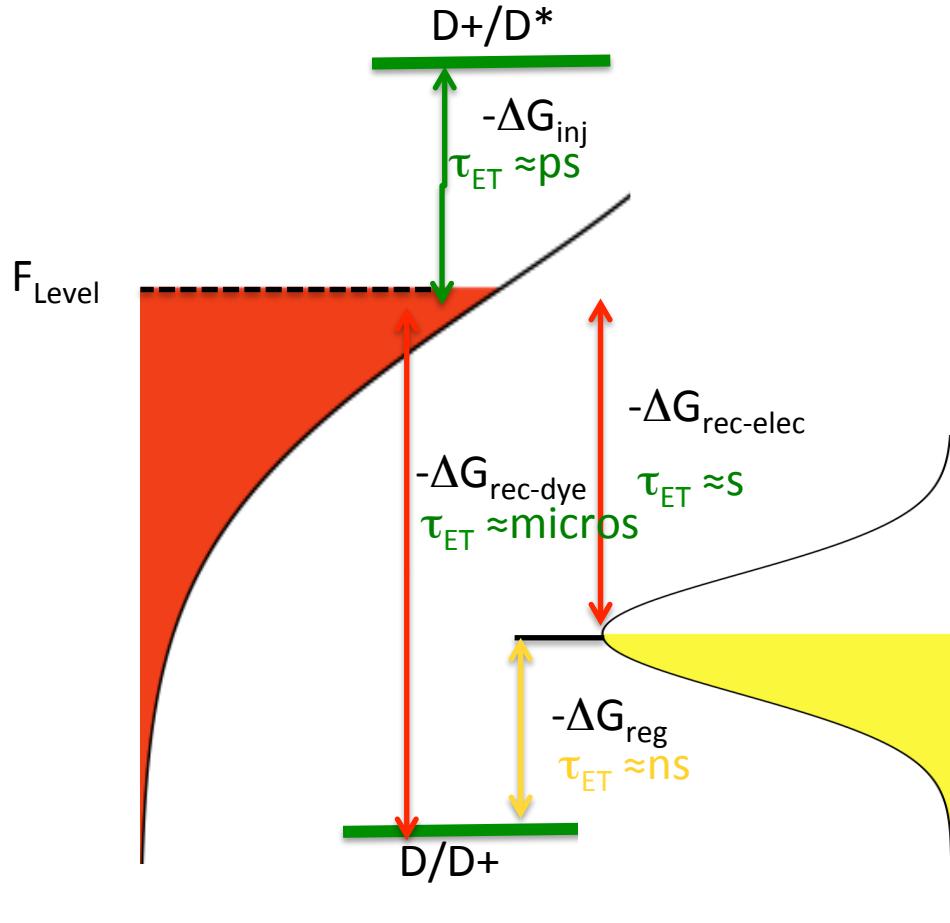
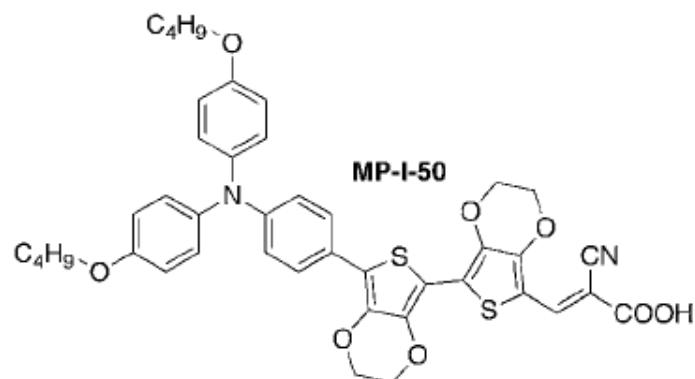
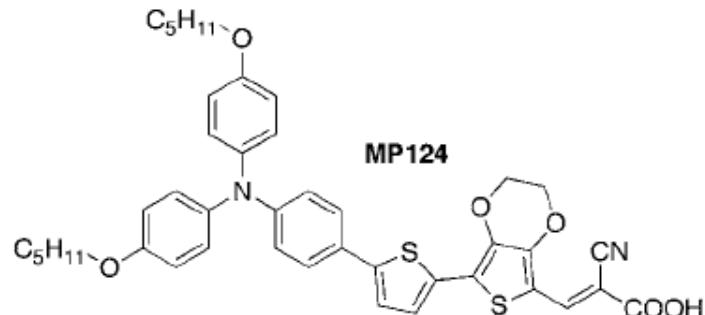


Potential/V vs.NHE





## Dye Sensitized Solar Cells ( DSSC)



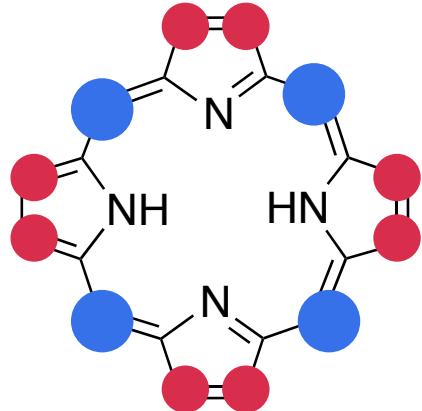
J Am Chem Soc (2008) vol. 130 (41) pp. 13558-13567

Energ Environ Sci (2011) vol. 4 (5) pp. 1820-1829

Angew Chem. Int. Ed. (2007) vol. 46 (44) pp. 8358-8362.

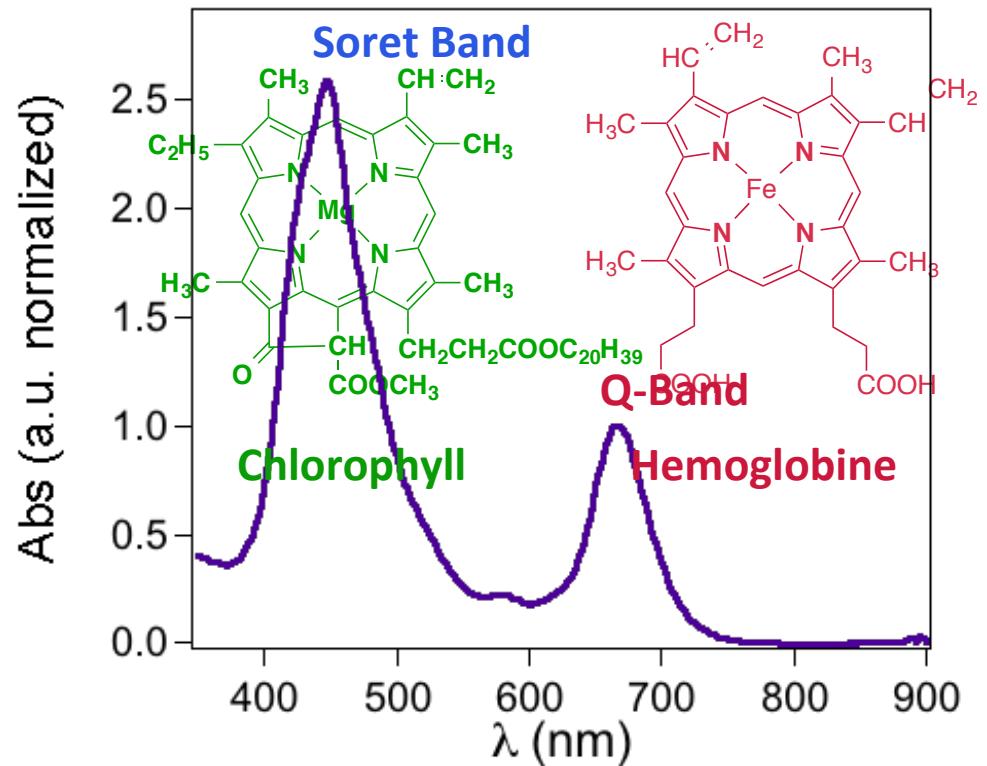


- 4 modified pyrrole connected at carbon  $\alpha$  by methine
- Huckel's rule
- High  $\epsilon$
- Present in Nature



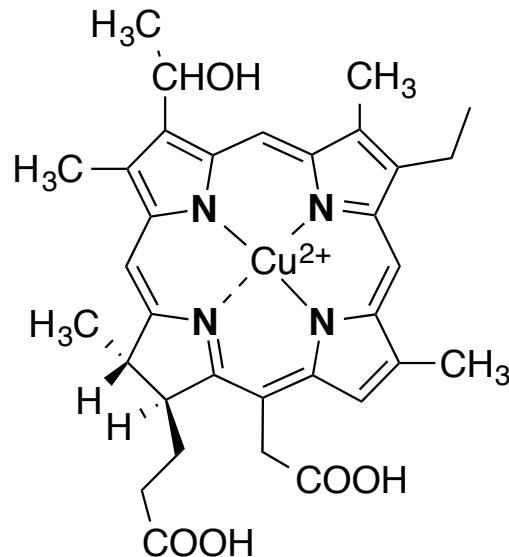
●  $\beta$ -positions

● meso-positions



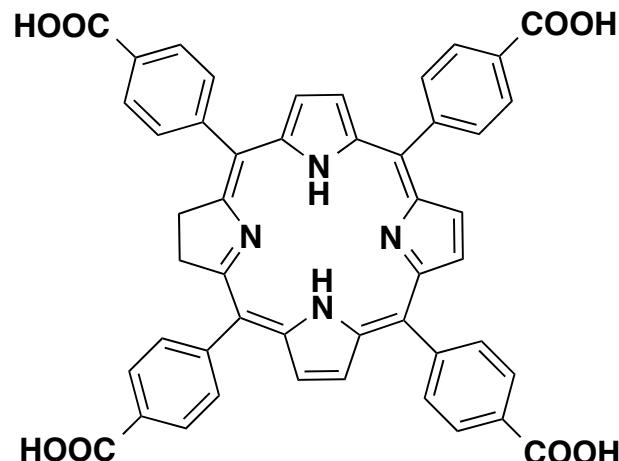


# Background on Porphyrins for DSSC



$$\eta=2.6\%$$

Cu-2- $\alpha$ -oxymesoisochlorin



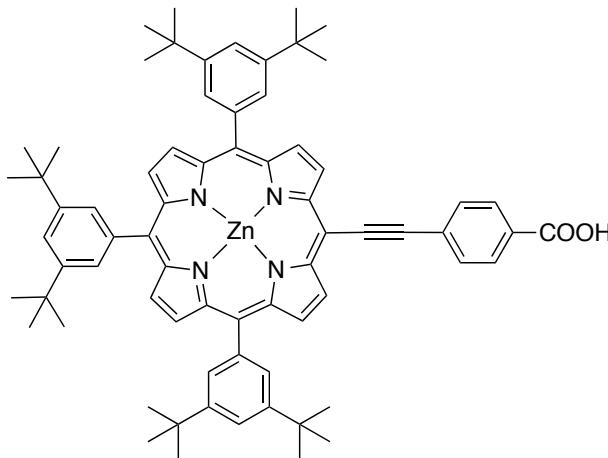
$$\eta=3.5\%$$

Kay, A.; Grätzel, M. *The Journal of Physical Chemistry* **1993**, *97*, 6272.

