

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

epalomares@iciq.es

Prof. Emilio Palomares



Barcelona Institute of
Science and Technology

AKNOWLEDGMENTS



Barcelona Institute of
Science and Technology



Generalitat
de Catalunya

European Research Council



<https://www.facebook.com/alwayspalomares/>

<https://twitter.com/palomaresgroup>

The biggest challenge...



The biggest challenge...



time line - Buscar con Go x Magdalena Skipper a Twi x

Twitter, Inc. [US] | https://twitter.com/Magda_Skipper/status/1014792178143584256

Aplicaciones Nature Chemistry Outlook Web Access Humor, inteligencia SABiDi - Biblioteca http://catalog.urv.cat The Diode Equation Diode Equation | PV Otros marcadores

Inici Moments Notificacions Missatges Cerca al Twitter Tuita X

Magdalena Skipper @Magda_Skipper

Can we imagine a solution to climate change without economics? - social science is key to global solution; Calhoun #ISClaunch

Tradueix el tuit

1:44 - 5 de jul. de 2018

3 retuits 8 agradaments

1 3 8

Tuita la teva resposta

Seamus McCelt @t1neq · 54 min

En resposta a @Magda_Skipper

Humans are screwing up so bad - problems are going to solve themselves (force upon them by the earth)

Tradueix el tuit

Qui seguir · Actualitza · Mostra-ho tot

- Orli Bahcall** @obahcall Segueix
- Manolis Dermitzakis** @de... Segueix
- Joe Pickrell** @joe_pickrell Segueix

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

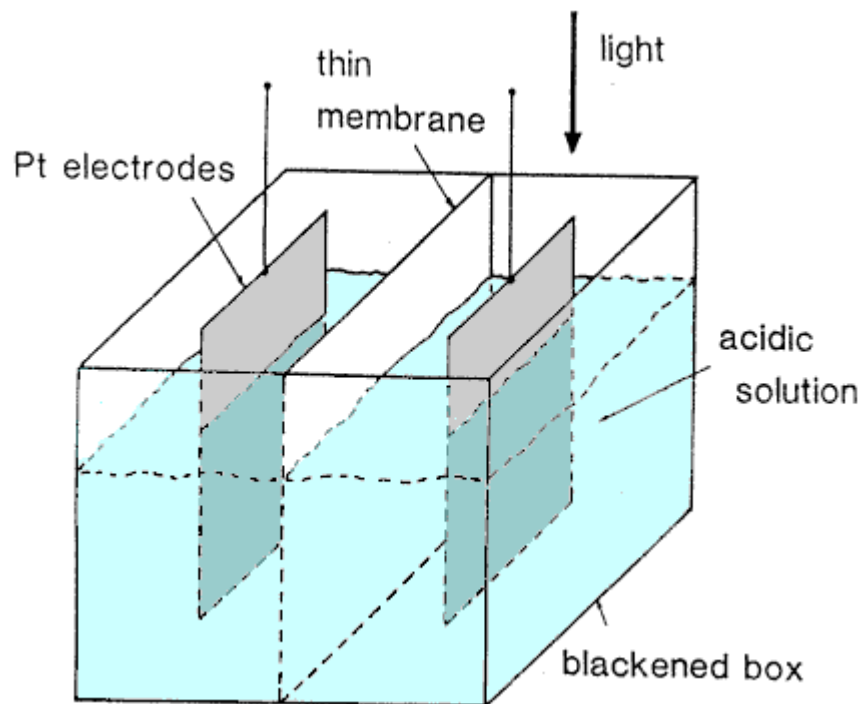
”

What occurs when light strikes on a material?



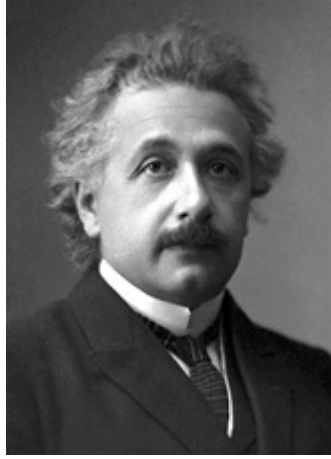
1839 (19 years old)

Photoelectric Effect



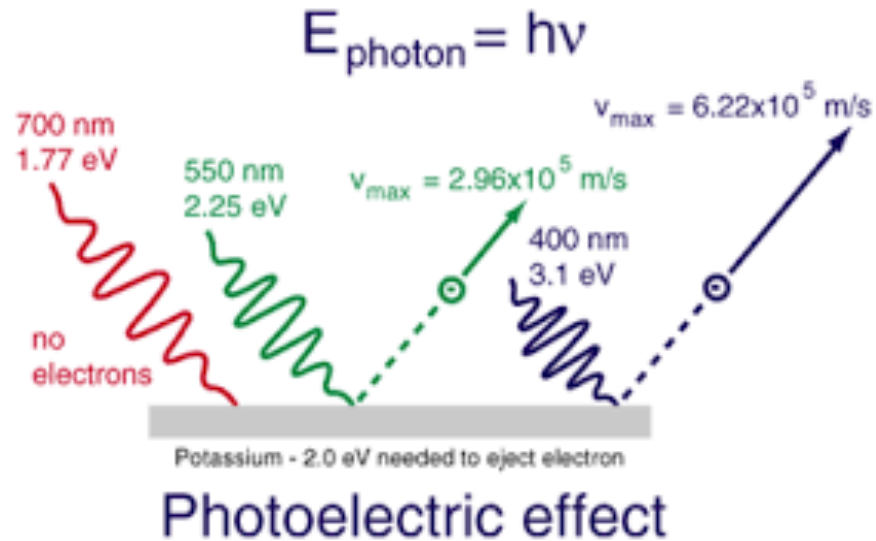
First photoelectrochemical cell with silver chloride in acidic media and illuminated while connected to Pt electrodes

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

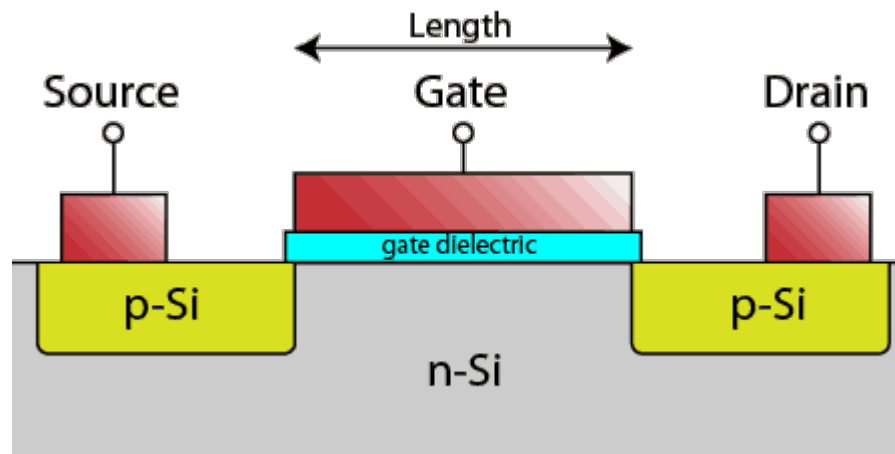


Bardeen

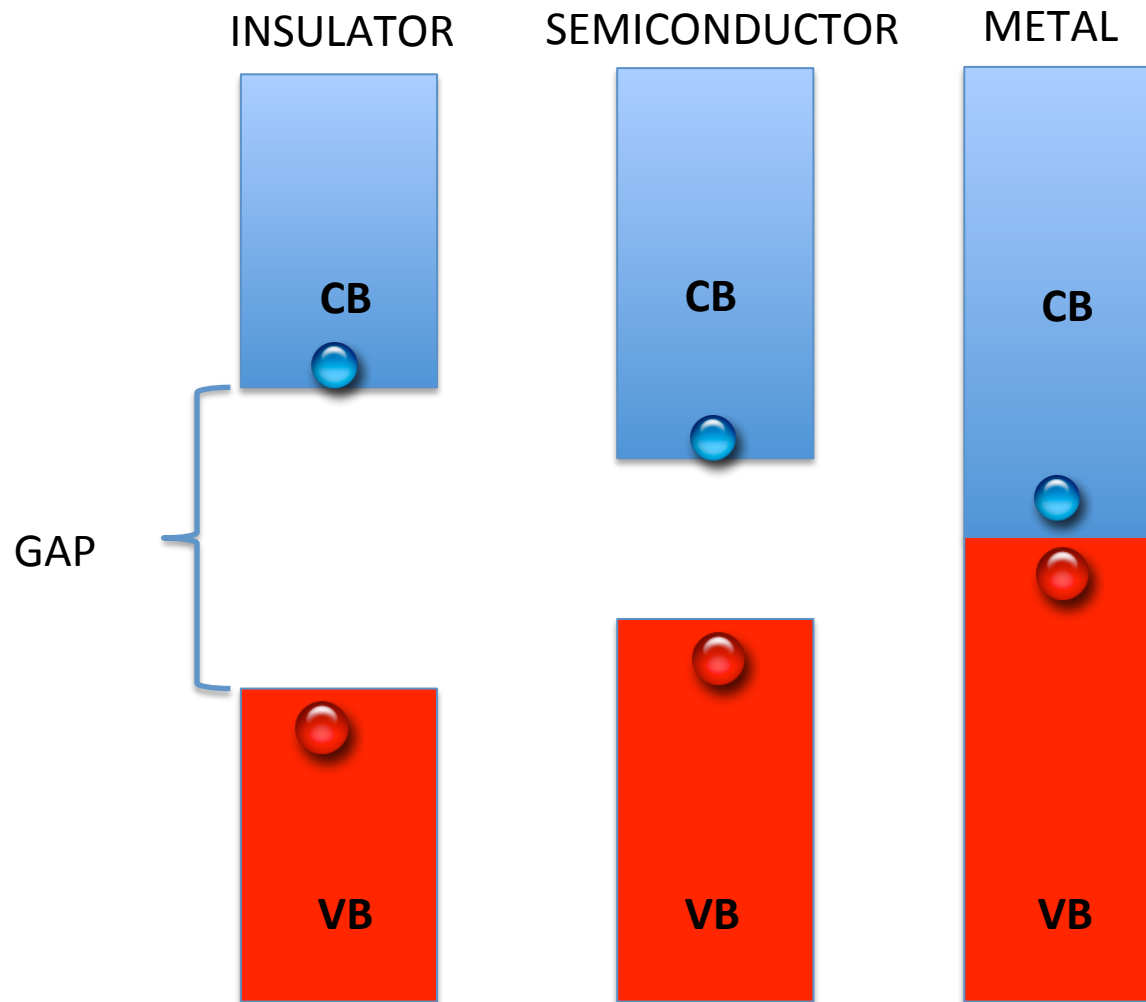


Brattain

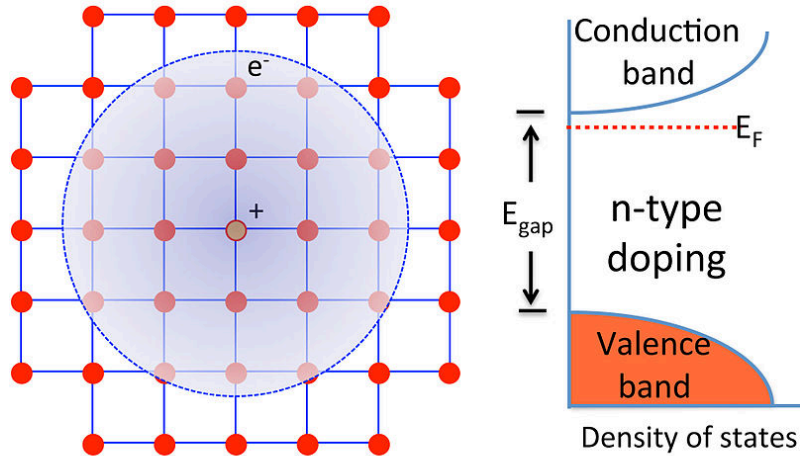
Physics Nobel Prize 1956



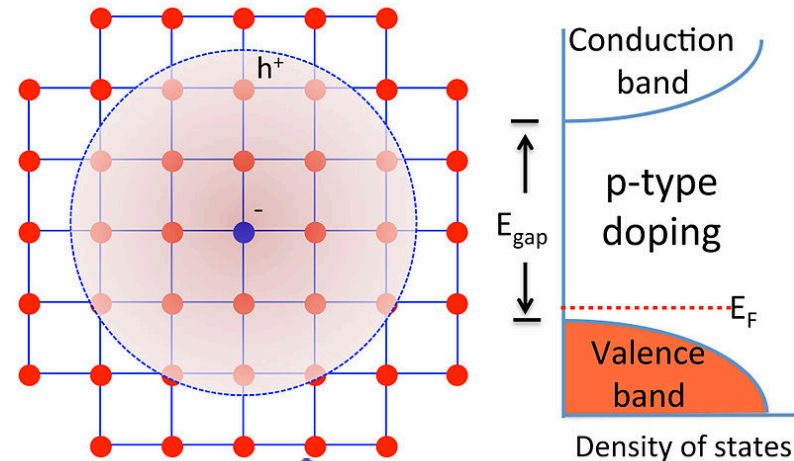
What is a semiconductor?



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

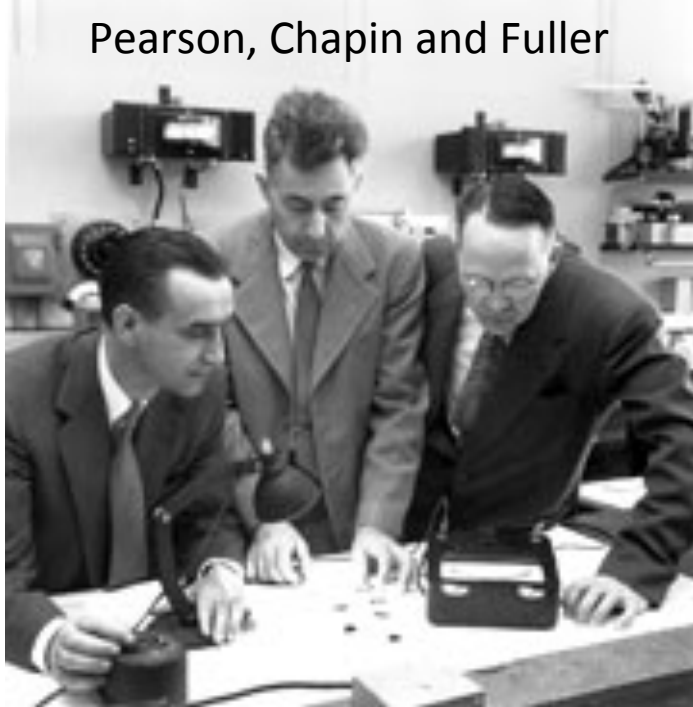
Basic electronic device that was the open door to integrated electronic circuits.

The P-N junction

What is a semiconductor?



