

# JORNADAS CIENTÍFICAS PROMETEO 2023

“PHOTOACTIVE MATERIALS”

13 de diciembre de 2023 10-13:30

CAMPUS BURJASSOT-PATERNA,  
EDIFICI: E.T.S. D'ENGINYERIA,  
Planta: 1 - SALÓN DE GRADOS JOAN PELECHANO



Organizado por: *Grupo de Reactividad Fotoquímica*

## Conferenciantes invitados



**Prof. Dario M. Bassani**  
(University of Bordeaux)



**Prof. Julio Lloret Fillol**  
Institut Català d'Investigació  
Química (ICIQ)



**Dr. Salvador Eslava**  
(Department of Chemical  
Engineering at Imperial  
College London)

# Programa

- ✓ 10: 00 / **Acto de Apertura de las Jornadas**
- ✓ 10:10 -10:50 / **Probing and powering molecular electronics using light**
  - **Prof. Dario M. Bassani**  
University of Bordeaux. Bordeaux
- ✓ 10:50-11:30 / **Artificial Photosynthesis as inspiration for Oxidation and Reduction Chemistry**
  - **Prof. Julio Lloret Fillol**  
Institut Català d'Investigació Química (ICIQ)
- ✓ 11:30-12:00 *Coffee-break*
- ✓ 12:00-12:40 / **Engineering photoelectrochemical and photocatalytic materials for solar fuels**
  - **Dr. Salvador Eslava**  
Department of Chemical Engineering at Imperial College London
  
- ✓ 12: 40- 12:50 | **Irene Pérez Herráez**  
Institute of Molecular Science, University of Valencia,  
N-acetyl-L-cysteine gold nanoclusters (AuNC@NAC) for selective detection of tetracycline
  
- ✓ 12:50- 13:00 | **Rita Cevallos Toledo**  
Institute of Molecular Science, University of Valencia  
Cooperative Sensitization Upconversion in Dye-Ln system
  
- ✓ 13:00- 13:10 | **Alejandro Cortés Villena**  
Institute of Molecular Science, University of Valencia  
Quantum-Confinement Effect of Perovskite Nanocrystals in Singlet Sensitization of BODIPY Dyes
  
- ✓ 13:10-13:20 | **Miguel Justo Tirado**  
Institute of Molecular Science, University of Valencia,  
Luminescent fibers of Au(I)-adamantylamine coordination polymer
  
- ✓ 13:20-13:30 | **Alessandro Ciccone**  
Institute of Molecular Science, University of Valencia,  
Photohealing of CsPbBr<sub>3</sub> nanocrystals by aryl bromide compounds



## Prof. Dario M. Bassani

### Biography

Dr. Bassani obtained a bachelor's degree in chemistry at the University of Louvain (Belgium), followed by PhD in Chemistry at Northwestern University under the guidance of F. D. Lewis. He entered the CNRS at the University of Bordeaux in 1997 after undertaking a postdoctoral fellowship first in Basel (Switzerland) with J. Wirz and then in Strasbourg with J.-M. Lehn. He leads a research group focused on the use of supramolecular interactions to control the photochemical and photophysical behavior of excited states in solution, in the solid, and on surfaces. Intermolecular communication in these assemblies is harnessed to give systems in which the reactivity, absorption, or emission reflects the ordering of the electro- and photo-active subunits. He is the recipient of several awards, including the Grammaticakis-Neumann Prize of the Swiss Chemical Society and is currently serving as editor-in-chief for Photochem. Photobiol. Sci.