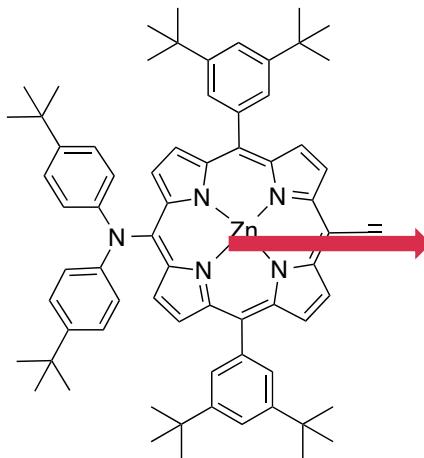
Cherian, S.; Wamser, C. C. *The Journal of Physical Chemistry B* **2000**, *104*,



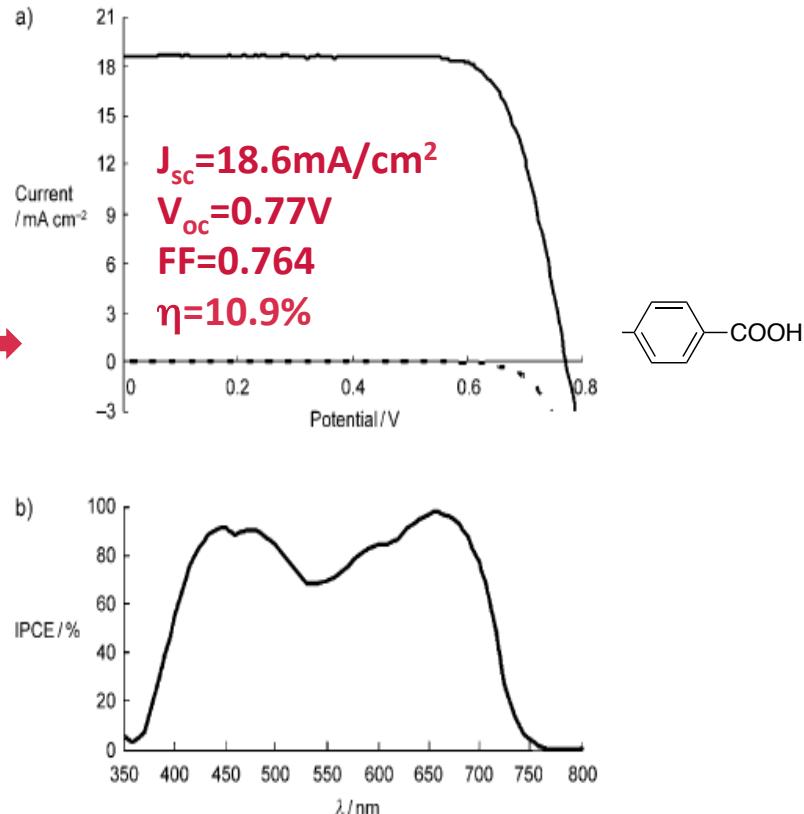
# Background on Porphyrins for DSSC



$\eta=4.34\%$   
YD0

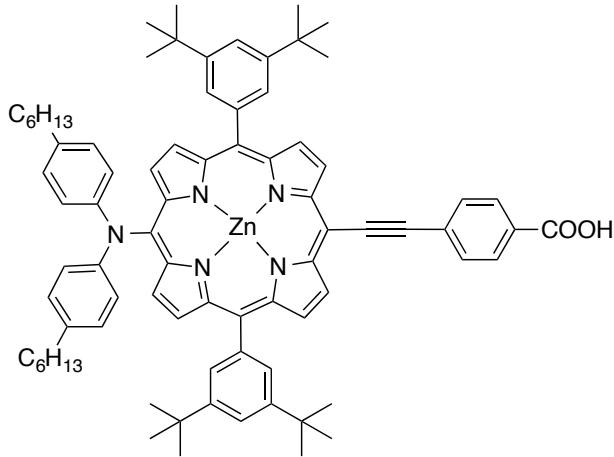


$\eta=6.15\%$   
YD1





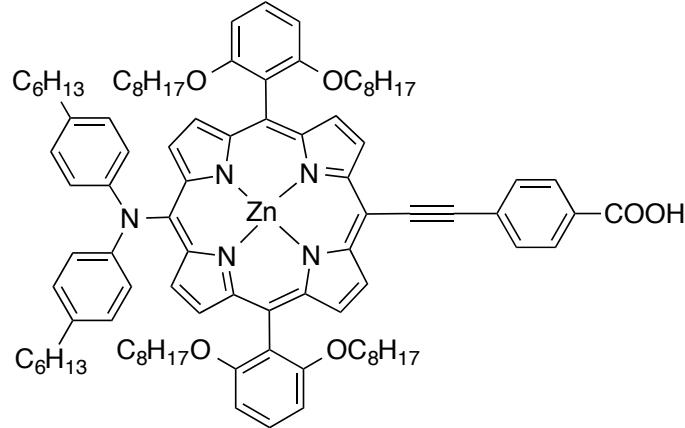
# DSSC at ICIQ\_Group Prof. Palomares



YD2

$$\eta = 8.4\% \text{ } (\text{Co}^{2+}/\text{Co}^{3+})$$

vs

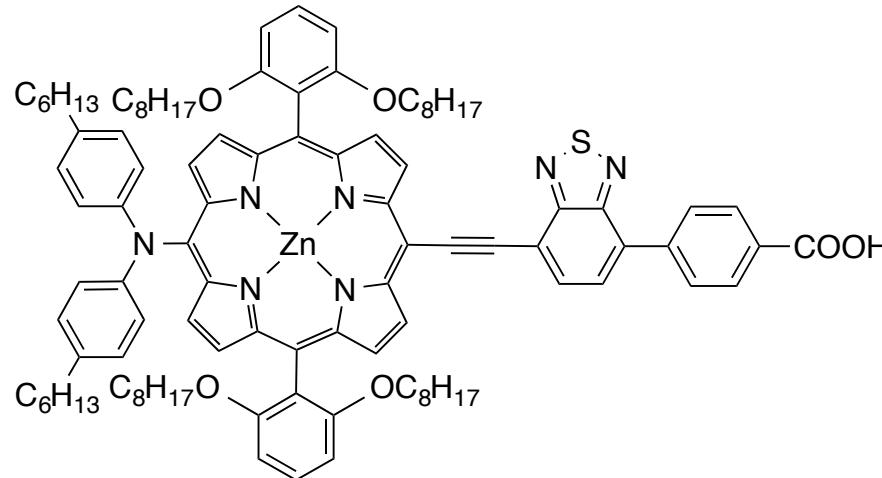


YD2-o-C8

$$\eta = 9.4\% \text{ } (I_3^-/I^-)$$

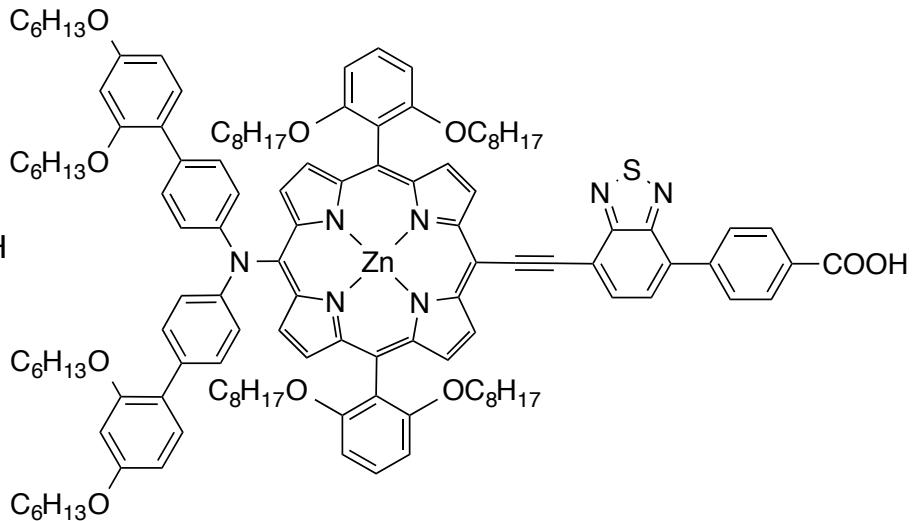
$$\eta = 11.9\% \text{ } (\text{Co}^{2+}/\text{Co}^{3+})$$

Yella, A.; Lee, H.-W.; Tsao, H. N.; Yi, C.; Chandiran, A. K.; Nazeeruddin, M. K.; Diau, E. W.-G.; Yeh, C.-Y.; Zakeeruddin, S. M.; Grätzel, M. *Science* **2011**, *334*, 629.



GY50

$\eta=12.75\% \text{ (Co}^{2+}/\text{Co}^{3+}\text{)}$



SM315

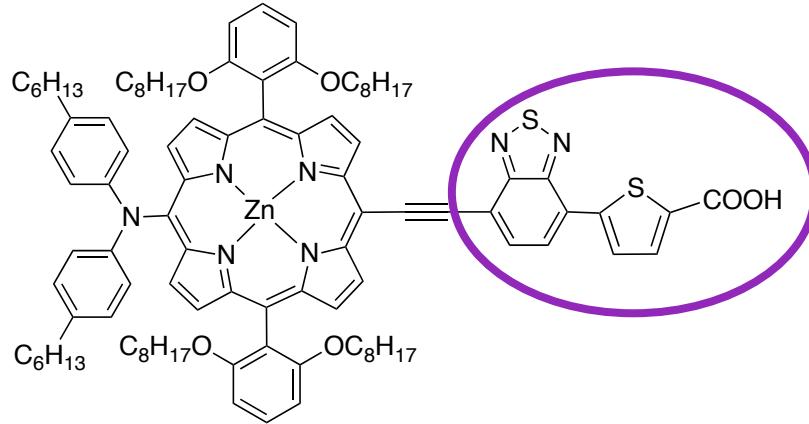
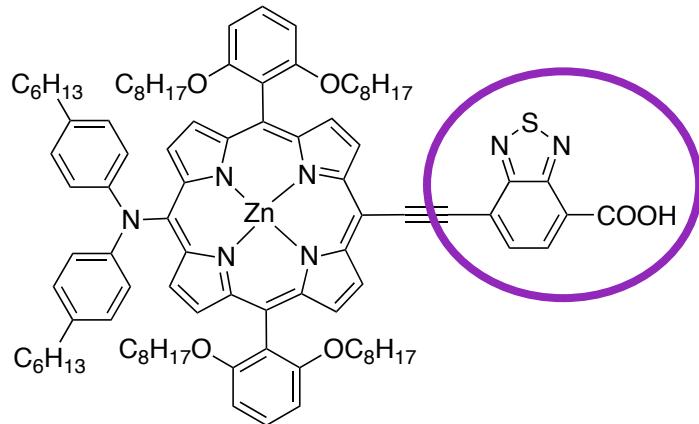
$\eta=13.0\% \text{ (Co}^{2+}/\text{Co}^{3+}\text{)}$

Yella, A.; Mai, C.-L.; Zakeeruddin, S. M.; Chang, S.-N.; Hsieh, C.-H.; Yeh, C.-Y.; Grätzel, M. *Angewandte Chemie International Edition* **2014**, 53, 2973.

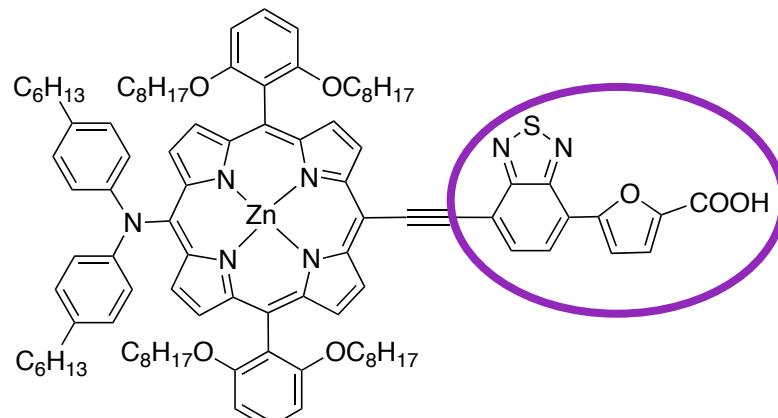
Mathew, S.; Yella, A.; Gao, P.; Humphry-Baker, R.; CurchodBasile, F. E.; Ashari-Astani, N.; Tavernelli, I.; Rothlisberger, U.; NazeeruddinMd, K.; Grätzel, M. *Nat Chem* **2014**, 6, 242.