Pearson, Chapin and Fuller

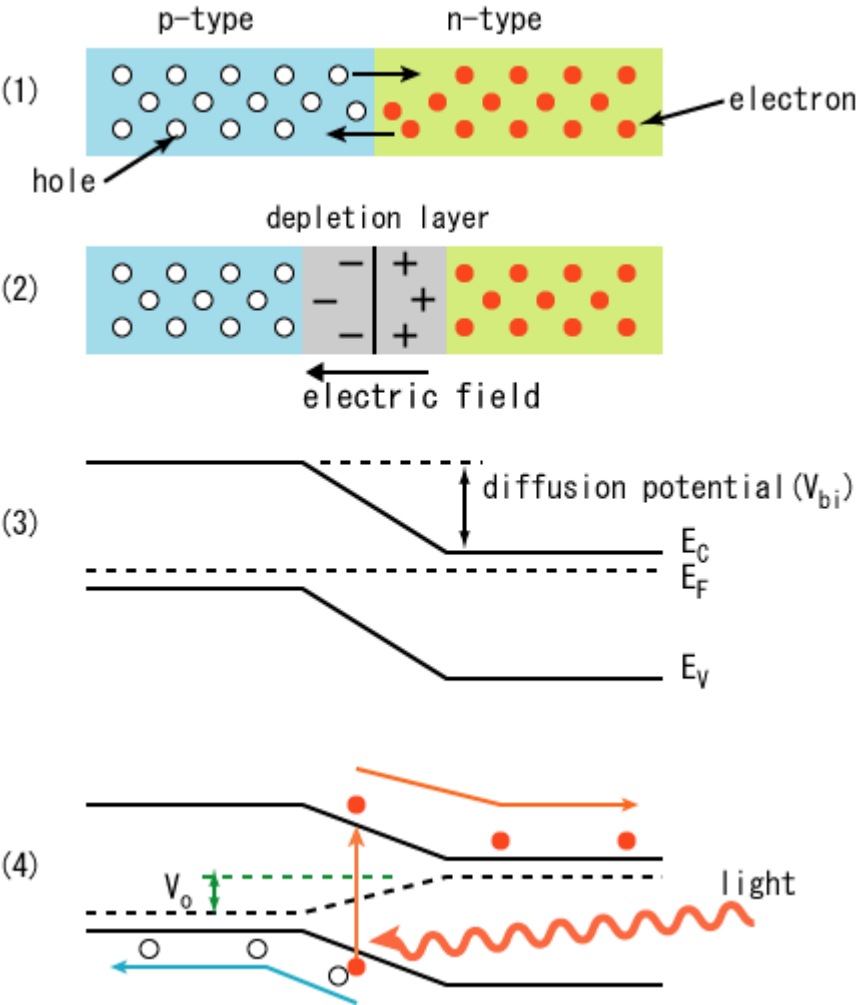


1954-First Practical Solar Cell with efficiency of 6%

FIRST SOLAR CELL.

The P-N junction

What is a semiconductor?



What is a semiconductor?



Heeger



MacDiarmid



Shirakawa

Chemistry Nobel Prize 2000

"for the discovery and development of conductive polymers".

**New game, new rules,
new science**



Barcelona Institute of
Science and Technology

What is a semiconductor?



Heeger

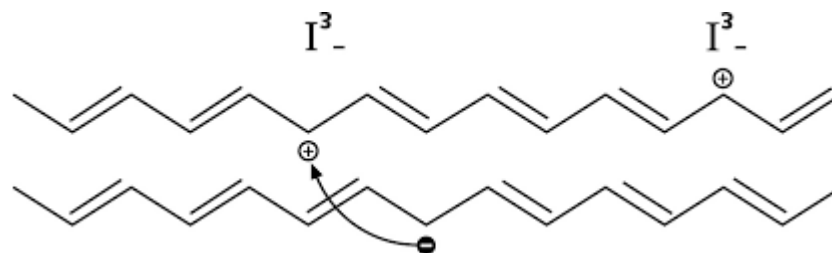


MacDiarmid



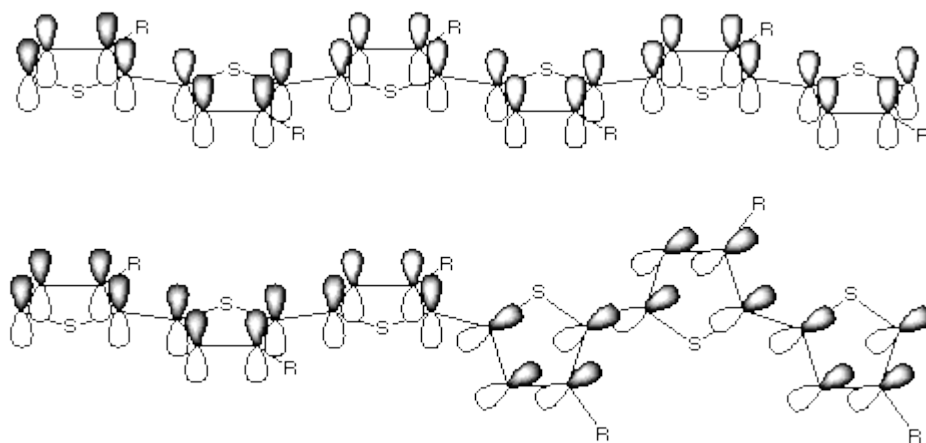
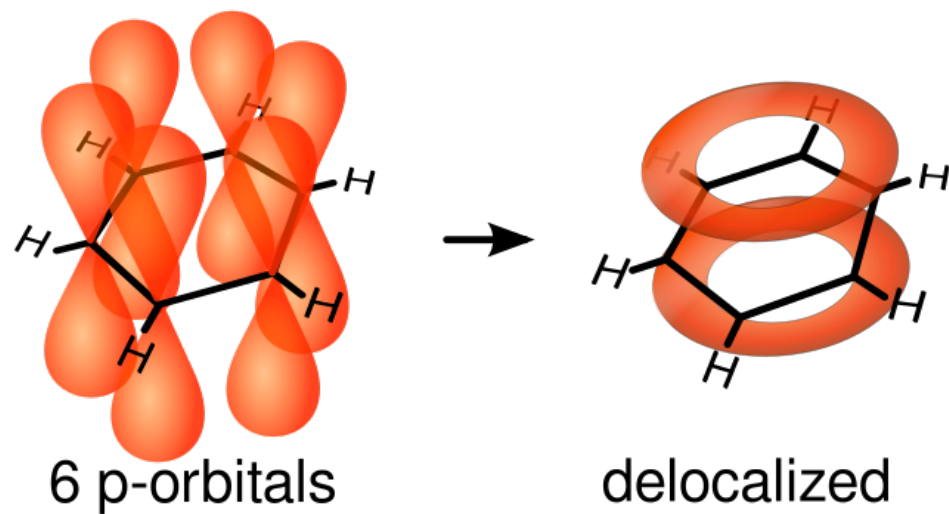
Shirakawa

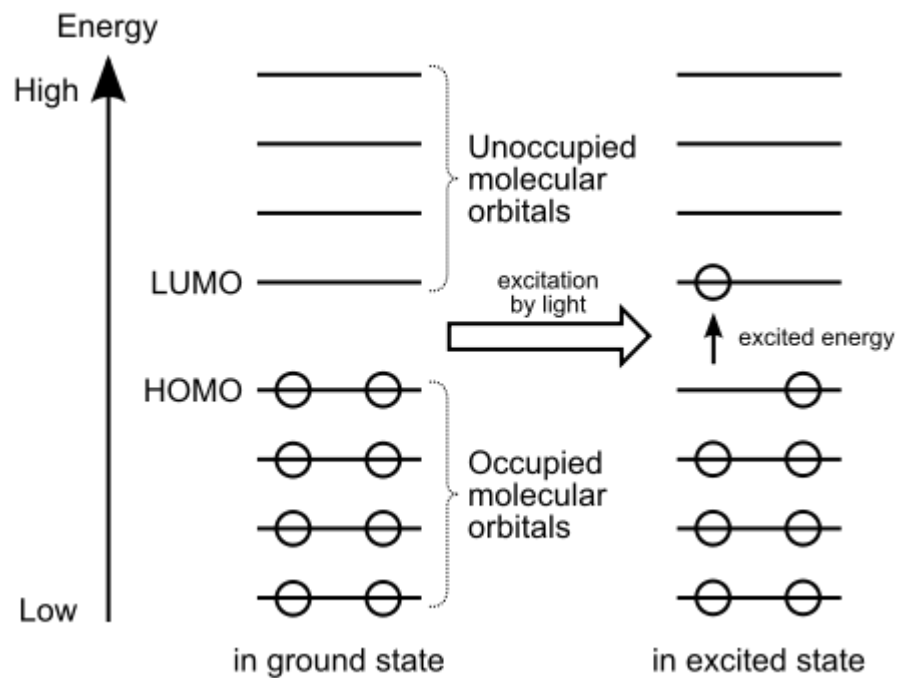
Chemistry Nobel Prize 2000



Polaron

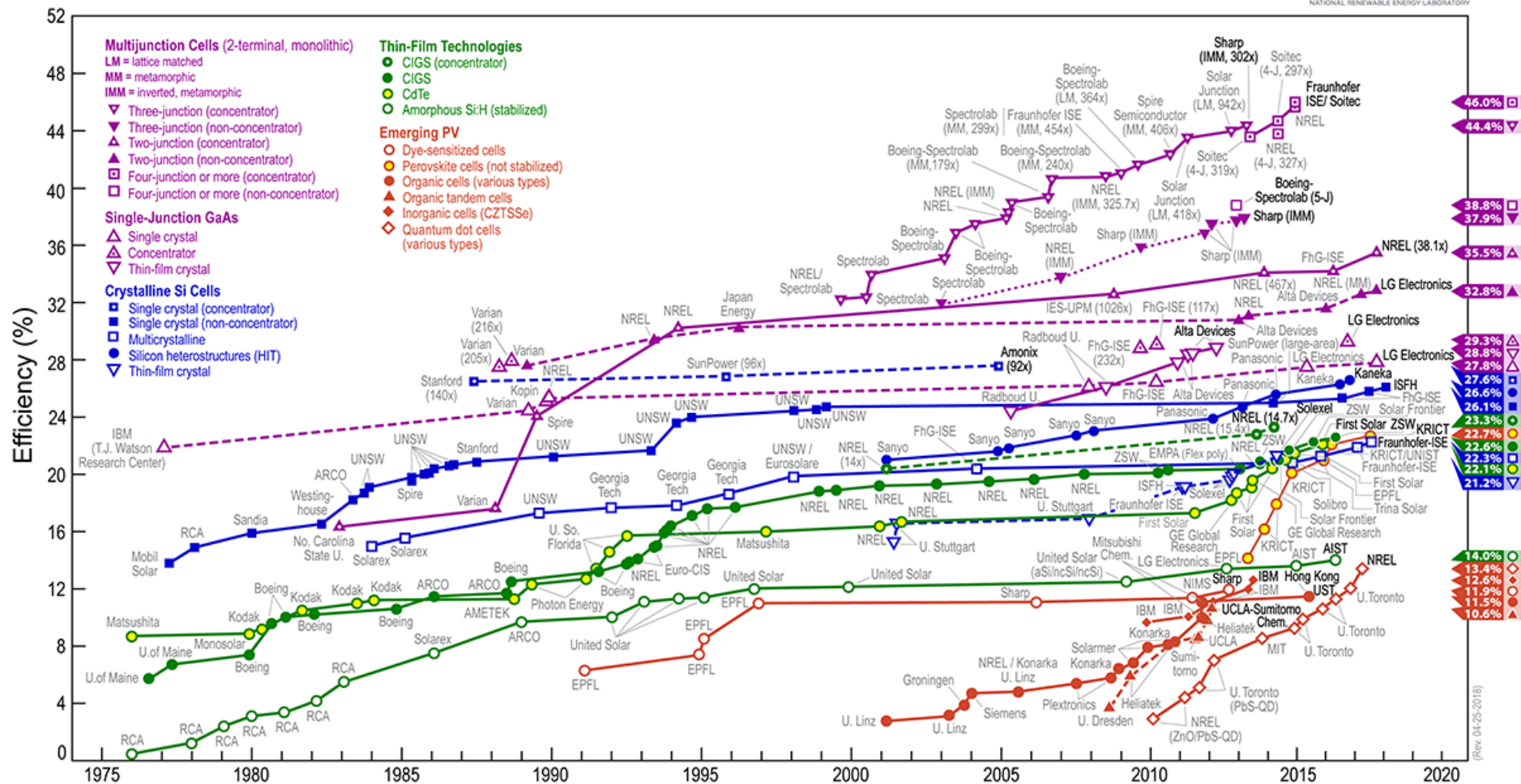
What is a semiconductor?





Solar Power.

