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EXCELENCIA
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27-28th april 2022

2nd meeting Excellence Network of the

RED moDe fotovoltaica

MATERIALES ORGÁNICOS DISRUPTIVOS PARA ENERGÍA FOTOVOLTAICA

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN
AGENCIA ESTATAL DE INVESTIGACIÓN
EUROPEAN UNION
STRUCTURAL FUNDS

preface

The energetic dependence of Europe, and the problems arising from this fact, has dangerously been increased with the recent invasion of Ukraine by the Russian army. This violent act is causing from the beginning of the invasion a number of war crimes which have been denounced not only by the Ukraine authorities but also by the international community. With this written we claim and support the human rights.

From a scientific viewpoint, decarbonization of energy sources is an urgent requirement in order to preserve the existence of our planet. In this regard, solar energy is free, clean, inexhaustible and the most socializing manner of energy since it spreads all over the Earth surface (www.iea-pvps.org). Thus, solar energy is among the best solutions to face the global energy crisis and environmental degradation. Actually, photovoltaics offers a feasible and promising solution to overcome the energy problem, by harvesting and converting solar energy into electrical power. In the frame of a joint multidisciplinary effort, current results have led not only to a remarkable improvement in device efficiencies, but also in reducing substantially fabrication costs. It is important to remark that the 2021 United Nations Climate Change Conference, more commonly referred to as COP26, was held at the SEC Centre in Glasgow, Scotland, United Kingdom, last November 2021. This pact reaffirms the former Paris Agreement (2015) temperature goal of holding the increase in the global average temperature to well below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C above pre-industrial levels, and recognizes that limiting global warming to 1.5 °C requires rapid, deep and sustained reductions in global greenhouse gas emissions, including reducing global carbon dioxide emissions by 45 per cent by 2030 relative to the 2010 level and to net zero around midcentury, as well as deep reductions in other greenhouse gases. However, achieving the target is not ensured, as with existing pledges the emissions in the year 2030 will be 14% higher than in 2010.

In this 2nd meeting Excellence Network of the *Red MODE-Fotovoltaica* (Materiales Orgánicos Disruptivos para Energía Fotovoltaica) participate members of the thirteen groups that constitute the Red, in a meeting to be held at the IMDEA Nanociencia institute in Madrid during April 27-28th, 2022. The aim of this multidisciplinary thematic Red is gathering the efforts to optimize the means for the future development of this important field in our country, as well as developing disruptive photo and electroactive materials for their further application in efficient photovoltaic devices.

We cordially invite you to enjoy this scientific meeting and its appealing scientific program with 14 invited lectures, and 11 contributed oral communications, and scientific discussions. We welcome all of you to Madrid, the city that never sleeps.

Nazario Martín
Symposium Chairman
Professor of Chemistry
Complutense University
Vice-Director of IMDEA-Nanoscience

Agustín Molina
Symposium Co-chairman
Ramon & Cajal Researcher
Department of Organic chemistry
Complutense University

programme

27th april

11.00-11.10

Opening remarks

11.10-11.40

Miquel Solà
“Photoinduced electron transfer in complexes of C60 and [n]cycloparaphenylenes“

11.40-12.10

Enrique Ortí
“Materials for perovskite solar cells: A theoretical insight”

12.10-12.40

Juan Galisteo
“Photo-induced processes in lead-halide perovskites”

12.40-12.55

Inés García-Benito
“Interface engineering for stable and efficient perovskite solar cells”

12.55-13.10

Catarina Ferreira
“Perovskite photovoltaic cells for stray light recycling to improve energetic efficiency in illumination devices”

13.10-15.00

Lunch

15.00-15.30

Mónica Lira/Masoud Karimipour
“Towards high stability lead halide perovskite solar cells by means of composition optimization and interface modification”

15.30-16.00

Cristina Roldán-Carmona
“Evaporated Perovskites Solar Cells”

16.00-16.30

Emilio Palomares
“Molecular approaches to energy conversion”

16.30-16.45

Arghanoon Moeini
“Optimization of low band-gap perovskite for photovoltaics”

16.45-17.00

María Morán Pedroso
“The role of the atmosphere on the photophysics of ligand-free lead-halide perovskite nanocrystals”

17.00-17.30

Coffee Break

17.30-18.00

Giovanni Bottari
"Novel photo- and electro-active conjugates based on tetracyanobuta-1,3-diene and cyclopenta[hi]aceanthrylene"

18.00-18.30

Pilar de la Cruz
"Molecular engineering of small molecules for highly efficient organic solar cells"

18.30-19.00

David Curiel
"Perovskite solar cells with small molecule self-assembled hole transporting layers"

19.00-19.15

Jorge Labella
"Subphthalocyanine-based electron-transport materials for perovskite solar cells"

19.15-19.30

Gibu George
"Effect of photoinduced electron transfer in ϖ-extended macrocycles"

27th
april

programme

28th april

10.00-10.30

David Casanova
"Electronic structure and photophysics of the BODIPY monomer and an orthogonal dimer"

10.30-11.00

Andrea Cabrera-Espinoza
"Photo-crosslinked fullerene-based hole transport material for humidity-resistant perovskite solar cells "

11.00-11.30

José Manuel Marín-Beloqui
"Triplet-charge annihilation in a small molecule donor:acceptor blend as a major loss mechanism in organic photovoltaics"

11.30-11.45

Javier Urieta-Mora
"Improving the long-term stability of doped spiro-type hole-transporting materials in perovskite solar cells"

11.45-12.00

Isidora Susic
"Quadruple-cation wide bandgap perovskite solar cells with enhanced thermal stability"

12.00-12.30

Coffee break

12.30-12.45

José Sánchez
"Dibenzofulvene-based molecules as hole extracting interlayer for perovskite solar cells"

12.45-13.00

Antony Stasyuk
"Molecular bowls as electron donors in photoinduced electron transfer reactions"

13.00-13.15

Wenhui Li
"New modified Spiro-OMeTAD molecule used as self-assembled monolayer (SAM) for efficient inverted perovskite solar cells"

13.15-13.30

Aitor Diaz-Andres
"Electronic structure and aromaticity in excimer and excited multimers"

13.00-13.30

Carles Ros
"Nano-photonic configurations to transform sunlight into other forms of energy"