# DSSC at ICIQ\_Group Prof. Palomares



LCVC02

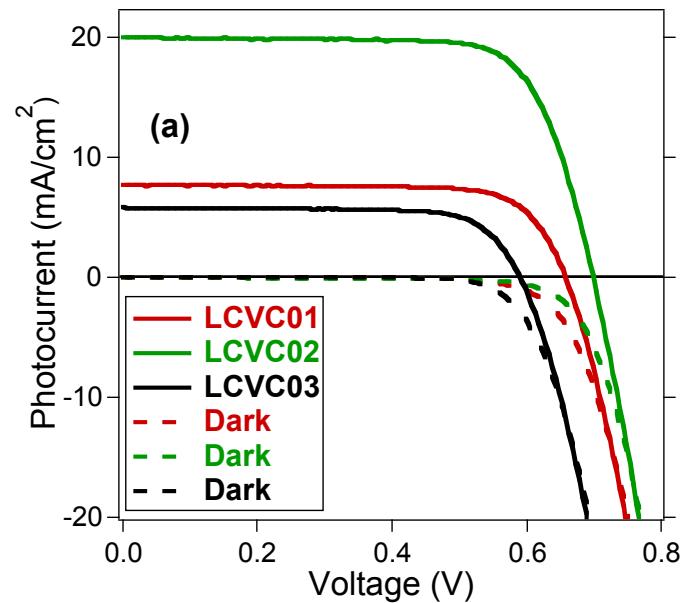
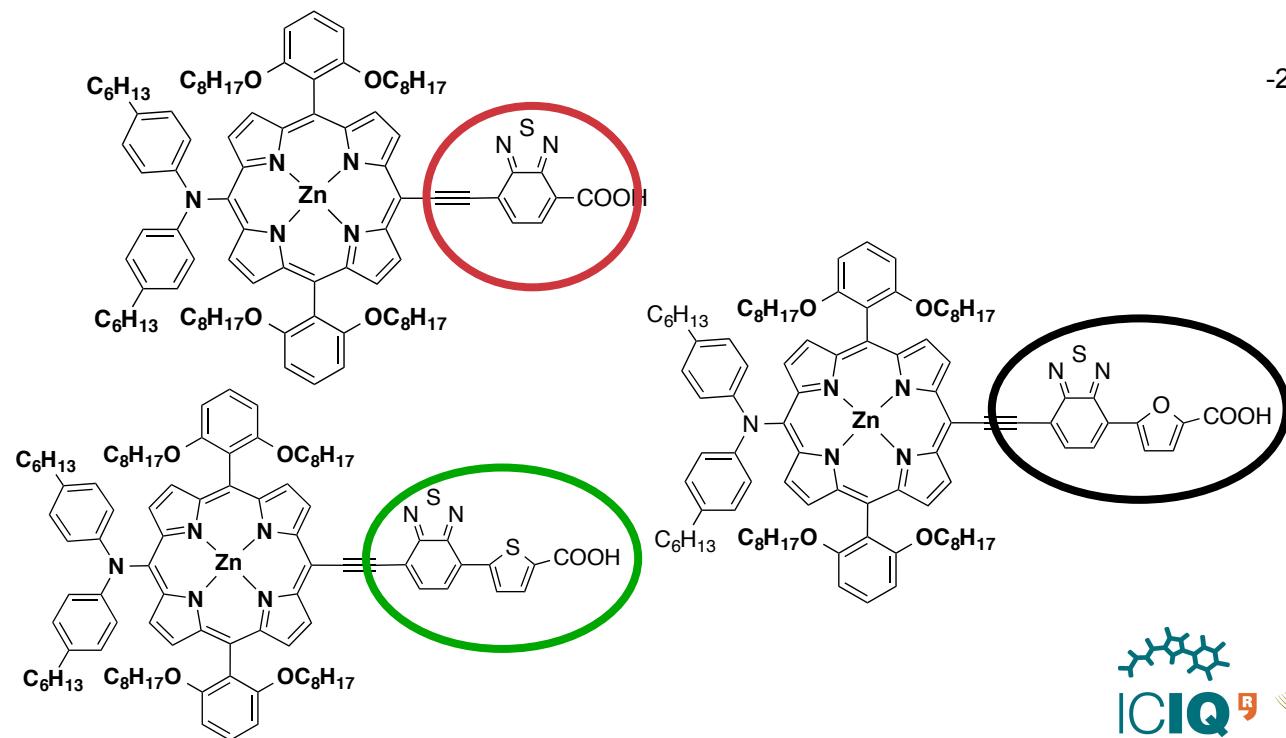


LCVC03



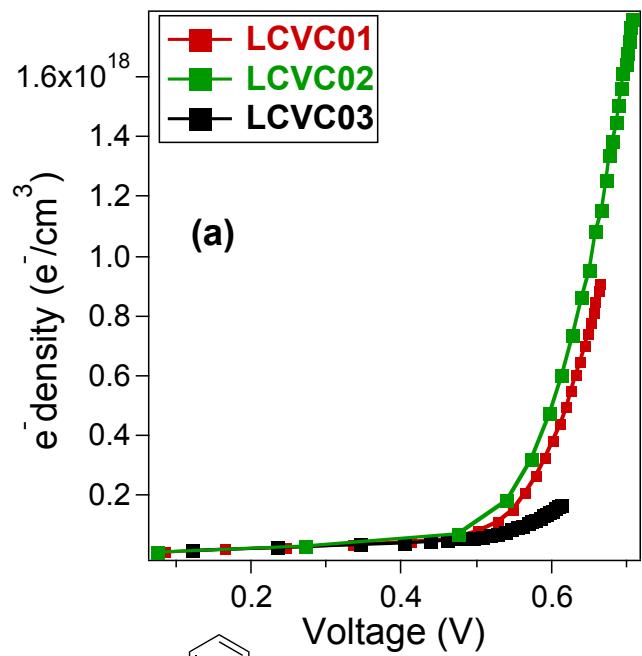
## Photovoltaic parameters of LCVC01, LCVC02 and LCVC03

Dye	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	FF (%)	$\eta$ (%)
LCVC01	0.65	7.69	75.40	3.84
LCVC02	0.70	20.00	74.41	10.41
LCVC03	0.58	5.81	74.42	2.55

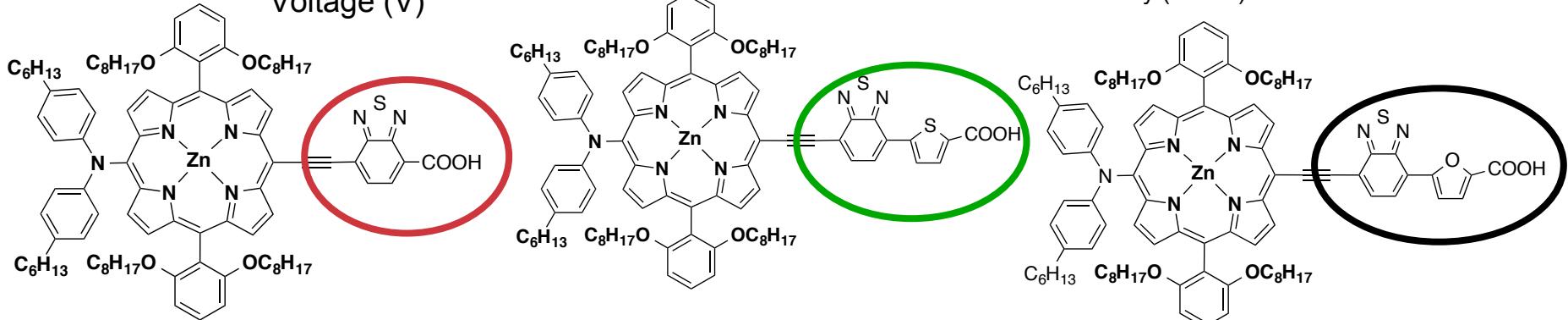
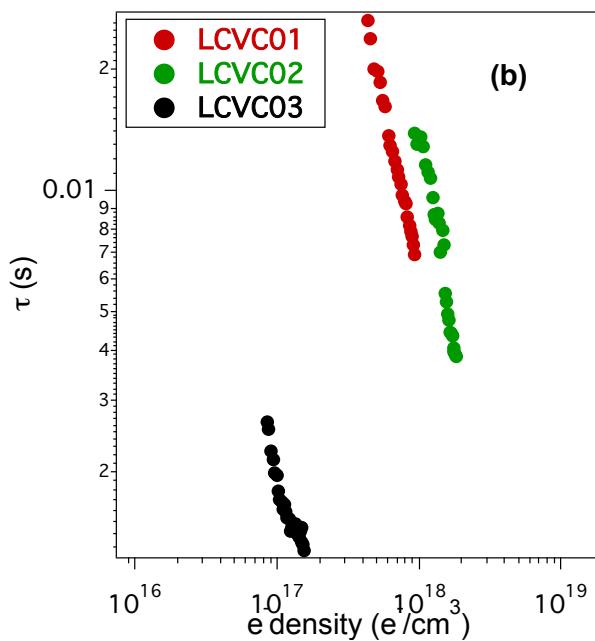




CE



TPV





## DSSC from lab to fab.



The EPFL's Convention Center (Lausanne, Switzerland) has 300 m<sup>2</sup> of dye-sensitized solar cells integrated to its façade and it represents the first application of such technology to a public building. The EPFL's Convention center will open on April 2014.



A Robust Organic Dye for Dye Sensitized Solar Cells Based on Iodine/Iodide Electrolytes Combining High Efficiency and Outstanding Stability

Damien Joly<sup>1</sup>, Laia Pellejà<sup>2</sup>, Stéphanie Narbey<sup>3</sup>, Frédéric Oswald<sup>3</sup>, Julien Chiron<sup>4</sup>, John N. Clifford<sup>2</sup>, Emilio Palomares<sup>2,5</sup> & Renaud Demadral<sup>1</sup>