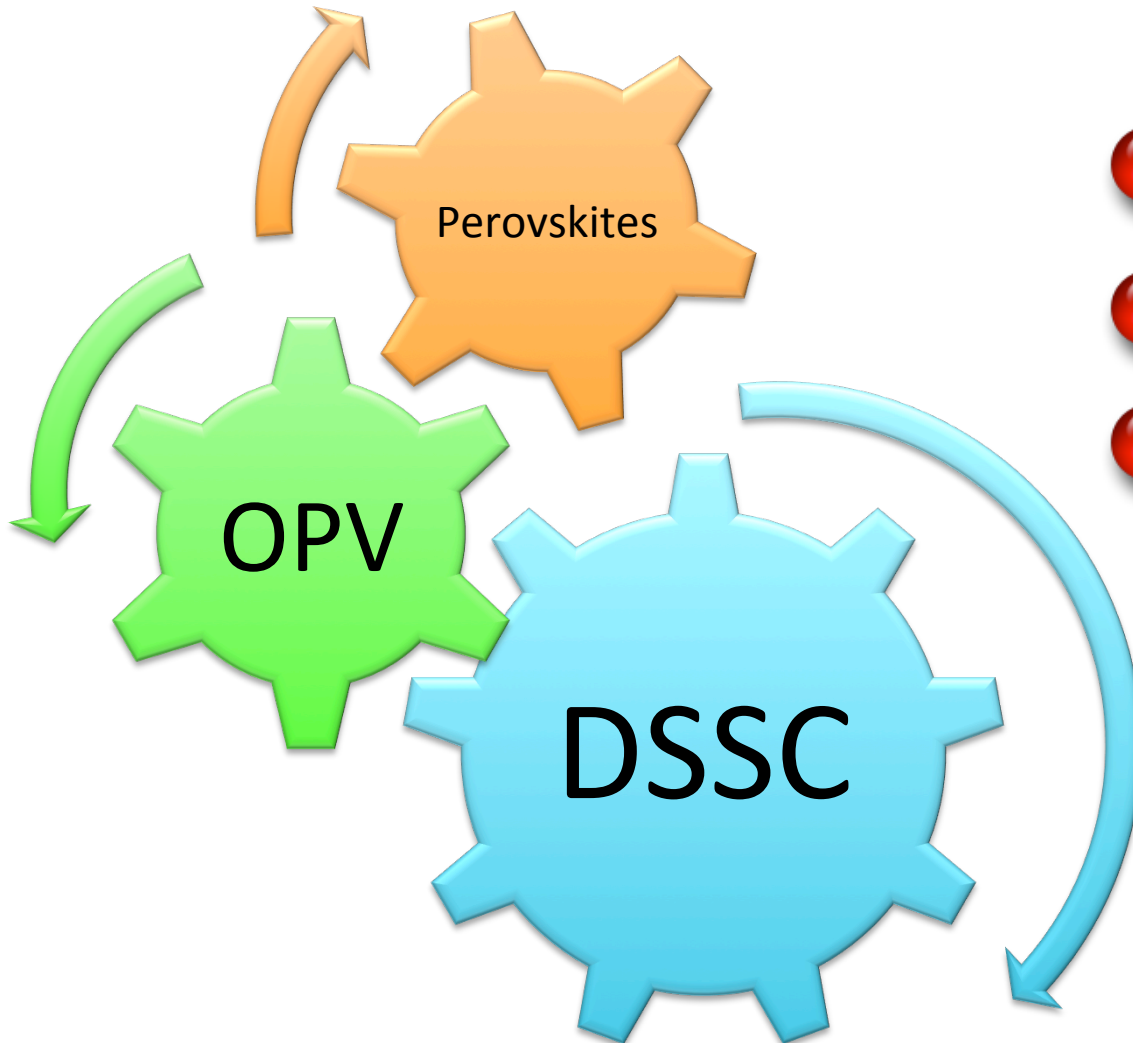
Best Research-Cell Efficiencies



Barcelona Institute of Science and Technology



Third generation PV. Powering the World with Solar Energy



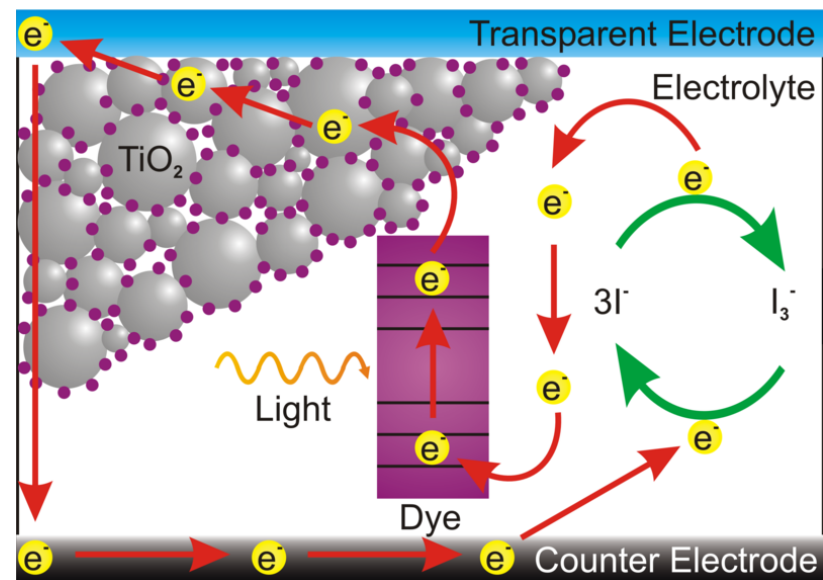
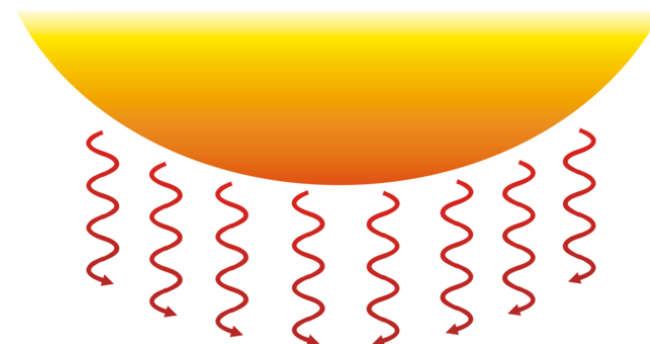
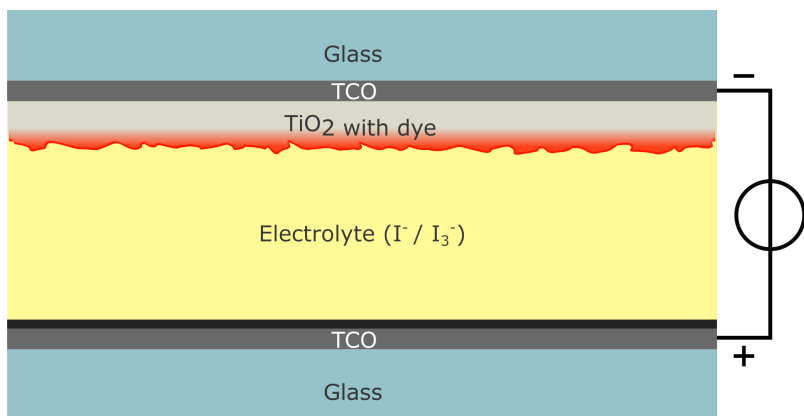
- Low-Cost
- Efficient
- Durable



Dye Sensitized Solar Cells (DSSC)



O'Regan & Grätzel



A low-cost, high-efficiency solar cell based on dye-sensitized colloidal TiO₂ films

B O'Regan, M Grätzel

Nature 353 (6346), 737-740

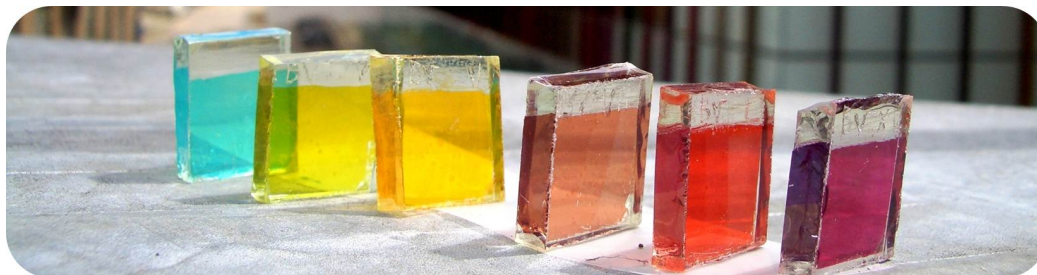
Over 28.000 citations!!!!



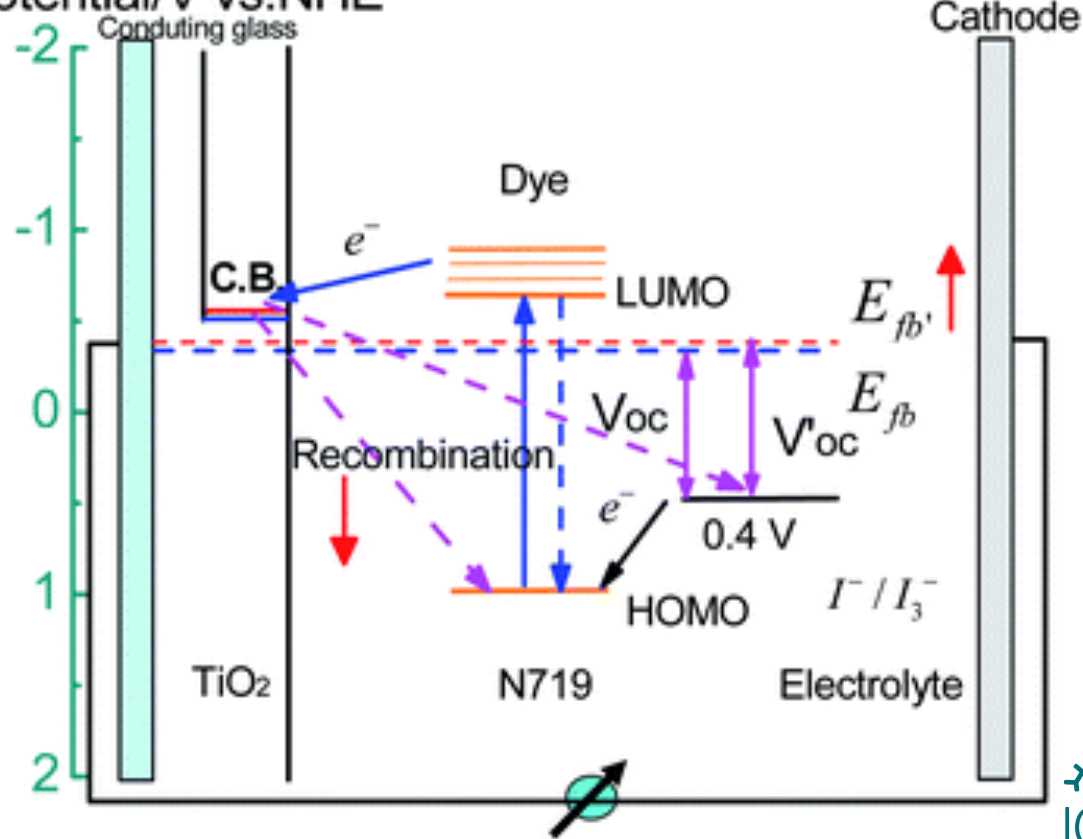
Barcelona Institute of
Science and Technology



Dye Sensitized Solar Cells (DSSC)

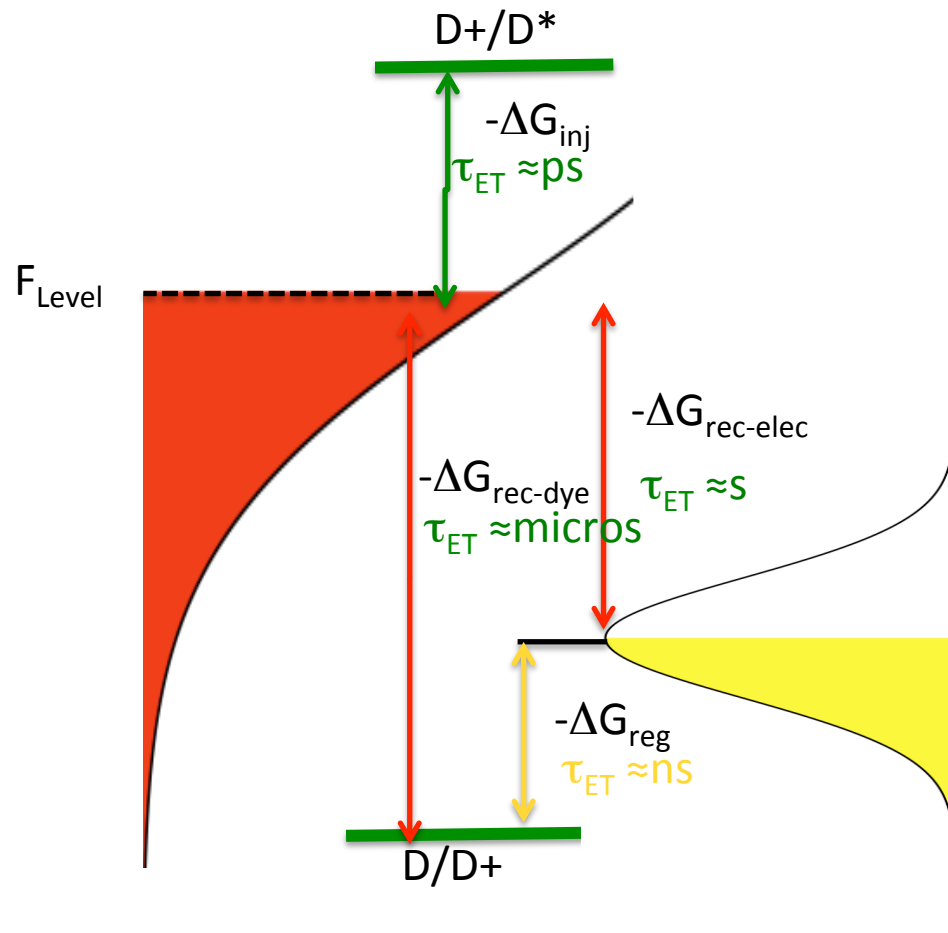
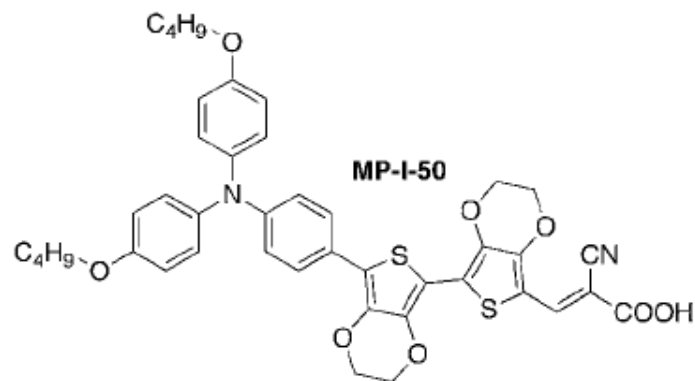
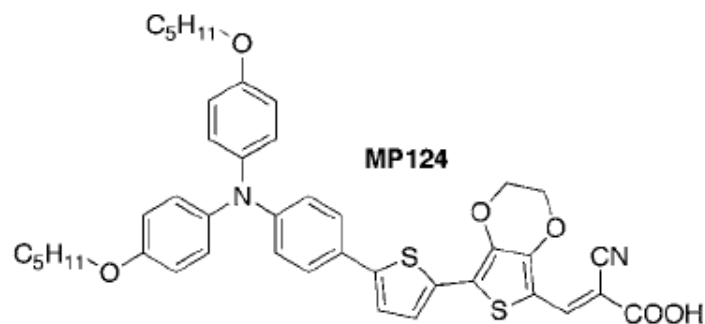


Potential/V vs.NHE





Dye Sensitized Solar Cells (DSSC)



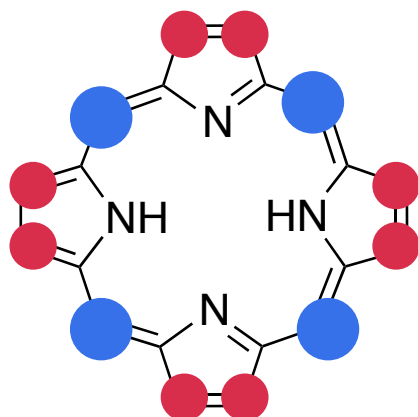
J Am Chem Soc (2008) vol. 130 (41) pp. 13558-13567

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

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

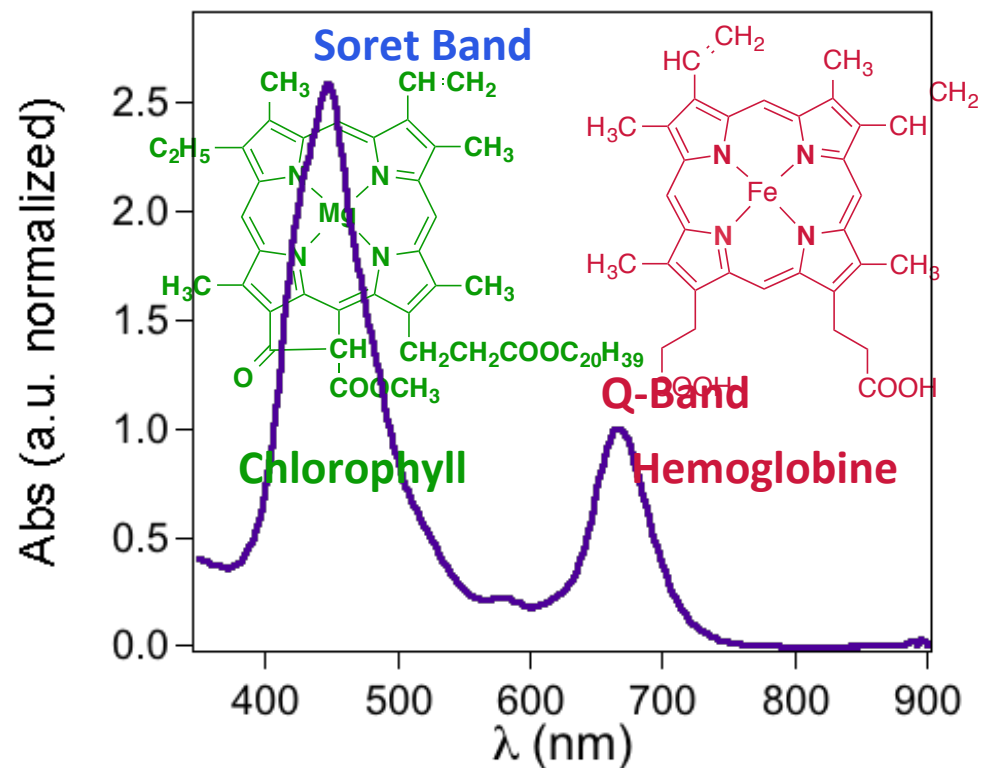


- 4 modified pyrrole connected at carbon α by methine
- Huckel's rule
- High ϵ
- Present in Nature