### Probing and powering molecular electronics using light - Dario M. Bassani

#### Abstract:

Molecular electronics was born from the concept of using finite molecular orbitals to simulate the basic operational principles of silicon-based devices.[1] More recently, and with the promise of new systems for sensing and energy conversion, the field grew to encompass organic or hybrid organic-inorganic materials such as conjugated polymers and perovskites that possess extended or infinite structures with highly delocalized orbitals. In some of these systems, light can be used to probe or trigger events linked to charge transfer processes, or changes within the active layer. To illustrate this, we will examine how light can be used to commute aromatic oligoamide foldamers between conductive and non-conductive states. These foldamers spontaneously adopt a helical conformation that is particularly conducive to long-distance p-type charge transport,[2] and can be rendered n-type by metalation.[3] However, their robustness makes them challenging for applications requiring a response to outside stimuli such as sensing or photocommuration. In perovskites, light is converted to electrical energy with record-breaking efficiencies. To date, these materials are still particularly prone to damage by moisture and ion diffusion. We can use spectroscopic techniques to follow the diffusion of protons and show that this process is also light-activated.[4] An interesting application of this finding is in rapidly screening the efficiency of novel protective barriers without the need of time-consuming ageing studies.[5] Time permitting, we will discuss uses of "stealth dopants" to irreversibly dope the bulk of hybrid perovskite materials in view of tailoring their electronic properties.[6]

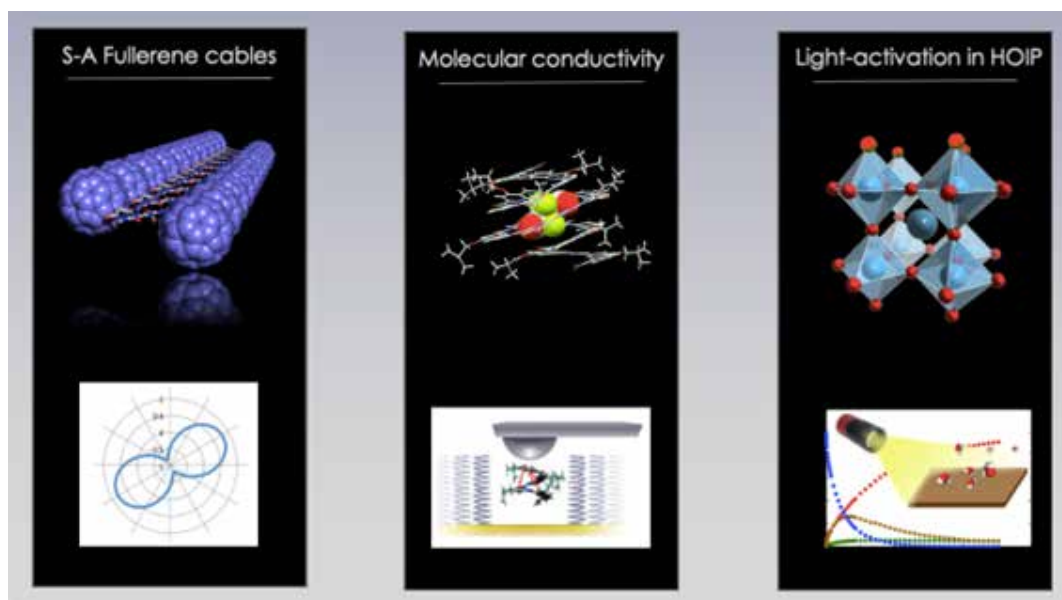


Figure 1. Probing and controlling supramolecular assemblies for applications in molecular electronics.



## Prof. Julio Lloret Fillol

### Biography

Julio Lloret-Fillol graduated in Chemistry from the University of Valencia (2001), where he obtained his PhD in 2006 under the supervision of Prof. Pascual Lahuerta and Prof. Julia Pérez-Prieto (2006), focusing on catalysis and organo-metallic chemistry. Then, he moved to the University of Heidelberg under the supervision of Prof. Lutz Hans Gade as Marie Curie postdoc fellow. He returned to Spain in 2010 thanks to the Ramón y Cajal program, starting his independent career at the University of Girona, researching water oxidation with iron molecular complexes. In 2014, he became a Young Research Group Leader at the Institut de Química Computacional i Catàlisi (UdG), and, since late that year, he started as Group Leader at the Institut Català d'Investigació Química (ICIQ).

In 2015, he was appointed ICREA Professor at the Institución Catalana de Investigación y Estudios Avanzados (ICREA) and received a grant from the European Research Council Consolidator Grant (ERC-CoG) to investigate photocatalytic reduction and artificial photosynthesis.

His scientific interests include chemical reactivity, synthetic methodology, artificial photosynthesis, catalysis in general, computational chemistry, and the study of reaction mechanisms. He is also interested in automation technologies applied to chemistry. His research group has specialized since 2015 in photo- and electrocatalysis to develop new reactivity in the context of artificial photosynthesis for the synthesis of fuels and fine chemicals, including water oxidation and water and CO<sub>2</sub> reduction, as well as exploring these concepts to develop organic reactivity. We have developed new catalysts directly on electrodes to produce green hydrogen through electrolysis, as well as in the design of devices for their study.

