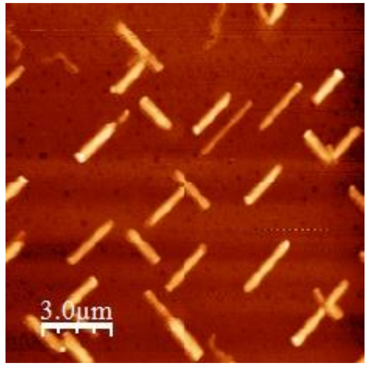
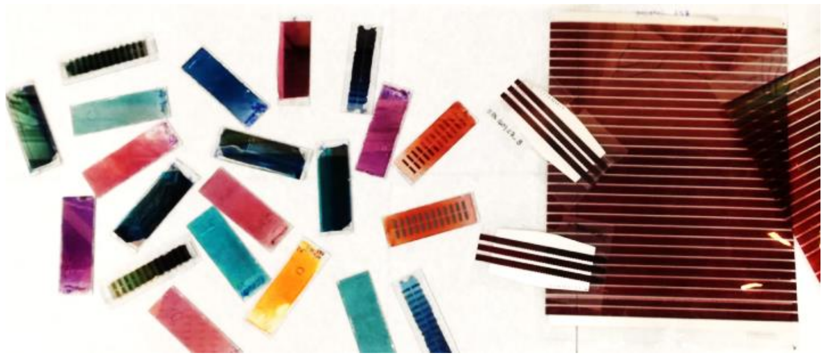
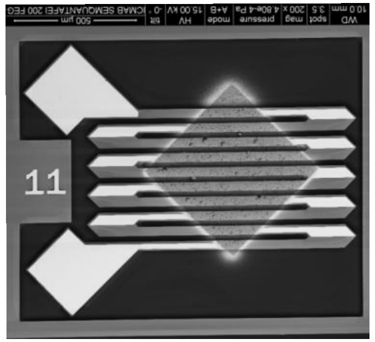
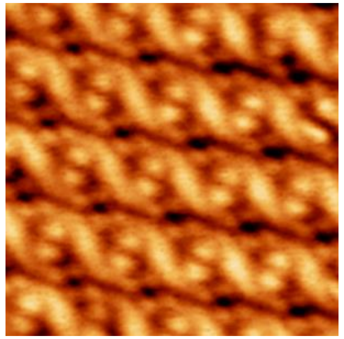
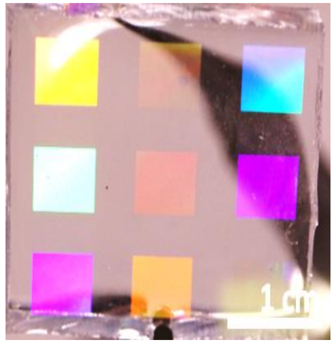
Materials for energy conversion: Research at ICMAB




Maria Isabel Alonso, Esther Barrena, Mariano Campoy-Quiles, Mariona Coll, Josep Fontcuberta, Alejandro Goñi, Agustín Mihi, Juan Sebastián Reparaz, Riccardo Rurali

Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Spain

MATENER 2018
Severo Ochoa Summer School on Materials for Energy
September 20th 2018

https://departments.icmab.es/

INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA

EXCELENCIA SEVERO OCHOA

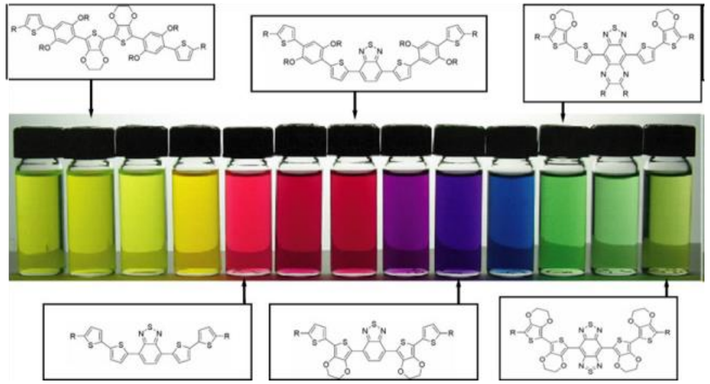
CSIC

Main subjects

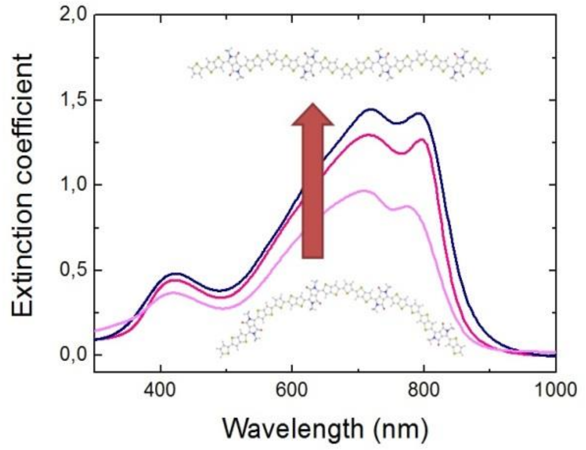
- Research on photovoltaics: organic, inorganic, hybrid
- Light management with photonic structures
- Thermoelectric structures: organic, inorganic, hybrid
- Thermal transport: theory and experiment

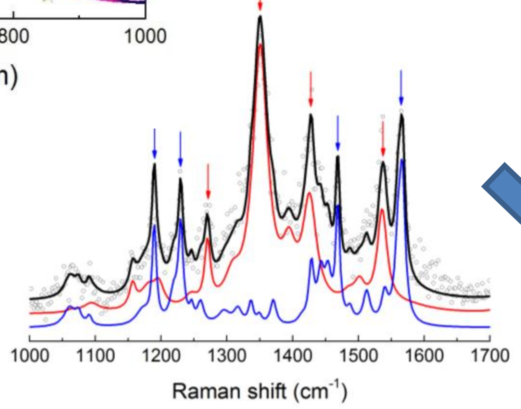
Organic photovoltaics

https://departments.icmab.es/nanopto

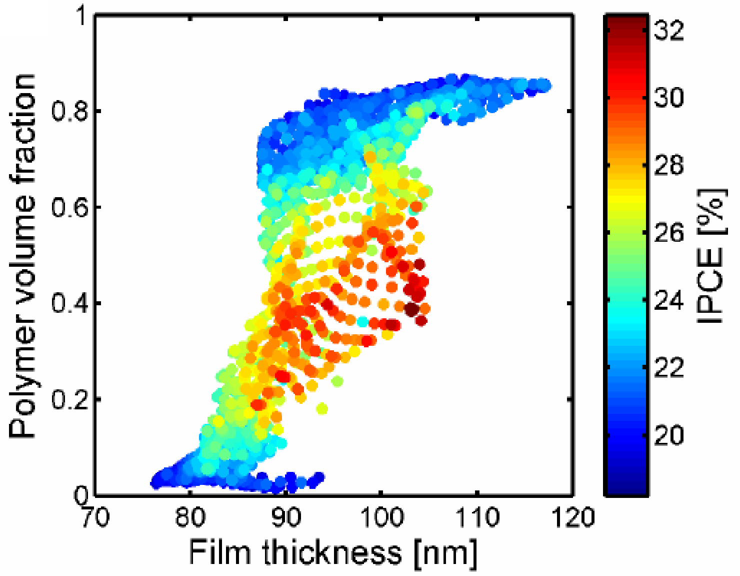


Fundamental properties

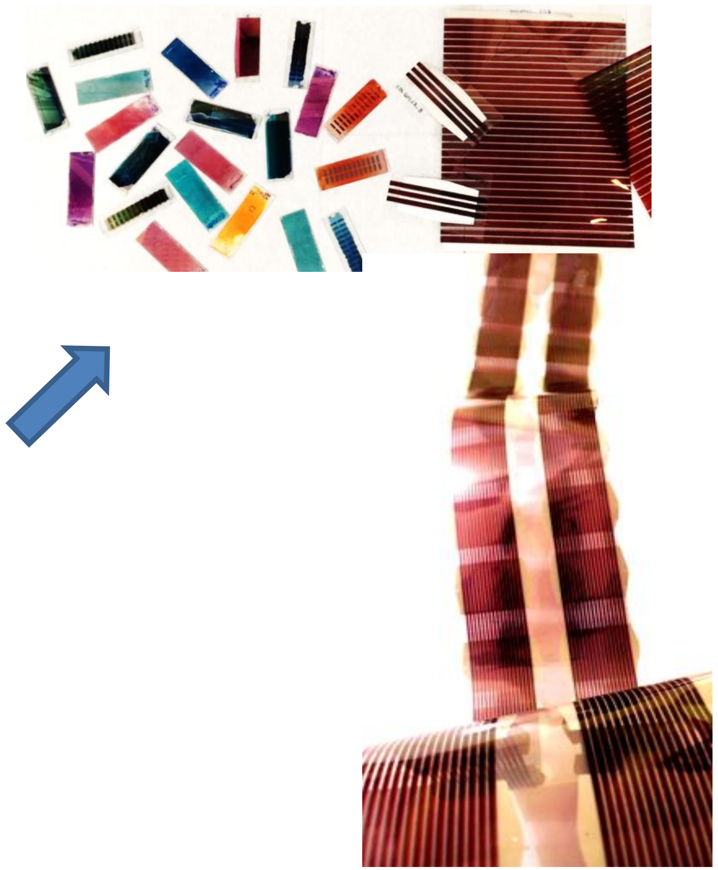




High throughput screening



Upscaling



Vezie et al *Nature Materials*, 15 (2016) 746
Sanchez-Diaz et al *Adv. Elect. Mater*. 1700477 (2018)
Alonso & Campoy *Springer Ser. Surf. Vol 52,* 335 (2018)