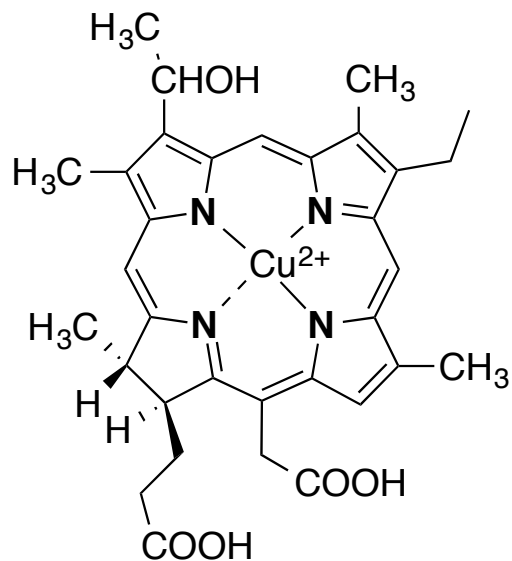
● β -positions

● meso-positions



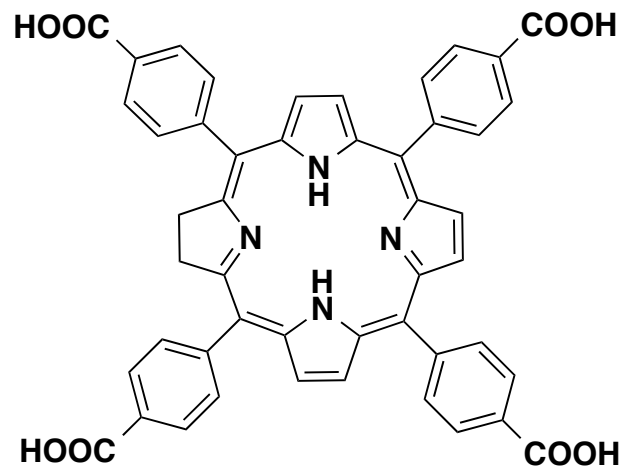


Background on Porphyrins for DSSC



$\eta=2.6\%$

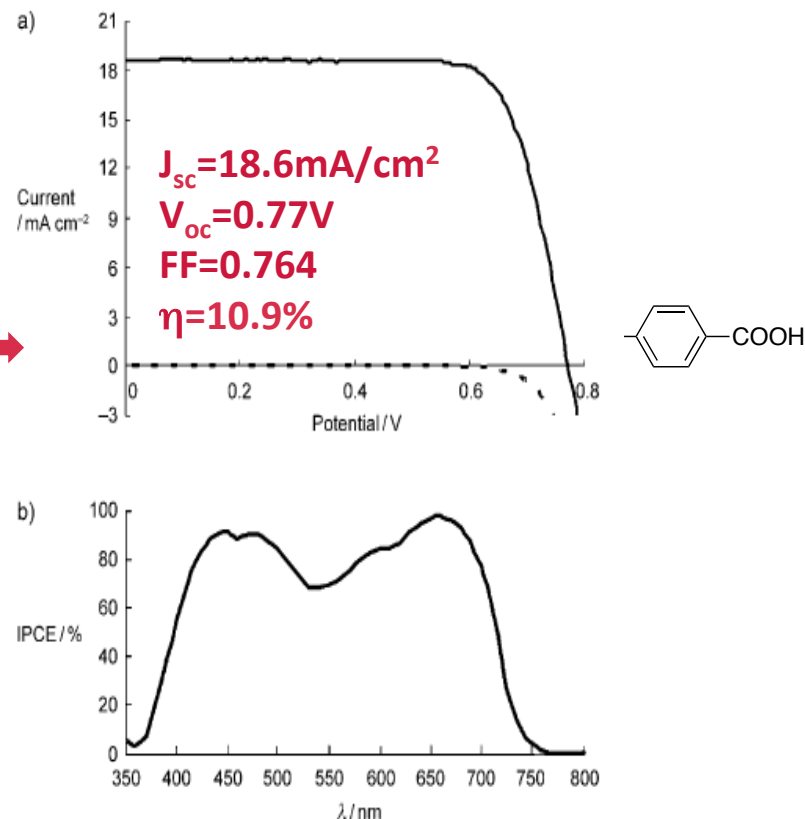
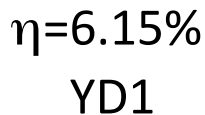
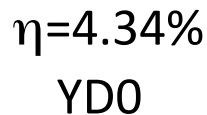
Cu-2- α -oxymesoisochlorin



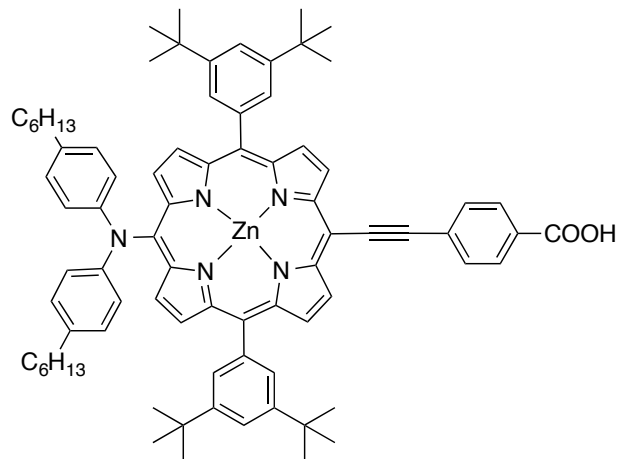
$\eta=3.5\%$

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,



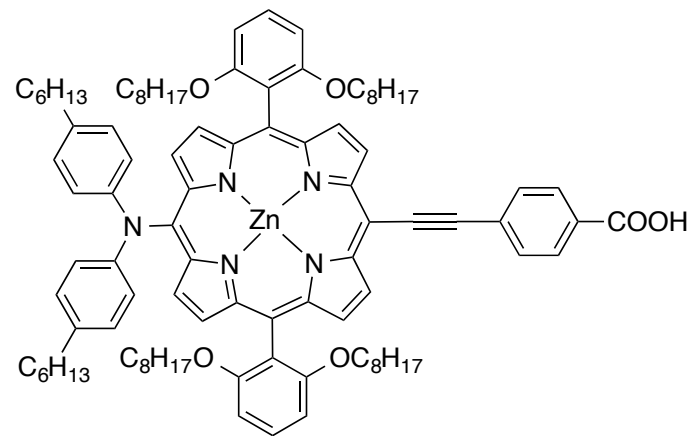
Beisho, C.T.P.; Zakeer, R.; Chis, M.; Lyche, C.; Vlach, G.; Gräzel, M.C.; Angel, W.; De, E.; Siell, D.; Fom, L.; Edition **2010**, 49, 6646. *Journal of Materials Chemistry* **2010**, 20, 1127.



YD2

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

Vs

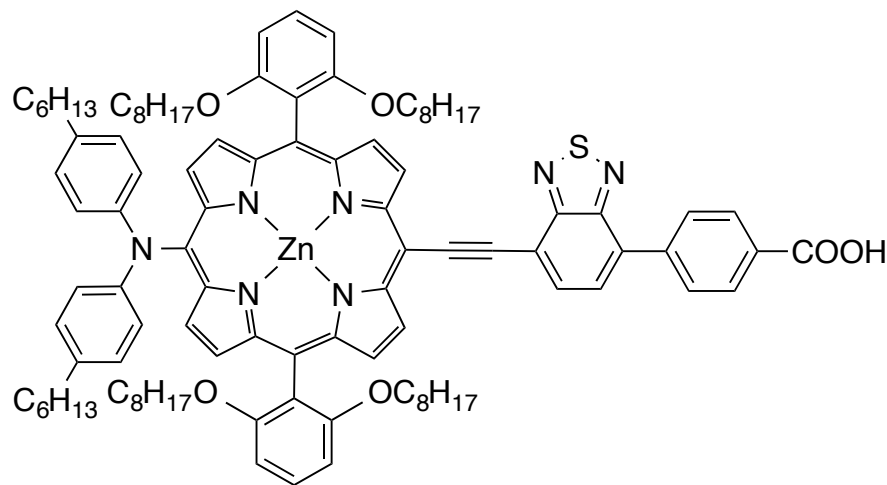


YD2-o-C8

$$\eta = 9.4\% (\text{I}_3^-/\text{I}^-)$$

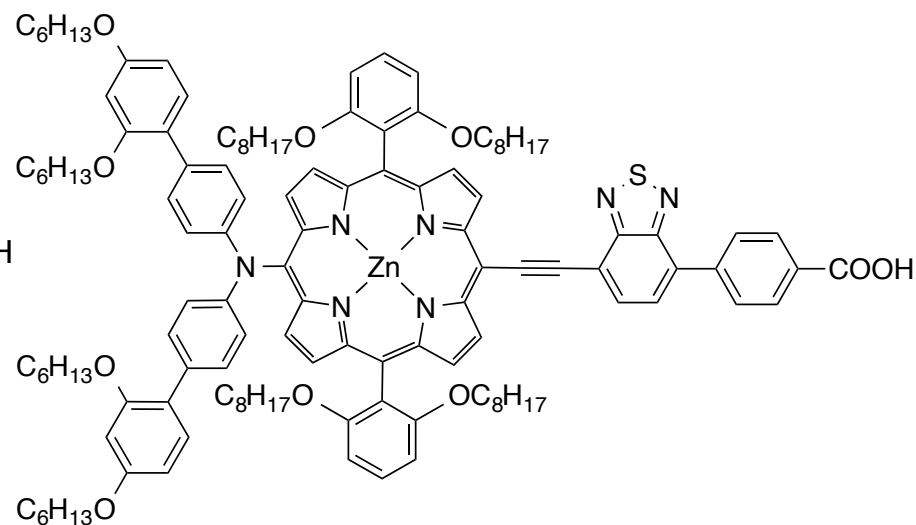
$$\eta = 11.9\% (\text{Co}^{2+}/\text{Co}^{3+})$$

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

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



SM315

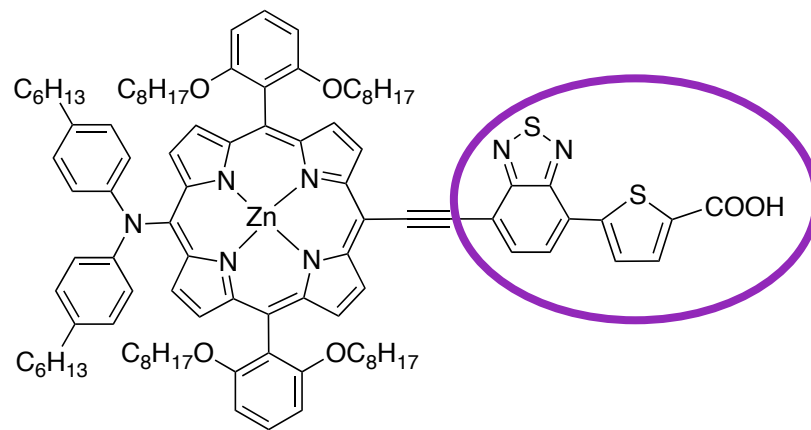
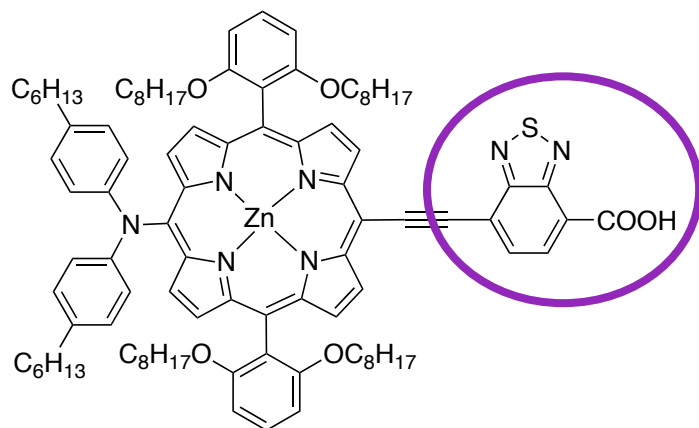
$$\eta = 13.0\% (\text{Co}^{2+}/\text{Co}^{3+})$$

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.

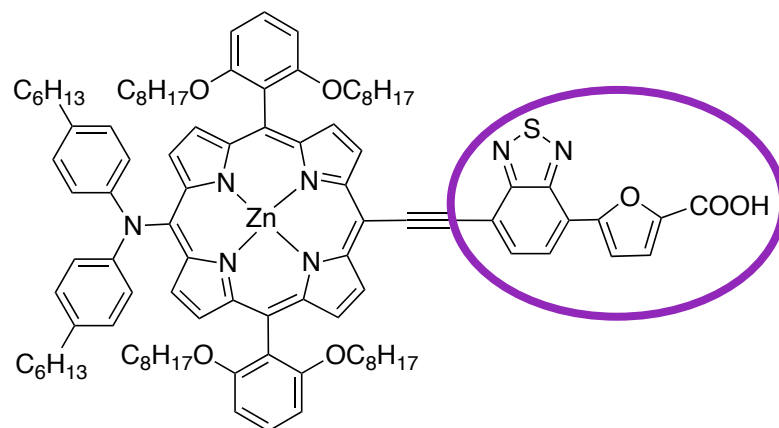
Mathew, S.; Yella, A.; Gao, P.; Humphry-Baker, R.; Curchod Basile, F. E.; Ashari-Astani, N.; Tavernelli, I.; Rothlisberger, U.; Nazeeruddin Md, K.; Grätzel, M. *Nat Chem* **2014**, 6, 242.



DSSC at ICIQ_Group Prof. Palomares



LCVC02



LCVC03

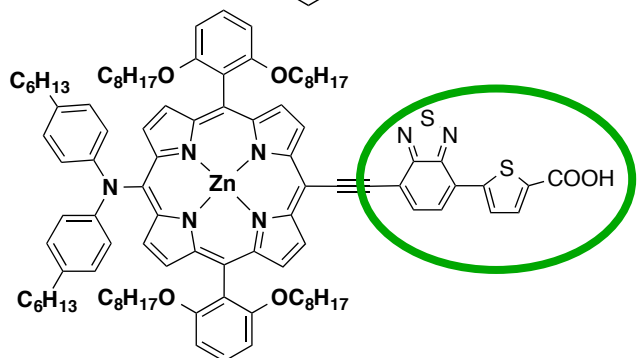
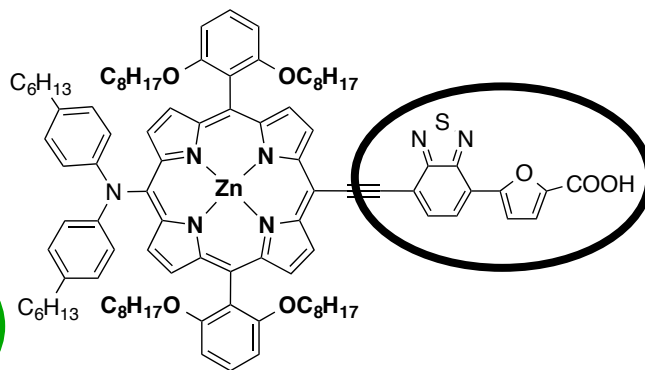
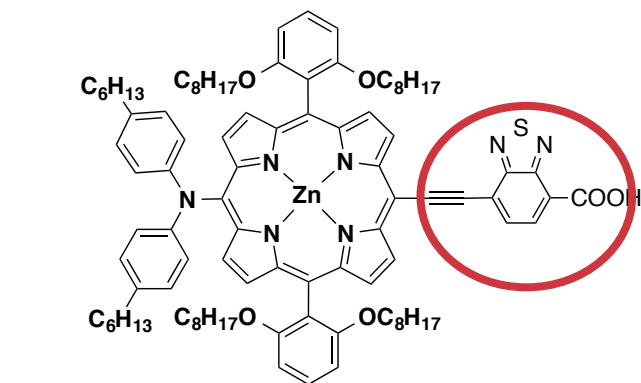
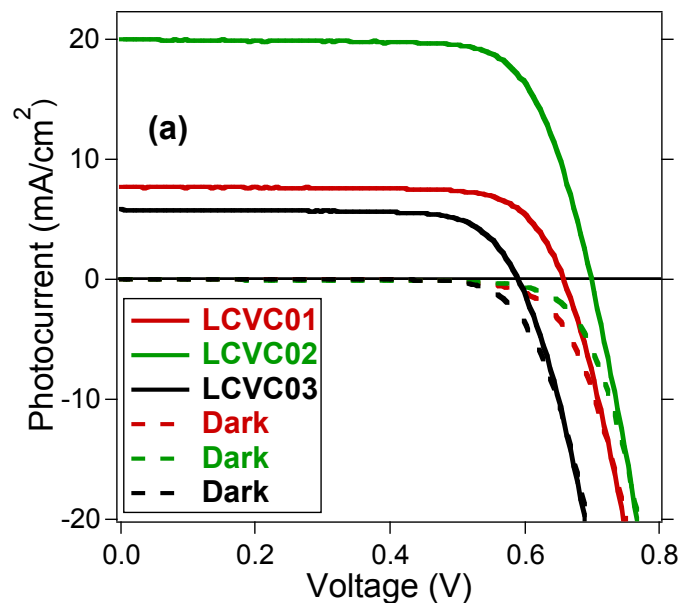