13:30

Closing remarks

2nd meeting Excellence Network
of the **Red MODE-Photovoltaics**

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abstracts

Photoinduced electron transfer in complexes of C_{60} and [n]cycloparaphenylenes

M. Solà[1], O. A. Stasyuk, A. A. Voityuk[1], A. J. Stasyuk[1]

[1] Institut de Química Computacional and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany, 69, 17003 Girona, Spain

A well-known disadvantage of using fullerenes as a component of photovoltaic devices is their tendency towards self-aggregation that makes difficult to develop photovoltaic materials with the desired properties.[1] Thanks to the concave-convex complementarity, fullerenes are an ideal guest molecule to form stable complexes with various macrocyclic host molecules[2] such as cyclodextrines, calix[8]arenes or cycloparaphenylenes (CPP, Figure 1). The formation of such host-guest complexes effectively suppresses fullerene aggregation and thereby facilitates the conversion of light into electricity. A number of supramolecular donor-acceptor (DA) complexes of CPP with various fullerenes including endohedral species have been reported to be capable of photoinduced electron transfer (PET). In such complexes, CPPs act as an electron donor. Using the TD-DFT approach, we have studied the PET in $C_{60}\subset$[10]CPP complex with and without encapsulated Li^+, in perfluorocycloparaphenylene (PFCPPs, $C_{60}\subset$[10]PFCPP), and in some nano-Saturn complexes of C_{60}.[3] Our results show that in most of these inclusion complexes fast PET is possible. The charge-separated states with the electron transfer from the host to the C_{60} unit can be efficiently populated through the decay of the locally excited states and occurs in sub-nanosecond time scale.

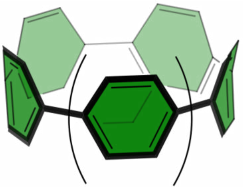

Figure 1. The [n]cycloparaphenylenes ([n]CPP).

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2 Q. Shi *et al. Chem. Commun.* **2021**, *57*, 12379-12405

3 a) A. J. Stasyuk *et al. Chem. Commun.* **2019**, *55*, 11195-11198; b) O. A. Stasyuk *et al. Phys. Chem. Chem. Phys.* **2021**, *23*, 2126-2133; c) O. A. Stasyuk *et al. Chem. Eur. J.* **2021**, *27*, 8737-8744; d) O. A. Stasyuk *et al. ChemPhysChem*, submitted.

Materials for perovskite solar cells: a theoretical insight

Enrique Ortí, Jesús Cerdá, Joaquín Calbo and Juan Aragó

Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, c/Catedrático José Beltrán, 2, 46980 Paterna (Valencia), Spain

e-mail: enrique.orti@uv.es

Hole-transporting materials (HTMs) are a crucial component in obtaining high power conversion efficiencies (PCEs) in perovskite-based solar cells (PSCs). They play the important roles of extracting the photogenerated holes, formed within the perovskite film, and transporting them to the electrodes. Among the wide number of chemical structures proposed as HTMs for PSCs, small organic molecules have received special attention with spiro-OMeTAD (2,2′,7,7′-tetrakis(*N*,*N*-di-*p*-methoxyphenylamine)-9,9′-spirobifluorene) as a reference.[1] In this communication, we first focus on how the donor ability and hole reorganization energy change with the chemical structure of the HTM. π-Extended, sulfur-rich compounds, such as the anthracene-tetrathiophene ATT-OMe system displayed in Figure 1a, that have been used as HTMs in PSCs achieving remarkable PCEs, are theoretically described.[2] Second, we investigate a series of HTMs based on fused polyheteroaromatic molecules incorporating 7-azaindole terminal moieties bearing hydrogen-bond donor and hydrogen-bond acceptor sites (Figure 1b). The 7-azaindole units induce the hydrogen-bond self-assembly of the conjugated molecules thus increasing the supramolecular ordering in the HTM layer. The effects of this ordering on the charrier transport in the HTM semiconducting layer are theoretically discussed.[3] Third, we briefly present how the optical properties (energy bandgap) of $Cs_2AgBiBr_6$ lead-free double perovskites can be tuned by substituting the monovalent Ag^{1+} and trivalent Bi^{3+} cations by divalent Sn^{2+}, Ge^{2+} and Zn^{2+} cations.[4]

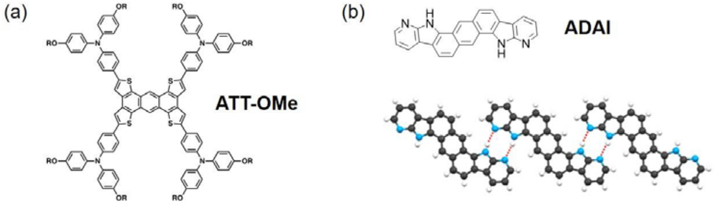

Figure 1. Chemical structure of the sulfur-rich ATT-OMe (a) and the H-bond-promoting ADAI (b) HTM molecules. Both HTMs are based on an anthracene central core.

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Photo-induced processes in lead-halide perovskites

Juan F. Galisteo López

Multifunctional Optical Materials - Instituto de Ciencia de Materiales de Sevilla

The potential of lead halide perovskites as a material to build state of the art optoelectronic devices, from solar cells to LEDs or photodetectors, by low temperature processing from earth-abundant materials is acknowledged nowadays after a decade of scientific and technological progress. Nevertheless, one of the main bottlenecks for their commercialization comes from its stability, or the lack of, under different external stimuli. Perhaps one of the more pressing is that related with photo-induced changes of the material that can severely affect its performance in a device, something particularly relevant for a material that has revolutionized the field of photovoltaics over the past years.

At the Multifunctional Optical Materials group we have devoted a research line to the study of the changes in the optical and structural properties that lead halide perovskites undergo when exposed to external illumination. Exploring different morphologies, from thin films to single crystals or nanocrystals, and compositions, we have established a number of factors that influence how external irradiation affects the material, from light intensity to the atmosphere surrounding the sample. In this presentation I will discuss how different photo-induced processes take place, from emission activation to darkening, and the possible driving forces behind them. Further, I will discuss how these processes may affect other phenomena observed in this type of materials such as blinking in nanocrystals or phase segregation in mixed-halide samples.

While photo-induced processes can be viewed as an obstacle for the commercialization of this material, understanding its physical origins may represent a means to further improve their performance if we can “tame” these processes.