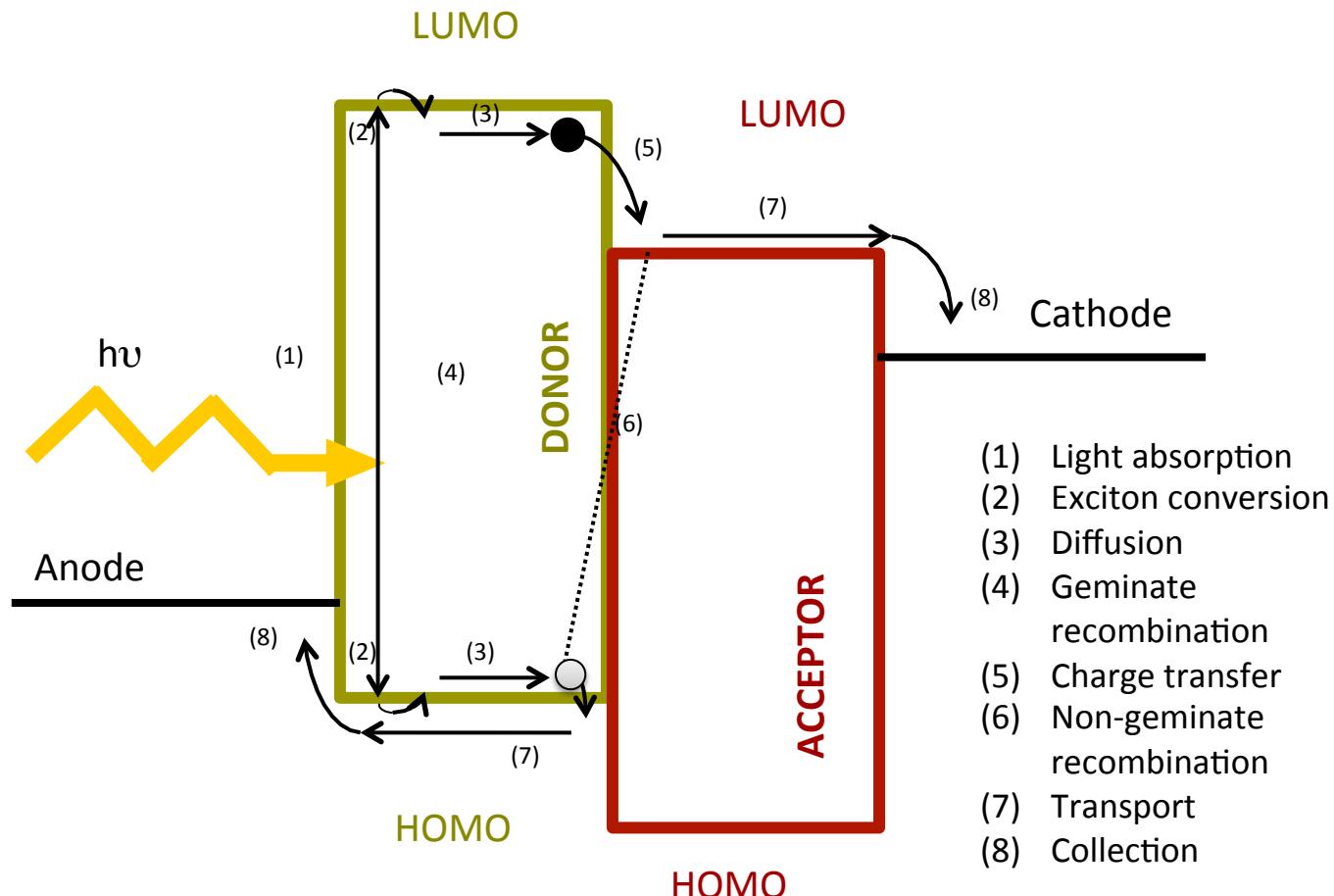
Windows of the EPFL's Convention Center



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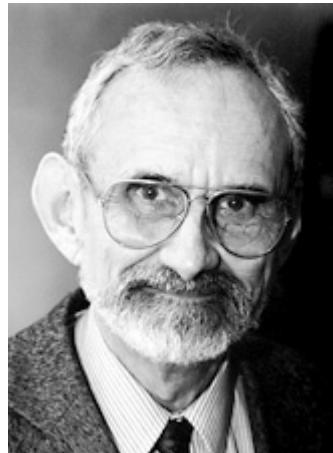


## Small molecule Organic Solar Cells

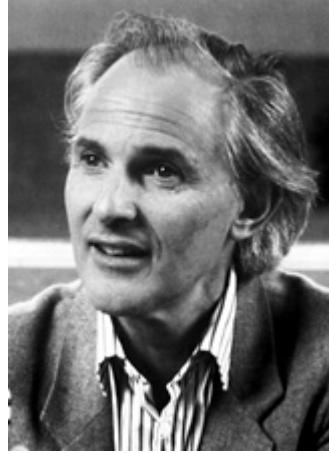




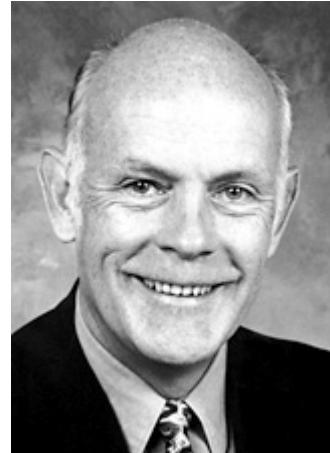
## Organic solar cells



Curl Jr.



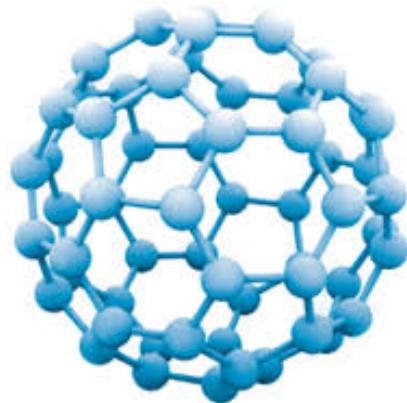
Kroto



Smalley

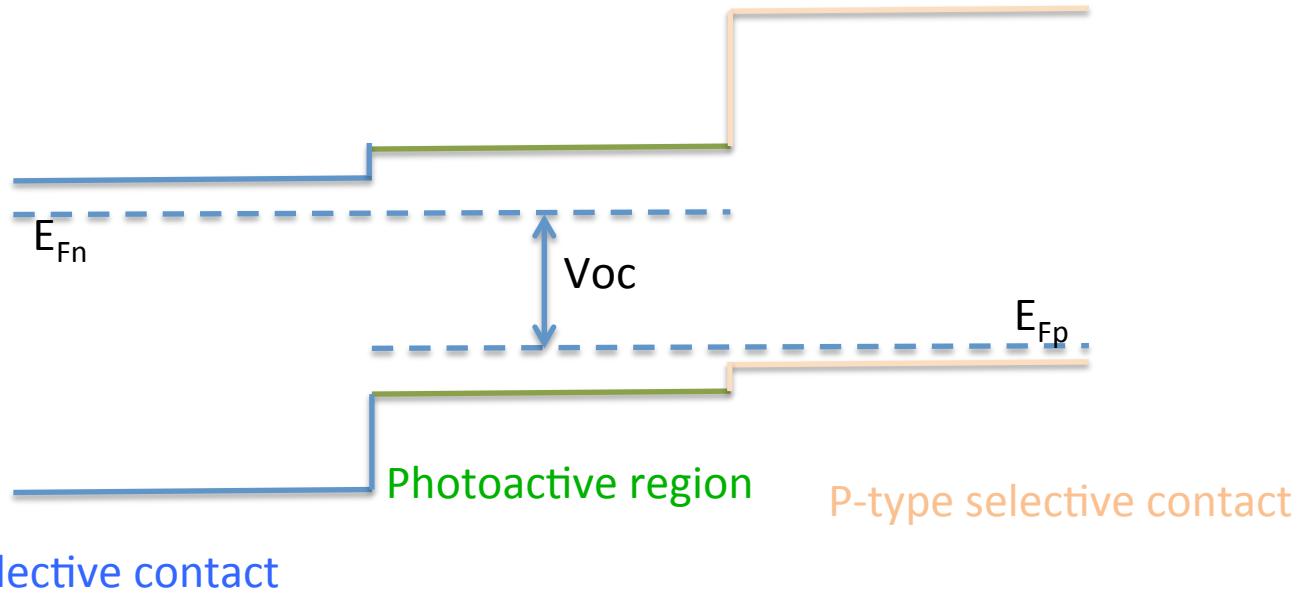
Chemistry Nobel Prize 1996

*"for their discovery of fullerenes".*





## Double Heterojunction Solar Cell

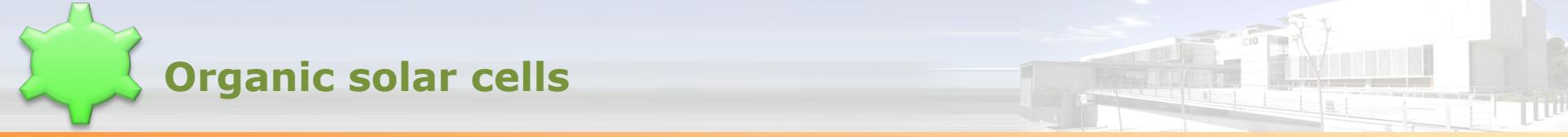


Contacts are often wide-band gap materials which need to be of sufficient electronic quality to support the quasi-Fermi level separation in the high quality narrow-gap active layer

To achieve maximum  $V_{oc}$  electron –hole recombination at the contacts must be minimized.

There are **TWO major recombination pathways:**

- 1.- In the surface of the active layer
- 2.- At the bulk of the active layer.



Friend



Nelson



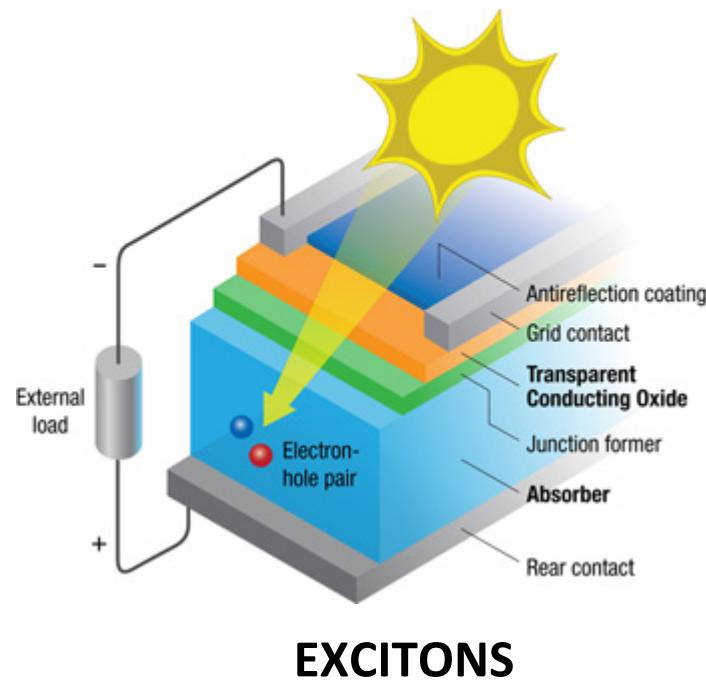
Brabec



Leo



Sariciftci



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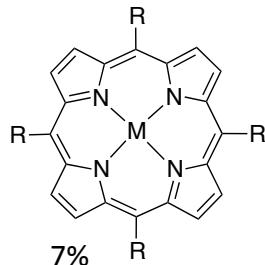




# Organic solar cells

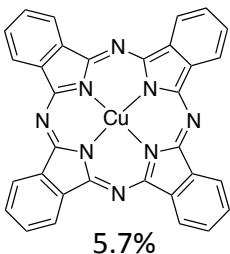


## Small-molecule based donors:



Porphyrins

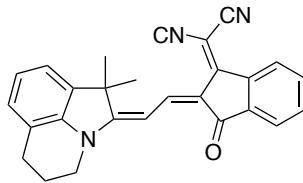
Qin et al., *Energy & Environ. Sci.* **2014**, 7, 1397-1401.



5.7%

Phthalocyanines

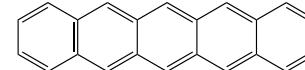
Xue et al., *Appl. Phys. Lett.* **2004**, 85, 5757-5759.



6.1%

Merocyanines

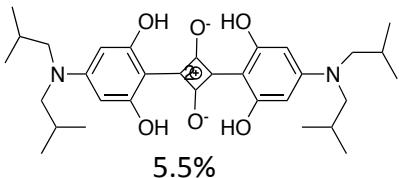
Steinmann et al., *Adv. Energy Mater.* **2011**, 1, 888-893.



2.7%

Polyacenes

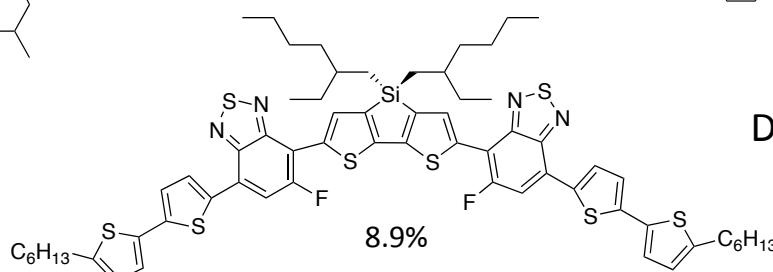
Yoo et al., *S., Appl. Phys. Lett.* **2004**, 85, 5427-5429.



5.5%

Squarines

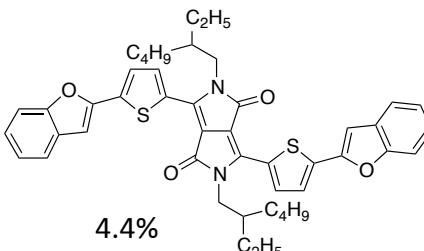
Wei et al., *Adv. Energy. Mater.* **2011**, 1, 184-187



8.9%

D-A structures (“push-pull”)

Kyaw et al., *Nano Lett.* **2013**, 13, 3796-3801.