Contact: mcampoy@icmab.es

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CSIC

Organic photovoltaics

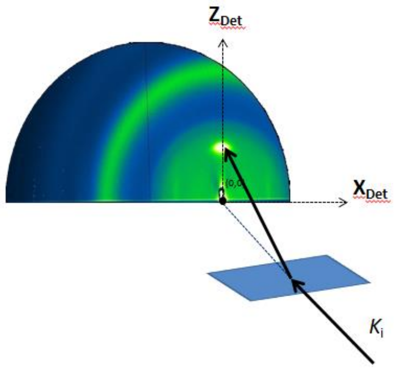
https://departments.icmab.es/surfaces

PHYSICAL CHEMISTRY OF SURFACES AND INTERFACES

Goal: Understanding the electronic and structural properties of organic solar cells at the nanoscale

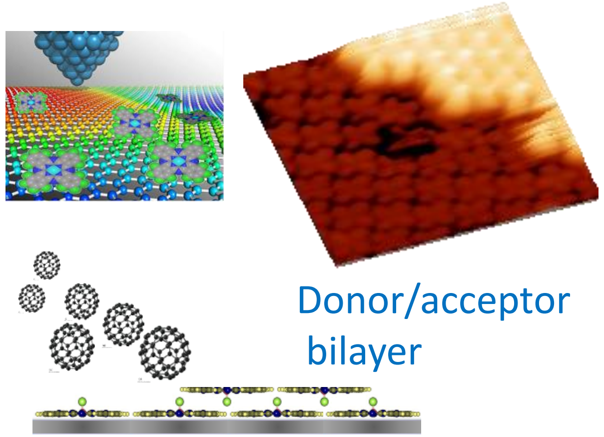
Focus: Organic-organic interfaces and molecular doping

Structure by GIXD



Real-time studies

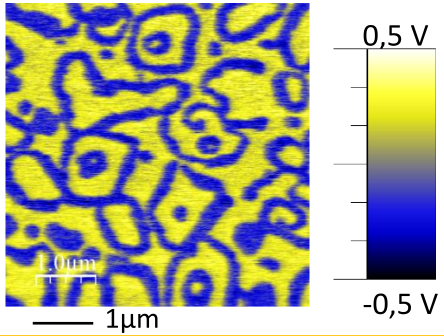
Molecular-scale studies



Donor/acceptor bilayer

Electronic properties -Kelvin Probe Force Microscopy / UPS

Surface potential of a dopant/organic interface



MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

Novel and optimized interfaces for responsive molecular-based devices -OPTIMODE

HORIZON 2020

Spins for Efficient Photovoltaic Devices based on Organic Molecules

SEPOMO

ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA EXCELENCIA SEVERO OCHOA CSIC

Contact: ebarrena@icmab.es

Inorganic photovoltaics: Photoferroelectrics

https://departments.icmab.es/mulfox

LABORATORY OF MULTIFUNCTIONAL THIN FILMS AND COMPLEX STRUCTURES

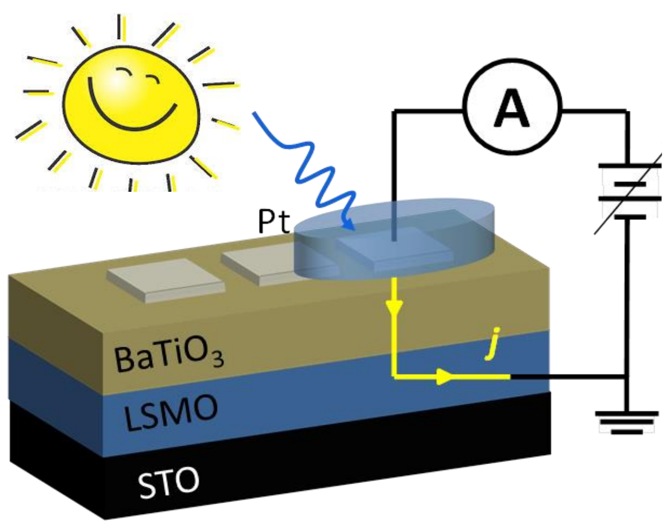
Josep Fontcuberta, Ignasi Fina, F. Sánchez, G. Herranz, J. Gázquez, F. Macià et al.

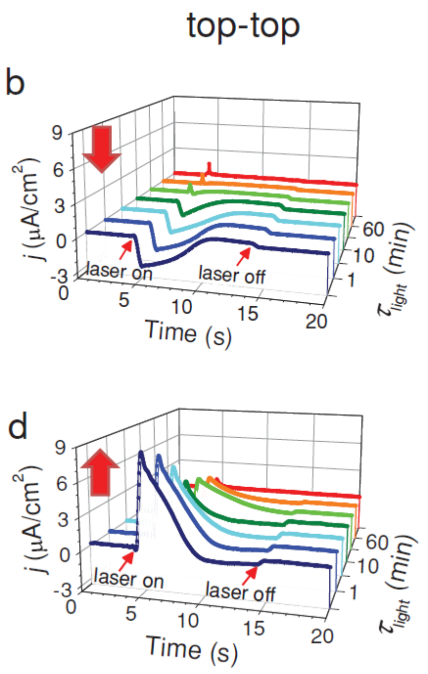
Objectives:

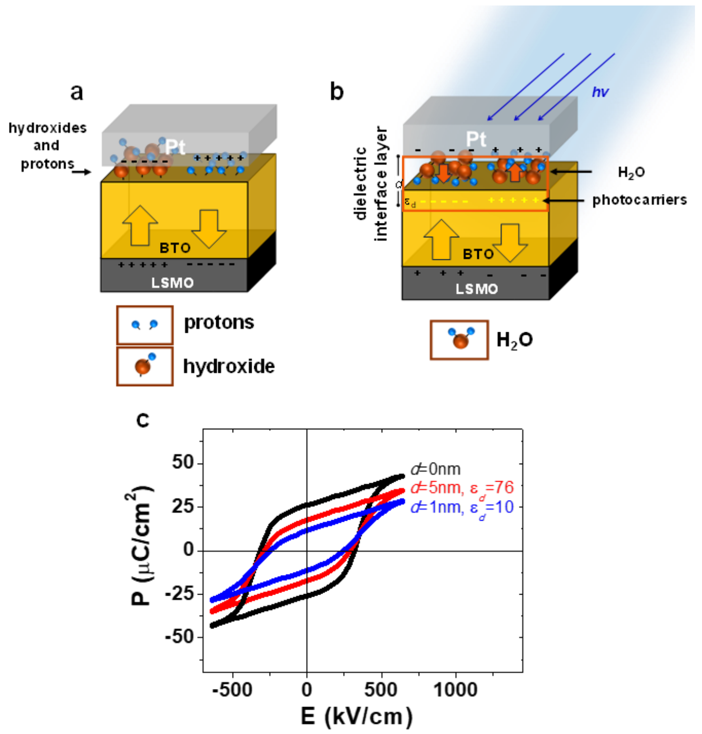
- Understanding the role of **internal electric fields** in ferroelectrics on **photo-currents** and the role of work function of metal electrodes.
- Enhancing photoabsorption of large band gap ferro-electric by defect and band **engineering**. *Collaboration with M. Coll & A. Fuertes on this topic*.

Methods:

- Epitaxial thin films by Pulsed Laser Deposition.







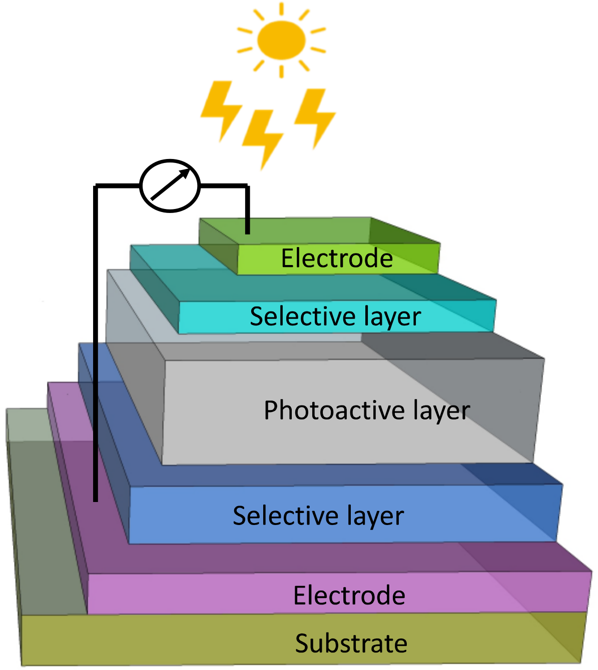
- *Both the direction of the photocurrent and its time-dependence can be selectively engineered by exploiting the competition between coexisting internal electric fields*
  Fanmao Liu, Ignasi Fina et al. Adv. Electron. Mater. 1, 1500171 (2015);
- *Photoinduced charges modify the screening of ferroelectric polarization and thus photoresponse of ferroelectrics*
  Fanmao Liu, Ignasi Fina et al. ACS Materials and Interfaces 10, 23968 (2018)

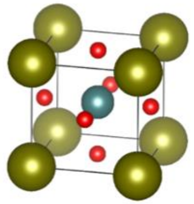
Contact: fontcuberta@icmab.es

ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA EXCELENCIA SEVERO OCHOA CSIC

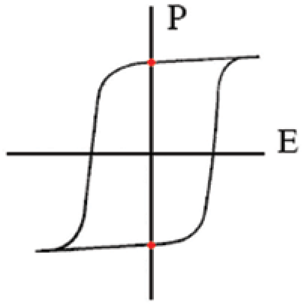
Cost-efficient chemical methodologies for all-oxide next generation PV

Goal: Design of an **all-oxide** photovoltaic device based on ferroelectric perovskite oxide materials as photoactive layer to fully match the solar spectrum while maintaining high stability, non-toxicity and device simplicity by **low-cost chemical methodologies.**





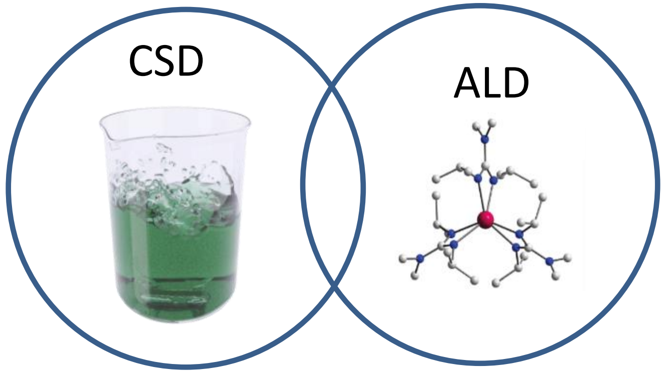
Ferroelectric Perovskite Oxide



- ✓ High stability
- ✓ Composition flexibility
- ✓ Ferroelectricity-driven mechanism for solar energy conversion

P. Lopez-Varó, M.Coll et al. Physics Reports 653,1-40, (2016)

Chemical deposition techniques....