Interface engineering for stable and efficient perovskite solar cells

I. García-Benito,[a,b] A. A. Sutanto,[b] M. K. Nazeeruddin,[b] G. Grancini[b]

[a]*Dto. Química Orgánica, Facultad C. Químicas, Universidad Complutense de Madrid,*
Av. Complutense s/n, 28040 Madrid, Spain.
[b]*Group of Molecular Engineering of Functional Materials, Institute of Chemical Sciences and*
Engineering, EPFL Valais Wallis, Rue de l'Industrie 17, CP 440, CH-1951 Sion, Switzerland.

Perovskite solar cells (PSCs) are the most emerging area of research among new generation photovoltaic technologies, owning to their power conversion efficiency (PCE) up to recently certified 25.5%[1] and low processing cost. Since the first-time reported all-solid state PSCs in 2012,[2] important enhancements have been done in the deposition methods, chemical composition, and synthesis technique, among others. However, the stability of PSCs has been a long-standing question.[3]

Engineering two-/three-dimensional (2D/3D) PSCs is a popular strategy for fabricating efficient and stable devices. Nevertheless, the precise function of the 2D/3D interface in controlling the durability of the solar device is still vague. Interestingly, we revealed a dynamical structural mutation of the 2D/3D interface employing a series of thiophene-based cations (2-TMAI, 3-TMAI, and 2-TEAI) as building blocks for layered 2D perovskites. As a result, we demonstrated that the specific choice of the organic barriers can lead to structurally stable and robust 2D overlayers with a decisive role in improving device stability under illumination.[4]

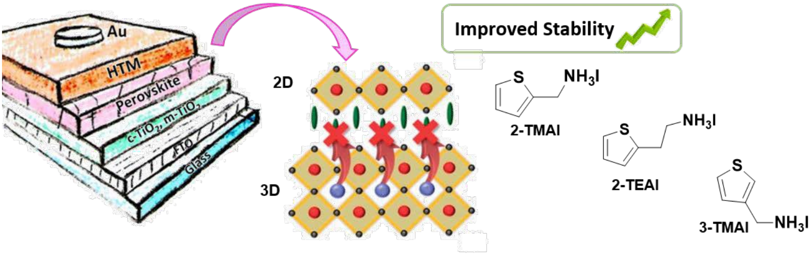

Figure 1. 2D/3D perovskite solar cell: Innovations at the interface.

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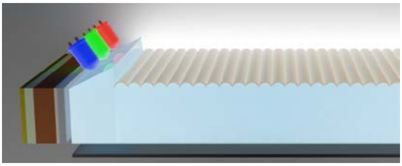
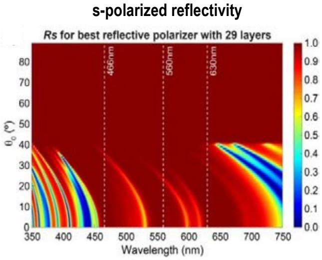
Perovskite photovoltaic cells for stray light recycling to improve energetic efficiency in illumination devices

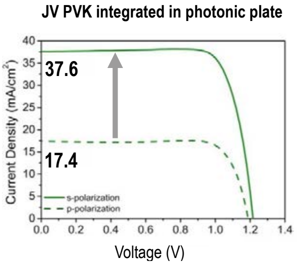
Catarina Ferreira[1], Guillermo Martínez-Denegri[1], Jordi Martorell[1,2]

[1]*ICFO – Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain*
[2]*Departament de Física, Universitat Politècnica de Catalunya, 08222 Terrassa, Spain*

Energetic efficiency in many illumination devices is far from optimal. For instance, in liquid crystal displays (LCDs) a large fraction of the emitted light is lost in the different optical elements used for the image formation, specially in the absorbing polarizers. To mitigate this issue, we designed a photonic plate capable of emitting diffuse and polarized light and we proved that perovskite (PVK) photovoltaic cells are ideal to recycle the stray light back into an electric power in such system. This is attributed to the unique combination of low *Voc* losses with a wide range of tunability of the PVK bandgap. Indeed, when we incorporated wide bandgap perovskite photovoltaic cells in optoelectronic illumination devices we achieved a high power conversion efficiency, of 37.5%, when recycling stray light back into electricity. We were thus able to demonstrate that appropriately tuned wide bandgap PVK cells are ideal to recycle stray light and to improve energetic efficiency in illumination devices where the light is obtained from narrowband sources, even when the overall light emission spans a broad wavelength range.







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Towards high stability lead halide perovskite solar cells by means of composition optimization and interface modification

Masoud Karimipour and Monica Lira-Cantu

Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and the Barcelona Institute of Science and Technology (BIST), Building ICN2, Campus UAB, E-08193 Bellaterra, Barcelona, Spain

In the last decade, lead halide perovskite solar cells have shown extreme capability of being future of photovoltaic energy by reaching power Conversion efficiencies (PCE) up to 25.6%. Despite of the significant success in the increase of efficiency and performance, the stability of the device under operational conditions has remained unmitigated. To reconcile the device with commercial standards, one needs to envisage both internal and external stressors responsible for the device degradation. Here, we have aimed to resolve the internal stressor issues by optimization of composition of the perovskite layer while its resultant device keeps yielding high PCE (~20%) but lower hysteresis and controlled ion migration. For resolving external stressors most known O2 and H2O, and voltage in operational conditions, we have implemented a series of passivation strategies at the interface of Spiro-OMeTAD and perovskite film using both ligand binding molecules and two dimensional (2D) nanosheets. Our results show that application of 2D materials and appropriate choice of ligand can harness the moisture degradation significantly and lead to the increase of stability of the devices.

Evaporated Perovskites Solar Cells

Cristina Roldán Carmona[a]

[a]*École Polytechnique Fédérale de Lausanne*

The rapid improvement in the power conversion efficiency (PCE) of perovskite solar cells (PSCs) has prompted interest in bringing the technology toward commercialization. Capitalizing on existing industrial processes facilitates the transition from laboratory to production lines. In this work, we prove the scalability of thermally co-evaporated MAPbI3 layers in PSCs and mini-modules. Using photoluminescence as a detection tool we study the effect of interface materials on the light emission properties. With a combined strategy of active layer engineering, interfacial optimization, surface treatments, and light management, we demonstrate PSCs (0.16 cm2 active area) and mini-modules (21 cm2 active area) achieving record PCEs of 20.28% and 18.13%, respectively. Un-encapsulated PSCs retained ~90% of their initial PCE under continuous illumination at 1 sun, without sample cooling, for more than 100 h. Looking toward tandem and building integrated photovoltaic applications, we have demonstrated semi-transparent mini-modules and colored PSCs with consistent PCEs of ~16% for a set of visible colors. Our work demonstrates the compatibility of perovskite technology with industrial processes and its potential for next-generation photovoltaics.