Barcelona Institute of
Science and Technology



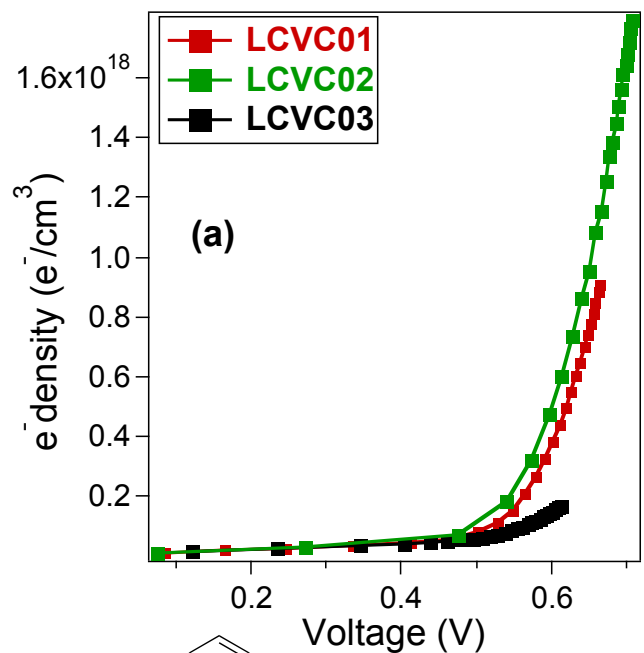
Photovoltaic parameters of LCVC01, LCVC02 and LCVC03

Dye	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	η (%)
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

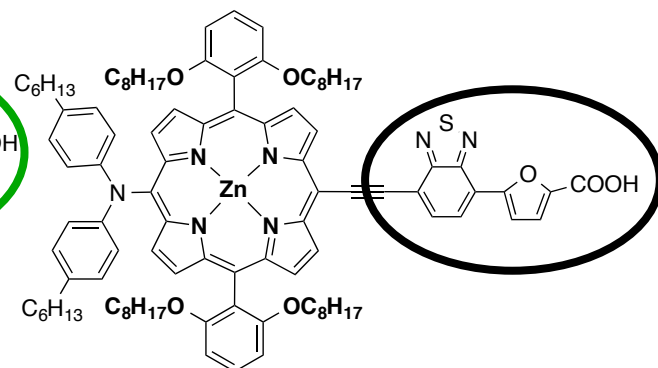
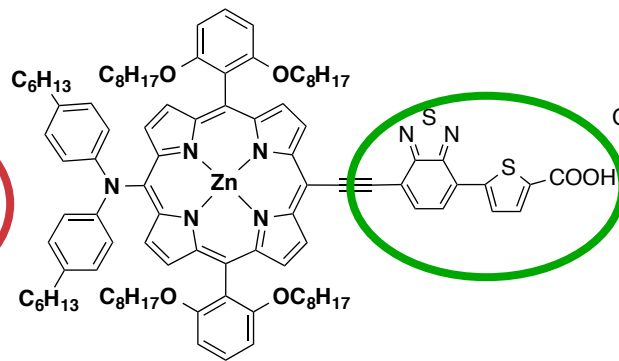
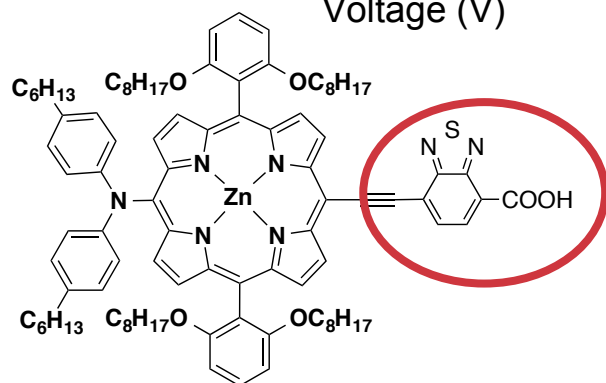
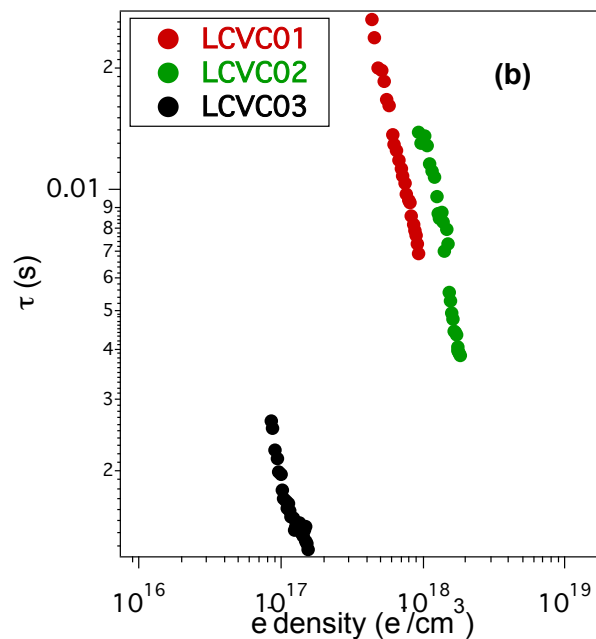




CE



TPV





DSSC from lab to fab.



The EPFL's Convention Center (Lausanne, Switzerland) has 300 m² 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.

SCIENTIFIC
REPORTS



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

Damien Joly¹, Laia Pellejà², Stéphanie Narbey³, Frédéric Oswald³, Julien Chiron⁴, John N. Clifford², Emilio Palomares^{2,5} & Renaud Demadrille¹

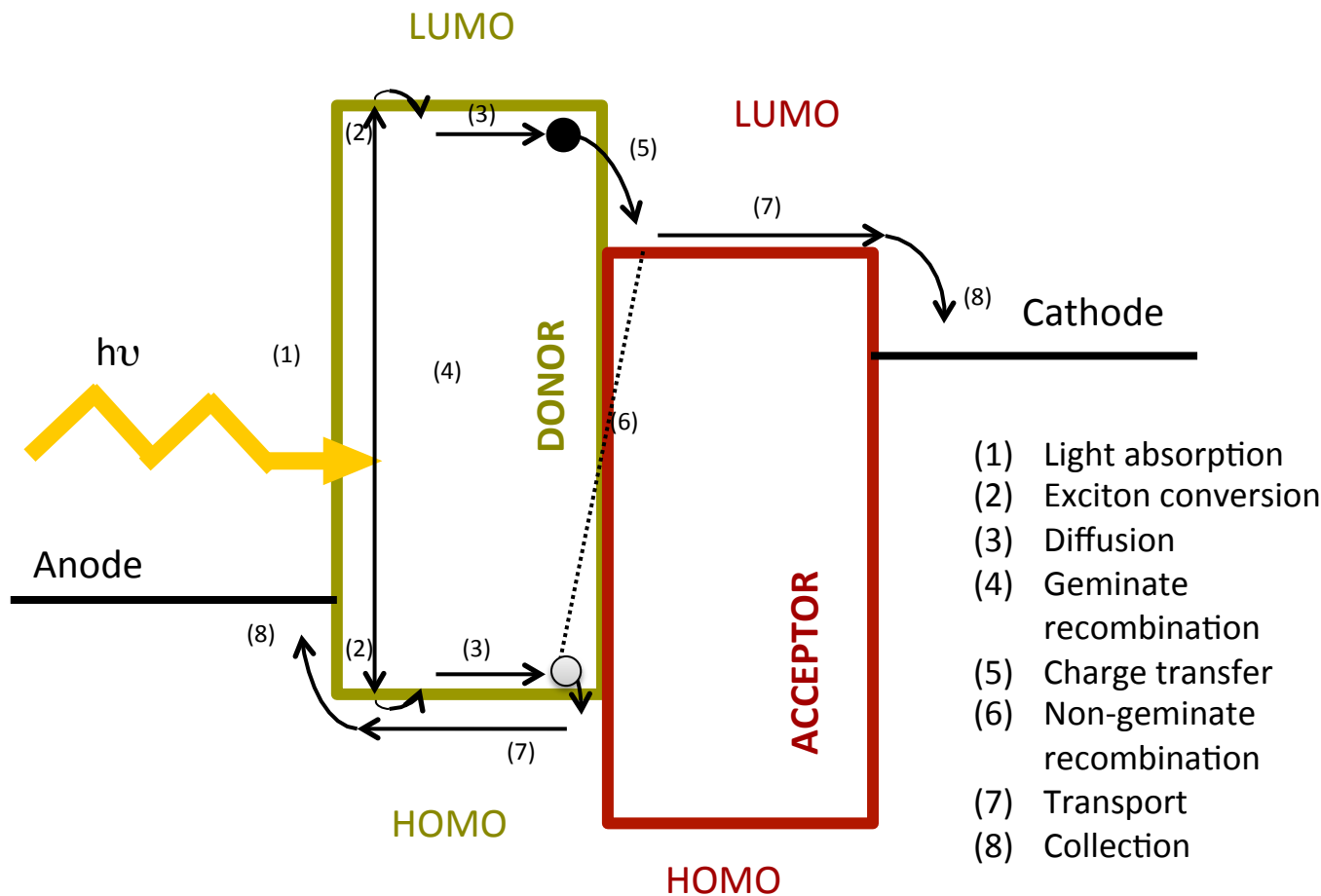
Windows of the EPFL's Convention Center

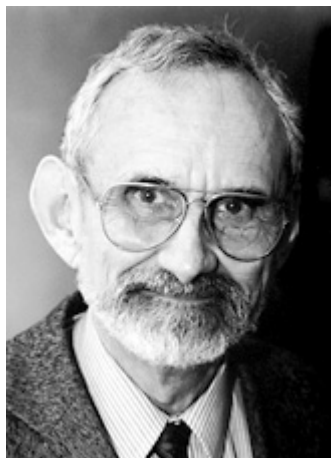


Barcelona Institute of
Science and Technology

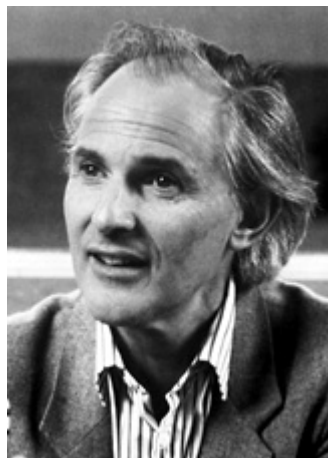


Small molecule Organic Solar Cells

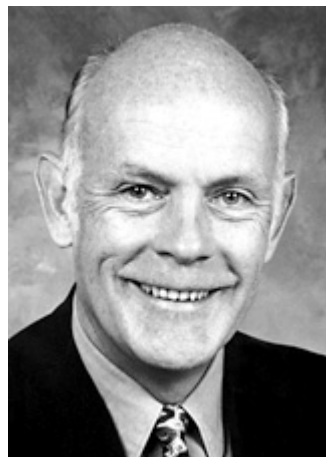




Curl Jr.



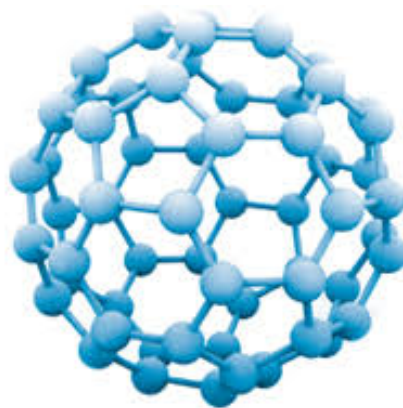
Kroto



Smalley

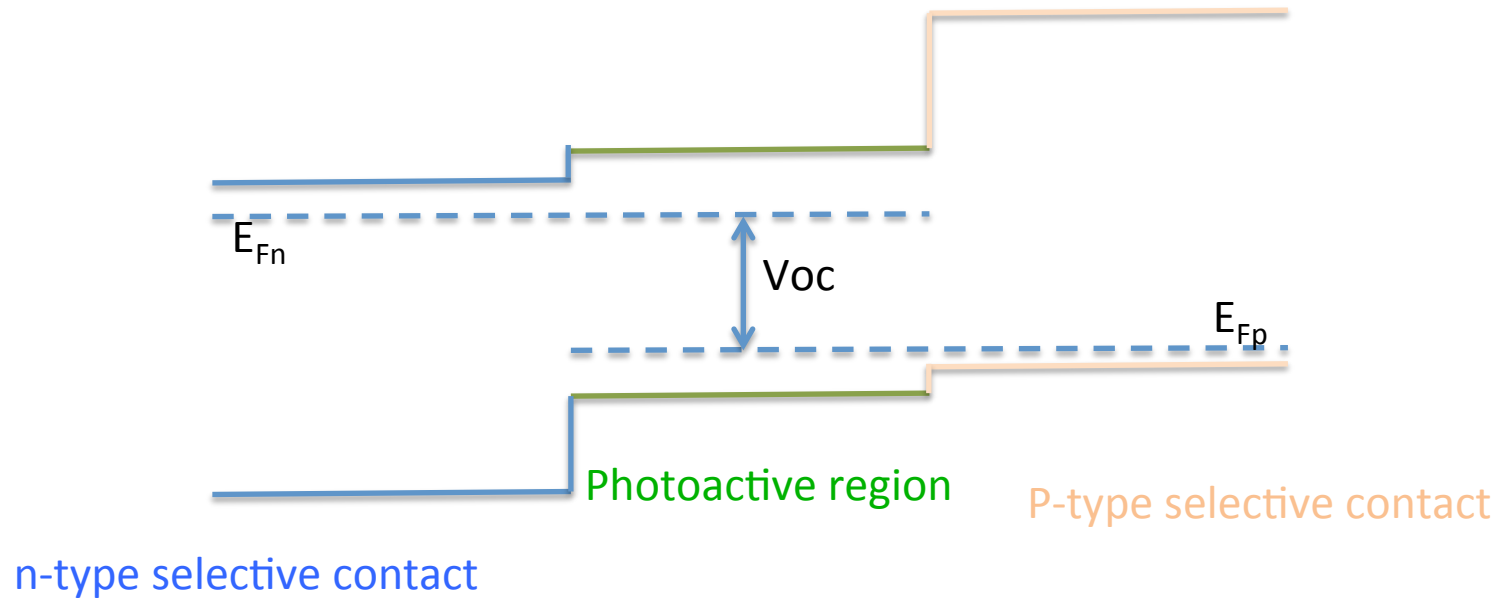
Chemistry Nobel Prize 1996

"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.