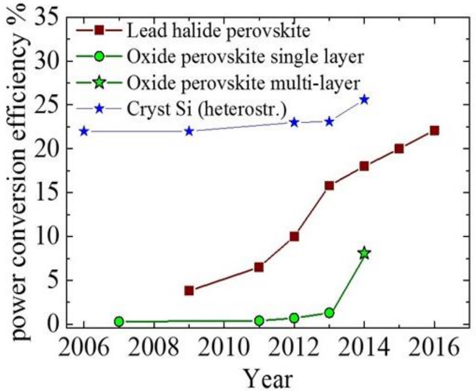
Develop new compositions with visible light absorption

...enables band gap tuning towards visible

$BiFeO_3$ —Co→ $BiFe_{1-x}Co_xO_3$

For enhanced efficiency

- *M.Coll, P. Machado, M. Scigaj*



https://departments.icmab.es/suman

Contact: mcoll@icmab.es

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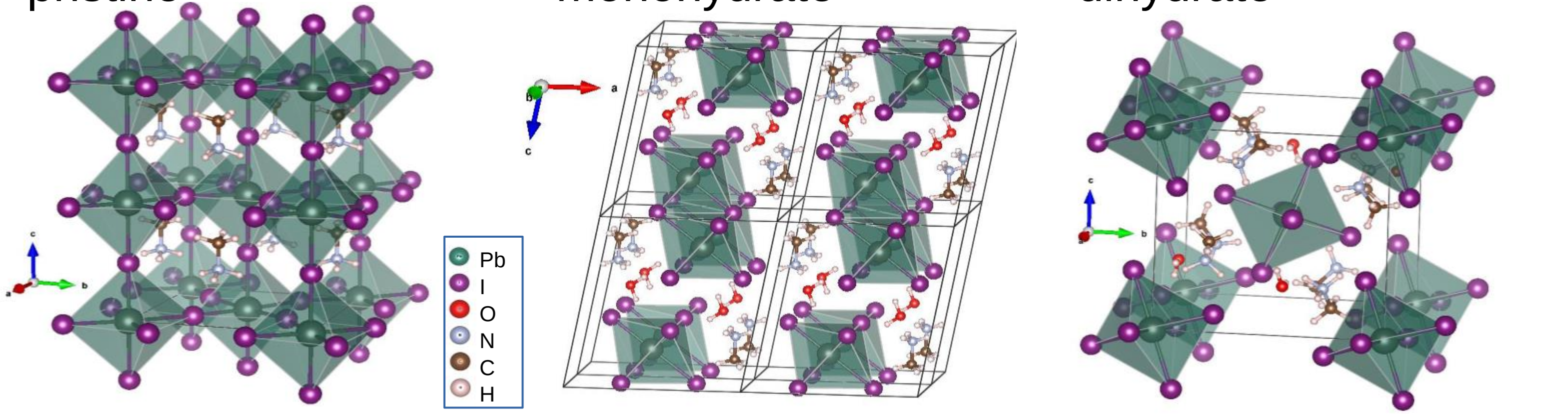
CSIC

Hybrid perovskites: Ellipsometry

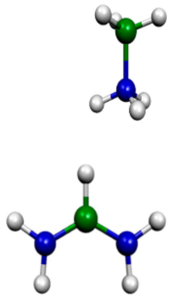
https://departments.icmab.es/nanopto

pristine monohydrate dihydrate



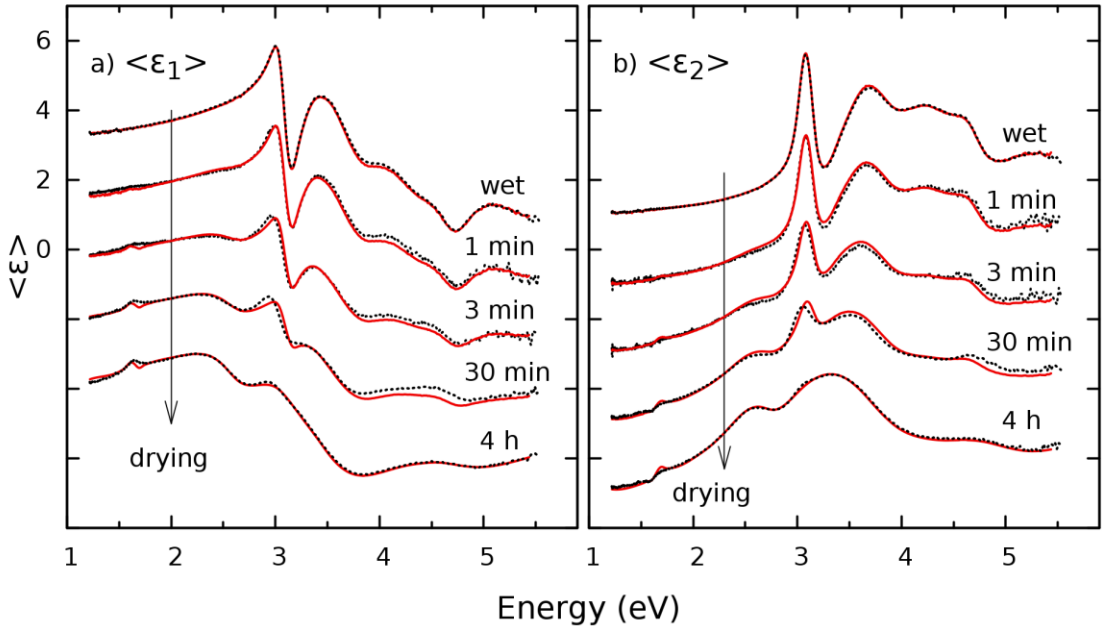
Reversible process / decomposition

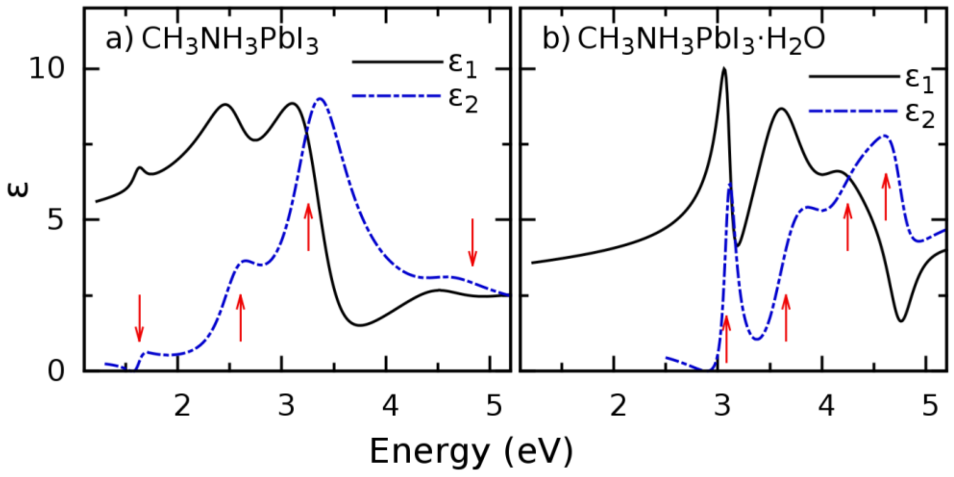
Increasing stability



MA^+ = methylammonium (CH3NH3+)

FA^+ = formamidinium (CH(NH2)2)+

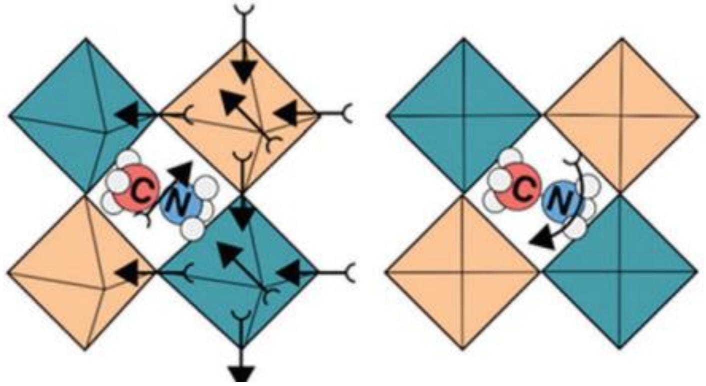




Leguy et al., Chem. Mater. **27** 3397 (2015)