Molecular approaches to energy conversion

Prof. Emilio Palomares
ICIQ-BIST. Avda. Països Catalans, 16. Tarragona. E-43007. Spain.
epalomares@iciq.es

During my lecture I will present our latest results[1,2] on the characterization of different type of solar cells from DSSC and OPV to MAPI using advanced photo-induced time resolved techniques. Using PICE (Photo-induced charge extraction), PIT-PV (Photo-induced Transient PhotoVoltage) and other techniques, we have been able to distinguish between capacitive electronic charge, and a larger amount of charge due to the intrinsic properties of the perovskite material. Moreover, the results allow us to compare different materials, used as hole transport materials (HTM), and the relationship between their HOMO and LUMO energy levels, the solar cell efficiency and the charge losses due to interfacial charge recombination processes occurring at the device under illumination. These techniques and the measurements carried out are key to understand the device function and improve further the efficiency and stability on perovskite MAPI based solar cells.

Figures

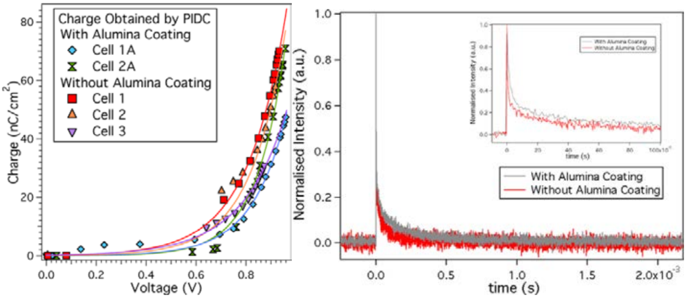

Figure 1. Measured charge in complete devices (left) using PIDC (Photo Induced Differential Charging) and the measured PIT-PV (Photo Induced Transient Photovoltage) decays for two solar cells with different TiO2/MAPI interface.

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Optimization of low band-gap perovskite for photovoltaics

Arghanoon Moeini

Universitat de Valencia, Instituto de Ciencia Molecular (ICMOL)

Fabrication of a stable low band-gap perovskite has always been proved challenging for photovoltaics applications. The objectives of this work have been, to develop a high-quality low-bandgap perovskite with mixed tin-lead (Sn-Pb), optimize the device, and make a semi-transparent structure as a photodiode.

The main bottlenecks of the aforementioned solar cells are prevention of Sn oxidation and fabrication of a fine perovskite surface to address the device's low stability and Voc. The optimization for perovskite with a formula of FA0.7 MA 0.3Pb0.5 Sn0.5 I3 has been exercised by means of wet deposition. Different methods such as solvent engineering, changing precursor concentration and various deposition processes have been tested. Also, different additives have been used to suppress Sn oxidation in the device. The solar cell characteristics have been improved up to 60%.

Perovskite photodetectors are a promising technology for imaging applications, due to their high performance, tunable absorption spectrum, and large area processability. New applications require devices with properties such as transparency, near-infrared (NIR) absorption, or scalability. Here, we have also fabricated semitransparent NIR perovskite photodetectors based on tin-lead (Sn-Pb) hybrid perovskites, by using very thin film perovskite layers (200 nm) and transparent indium tin oxide (ITO) electrodes. The top ITO contact was processed via pulsed layer deposition (PLD) with no damage to the underlying stack. The photodetectors have a full-stack transmission of over 48% in the NIR (between 780 and 1100 nm) and exhibit good performance with a dark current of 1.74·10-2 mA/cm2 (at -0.2 V), the external quantum efficiency of 23% and 13%, and detectivity of 6.6·1010 and 4.2·1010 Jones (at -0.2 V), at 850 and 940 nm, respectively. The performance of these devices makes them good candidates to be used as photodetectors for NIR applications or as bifacial devices.

The role of the atmosphere on the photophysics of ligand-free lead-halide perovskite nanocrystals

María Morán Pedroso

Multifunctional Optical Materials - Instituto de Ciencia de Materiales de Sevilla

Lead-halide perovskite (LHP) nanocrystals (NCs) have emerged as a relevant material for optoelectronic applications from LEDs (due to their large quantum yield) to solar cells. Prior to incorporating them into a device, a precise understanding of their optoelectronic properties and how they interact with light is fundamental. Most studies usually rely on colloidal suspensions of NCs where it is not possible to disentangle the effects of solvents or ligands.

In this work, we study the optical properties of ligand-free LHP NCs synthesized in the pores of nanoporous metal-oxide matrices by spin coating a solution of LHP precursors that allow us to control the NC load and size. The time evolution of LHP NCs photoluminescence (PL) under different atmospheres is considered. PL was monitored and compared with XPS measurements. We observe that defect healing and creation take place simultaneously. Comparing samples with different size and load lead us to associate PL activation with bulk processes and PL darkening with surface degradation.

Molecular engineering of small molecules for highly efficient organic solar cells

Pilar de la Cruz, Fernando Langa

Universidad de Castilla-La Mancha, Instituto of Nanociencia, Nanotecnología y Materiales Moleculares (INAMOL), Campus de la Fábrica de Armas, Toledo, Spain. Tel: 34 9252 68843.

E-mail: fernando.langa@uclm.es

Organic solar cells (OSCs) based on solution-processed bulk heterojunction (BHJ) active layers have emerged as promising solutions for the conversion of solar energy into electrical energy in building and indoor applications due to their unique advantages, such as being lightweight and semitransparent and the possibility of being processed by low-cost roll-to-roll methods. The BHJ active layer employed for OSCs consists of a blend of an electron-donating material and an electron-accepting material creating internal donor-acceptor heterojunctions, and their optical and electrochemical properties are very important for the realization of a high-power conversion efficiency (PCE).