4.4%

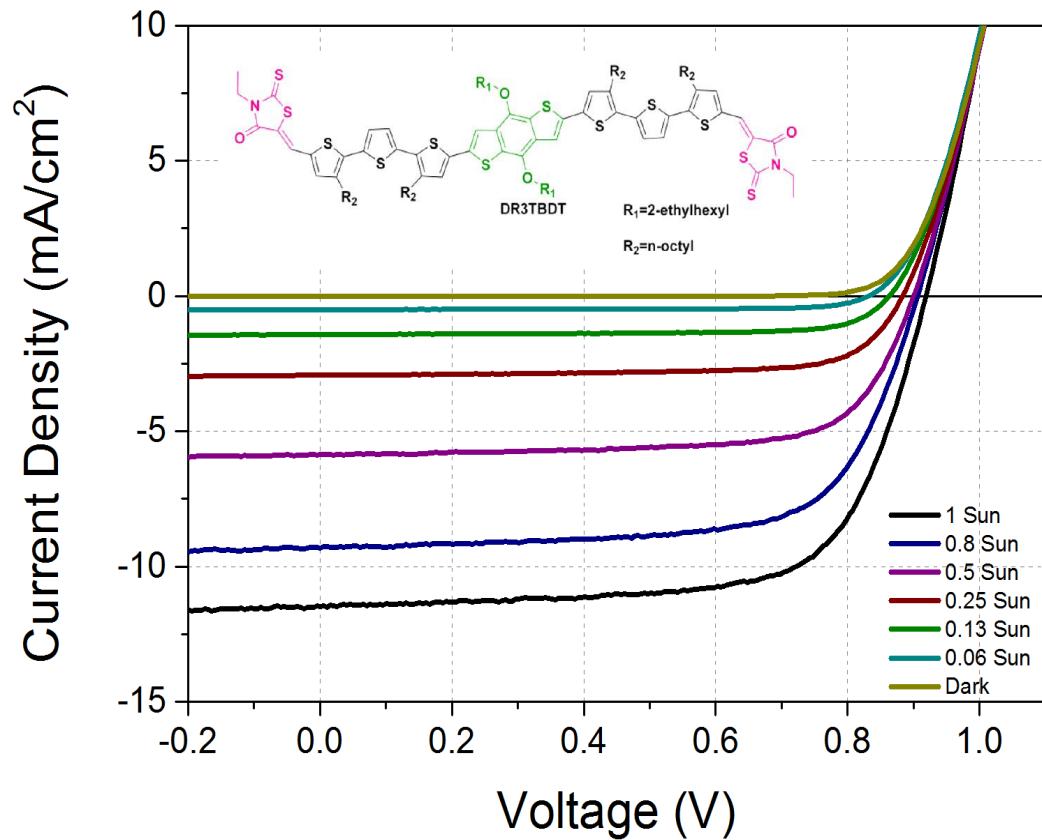
Diketopyrrolopyrroles

Walker et al., *Adv. Funct. Mater.* **2009**, 19, 3063-3069.



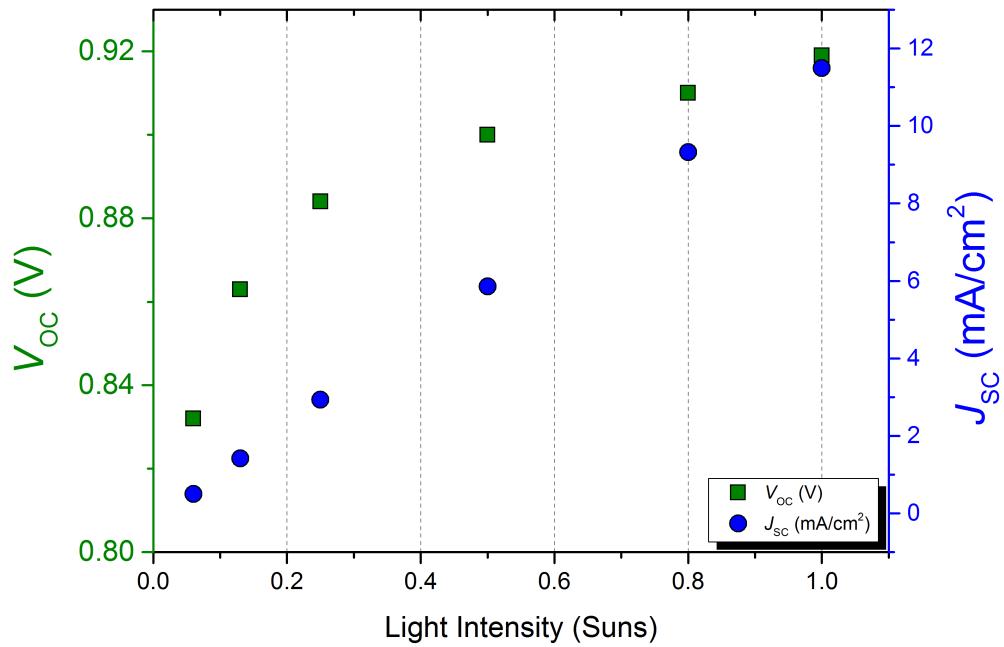
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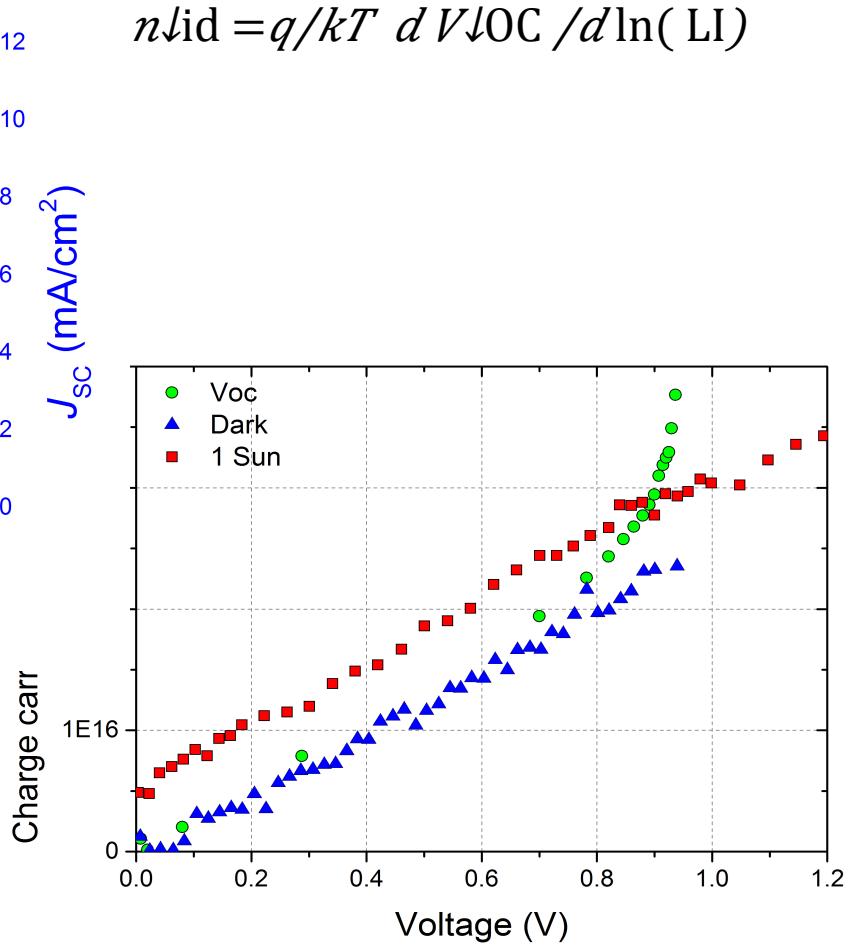


# OSC at ICIQ\_ Palomares group



$$n \downarrow id = q/kT \cdot dV \downarrow OC / d \ln(LI)$$

(a)

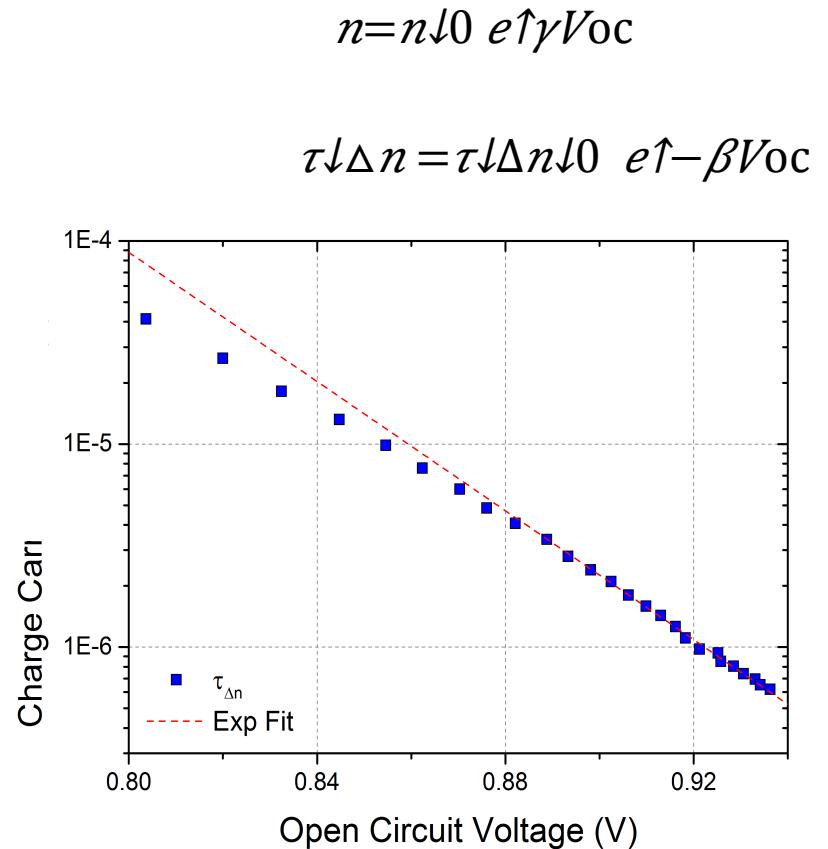
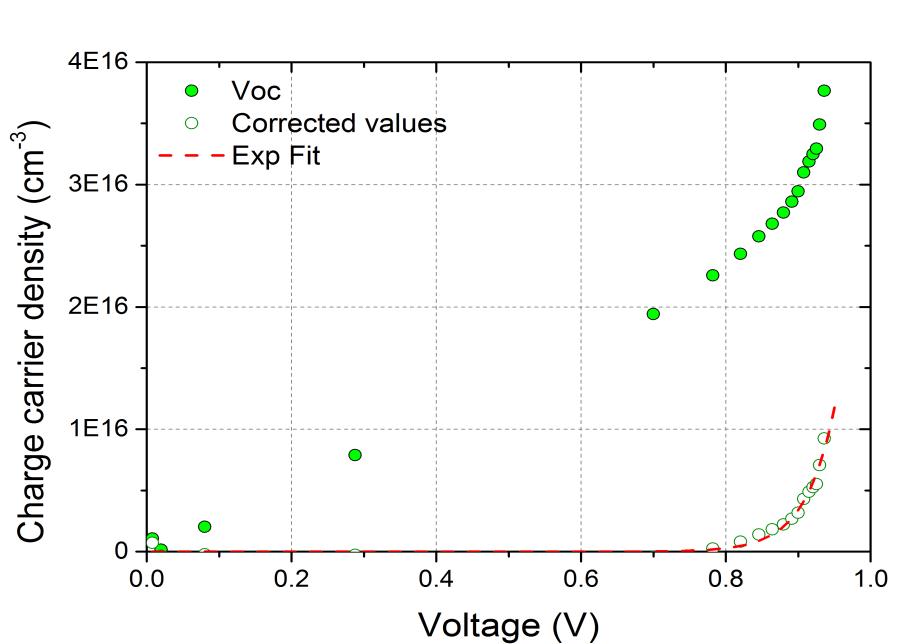