Contact: isabel@icmab.es

Hybrid perovskites: Using pressure and temperature to unravel the structural-optical/vibrational-properties relationship



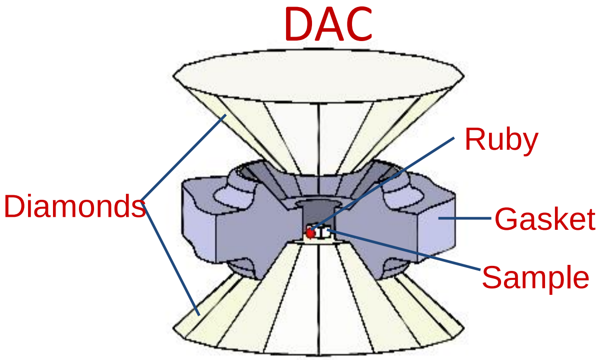
$MA_{1-x}FA_xPbX_3$ (X=Cl, Br, I)

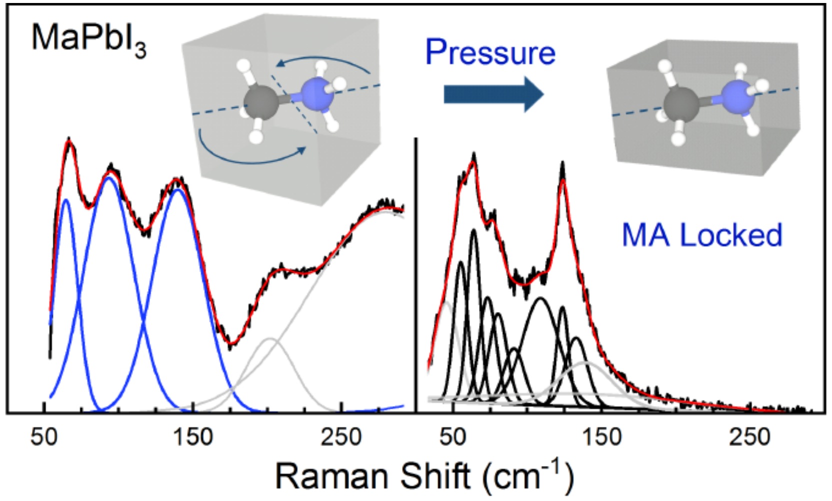
Tailoring fundamental properties

Focus: Interplay between organic & inorganic degrees of freedom

x : Organic cation composition (0—1)
T : Temperature (10—380 K) but ambient pressure
P : Hydrostatic pressure (0—15 GPa) but room temperature

Techniques: Photoluminescence (PL) & Raman,
He flow cryostat & diamond anvil cell (DAC)





Organic cation dynamic disorder

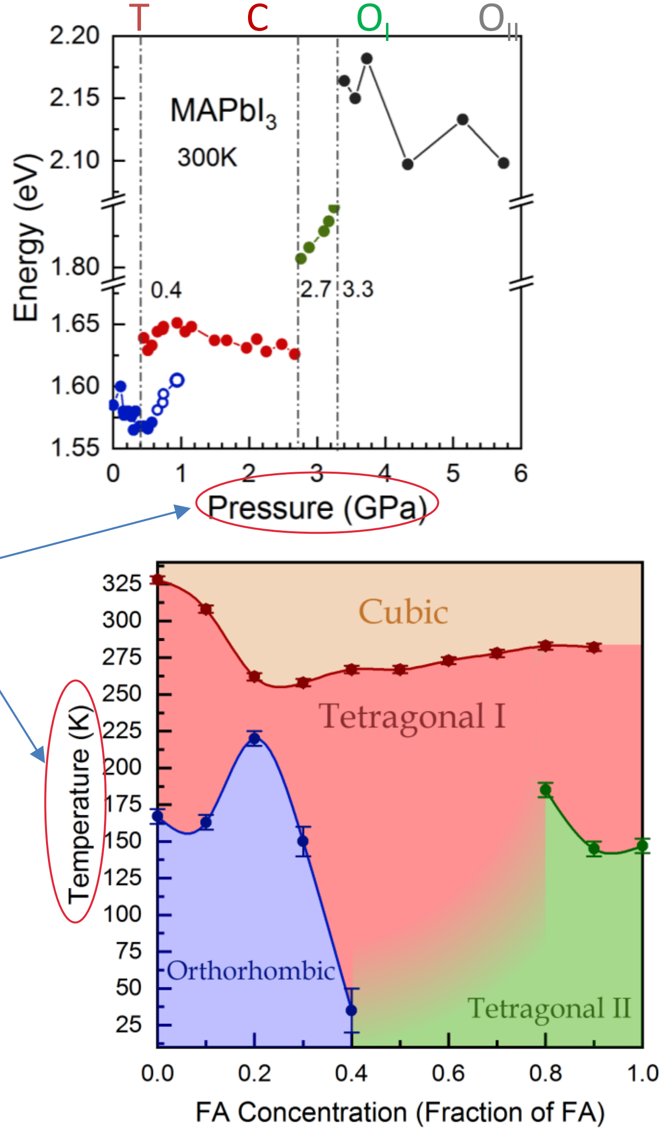
Influence on inorganic cage phonon modes

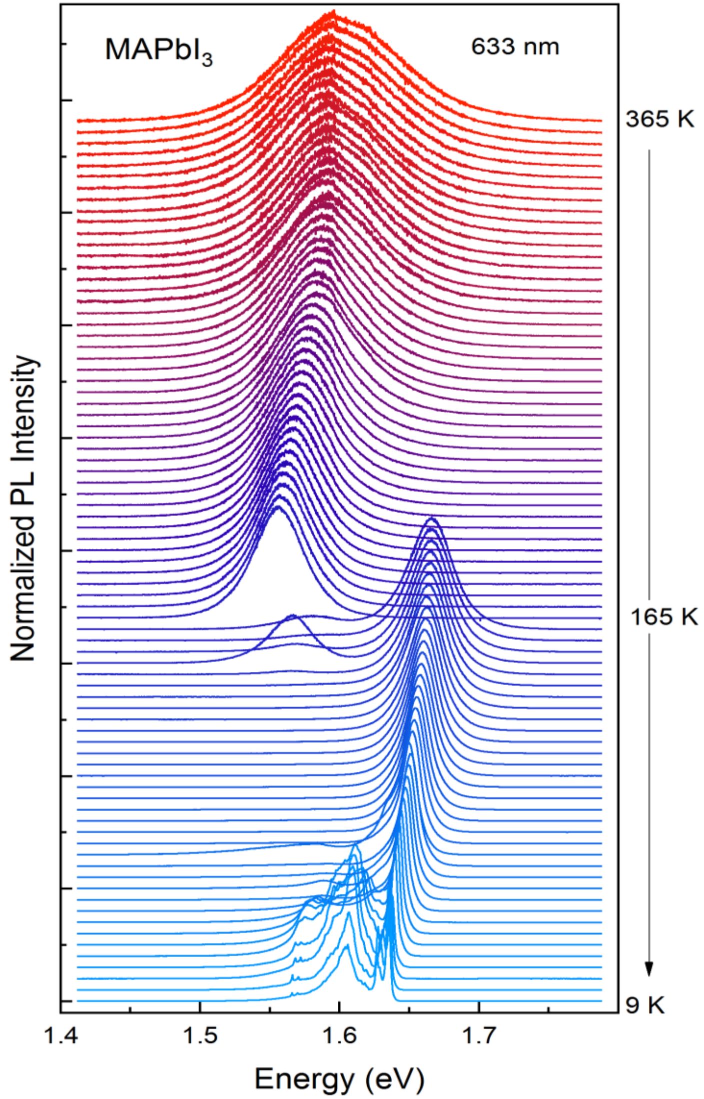
Leguy et al., Phys. Chem. Chem. Phys. **18** 27051 (2016)

Contact: goni@icmab.es

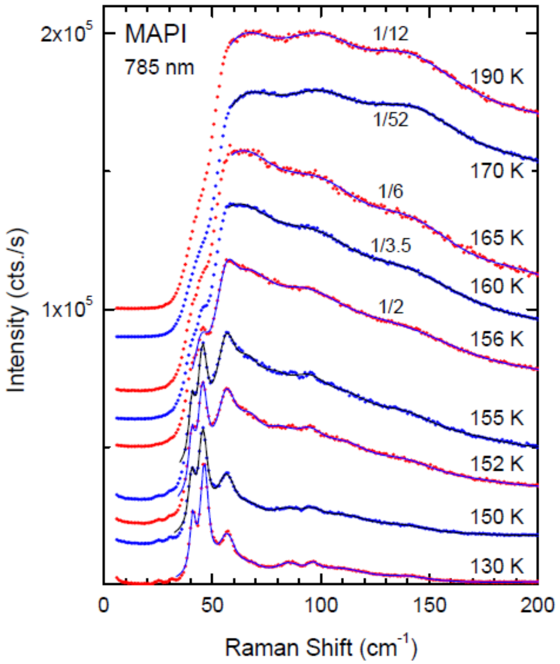
Hybrid perovskites: Using pressure and temperature to unravel the structural-optical/vibrational-properties relationship

Phase transitions





Temperature: Dynamic disorder due to unlocking of MA cations causes huge inhomogeneous broadening of cage modes