The optical and electrochemical properties of porphyrins can be adjusted by molecular design and functionalization on the b or meso positions of the porphyrin ring as well as by introduction of different central metal ions.

Although the pioneering use of porphyrins in OSCs was disappointing, as reported efficiencies were very low; the situation has changed over the last five years as Zn-porphyrins with ABAB structures linked to acceptor units, having relatively long-lived singlet excited states, have been successfully used as donors or acceptors, resulting in increased efficiencies.

In the other hand, diketopyrrolopyrrole (DPP), present excellent properties as strong electron acceptor capacity, small band gap, as well as high electronic mobility and low LUMO. Thus, DPP is an outstanding core for the preparation of non-fullerene acceptors.

In this talk, I´ll present our recent results on the design of new A−D−A or D-A-D small molecules based on porphyrins or DPP having broad absorption (up to 1000 nm) and affording, in some cases, voltage higher than 1V, reaching efficiencies close to 16%.

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Novel photo- and electro-active conjugates based on tetracyanobuta-1,3-diene and cyclopenta[*hi*]aceanthrylene

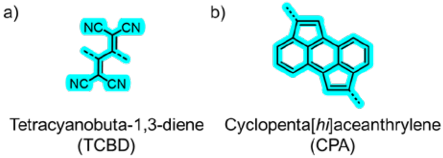
Giovanni Bottari[a], Luis M. Mateo, Alvaro Corrochano, Tomás Torres, Samara Medina Rivero, Juan Casado, Laura Calió, Hernán Míguez.

[a]*Universidad Autónoma de Madrid, IMDEA Nanociencia*

In this talk, I will start presenting some recent examples from our group on the preparation and study of novel photo- and electro-active conjugates based on tetracyanobuta-1,3-diene (TCBD) (Figure 1a) [1] and cyclopenta[*hi*]aceanthrylene (CPA) (Figure 1b),[2] two interesting molecular fragments with unique structural and electronic features.

Next, I will introduce some recent examples of TCBD- and CPA-based derivatives resulting from our collaboration with some members of MODE FOTOVOLTAICA.

Figure 1



Tetracyanobuta-1,3-diene (TCBD)

Cyclopenta[*hi*]aceanthrylene (CPA)

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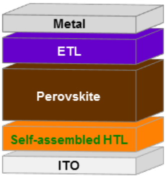
Perovskite solar cells with small molecule self-assembled hole transporting layers.

David Curiel

Multifunctional Molecular Materials Group, Department of Organic Chemistry, Faculty of Chemistry, Campus of Espinardo, University of Murcia, 30100 Murcia, Spain

Since the first reports about perovskite solar cells the remarkable improvement of their efficiency has turn these photovoltaic devices into a very promising technology. Part of the progress in the perovskite solar cells performance is associated to the development of interfacial layers that contribute to the selective charge extraction and transport, protection of the active layer and adjustment of the thin film morphology.[1,2]

Despite the large number of materials that have been assessed as hole and electron transporting layers, the use of self-assembled materials has barely been explored. Nevertheless, self-assembly processes could allow a better control of the molecular organization within the transport layers and subsequently of the morphology and charge transport properties.[3,4] Accordingly, polyheteroaromatic small molecules have been rationally designed to evaluate the effect of self-assembly when they are incorporated as dopant-free hole transporting layers (HTLs) and passivating layers in different type of perovskite solar cells with lead-based, hybrid lead-tin and triple cation perovskite active layers.



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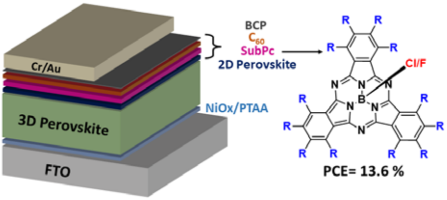
Subphthalocyanine-based electron-transport materials for perovskite solar cells

Jorge Labella[a], Cristina Momblona, Mohammad Khaja Nazeeruddin, Tomás Torres

[a]Universidad Autónoma de Madrid

Non-fullerene ETMs are emerging as a hot topic in the field of perovskite solar cells (PSCs). Herein, we evaluate the potential of subphthalocyanines (SubPcs) as ETMs in PSCs.[1,2] To this end, ETMs based on SubPcs with different axial and peripheral substituents have been incorporated in *p-i-n* PSCs, where the perovskite is deposited by either solution processing (CsFAMAPbIBr) or thermal evaporation (MAPI). The device performance, morphology, and stability of these devices are analyzed using several techniques, and the interfacial effects induced by the SubPcs are studied using PL and TR-PL.

Figure 1



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Effect of photoinduced electron transfer in π-extended macrocycles

G. George[a], A. J. Stasyuk[a], M. Solà[a]

[a] Institut de Química Computacional and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany, 69, 17003 Girona, Spain

Fullerene based inclusion complexes of cycloparaphenylenes (CPP) are promising candidate for the development of photovoltaic devices. Photophysical properties of CPPs can be tuned substantially by changing both the inner and outer subunits.[1] Du and co-workers recently reported the synthesis and photophysical properties for a series of π-extended crown-shaped macrocycles bearing conjugated segments of different sizes (Figure 1).[2,3,4] The photoinduced charge separation in these series of C_{60} fullerene encapsulated π-conjugated molecular crowns complexes has been studied in detail using the TD-DFT approach. In these inclusion complexes fast photoinduced electron transfer has been revealed. The charge-separated states with the electron transfer from the crown to the C_{60} unit can be efficiently populated through the decay of the locally excited states and occurs in sub-nanosecond time scale.

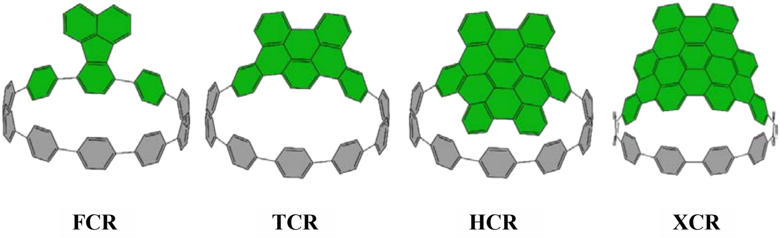

Figure 1. The series of π-conjugated molecular crowns.