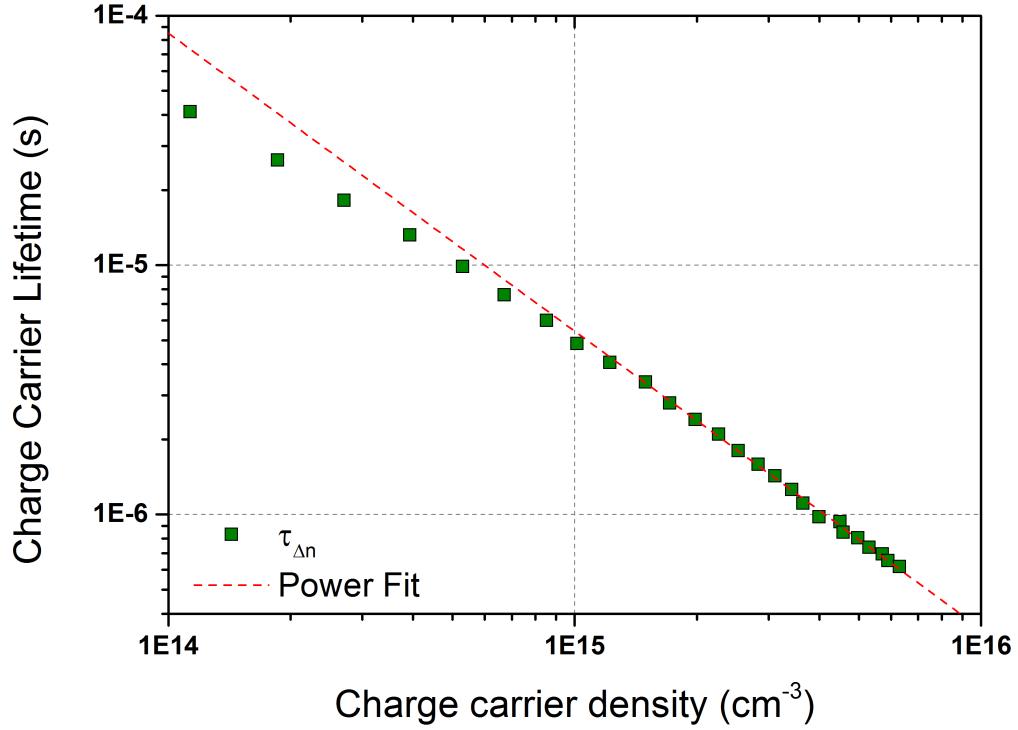
$$n \downarrow dark = Q/edA = C \downarrow geo / edA V$$

$$C \downarrow geo = edA d n \downarrow dark / d V$$



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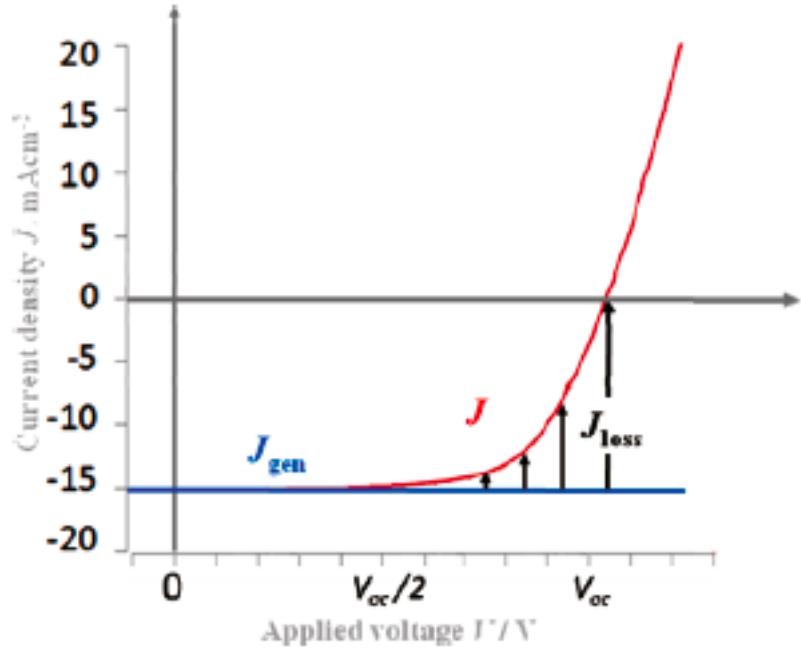




$$dn/dt = -kn\uparrow\phi$$



From Ryan et al. 2013 ( below)

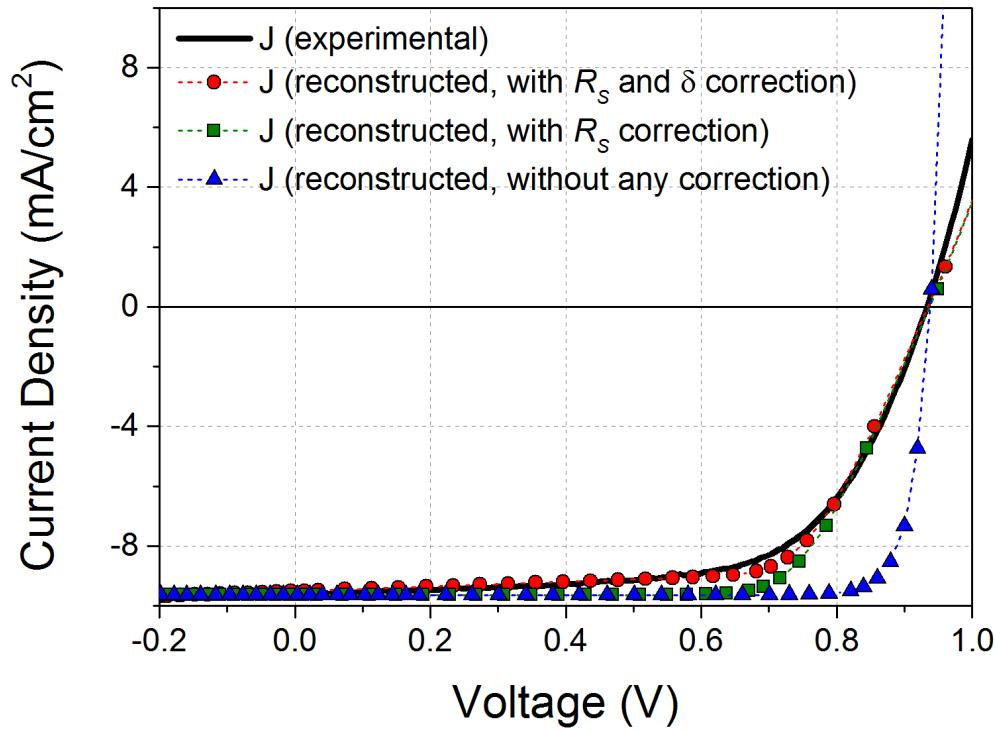


$$J_{loss} = de n / (1 + \lambda) \tau \Delta n + V / AR \downarrow sh$$

$$J_{loss} = \frac{edn}{\tau_n} \quad J = J_{gen} + J_{loss}$$

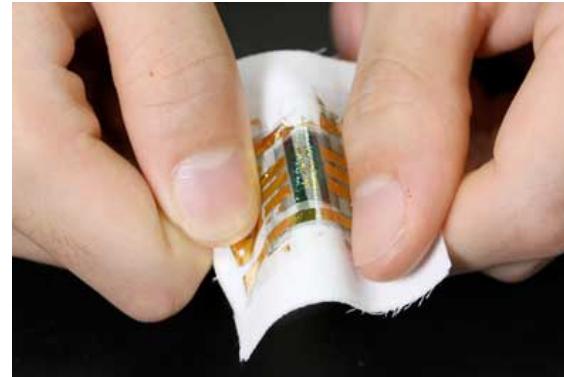
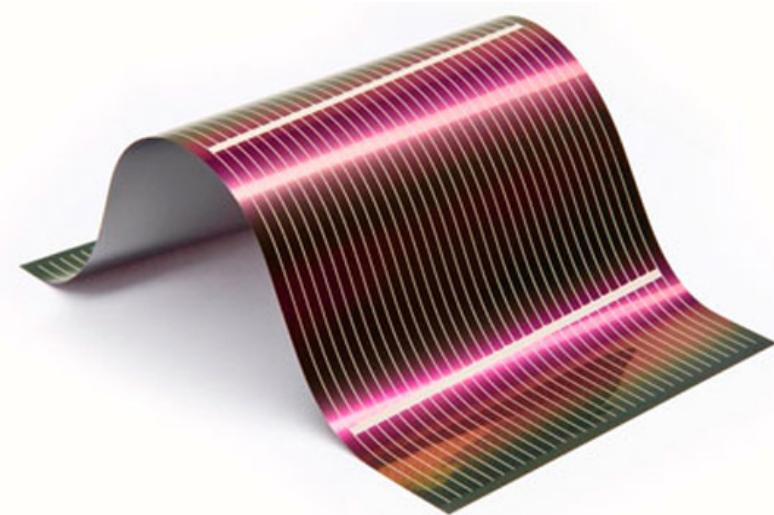
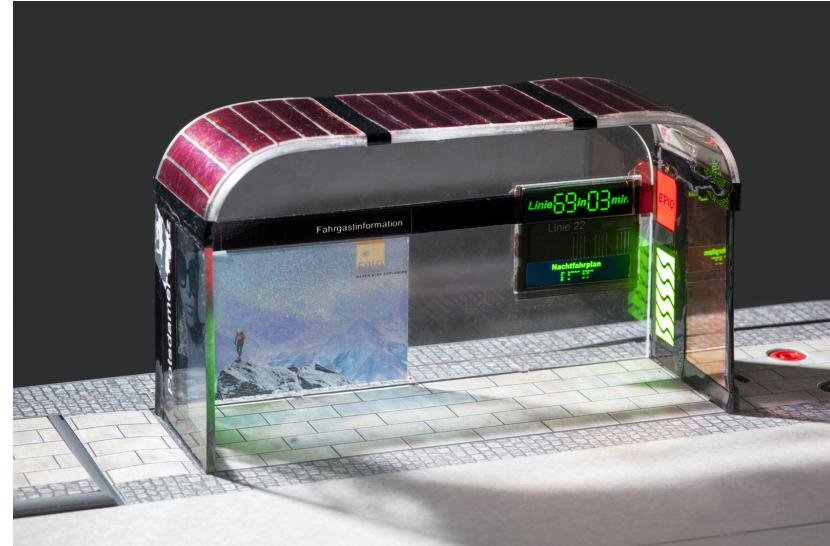
Maurano et al. Transient Optoelectronic Analysis of Charge Carrier Losses in a Selenophene/Fullerene Blend Solar Cell.  
J. Phys. Chem. C (2011) vol. 115 pp. 5947

Ryan et al. Nongeminate Recombination Dynamics–Device Voltage Relationship in Hybrid PbS Quantum Dot/C<sub>60</sub> Solar Cells. J. Phys. Chem. C (2013) vol. 117 pp. 17470-17476





# OSC from Lab to Fab





# OSC from Lab to Fab

<https://youtu.be/RyVjAw1Jjck>

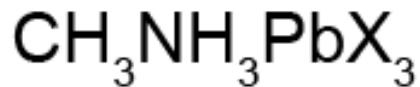
The screenshot shows a YouTube search results page with the query '(2) Faces of Chemistry'. The main video thumbnail features the title 'FACES OF CHEMISTRY' and 'RSC Advancing the Chemical Sciences'. Below the video, the caption reads: 'Faces of Chemistry: Organic solar cells (BASF) - Video 1 (11+)'. The video has 10,910 visualizaciones and was published on March 29, 2012. The video player shows a progress bar at 0:08 / 3:46. A 'SUSCRIBIRSE 42 MIL' button is visible. To the right, there are several recommended videos:

- 'Faces of Chemistry: Organic solar cells (BASF) - Video 2...' by Royal Society Of Chemistry (133 mil visualizaciones)
- '16 animales que te helarán la sangre' by Robe - Un Suspiro Acompasado (Recomendado para ti)
- 'Robe - Un Suspiro Acompasado' by robeextremoVEVO (Recomendado para ti)
- 'Cómo funciona una central de energía solar' by Marcos Gchu (47 mil visualizaciones)
- 'Solar energy / Solar photovoltaics / Photovoltaic...' by Thomas Schwenke (732 mil visualizaciones)