Contact: goni@icmab.es

Main subjects

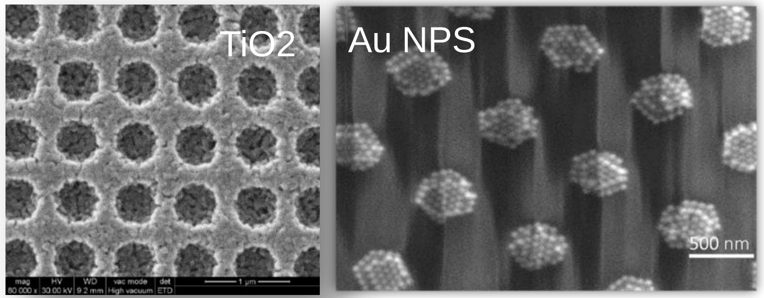
- Research on photovoltaics: organic, inorganic, hybrid
- Light management with photonic structures
- Thermoelectric structures: organic, inorganic, hybrid
- Thermal transport: theory and experiment

Light management with photonic structures:
Soft nanoimprinting lithography in our lab

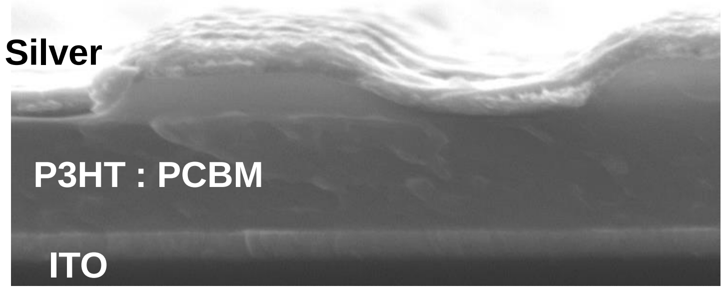
ENLIGHTMENT erc European Research Council

https://departments.icmab.es/nanopto

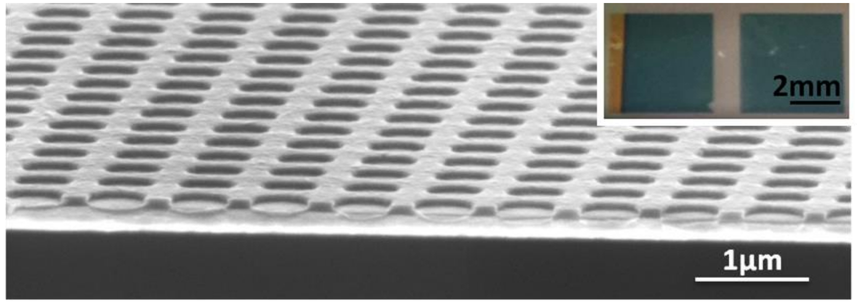
1 Nanoparticles (TiO2, Au, ...)



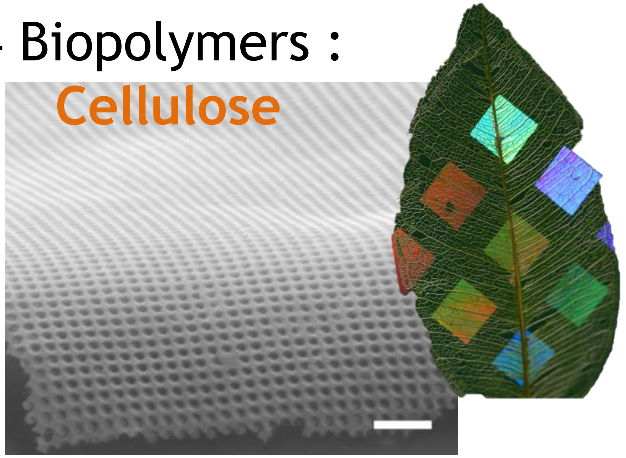
2 Resists, polymers etc



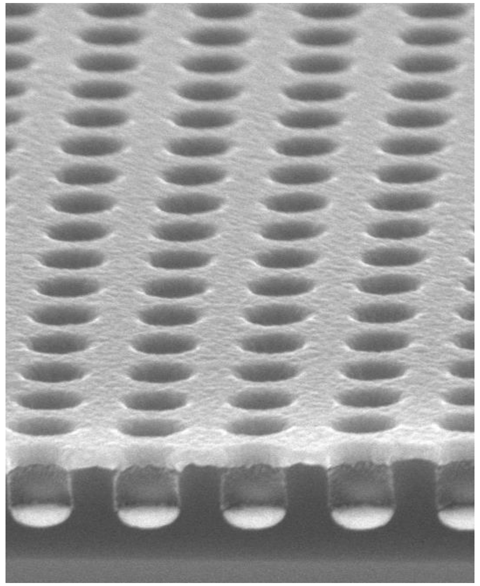
3 Germanium



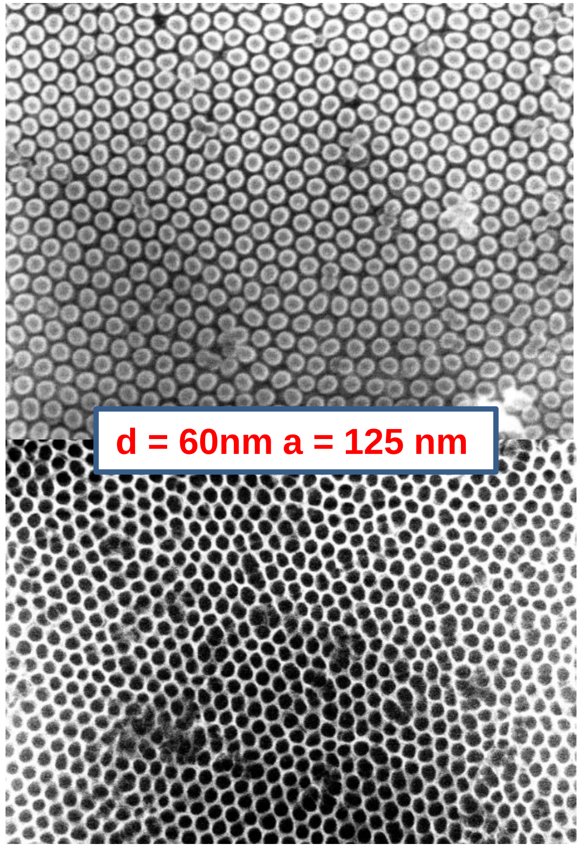
4 Biopolymers :



5 Metal coated



6 Small Features



Contact: amihi@icmab.es

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CSIC

Main subjects

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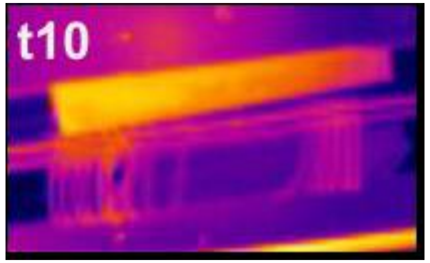
- Thermoelectric structures: organic, inorganic, hybrid
- Thermal transport: theory and experiment

Organic thermoelectrics

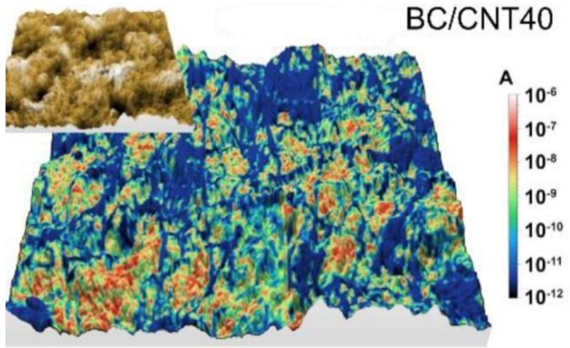
https://departments.icmab.es/nanopto

Fundamental properties

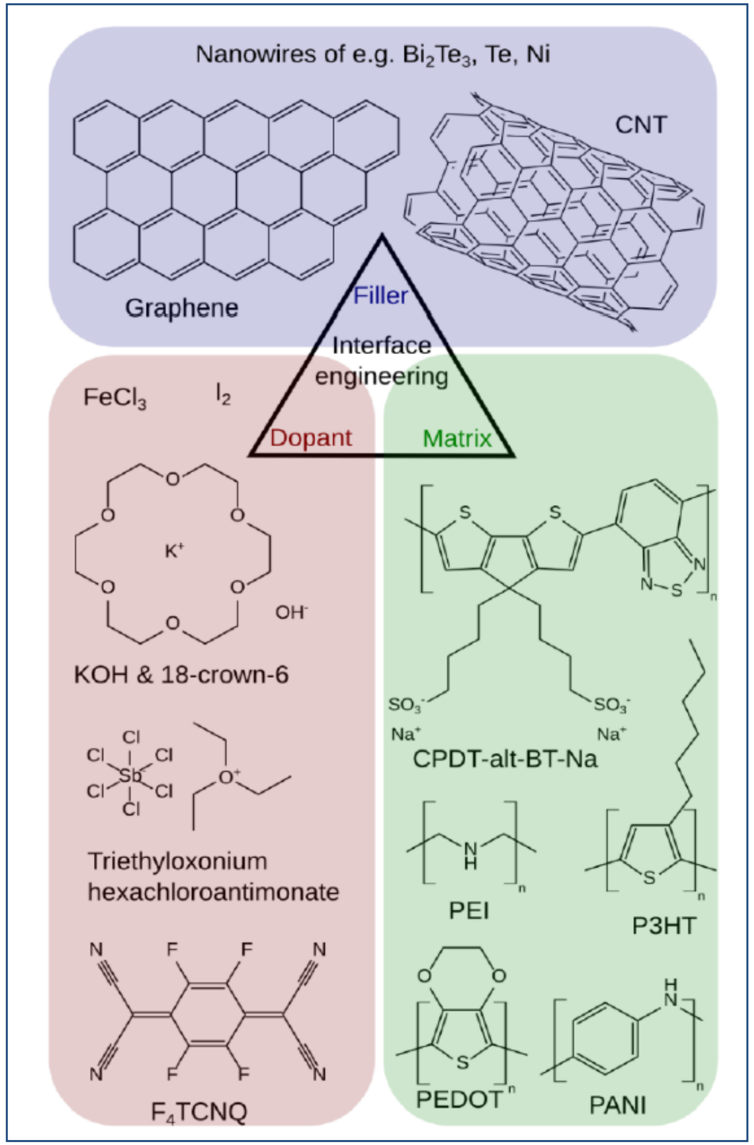
thermal



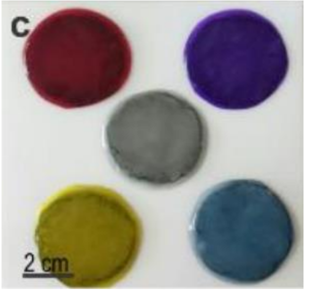
electrical

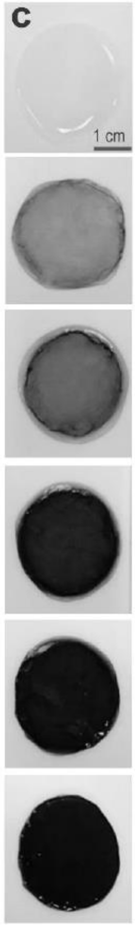


Keifer et al *Advanced Science*, 4 (2017) 1600203
Dörling et al *Advanced Materials*, 28 (2016) 2782
Bounioux et al *Energy Environ. Sci.*,6 (2013) 918