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Electronic structure and photophysics of the BODIPY monomer and an orthogonal dimer

David Casanova

Donostia International Physics Center, DIPC; Manuel Lardizabal 4, 20018, Donostia, Euskadi, Spain
IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Euskadi, Spain

In this presentation I will describe and rationalize the electronic structure of BODIPY combining a variety of quantum chemistry methods and computational tools. Examination of the obtained results using state-of-the-art electronic structure analyses provides a new and complete interpretation of the nature of low-lying electronic states in BODIPY and elucidates the limitations of excited-state methods in the computation of T_1 and S_1 energies. Our analysis [1] identifies the important role and physical origin of the mild open-shell character in the BODIPY ground state, and provides guidelines for the accurate quantification of the T_1/S_1 gap, which is extremely relevant for the computational investigation of the photophysical properties of BODIPY and its derivatives.

These results will be used to investigate triplet state generation in an orthogonal BODIPY dimer by combining delayed photoemission techniques with electronic structure calculations [2]. Our analysis describes different competing deactivation channels beyond prompt radiative decay. In particular, we identify charge-transfer (CT) mediated intersystem crossing (ISC) as the most likely mechanism for the triplet state generation in this system. Interestingly, the dependence of the yield of triplet state population and emission profiles with the solvent polarity evidences the decisive role of the CT configuration in the fate of the photoactivated dimer, controlling the relative ISC, reverse ISC, and internal conversion efficiencies.

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Photo-crosslinked fullerene-based hole transport material for humidity-resistant perovskite solar cells

Andrea Cabrera-Espinoza, Juan Luis Delgado*

POLYMAT, University of the Basque Country UPV/EHU, Avda. Tolosa 72, Donostia - San Sebastián 20018, Spain.

Perovskite solar cells (PSCs) are recognized as one of the most promising technologies to convert solar energy into electricity. To date, PSCs have achieved a record power conversion efficiency (PCE) of 25.5%, surpassing the PCE of simple silicon-based solar cells (23.3%).1 In a PSC, the perovskite is sandwiched by the electron transport layer (ETL) and the hole transport layer (HTL), and these last two layers are in contact with the cathode and the anode, respectively. In the regular configuration, the hole transport material (HTM) is processed on top of the perovskite film, as shown in Figure 1.2

To reach high efficiencies with remarkable stability in a regular PSCs, the HTMs are critical in promoting the charge extraction and transport as well as protecting the perovskite layer.3 The most relevant HTMs involve triarylamine derivatives, such as poly(triarylamine) (PTAA) and 2,2′,7,7′-tetrakis-(N,N-di-p-methoxyphenylamine)-9,9′-spiro-bifluorene (Spiro-OMeTAD). These HTMs not only are expensive but also reveal low hole mobility and conductivity. Thus, dopants such as Li-TFSI, t-BP and FK209 should be incorporated to improve the electronic properties. However, these additives are highly hygroscopic and accelerate the degradation of the perovskite layer.4 Consequently, seeking for new dopant-free HTMs that provide stability to the solar cells is of vital importance in this field.

In a previous study, our group reported the first free-dopant fullerene-based HTM (FU7) with 12.5 ± 0.8% of efficiency, which is higher than the efficiency of the devices based on un-doped Spiro-OMeTAD (2.3 ± 0.9%).5 In this work, chains ended in allylic groups were introduced into the molecular structure of FU7 through the synthesis of F-T12. The allylic groups were subjected to in situ photo-crosslinking with pentaerythritol tetrakis(3-mercaptopropionate) (PETMT), generating a cross-linked conductive layer. This layer allowed to obtain devices with 15.10 ± 0.08% of PCE, value higher than devices made with un-crosslinked layer (13.2 ± 0.2%) and more importantly, the hydrophobic surface of crosslinked layer enhanced the stability under environmental conditions.

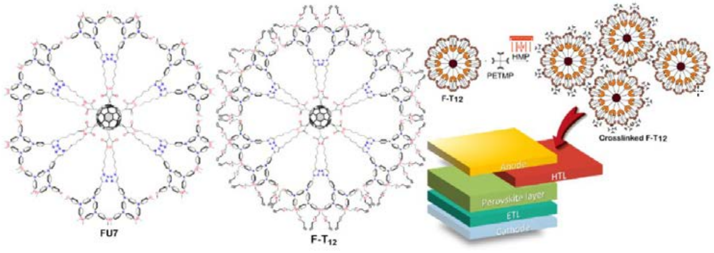

Figure 1. Molecular structure of **FU7** and **F-T$_{12}$**. Crosslinking reaction. Regular PCSs.

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Triplet-charge annihilation in a small molecule donor: acceptor blend as a major loss mechanism in organic photovoltaics

José Manuel Marín-Beloqui*,[a,b] Tracey M. Clarke*[b]
a) Department of Physical Chemistry, University of Málaga, 29071, Málaga, Spain.
b) Department of Chemistry, University College of London, WC1H 0AJ, London, United Kingdom

Organic photovoltaics (OPV) are close to reaching a landmark 20% device efficiency.[1] One of the proposed reasons that OPVs have yet to attain this milestone is their propensity toward triplet formation.

In this talk,[2] the small molecule donor, DRCN5T, is studied using a variety of spectroscopy techniques, and blended with both fullerene and non-fullerene acceptors. Specifically, picosecond and microsecond transient absorption and Raman spectroscopies are focused on. Despite DRCN5T's ability to achieve OPV efficiencies of over 10%,[3] it generates an unusually high population of triplets. These triplets are primarily formed in amorphous regions via back recombination from a charge transfer state. As such, triplets have a dual role in DRCN5T device efficiency suppression: they both hinder free charge carrier formation and annihilate those free charges that do form.

Using microsecond transient absorption spectroscopy under oxygen conditions, this triplet-charge annihilation (TCA) is directly observed as a general phenomenon in a variety of DRCN5T: fullerene and non-fullerene blends. Since TCA is usually inferred rather than directly observed, it is demonstrated that this technique is a reliable method to establish the presence of TCA.

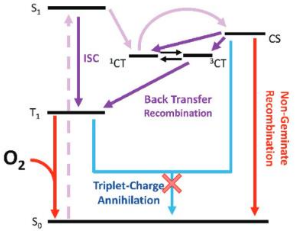

Figure 1. Summary of the processes occurring in DRCN5T blend systems under inert atmosphere (blue arrows) and under oxygen (red arrows and red cross). Purple arrows illustrate the processes that take place both under oxygen and inert atmospheres).