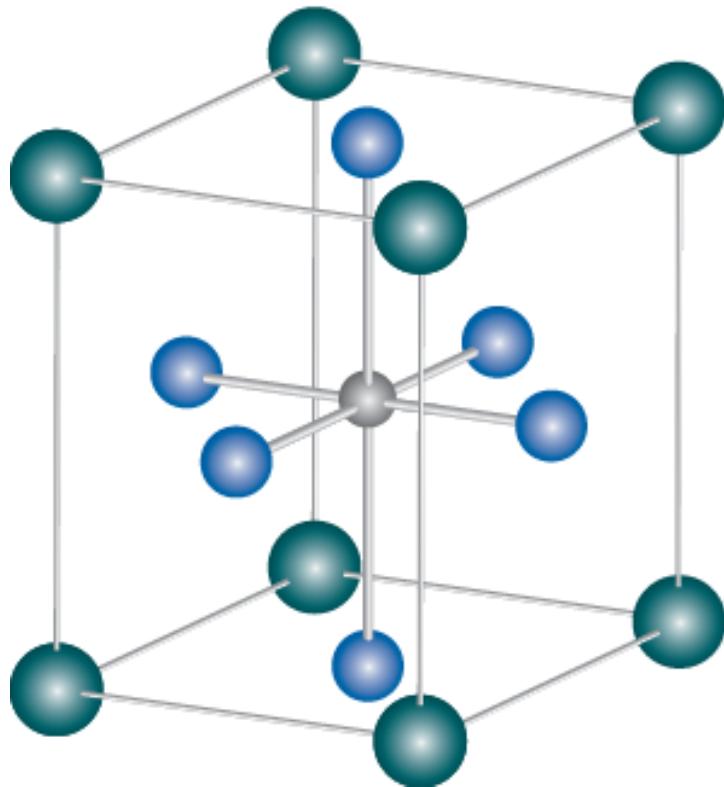
The bottom of the screen shows the Windows taskbar with various pinned icons and the system clock indicating 12:11 on 06/07/2018.



# Hybrid Perovskite Materials



[http://en.wikipedia.org/wiki/Perovskite\\_solar\\_cell](http://en.wikipedia.org/wiki/Perovskite_solar_cell)



- Methylammonium ion
- Halogen ion
- Lead ion

Kojima, Akihiro; Teshima, Kenjiro; Shirai, Yasuo; Miyasaka, Tsutomu (6 May 2009). "Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells". *Journal of the American Chemical Society* 131 (17): 6050–6051. [doi:10.1021/ja809598](https://doi.org/10.1021/ja809598)



# Hybrid Perovskite Materials



<https://www.youtube.com/watch?v=ZdpQgPJ1Plk>



# Hybrid Perovskite Materials



Miyasaka



Snaith



Park



Grätzel

***SUCCE HAS MANY FRIENDS...Failure is an orphan***

John F. Kennedy

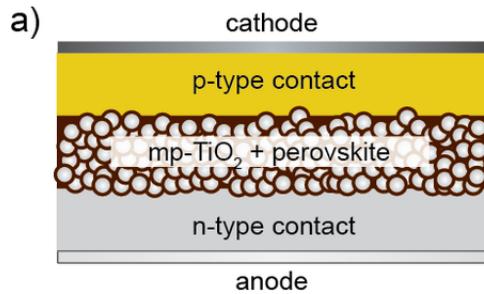
First solid ionic with semiconductor properties suitable for photovoltaics



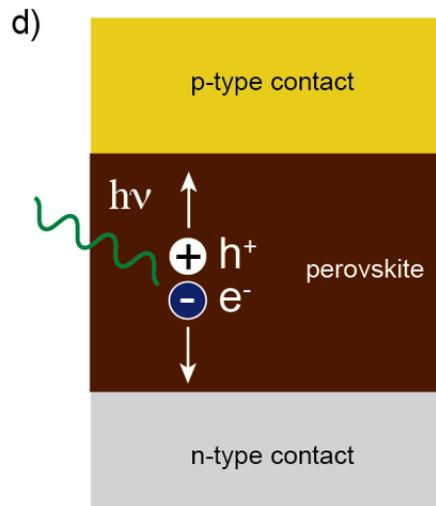
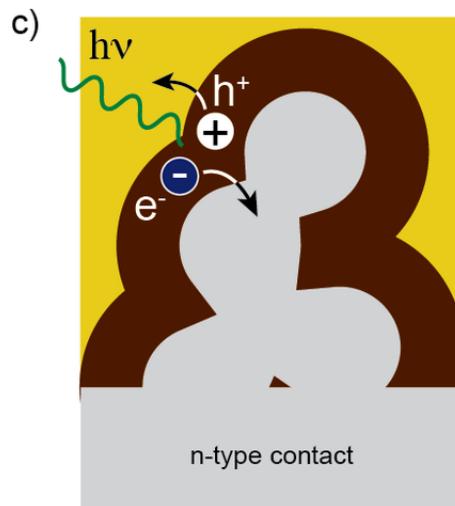
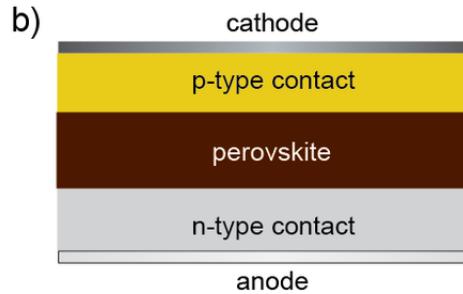
# Hybrid Perovskite Materials



## Sensitized perovskite solar cell



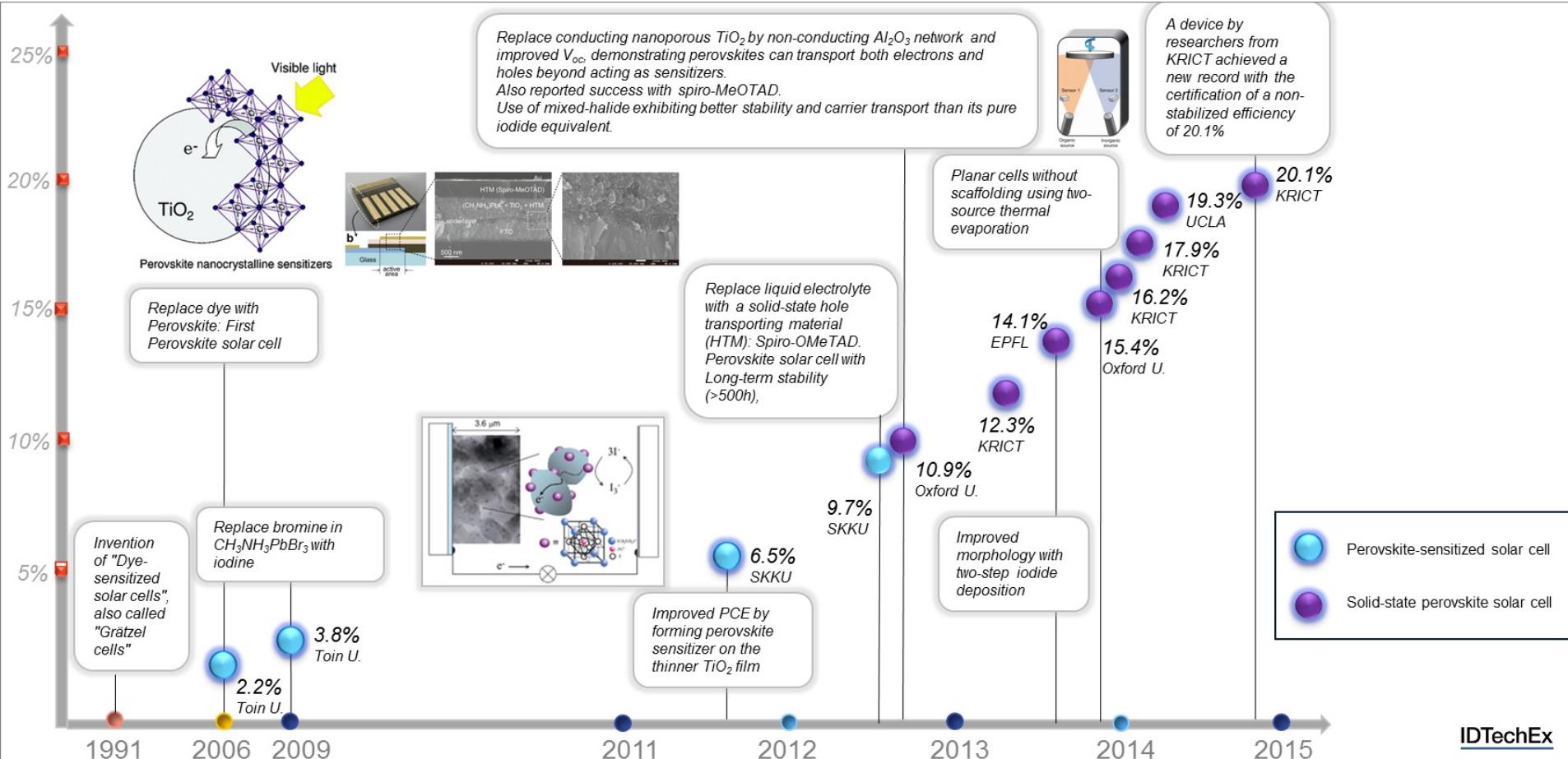
## Thin-film perovskite solar cell



Kojima, Akihiro; Teshima, Kenjiro; Shirai, Yasuo; Miyasaka, Tsutomu (6 May 2009). "Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells". *Journal of the American Chemical Society* 131 (17): 6050–6051. [doi:10.1021/ja809598](https://doi.org/10.1021/ja809598)