Materials processing and screening



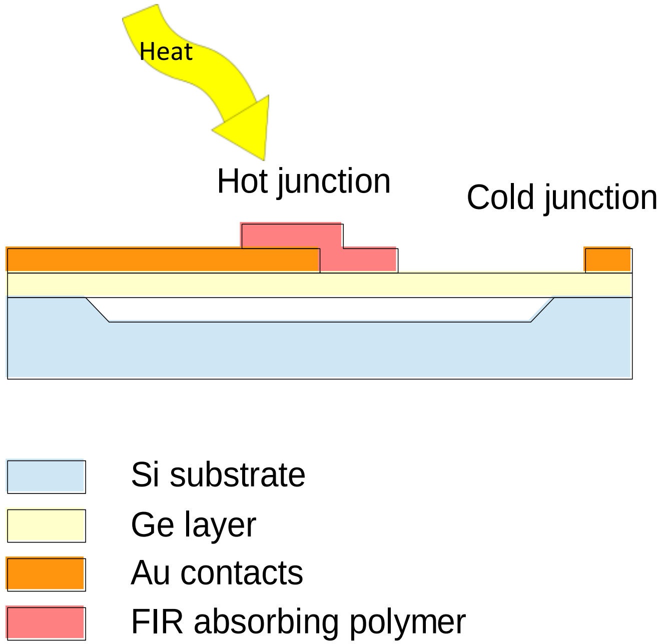


Doping gradients

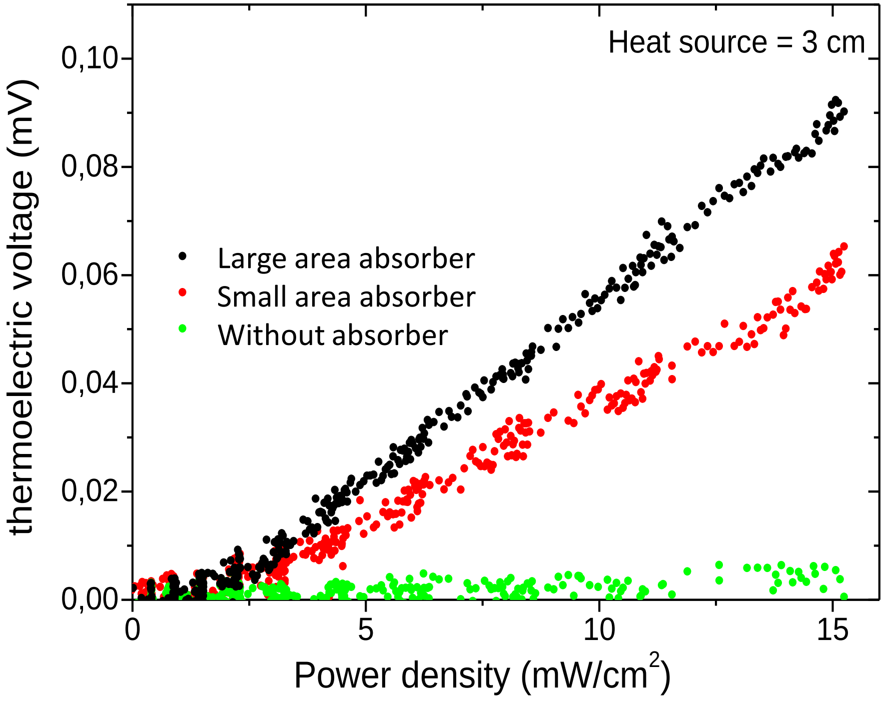
Contact: mcampoy@icmab.es

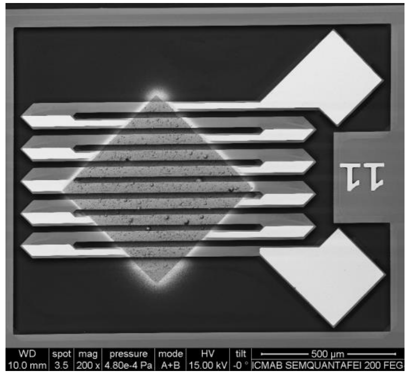
Inorganic and hybrid thermoelectrics

https://departments.icmab.es/nanopto

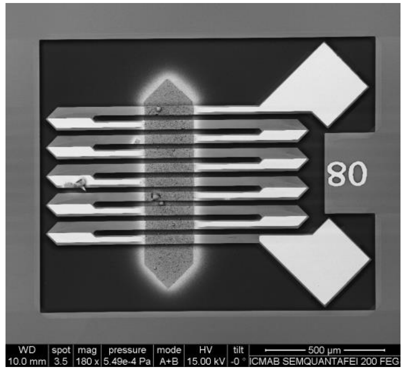


Thermoelectric Body-Heat Sensors Based on SiGe Membranes





Device: 10 pairs, large absorber
Resistance: 240 kΩ
Sensitivity: 6 μV/(mW/cm^2)
Responsivity: 5 V/W



Device: 10 pairs, small absorber
Resistance: 290 kΩ
Sensitivity: 4 μV/(mW/cm^2)
Responsivity: 5 V/W

Contact: goni@icmab.es

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CSIC

Main subjects

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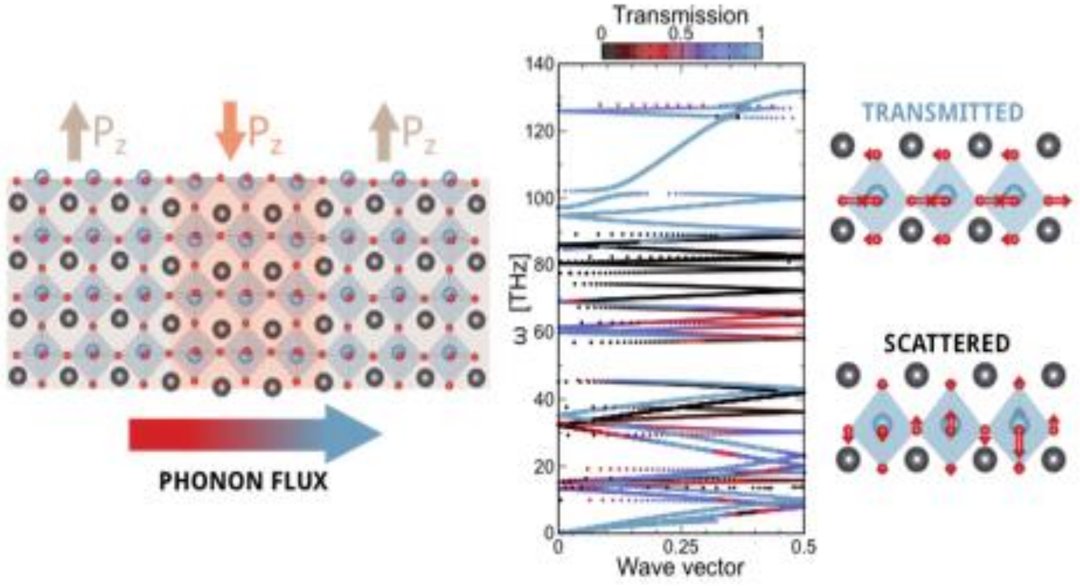
- Thermoelectric structures: organic, inorganic, hybrid
- Thermal transport: theory and experiment