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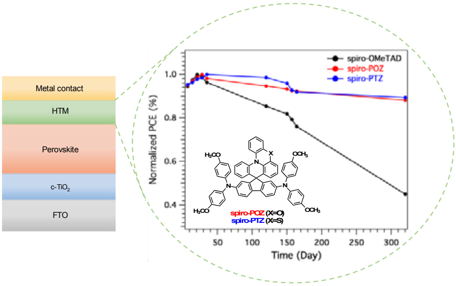
Improving the long-term stability of doped spiro-type hole-transporting materials in perovskite solar cells

J. Urieta-Mora[1,2], A. Molina-Ontoria[1], I. García-Benito, L. Illicachi,[2] J. Calbo,[4] J. Aragó[4], E. Ortí[4], M. K. *Nazeeruddin*[3], *N. Martín*[1,2]

1. Dpto. de Química Orgánica, Facultad de Química, Universidad Complutense, Madrid, Spain
2. IMDEA-Nanoscience, C/ Faraday, 9 28049, Madrid, Spain
3. École Polytechnique Fédérale de Lausanne, CH-1015 Sion, Switzerland
4. Instituto de Ciencia Molecular, Universidad de Valencia, Paterna, Spain

Perovskites solar cells (PSCs) have emerged, since 2009, as the most promising technology to replace silicon PV.[1] Outstanding results of PCE up to 25.7 % have been obtained using perovskites (eg. $MAPbI_3$) in just a few years of research.[2] The continuous improvement of the efficiency in PSCs has been achieved using commercially available spiro-OMeTAD as hole-transporting material (HTM). However, spiro-OMeTAD is an expensive material due to its difficult purification and multi-step synthesis which limits its future use in large-scale applications. Additionally, long-term stabilities have not been reached incorporating spiro-OMeTAD which is usually correlated with the use of hygroscopic p-dopants such as LiTFSi or FK-209. As a consequence, great efforts in the synthesis of alternative organic low-cost molecules for its application as HTMs have been reported in the recent years, including PAH-based, spiro-containing or dopant-free materials.[2] Our research group have recently reported two doped-HTMs based on electron-rich spiranic scaffolds, namely, 9H-quinolinophenoxazine (spiro-POZ) and 9H-quinolinophenothiazine (spiro-PTZ) which exhibit excellent solubility, optimal HOMO energy, and excellent thermal stability with glass transition temperatures higher than those measured for the reference material, spiro-OMeTAD.[3] The incorporation of both new HTMs into $[(FAPbI_3)_{0.87}(MAPbBr_3)_{0.13}]_{0.92}[CsPbI_3]_{0.08}$-based solar cells reached PCEs around 17% for mesoporous cells, and higher than 18% in planar configurations, matching the PCE of spiro-OMeTAD. Remarkably, doped spiro-POZ and spiro-PTZ exhibit excellent long-term stability in planar devices, retaining over 84% of their initial efficiency after more than 300 days of exposure to ambient conditions. Furthermore, after 1200 h under continuous 1 sun illumination, the PCE of the PSCs based on spiro-POZ and spiro-PTZ decreases by only 6% in sharp contrast to the poor performance of spiro-OMeTAD. Therefore, despite the doping conditions used for spiro-POZ and spiro-PTZ, excellent long-term PSC stabilities were achieved, making these materials to be among the most stable doped and dopant-free HTMs in PSCs.



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Quadruple-cation wide bandgap perovskite solar cells with enhanced thermal stability

Isidora Susic[a]

[a]*University of Valencia*

Metal halide perovskites have proven to be excellent semiconductors, with tuneable band gap, high absorption coefficients and large charge diffusion length. Multi-component lead halide perovskite compositions are widely studied in order to stabilize the perovskite phase, in particular for wide bandgap formulations. The vacuum-deposition of multi-component perovskites is not straightforward, as the number of precursors is in principle limited by the number of thermal sources available in the vacuum chamber. Here we present a process which allows to increase the complexity of the formulation of vacuum-deposited lead halide perovskites films by multi-source deposition and pre-mixing both inorganic and organic components. We apply it to the preparation of wide bandgap CsMAFA triple-cation perovskite solar cells, which are found to be efficient but not thermally stable. With the aim of stabilizing the perovskite phase, we add guanidinium (GA+) to the material formulation, and obtained CsMAFAGA quadruple-cation perovskite films with improved thermal stability, as observed by X-ray diffraction and rationalized by microstructural analysis. The corresponding solar cells showed similar performance with a remarkable thermal stability, when compared to the triple-cation perovskite devices. This work paves the way towards the vacuum-processing of complex perovskite formulations, with important implications not only for photovoltaics but also for other fields of application.

Dibenzofulvene-based molecules as hole extracting interlayer for perovskite solar cells

José G. Sánchez

Institut Catalá d'Investigació Quimica, Avda. Països Catalans, 16 43007 Tarragona, Spain

Solar photovoltaic energy (PV) has grown favorably in the last years. The advances in improving the efficiency of the different PV technologies encourage to investigate further enhancing PV devices. Among the different PV technologies, the perovskite solar cells (PSCs) are considered as a potential candidate for next-generation energy harvesting. PSCs are fabricated by a perovskite film sandwiched between two electrodes, an electron and a hole selective interlayers (ETL and HTL, respectively). Thus, the engineering of these interlayers plays an important role to obtain efficient devices.

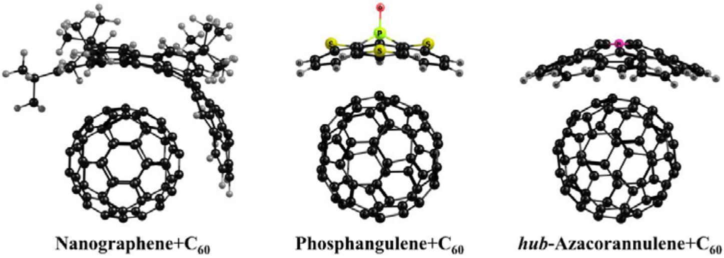
In this talk, I will show the development of dibenzofulvene-based (DBF) molecules as HTL for perovskite solar cells applications. I will also describe fabrication process of the photovoltaics devices, as well as the electrical and optical characterization. We discuss the effect of the different conjugated side chains of the DBF-based molecules on the performance of PSCs.