Organic solar cells



Friend



Nelson



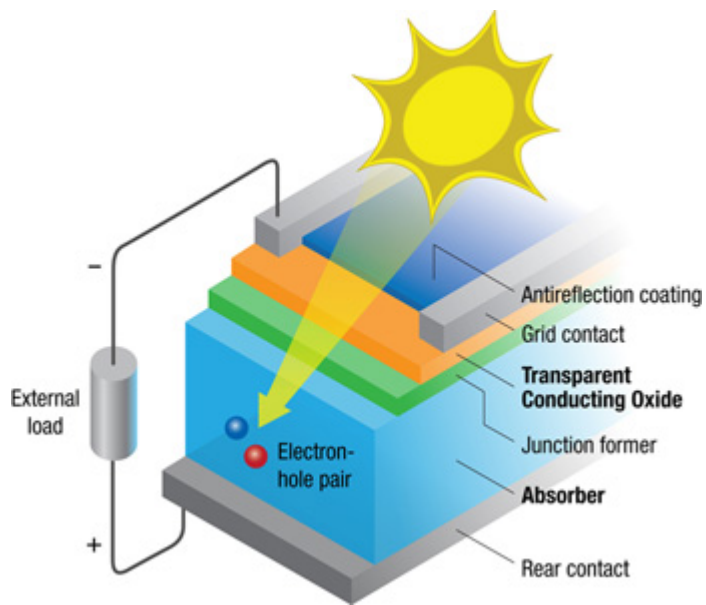
Brabec



Leo



Sariciftci



EXCITONS



Barcelona Institute of
Science and Technology

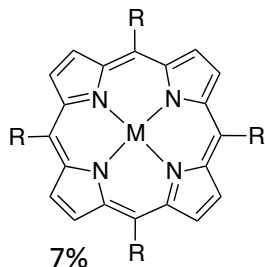




Organic solar cells

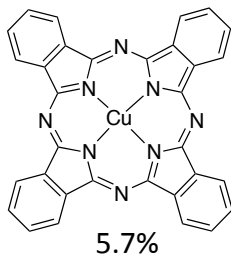


Small-molecule based donors:



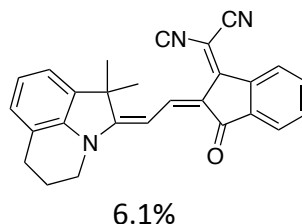
Porphyrins

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



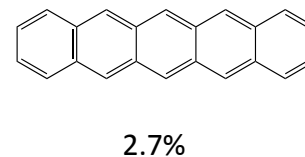
Phthalocyanines

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



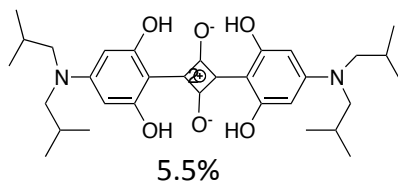
Merocyanines

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



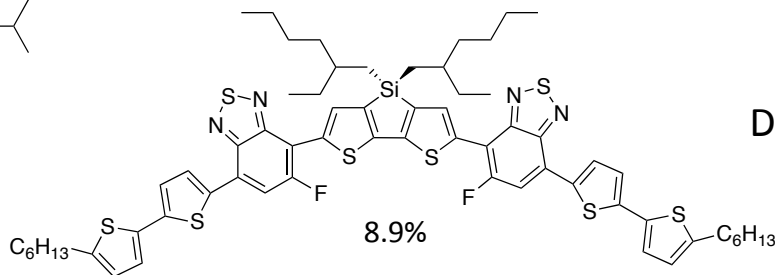
Polyacenes

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



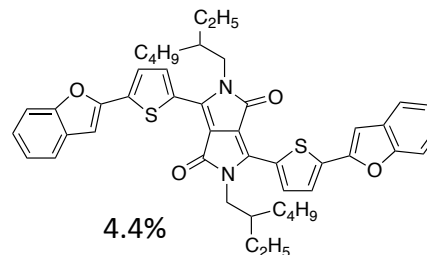
Squarines

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



D-A structures ("push-pull")

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

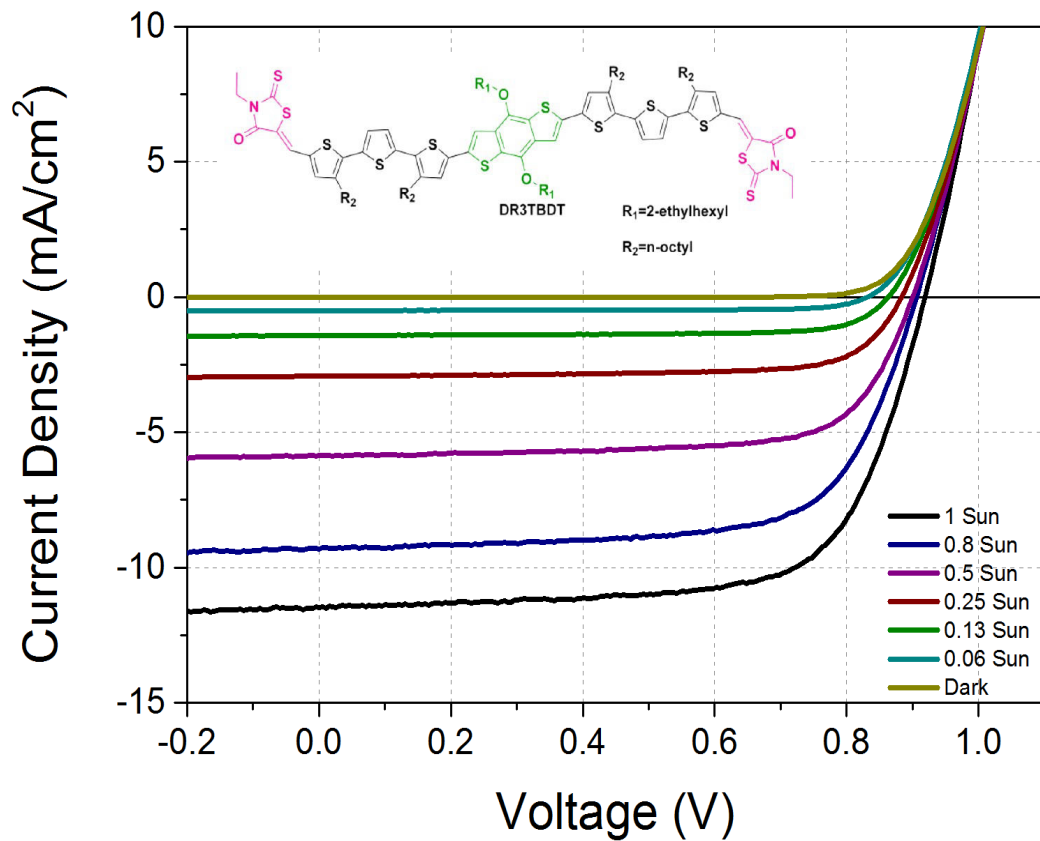


Diketopyrrolopyrroles

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

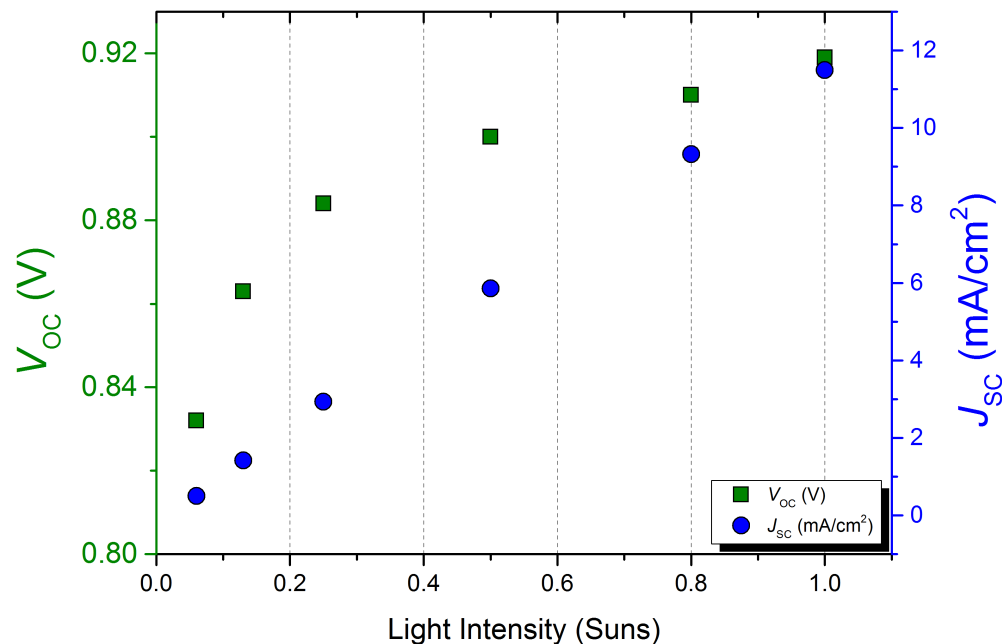


OSC at ICIQ_Palomares group





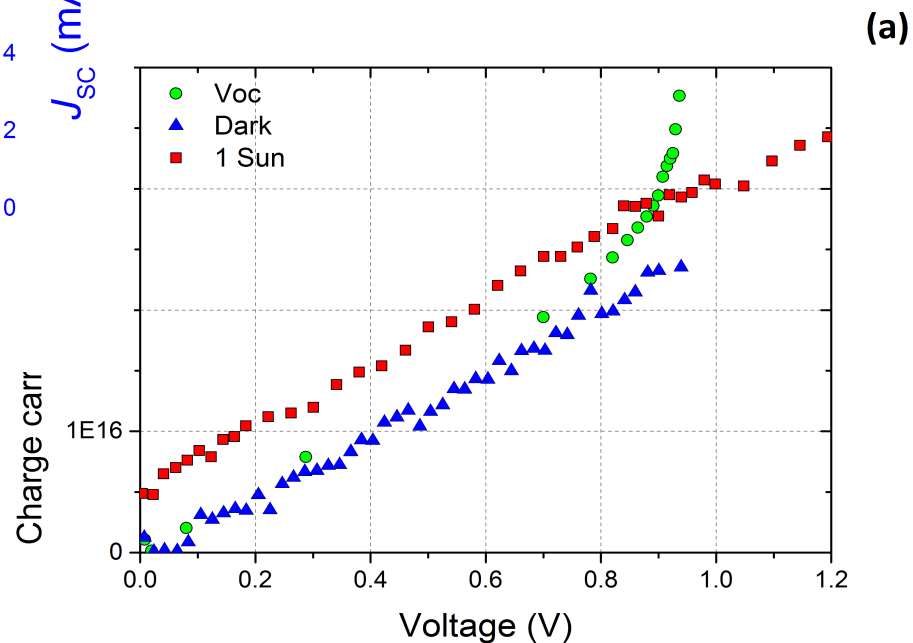
OSC at ICIQ_Palomares group



$$n \downarrow \text{dark} = q/kT \quad dV_{OC} / d \ln(LI)$$

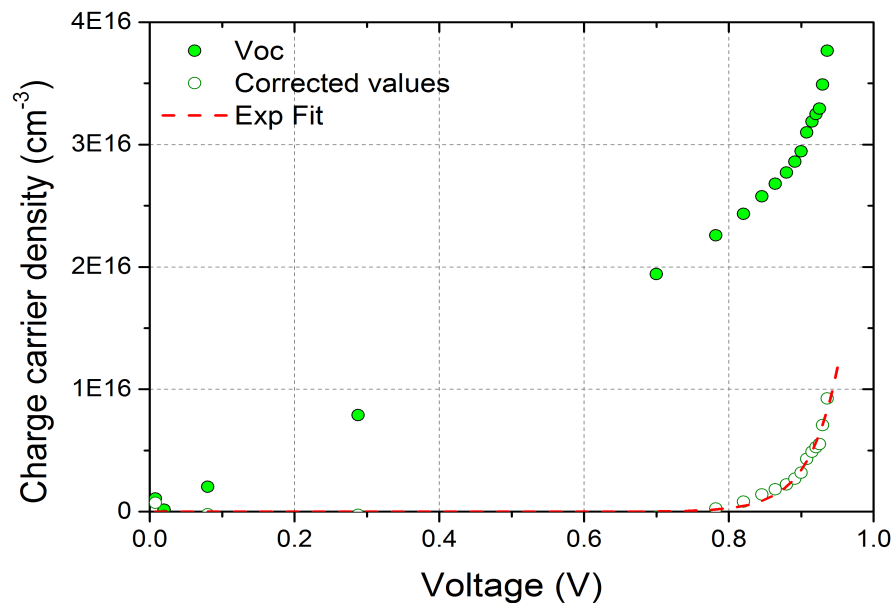
$$n \downarrow \text{dark} = Q/edA = C \downarrow \text{geo} / edA V$$

$$C \downarrow \text{geo} = edAd \quad n \downarrow \text{dark} / dV$$





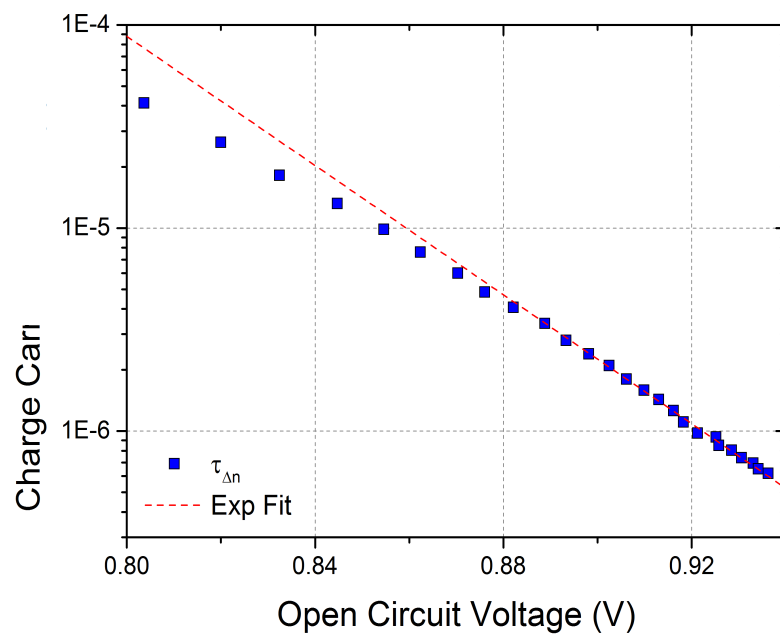
OSC at ICIQ_Palomares group



(b)

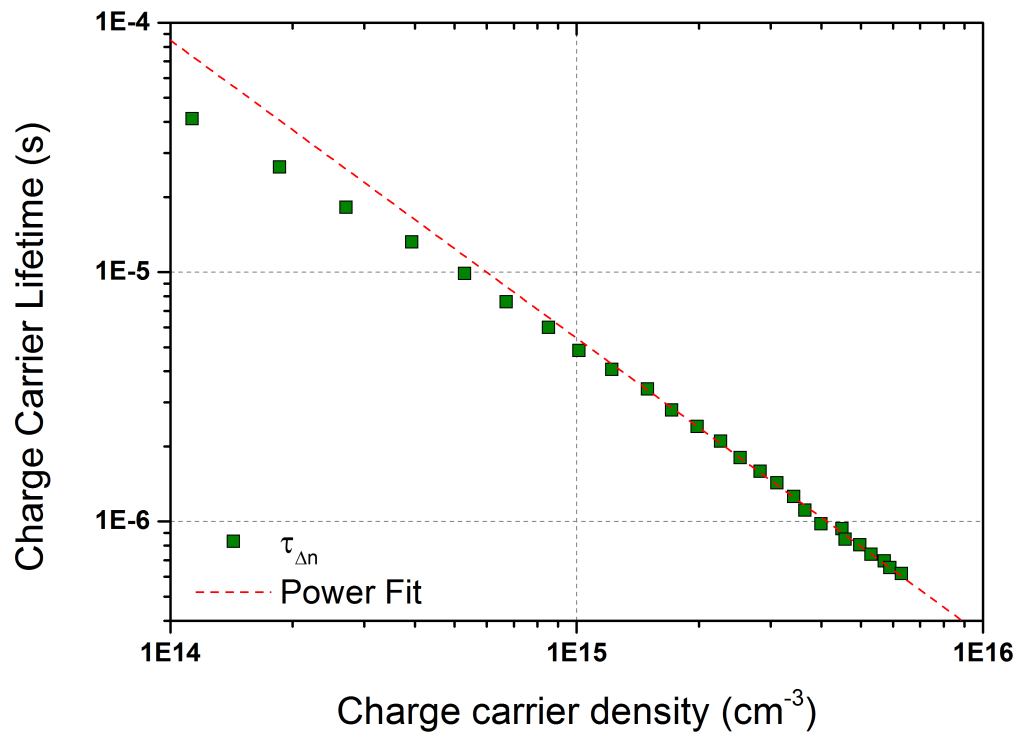
$$n = n_0 \exp(\gamma V_{oc})$$

$$\tau_{\Delta n} = \tau_{\Delta n_0} \exp(-\beta V_{oc})$$





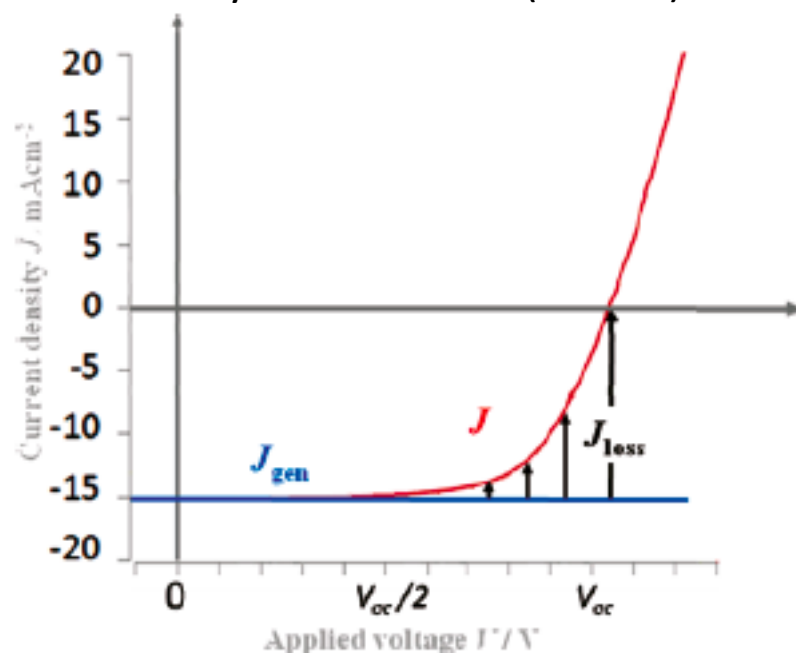
OSC at ICIQ_Palomares group



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



From Ryan et al. 2013 (below)