Nanoscale thermal transport : Theory

https://departments.icmab.es/mst

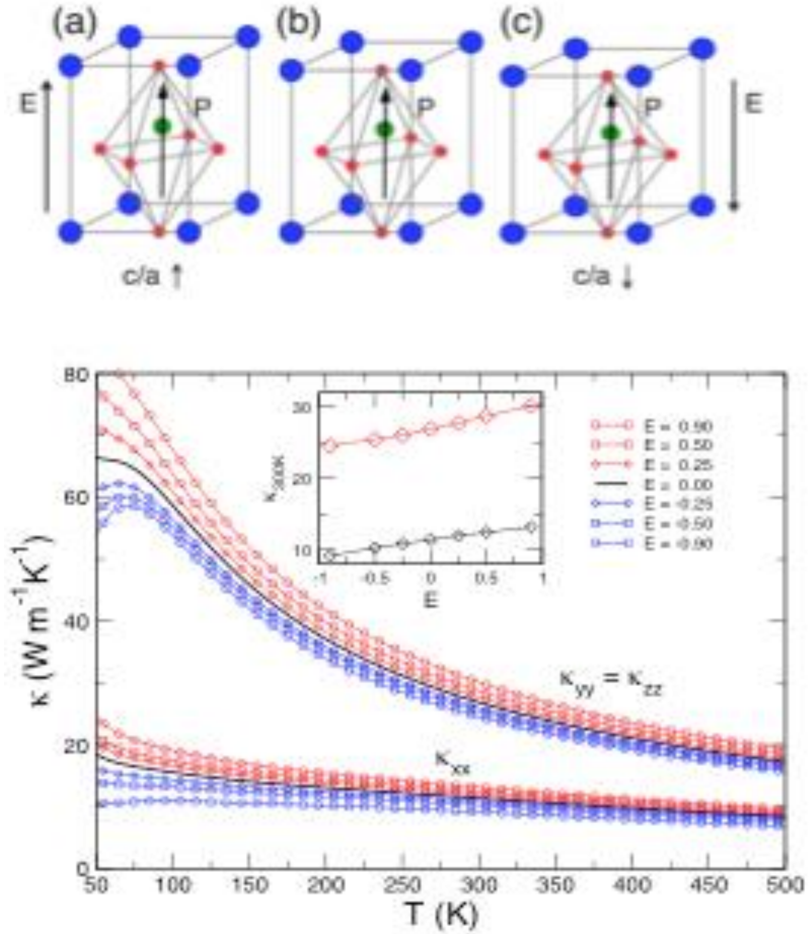
Phononic devices based on ferroelectric oxides

A phonon switch and polarizer based on ferroelectric domain walls



Seijas-Bellido et al., Phys. Rev. B **96** 140101(R) (2017)
Royo et al.. Phys. Rev. Mater. **1** 051402(R) (2017)

Towards an all-electric control of the heat flux



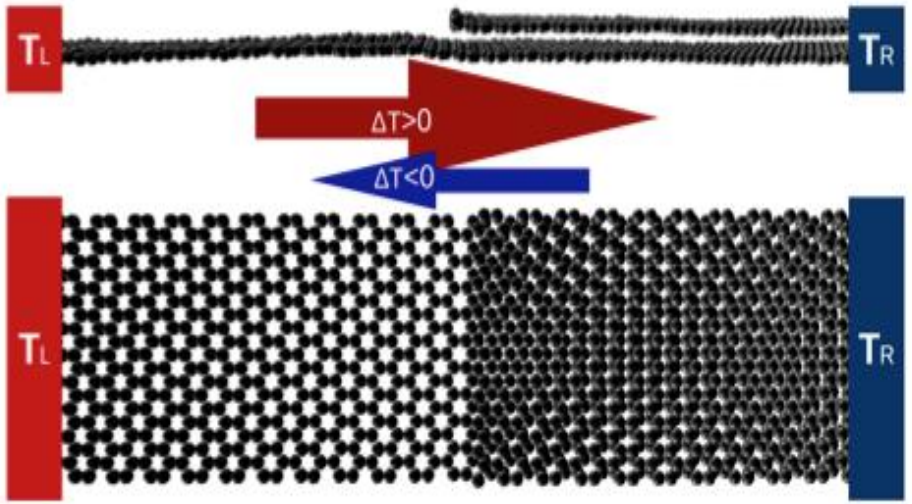
Contact: rrurali@icmab.es

Nanoscale thermal transport : Theory

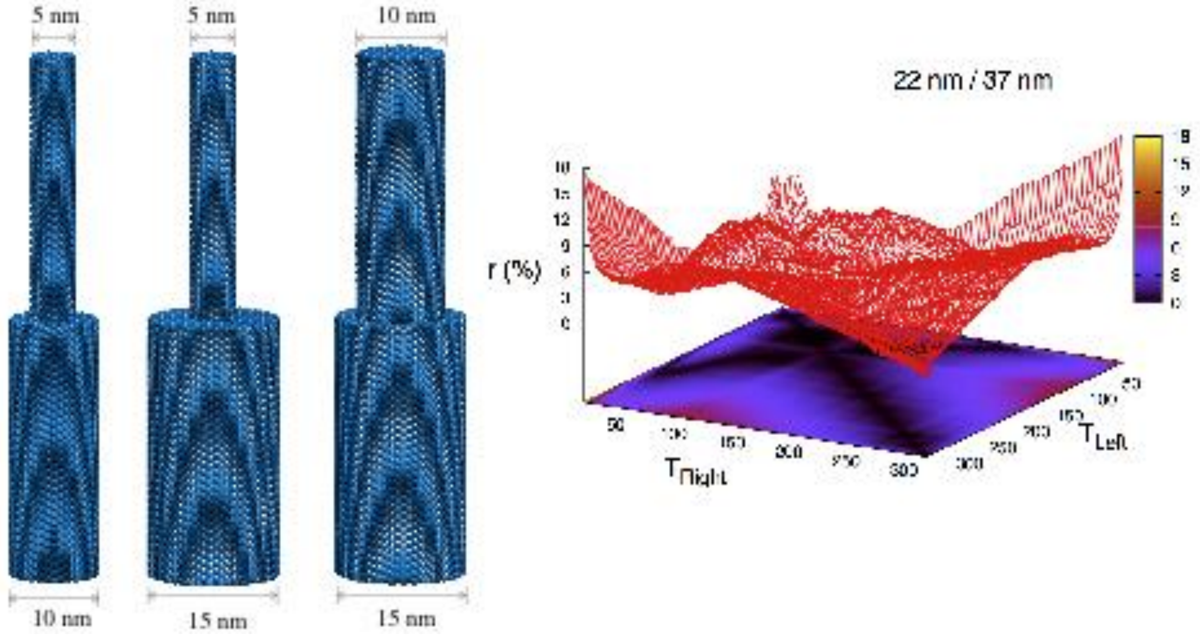
https://departments.icmab.es/mst

Nanostructured materials for heat rectification

2D materials heterostructures based thermal diodes



Semiconducting nanowires for heat rectification



Rurali et al.. Nano Lett. **15** 8255 (2015)

Contact: rrurali@icmab.es

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(Nanoscale) thermal transport : Experiment

https://departments.icmab.es/nanopto

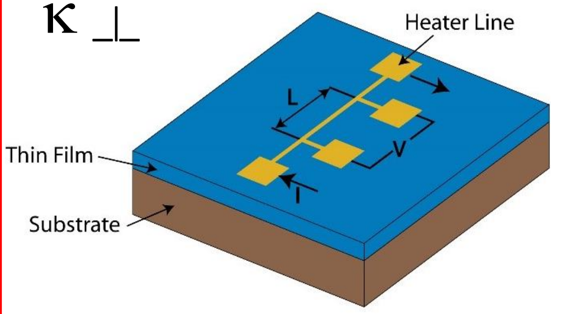
κ

THERMAL CONDUCTIVITY

Steady-state

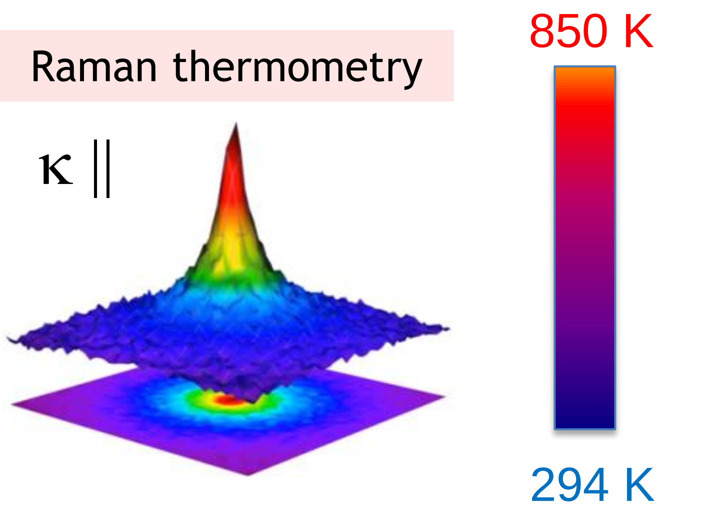
3 omega method

$\kappa \perp$



Raman thermometry

$\kappa \parallel$

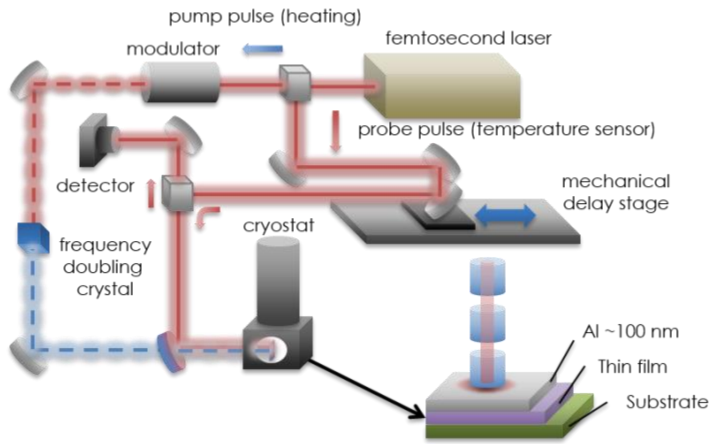


Time Domain

$\alpha = \kappa / \rho C_P$

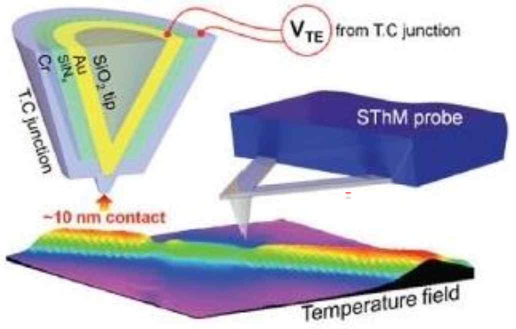
THERMAL DIFFUSIVITY

Time-domain thermoreflectance



J. S. Reparaz *et al.*; ***Rev. Sci. Instr. 85, 034901 (2014)***
M. R. Wagner, Graczykowski, J. S. Reparaz, *et al.*;
Nano Letters 16, 5661 (2016)
B. Graczykowski, A. El Sachat, J. S. Reparaz, *et al.*;
Nat. Comm. **8, 415 (2017)**