Molecular bowls as electron donors in photoinduced electron transfer reactions

A.J. Stasyuk,[a*] O.A. Stasyuk,[a] A.A. Voityuk[a] and M. Solà[a]

[a] The Institute of Computational Chemistry and Catalysis of the University of Girona,
C/ Maria Aurèlia Capmany 69, 17003, Girona, Catalonia, Spain

In recent decades, remarkable progress has been made in the field of organic synthesis. As a result, researchers have been able to synthesize compounds with complicated structures that could not be synthesized in the past, such as curved π-conjugated molecules.[1,2] In this work, we report the results of computational modeling and advanced analysis of the photoinduced processes in a series of C_{60} fullerene complexes with experimentally synthesized molecular bowls and curved nanographenes.[3-5] Our results demonstrate that introducing heteroatom (sulfur or nitrogen) into the bowl-shaped π-conjugated molecules and extending the π-conjugation can modulate their electron-transfer properties. Analysis of the ground and excited-state electronic properties of the complexes revealed that the propensity of a particular complex to photoinduced electron transfer (PET) is mainly determined by the electronic properties of the bowl. In most promising complexes, PET occurs in nano- to picosecond timescale.



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New modified Spiro-OMeTAD molecule used as self-assembled monolayer (SAM) for efficient inverted perovskite solar cells

Wenhui Li,[a] Maria Méndez,[a] Emilio Palomares*[ab]

[a] *Institute of Chemical Research of Catalonia (ICIQ-BIST), Avda. Països Catalans, 16, 43007 Tarragona, Spain.*
[b] *Catalan Institution for Research and Advanced Studies (ICREA), 08010 Barcelona, Spain.*

Organic hole selective materials are vital for high-performance perovskite solar cells. PTAA and Spiro-OMeTAD are two widely commercialized hole selective contacts (HSCs). In particular, PTAA shows high efficiencies in inverted perovskite solar cells (iPSCs), which are comparable with the record efficiencies of Spiro-OMeTAD in regular PSCs. However, using the low-cost Spiro-OMeTAD as HSC is meaningful for the cost-effective iPSCs compared to PTAA. This work modifies the commercial Spiro-OMeTAD by introducing carboxylic acid anchoring groups (Spiro-Acid) to form self-assembled monolayers (SAMs) as HSCs for iPSCs. We demonstrate the high-performance of Spiro-Acid based iPSCs with a power conversion efficiency (PCE) of 18.15%, which is comparable with PTAA based iPSCs, and with a remarkable stability under long-term illumination. Charge transfer and charge carrier dynamics are studied by using advanced characterization techniques to better understand the interfacial kinetics. Our results demonstrate that Spiro-Acid as HSCs has a great potential in low-cost, long-term stability and high performance iPSCs devices.

Electronic structure and aromaticity in excimer and excited multimers

Aitor Diaz-Andres[1], David Casanova[1,2]

[1]*Donostia International Physics Center, DIPC; Manuel Lardizabal 4, 20018, Donostia, Euskadi, Spain*

[2]*IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Euskadi, Spain*

In this presentation I will analyze the forces involved in the formation of the benzene excimer, its electron structure, and (anti)aromatic character [1]. Electronic wave functions are decomposed in terms of localized excitations and ion-pair configurations through diabatization, and we show that excimer (anti)aromaticity can be described as the linear combination of ground, excited, and ionic molecular states. Our analysis concludes that the benzene excimer must be characterized as antiaromatic, with weaker antiaromaticity than the molecular excited singlet. Moreover, we define a model electronic Hamiltonian for the excimer state and we use it as a building block for the extrapolation of electronic Hamiltonians in molecular aggregates. Benzene multimers present a nonuniform (anti)aromatic character, with the center of the column being antiaromatic and the edges behaving as aromatic. We also extend our study to the characterization of the triplet state benzene excimer and the benzene-tricyanobenzene exciplex. The implications of this work go beyond the study of the excimer, providing a general framework for the calculation and characterization of excited states in aggregates.

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Nano-photonic configurations to transform sunlight into other forms of energy

Carles Ros[1], Catarina Ferreira[1], Adrian Pinilla[1], Sidney Palardonio[1], Constanza Sansierra[1], Mingyu Zhang[1], Jordi Martorell[1,2]

[1]ICFO – Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain
[2]Departament de Física, Universitat Politècnica de Catalunya, 08222 Terrassa, Spain

70% of worldwide energy used today derives from fossil fuels. To change this, the production of fuels that are carbon neutral is viewed as the next step after solar energy consolidates as one of the most important sustainable energy sources on the planet.

Our research focuses in implementing light-management strategies for solar fuels production and energy harvesting and storage. 1D and 3D photonic structures are implemented to maximize the solar absorption and conversion for nanostructured metal oxide photoelectrodes in tandem with organic and perovskite solar cells. Photoelectrochemical (PEC) water splitting, CO_2 reduction and other novel strategies like hydrogen storage in the graphene basal plane are studied coupled by organic and inorganic cocatalysts.

In the ONPV group we consider several nano-photonic based approaches to obtain a broadband sunlight absorption for the most effective conversion of sunlight into storable chemical energy. Such approaches may consider, among others, $BiVO_4$, SnS_2 or other advanced photoelectrodes in tandem with non-fullerene transparent organic photovoltaic cells, a perovskite (PVK) solar cell, and a photonic nano-structuring for an optimally balanced and enhanced absorption.

Per molecule, hydrogen can store one of the largest amounts of chemical energy. This energy can be transformed into electricity in an environmentally clean procedure using a fuel cell. However, the challenge of storing such hydrogen in a small volume, as well as the lack of a hydrogen distribution infrastructure represent major drawbacks for a deployment of a hydrogen-based economy. In the ONPV research group we explore H atoms storage by chemically binding them to the carbon atoms of a 2-dimensional graphene like lattice, exploiting the safe and high hydrogen storage capacity provided by such graphene like structures. Particular emphasis is placed on the study of the dynamical evolution of the lattice morphology which is key to achieve a stable H storage as well as the reverse process of H desorption.

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C/ Faraday, 9
Ciudad Universitaria de Cantoblanco
28049 · Madrid (Spain)
www.nanociencia.imdea.org