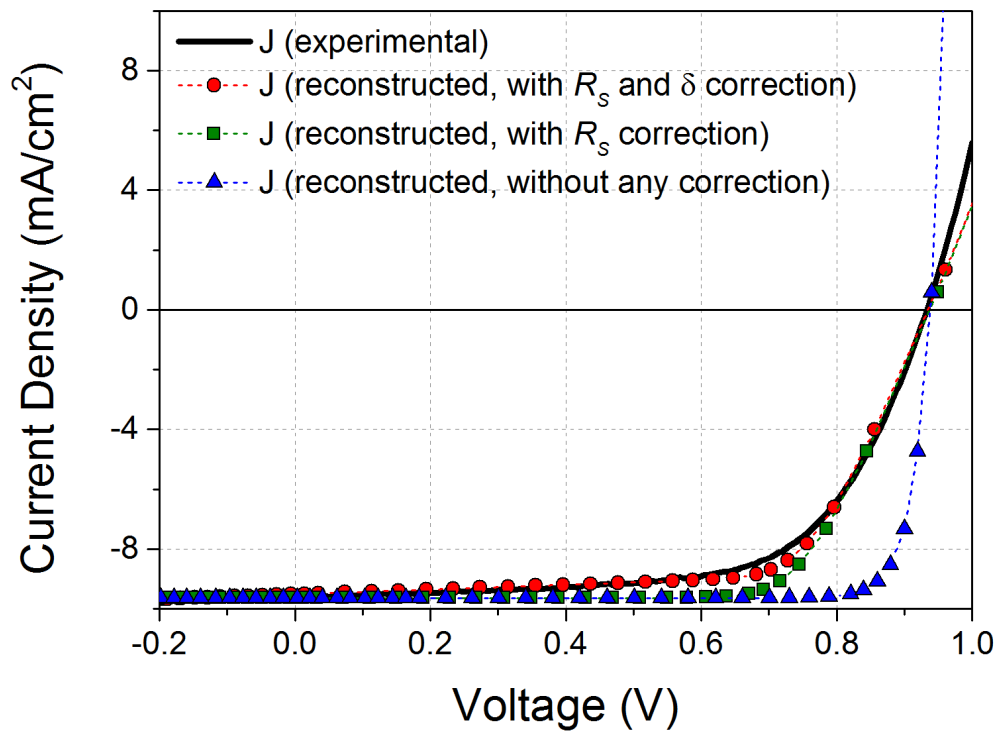


$$J_{loss} = d e n / (1 + \lambda) \tau \Delta n + V / A R \Delta s h$$

$$J_{loss} = \frac{e d n}{\tau_n} \quad J = J_{gen} + J_{loss}$$

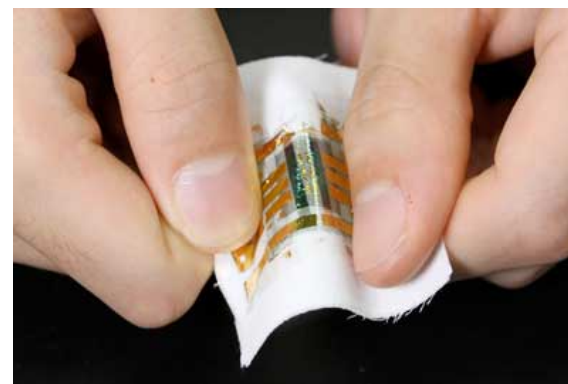
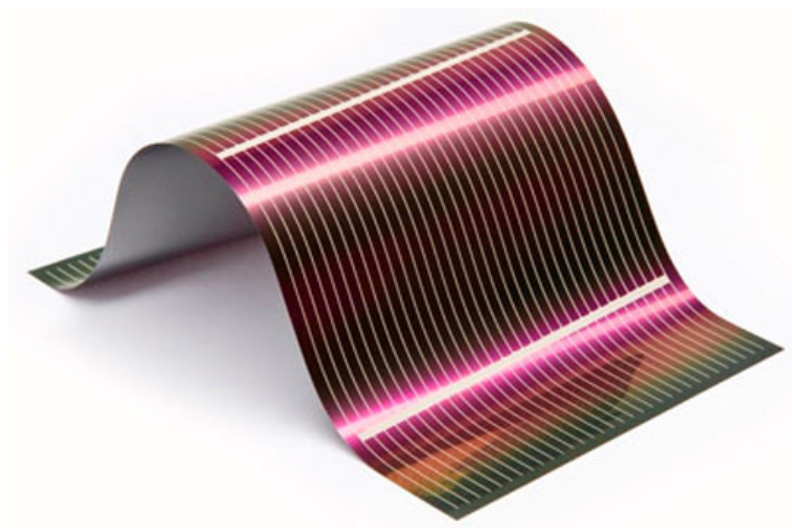
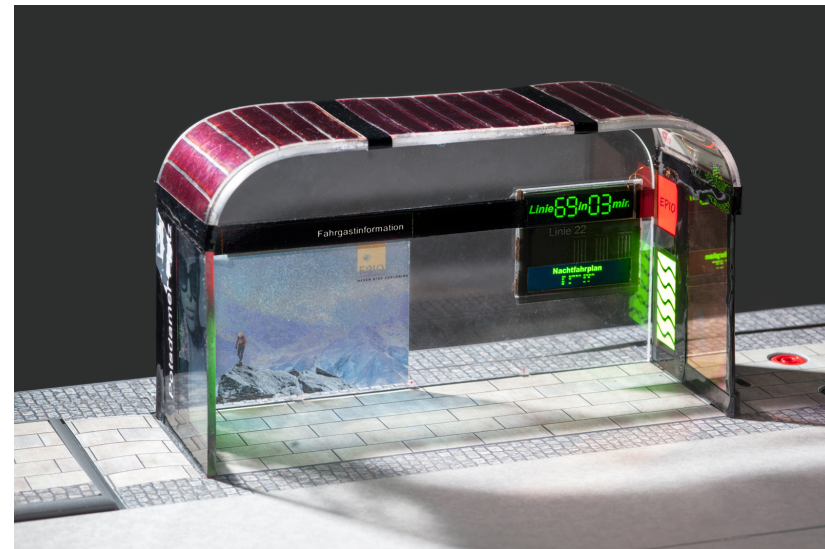
Maurano et al. Transient Optoelectronic Analysis of Charge Carrier Losses in a Selenophene/Fullerene Blend Solar Cell. J. Phys. Chem. C (2011) vol. 115 pp. 5947

Ryan et al. Nongeminate Recombination Dynamics–Device Voltage Relationship in Hybrid PbS Quantum Dot/C60 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>

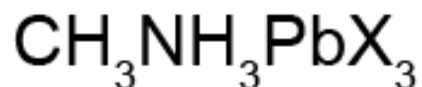
The screenshot shows a YouTube video player interface. The video title is "Faces of Chemistry: Organic solar cells (BASF) - Video 1 (11+)" with 10,910 views. The channel is "Royal Society Of Chemistry". The video player shows a blue background with the text "FACES OF CHEMISTRY" and "RSC Advancing the Chemical Sciences". Below the video, there are social media sharing icons and a red "SUSCRIBIRSE 42 MIL" button. To the right of the video player, there is a "Siguiente" (Next) section with a "REPRODUCCIÓN AUTOMÁTICA" (Automatic Playback) toggle. The next video is "Faces of Chemistry: Organic solar cells (BASF) - Video 2..." with 133,000 views. Below this, there are three more video recommendations: "16 animales que te helarán la sangre" (9:52), "Robe - Un Suspiro Acompasado" (9:06), and "Cómo funciona una central de energía solar" (5:53). The bottom of the screenshot shows a Windows taskbar with various application icons and a system clock showing 12:11 on 06/07/2018.



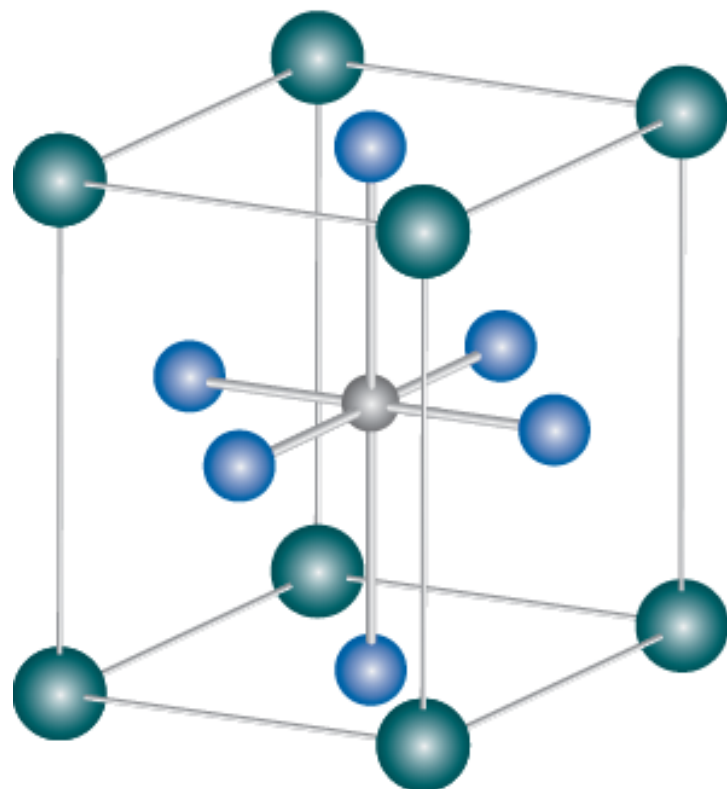
Barcelona Institute of Science and Technology



Hybrid Perovskite Materials



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>

The screenshot shows a web browser window with a YouTube video player. The video title is "Perovskite Solar Cell" and the description is "Perovskite Solar Cell - Frontier Energy Solution (2017)". The video has 14,727 views and 163 likes. The player shows a progress bar at 0:03 / 7:05. To the right of the video player, there is a "Siguiente" (Next) section with three video recommendations:

- Siguiente**
 - Spray Coated Perovskite Solar Cells** by BULLAKI, 4 mil visualizaciones, 4:13.
 - Everything you ever wanted to know about perovskite** by Science Magazine, 24 mil visualizaciones, 4:47.
 - Most efficient Solar Panels in 2018** by Synergy Files, 95 mil visualizaciones, 2:56.
- REPRODUCCIÓN AUTOMÁTICA** (toggle switch is on).
- Robe - Aproximadamente Robe** by robeextremoVEVO, Recomendado para ti, 4:12.



Hybrid Perovskite Materials



Miyasaka



Snaith



Park



Grätzel

SUCCESS HAS MANY FRIENDS...Failure is an orphan

John F. Kennedy

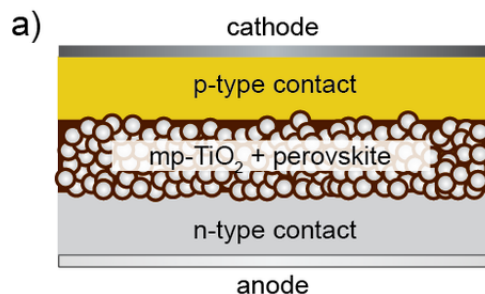
First solid ionic with semiconductor properties suitable for photovoltaics



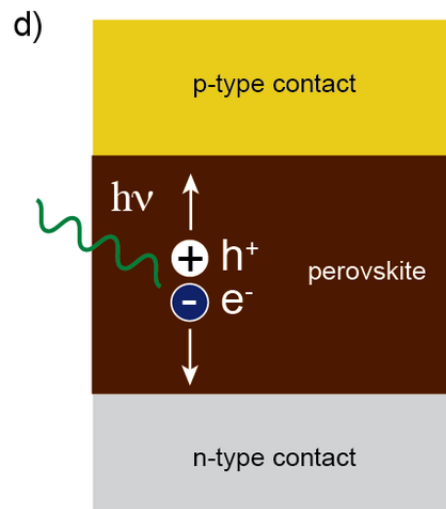
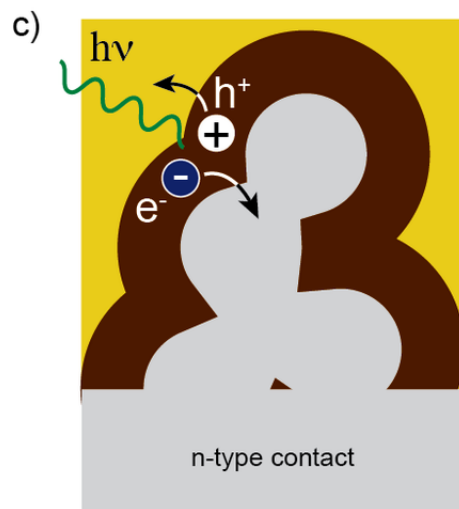
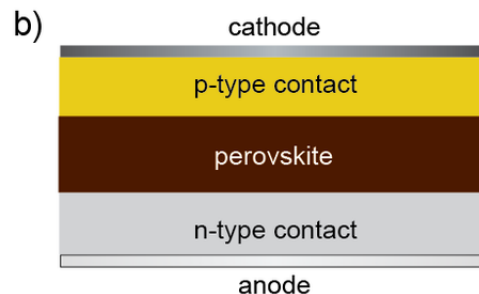
Hybrid Perovskite Materials



Sensitized perovskite solar cell



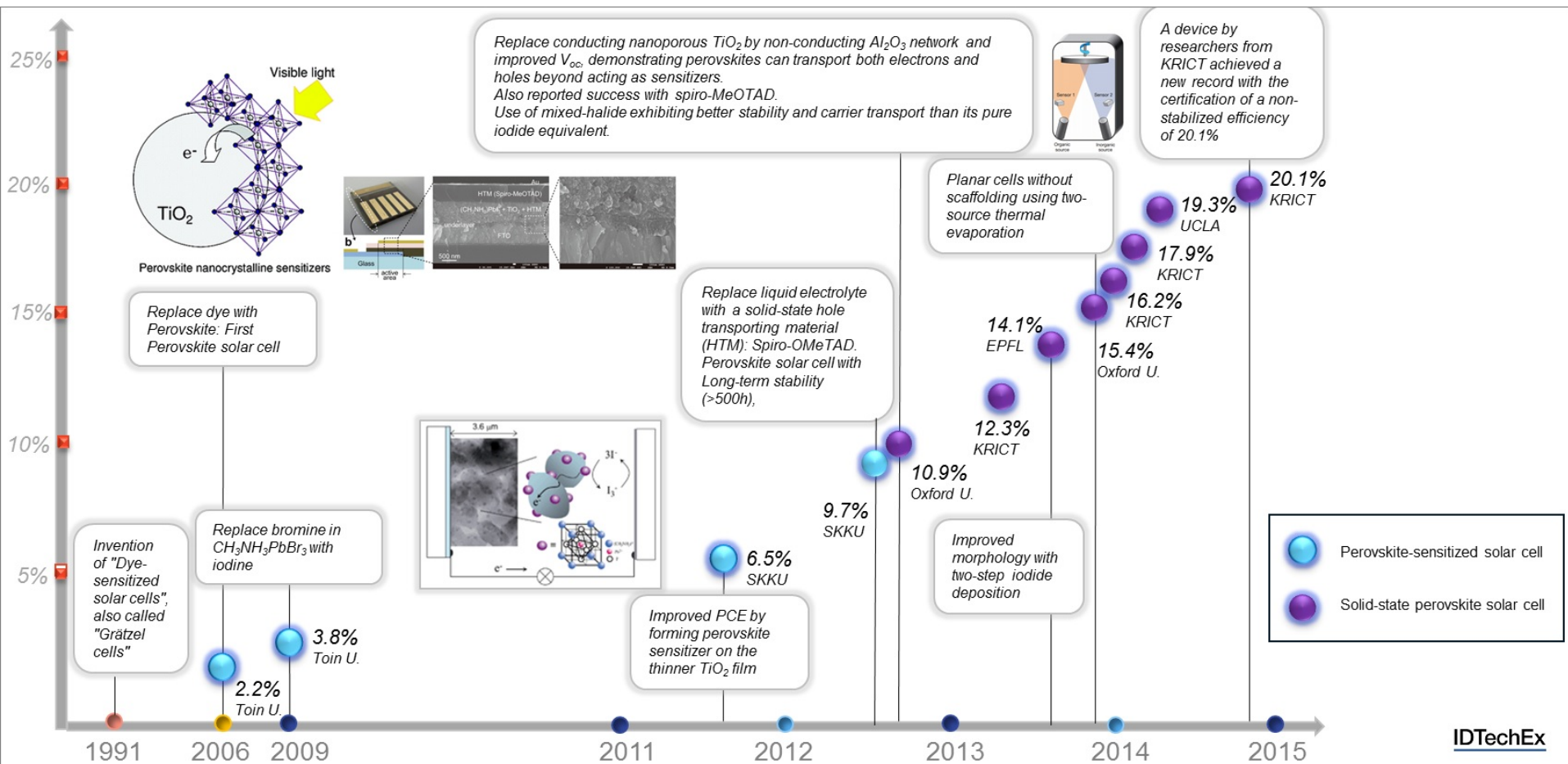
Thin-film perovskite solar cell



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)