Lloret-Fillol has published over 107 articles in high-impact journals and has been invited to more than 85 conferences. He has been active in technology transfer, holding eight patents and co-founding three spin-off companies. He co-founded Trellum Technologies (Chief Scientific Officer (CSO)), Gioxcat (Advisor), and most recently, JOLT Solutions (Chief Scientist (CS)). The latter secured Series A investment for industrializing electrode manufacture for Alkaline Electrolyzers. At JOLT, we are applying a new technology that we have patented for the growth of catalysts on surfaces in industrial manufacturing of electrodes to produce green hydrogen with alkaline electrolyzers.

The results of his research have been recognized in several awards, such as the Thieme Chemistry Journals Award, Young Academy of Europe, Young Researcher Award 2015, Young Researcher Award 2014 of the Organometallic Group of the RSEQ and the recent GEQO Award 2023 for Research Excellence.

### Artificial Photosynthesis as inspiration for Oxidation and Reduction Chemistry

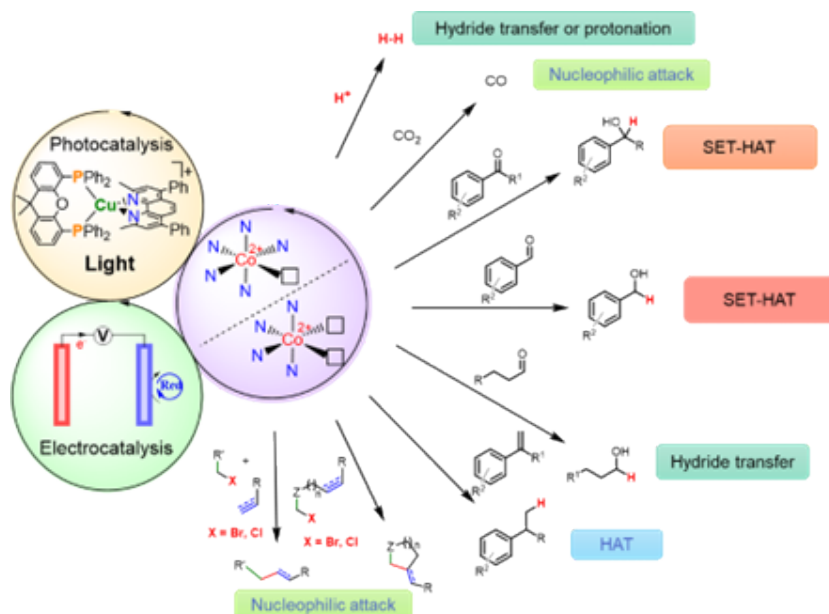
#### Abstract:

Inspired by natural photosynthesis, there is a vision that fuels and chemicals can be synthesized using Earth's basic elements (i.e., H<sub>2</sub>O, CO<sub>2</sub>, N<sub>2</sub>) and removable energy. This concept has given rise to the multidisciplinary field of artificial photosynthesis.<sup>2-4</sup> One of the most appealing research areas in this context is the mechanistic understanding of multi-electron, multi-proton processes, which are central to the transformation of small molecules in artificial photosynthesis. These studies have not only provided new insights into the processes, but also led to the discovery of new reactivity.

In this regard, we will discuss a procedure for the synthesis of water oxidation catalysts, and an ideal reaction to extract reductive equivalents. On the reductive side, we have discovered that well-defined coordination complexes based on the tacn moiety are highly efficient homogeneous catalysts for reducing water,<sup>1</sup> and CO<sub>2</sub> and organic substrates such as ketones, aldehydes, and olefins.<sup>3</sup> The low valent metal intermediates also promote the challenging visible-light reductive radical C-C bond formations from unactivated chloroalkanes, which opens new avenues in photoredox catalysis.<sup>4</sup> This presentation will discuss these aspects, and how to control the selectivity between water reduction and the reduction of organic functionalities. Mechanistic understanding was employed to develop new reactivity and even unlock the reactivity of the Ir-based photosensitizers.