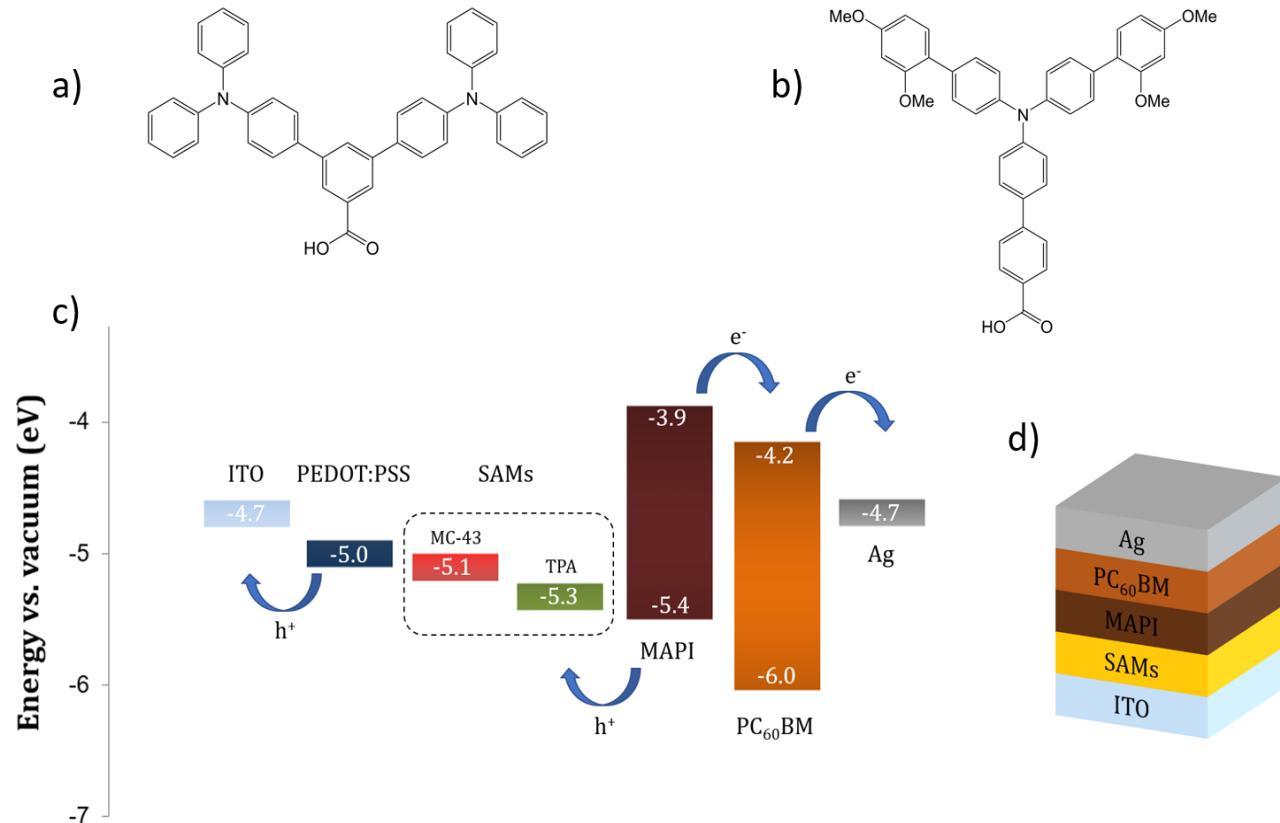


# Hybrid Perovskite Materials



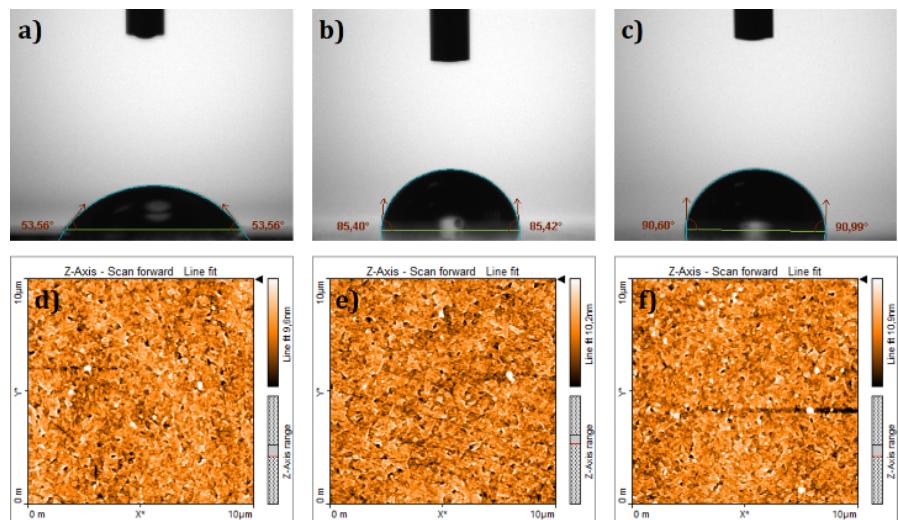
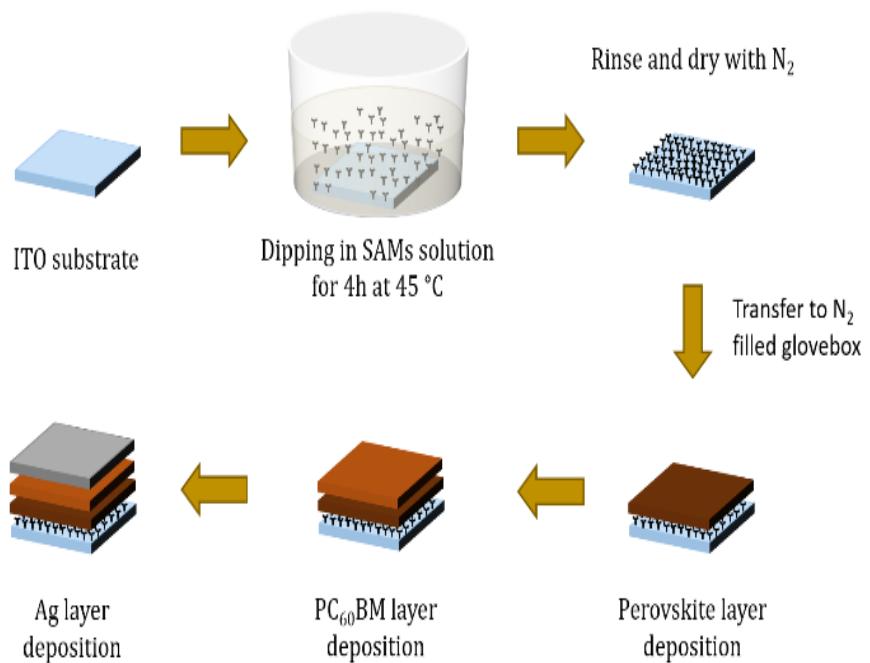


# Perovskites at ICIQ\_Palomares group



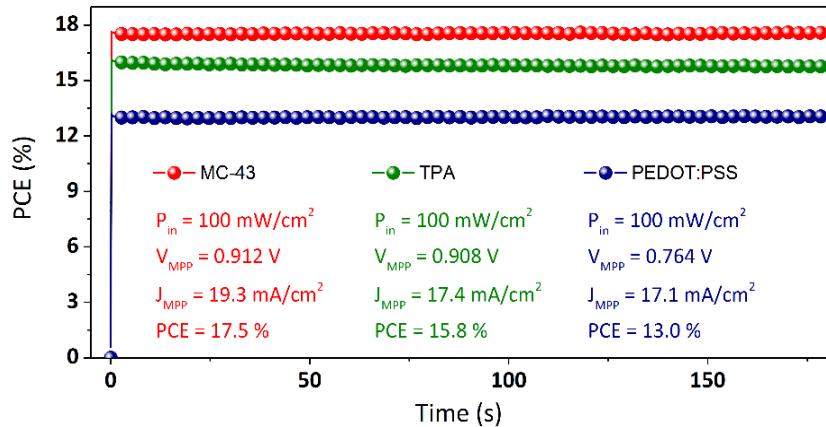
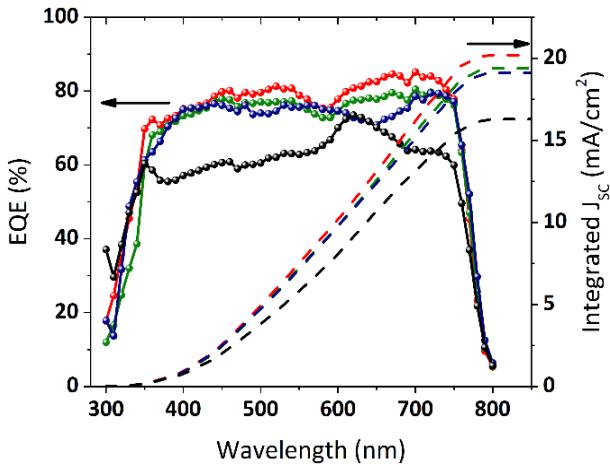
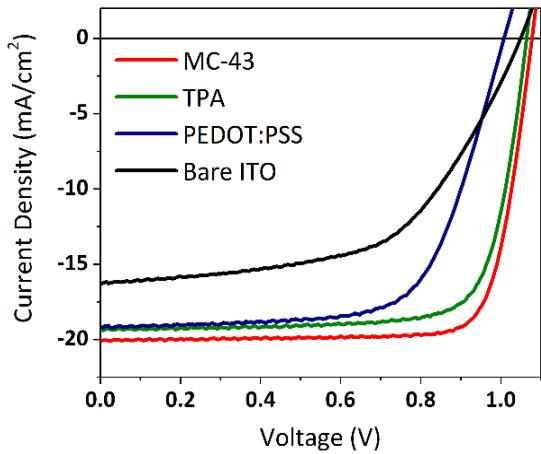


# Perovskites at ICIQ\_Palomares group





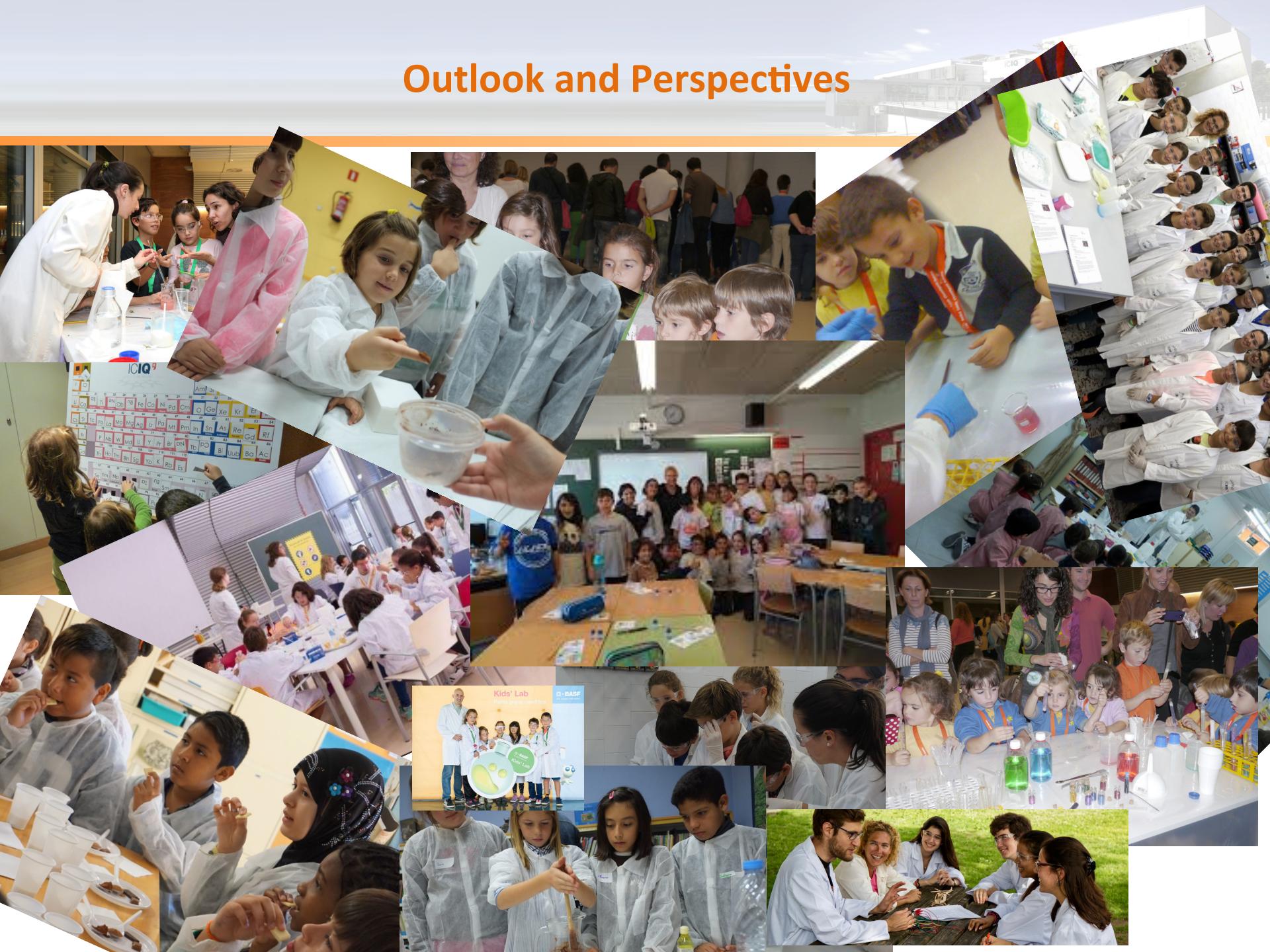
# Perovskites at ICIQ\_Palomares group



# Outlook and Perspectives



# Outlook and Perspectives



# Thank you for your attention.

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**EPalomaresGil** @EPalomaresGil

biòleg que fa química amb equips de física, pare de 3 príncipes i amant de la vida. No crec en el karma però si en les bones persones.

② Tarragona, Espanya

Tuits Tuits i respostes Continguts

EPalomaresGil @EPalomaresGil · 4 h I aquí un poc de la química dels focs artificials. @TGNAjuntament @TGNcultura @TGNturisme @SER\_TgnReus

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13:05 06/07/2018