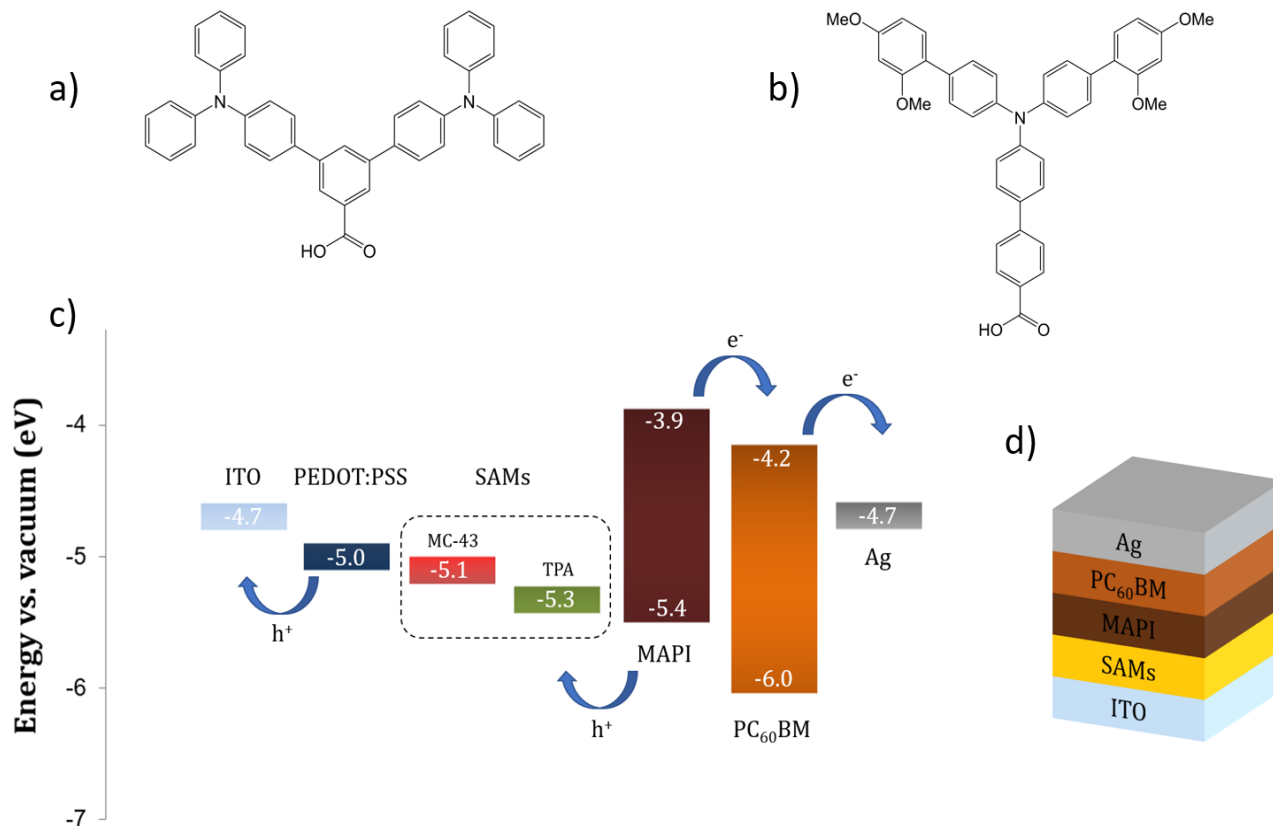


Hybrid Perovskite Materials



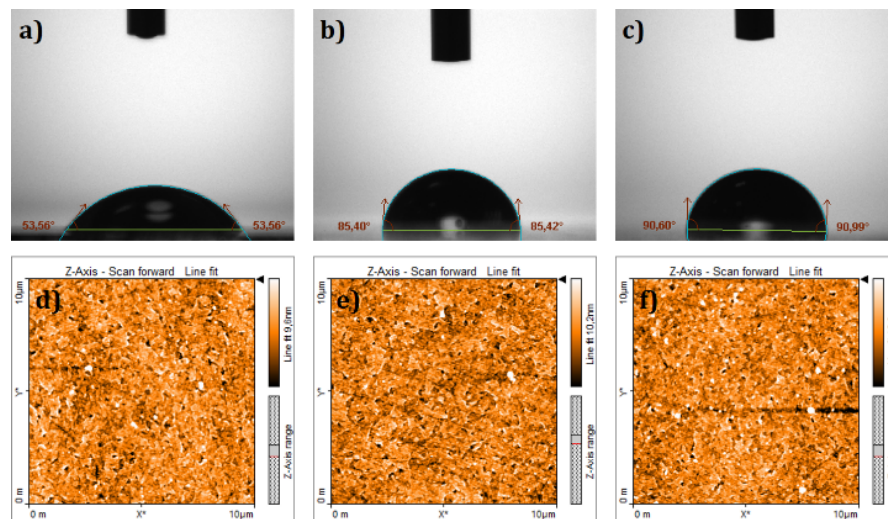
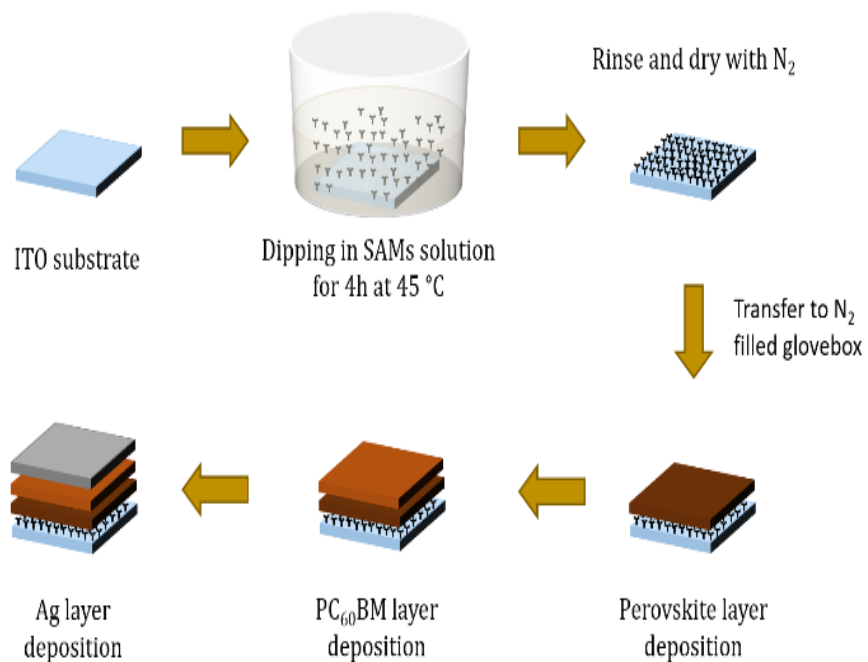


Perovskites at ICIQ_Palomares group



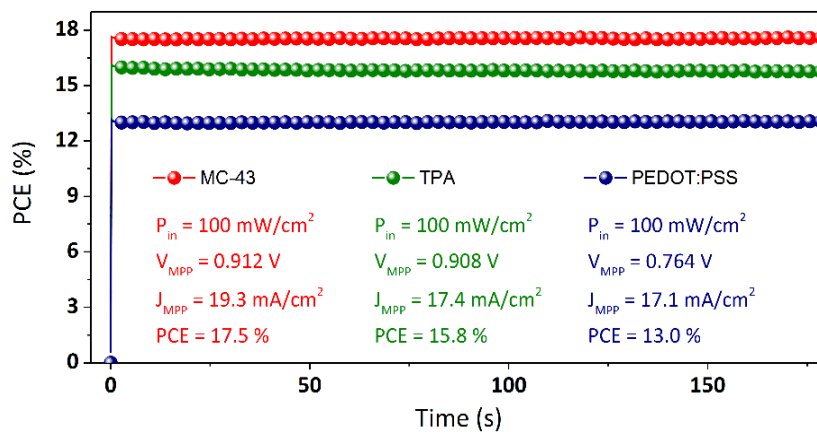
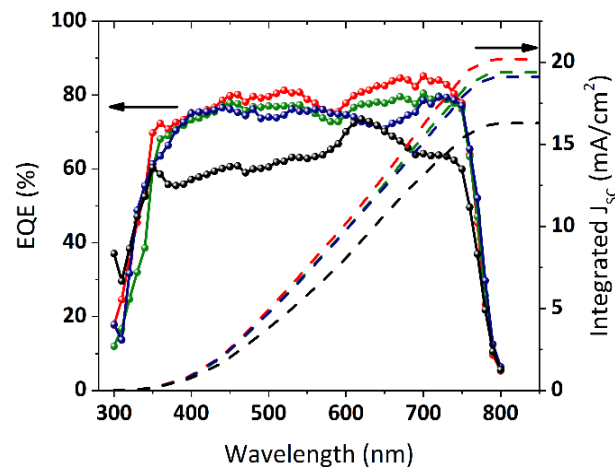
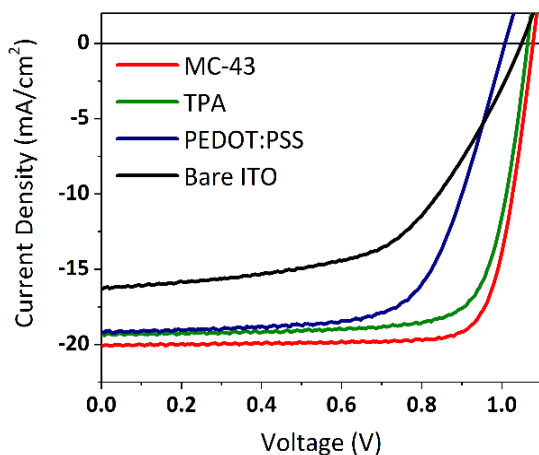


Perovskites at ICIQ_Palomares group



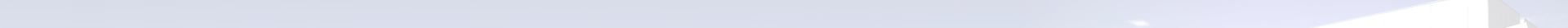


Perovskites at ICIQ_Palomares group

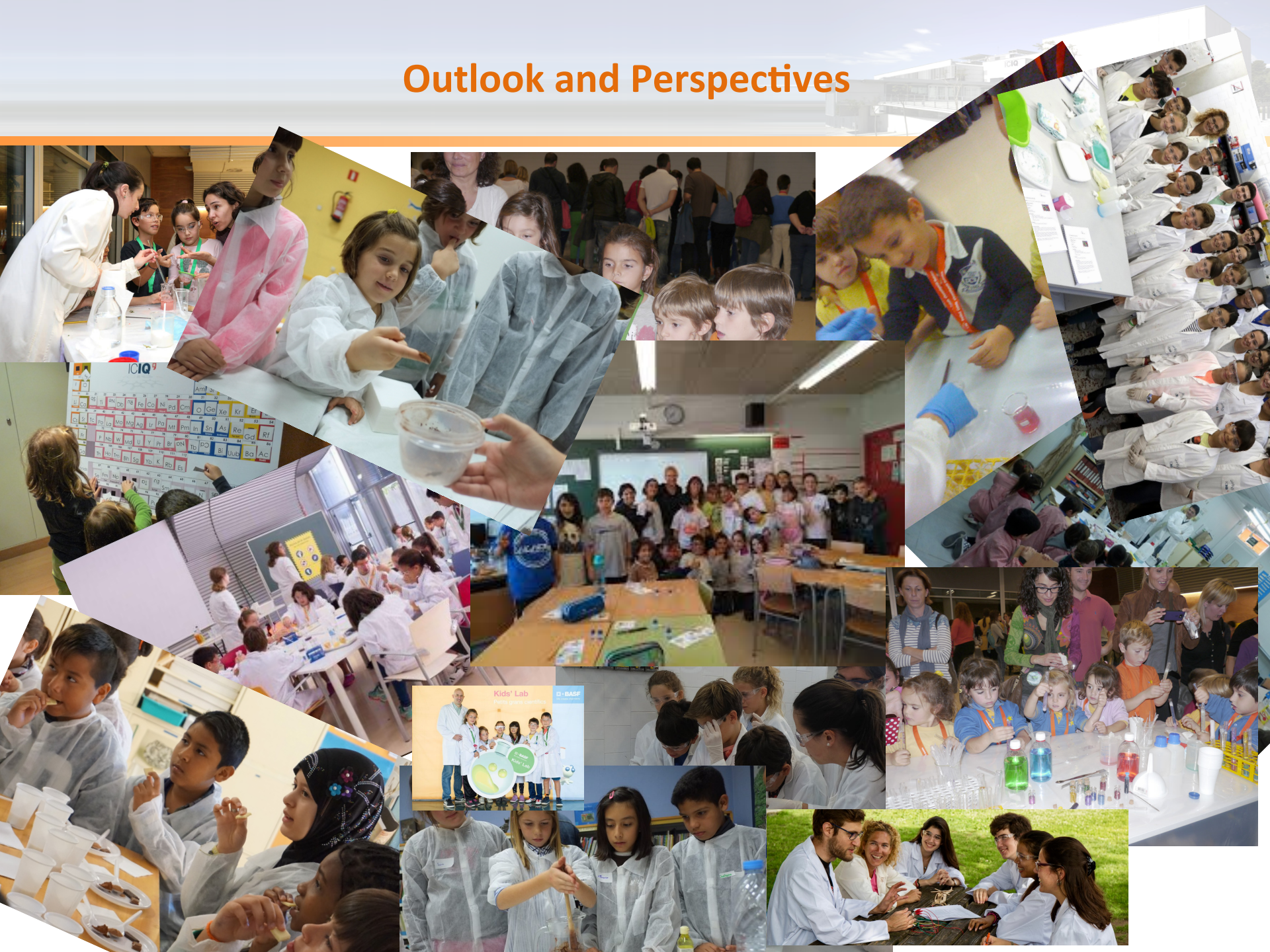


Outlook and Perspectives





Outlook and Perspectives



Thank you for your attention.

EPalomaresGil (@EPalomaresGil)

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

Torraçona, Espanya

Tuits 1.034 Seguint 176 Seguidors 166 Agradaments 1.415 Llistes 0 Moments 1

Tuits i respostes Continguts

EPalomaresGil @EPalomaresGil · 4 h
I aquí un poc de la química dels focs artificials. @TGNajuntament @TGNcultura @TGNturisme @SER_TgnReus

Qui seguir · Actualitza · Mostra-ho tot

Orchestra Sci. @Orchestra...
Segueix

GEQO RSEQ @geqo_rseq
Segueix