# Prof. Julio Lloret Fillol



## References

1. A) Boutin E., et al. *Chem. Soc. Rev.* 2020, 49, 5772. B) Pannwitz A., et al. *Chem. Soc. Rev.* 2021, 50, 4833.
2. A) Call A., et al. *Chem. Eur. J.* 2014, 20, 6171. B) Call A., et al. *Chem. Sci.* 2018, 9, 2609. C) Call A., et al., *ACS Catal.* 2019, 9, 5837.
3. A) Fernández S., et al. *J. Am. Chem. Soc.* 2019, 142, 120; B) Fernández S., Cañellas S., Franco F., Luis J. M., Pericàs MÀ, Lloret-Fillol J. *ChemElectroChem* 2021, 23, 4390.
4. A) Call A., Casadevall, C., Acuña-Pares, F., Casitas Montero, A., Lloret Fillol, J., *Chem. Sci.* 2017, 8, 4739; B) Call A., Lloret-Fillol J. *Chem. Commun.* 2018, 69, 9643. Casadevall C., et al. *Chem. Sci.* 2022, 13, 4270.
5. A) Claros M. et al. *Angew Chem* 2019, 58, 4869 B) Aragon, J. et al. *Angew. Chem.* 2022, e202114365.



## Dr. Salvador Eslava

### Biography

Dr Salvador Eslava is a Reader (Assoc. Prof.) in the Department of Chemical Engineering at Imperial College London since November 2019. He joined Imperial after five years as a Lecturer (Asst. Prof.) at University of Bath. He currently holds an EPSRC Fellowship on Interface Engineering for Solar Hydrogen and was recently awarded the Warner prize from the Institution of Chemical Engineers (IChemE). Before Bath, he was a research associate in the Materials Department at Imperial College London (2011-2014) working with Prof. E. Saiz on graphene and MOFs and in the Chemistry Department at The University of Cambridge (2009-2011), working with Professors Dominic Wright and Richard Lambert on titanium clusters. He defended his PhD degree in 2009 conducted in the Centre for Surface Chemistry and Catalysis (COK) at Katholieke Universiteit Leuven and IMEC, Belgium, in the group of Prof. Johan Martens working on zeolitic dielectrics. He holds a Taught Master in Materials Science from Università degli Studi di Pavia, Italy, and an MEng in Chemical Engineering from Autonomous University of Barcelona, Spain. He has published more than 75 articles and received £3m funding from EPSRC, The Royal Society, and Innovate UK.

### **Title: Engineering photoelectrochemical and photocatalytic materials for solar fuels**

#### **Abstract:**

Photoelectrochemical and photocatalytic conversion of water and carbon dioxide using solar energy offers a clean solution to the world energy requirements of a sustainable future. Achieving its full potential depends on developing inexpensive photoelectrodes and photocatalysts that can efficiently absorb solar light and drive the photoinduced charges to react with water and carbon dioxide. In this talk, I will present recent developments we have achieved in the preparation of inexpensive photoanodes, photocathodes and photocatalyst composites. For example, we have achieved nanostructured BiVO<sub>4</sub> functionalized with bismuthene and NiFeOx that influence surface states and boost 6 times their photocurrent performance. We have also achieved halide perovskites CsPbBr<sub>3</sub> photoanodes protected with printed carbon layers and graphite sheets and functionalized with NiFeOx water-oxidation electrocatalyst, achieving photoanodes of low onset potential of +0.4 V vs. RHE and photocurrents around 8 mA cm<sup>-2</sup> at 1.23 V vs. RHE for water oxidation. These, moreover, achieve operational stabilities for oxygen evolution above 100 h, inexpensively extended to weeks by replacement of the graphite protection or to months using alternative carbon allotropes. We will also present composites of halide perovskites, such as Cs<sub>2</sub>AgBiBr<sub>3</sub>/bismuthene and Cs<sub>3</sub>Bi<sub>2</sub>Br<sub>9</sub>/g-C<sub>3</sub>N<sub>4</sub>, for their use in the photocatalytic reduction of CO<sub>2</sub>. An extended characterization helps us relate their physical and charge-transfer properties to their performance, guiding us in their rational design for their optimization and future application.