Scanning probe microscopy



New objectives:
- Develop interferometric technique to visualize **heat propagation dynamics** at the nanoscale
- Implement **simultaneous sub-micrometer** and **picosecond resolution**

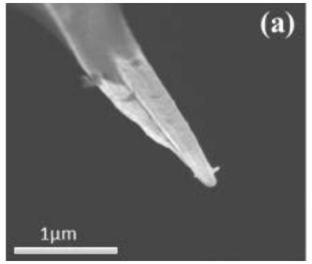
Contact: jsreparaz@icmab.es

ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA
EXCELENCIA SEVERO OCHOA
CSIC

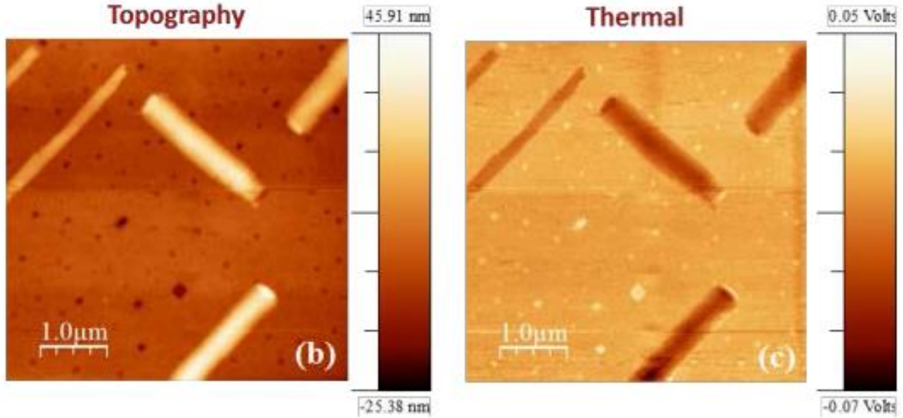
Nanoscale thermal transport: Experiment

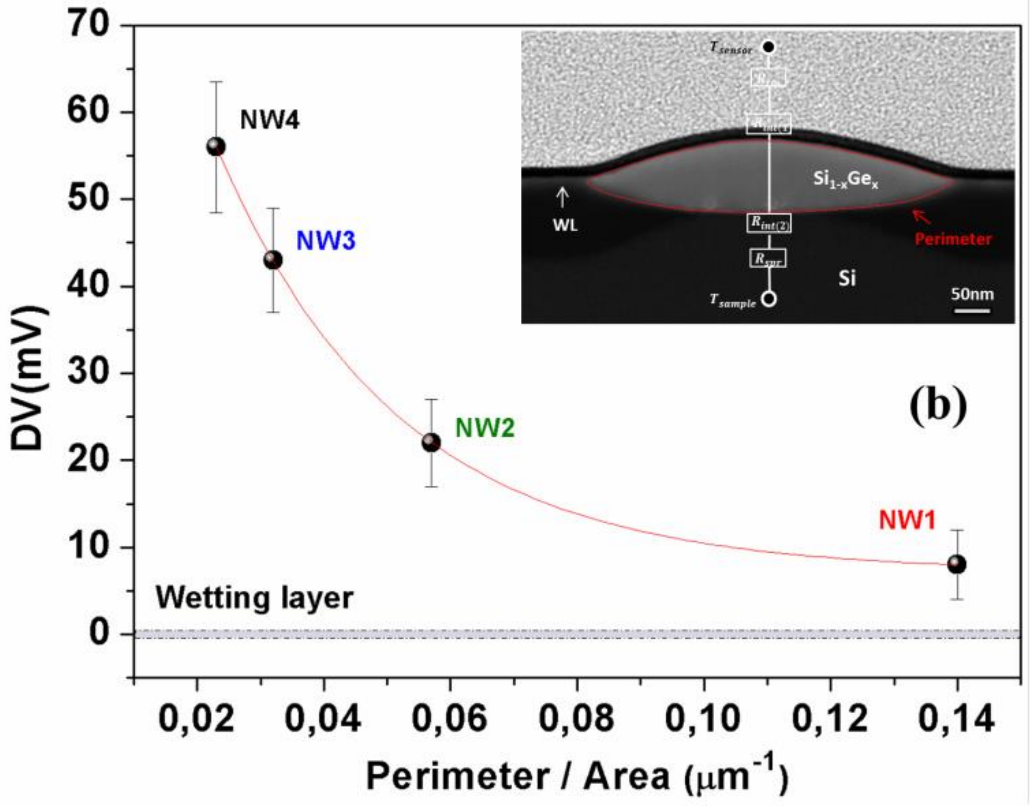
https://departments.icmab.es/nanopto

- Objective: Obtain *in-plane nanowires* and measure thermal properties
- Au-seeded VLS growth by Molecular Beam Epitaxy on Si (001)



- SThM performed in ambient using a Pt dual-wire thermal probe





El Sachat et al. Nanotechnology **28**, 505704 (2017)

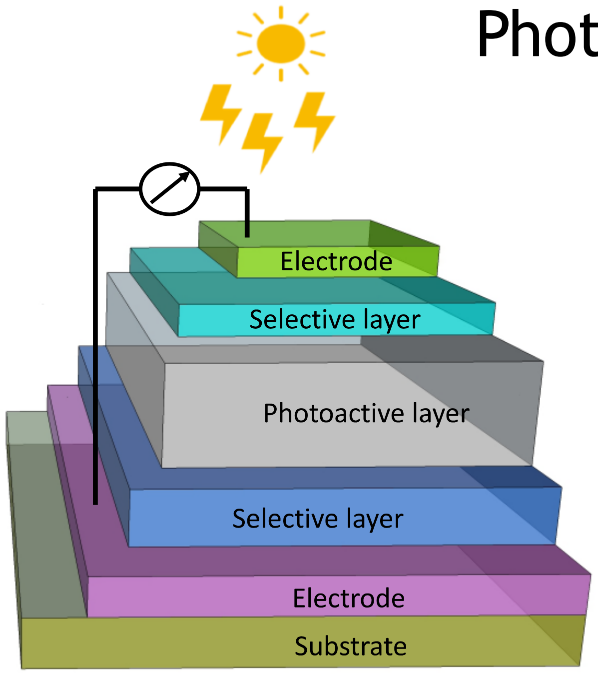
Contact: isabel@icmab.es

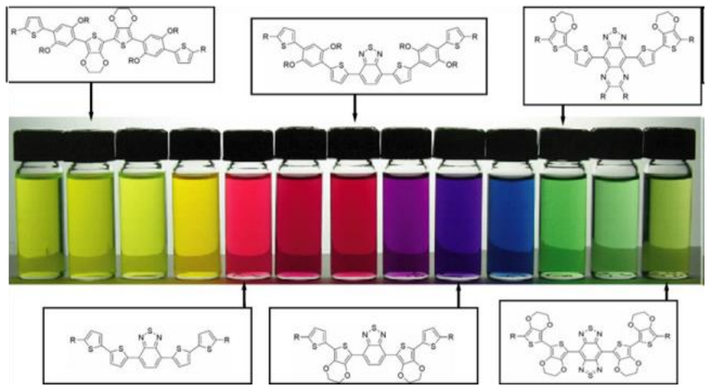
ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA EXCELENCIA SEVERO OCHOA CSIC

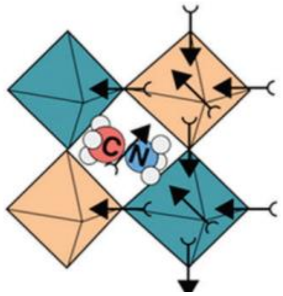
Summary

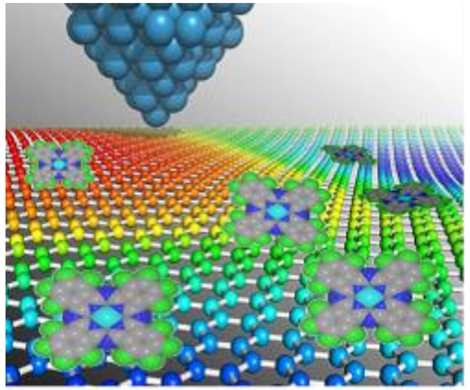
Maria Isabel Alonso, Esther Barrena, Mariano Campoy-Quiles, Mariona Coll, Josep Fontcuberta, Alejandro Goñi, Agustín Mihi, Juan Sebastián Reparaz, Riccardo Rurali

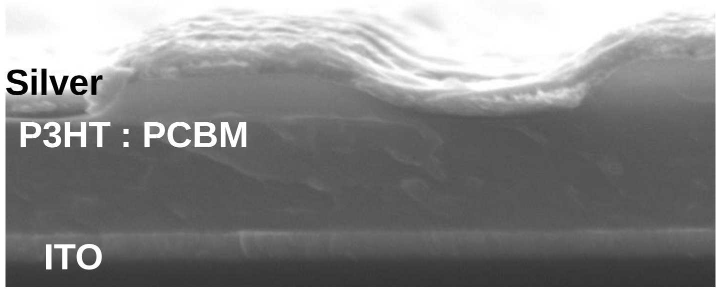
Photovoltaic











Thermoelectric