

Palomares Research Group



Group Leader: Emilio Palomares

Postdoctoral researchers: Georgiana Stoica/ Lydia Cabau/ Núria Fernández/ Rajesh Pudi

PhD students: Ilario Gelmetti / Cristina Rodríguez/ Jesús Jiménez/Alba Matas/ José Manuel Marín/ Sofía Paulo/ Daniel Fernández

Laboratory technicians: Santi Gené/ Antonio Moncho/ Werther Cambarau

Visiting students: David Millán / Jesús Idígoras /Oscar Ruiz

Administrative support: Eva Busto

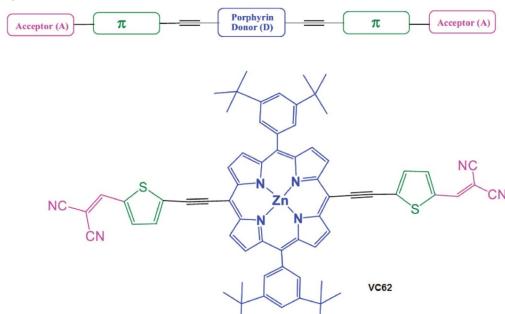
Abstract

The research on materials for energy and bio-applications are at the central core of our research. Since the group formation in 2006, our particular interest has been the development of third generation solar cells (DSSC, OPV, QDSC and Perovskite materials) and the detailed study of the interfacial

charge transfer reactions that limit the efficiency on these novel generation of solar cells.

On the other hand, we are devoted also to the development and study of novel fluorescence semiconductor materials for biomedical applications that advance on the application of nano-science to medicine.

During 2015 our group has focussed on the synthesis and characterization of organic semiconductor molecules that have been used as electron donor in solution processed organic solar cells using the fullerene derivative PCBM-C70 as electron acceptor moiety. **Scheme 1** illustrates the general A- π -Por- π -A of one of the different molecules families that we have synthesised.



Scheme 1: Zn-porphyrin (POR) as central core for efficient electron donor in bulk-heterojunction organic solar cells.

Moreover, we have continued our work on the application of dye sensitized solar cells to reach the 10% light-to-energy conversion target using our porphyrins as part of our deliverable list in our CRYMOSOL (CTQ-2013-47183R) project. **Figure 1.**

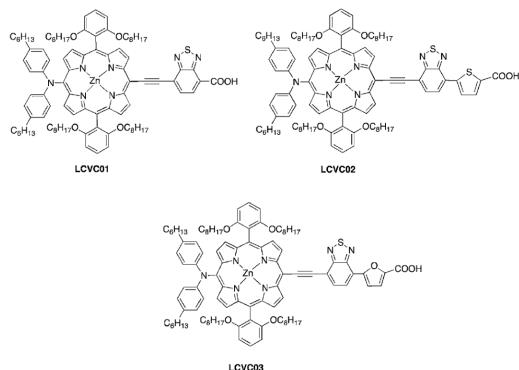


Figure 1. The set of asymmetric porphyrins synthetized as target molecules in CRYMOSOL. The LCVC02 achieved efficiencies over 10% at 1 sun.

Palomares group has also achieved within CRYMOSOL record efficiencies for methyl ammonium lead iodide (MAPI) perovskite solar cells. The MAPI, when processed either from

Articles

"Efficient bulk heterojunction solar cells based on solution processed small molecules based on the same benzo[1,2-b:4, 5-b']thiophene unit as core donor and different terminal units"

Nanoscale (2015), 7, 7692-7703

Vijay Kumar, C.; Cabau, L.; Koukaras, E. N.; Siddiqui, S. A.; Sharma, G. D.; Palomares, E.

solution leads to a solid with perovskite structure; for this reason these novel type of solar cells are known as perovskite solar cells.

The group has focused not only on making the most efficiency devices (14% under sun-simulated conditions of 100mW/cm²@ 1.5 AM G) but also to characterize for the first time the interfacial charge transfer recombination reactions that prevent the MAPI perovskite solar cell to reach its maximum theoretical efficiency of 25%. **Figure 2** illustrated several current vs voltage curves for MAPI perovskite solar cells and Al₂O₃ /m-TiO₂ modified MAPI solar cells.

JL-44-f35-1-reverse

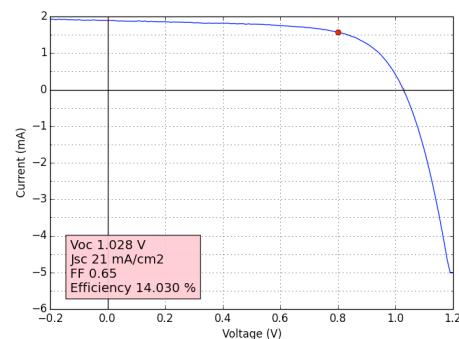


Figure 2. Current density vs voltage curve at 1 sun (100mW/cm²@ 1.5 AM G) and in the dark for a perovskite solar cell fabricated at ICIQ from solution processed methods.

Group Competitive Research Projects.

1. AGAUR-SGR-2014-763
2. MICINN CTQ-2013-47183R
3. EU-ERC-POC (2NanoSi)
4. SGR-project-207 2009

Group Industrial Research Projects.

1. HYPRINT-Torrejad
2. Perovskite materials. EURECAT.

"Synthesis, optical and electrochemical properties of the A- π -D- π -A porphyrin and its application as an electron donor in efficient solution processed bulk heterojunction solar cells"

Nanoscale (**2015**), 7, 179-189

Vijay Kumar, C.; Cabau, L.; Koukaras, E. N.; Sharma, G. D.; Palomares, E.

"Atomic species identification at the (101) anatase surface by simultaneous scanning tunnelling and atomic force microscopy"

Nat. Commun. (**2015**), 6, 7265

Stetsovych, O.; Todorovic, M.; Shimizu, T. K.; Moreno, C.; Ryan, J. W.; Leon, C. P.; Sagisaka, K.; Palomares, E.; Matolin, V.; Fujita, D.; Perez, R.; Custance, O.

"Optoelectronic Studies of Methylammonium Lead Iodide Perovskite Solar Cells with Mesoporous TiO₂: Separation of Electronic and Chemical Charge Storage, Understanding Two Recombination Lifetimes, and the Evolution of Band Offsets during J-V Hysteresis"

J. Am. Chem. Soc. (**2015**), 137, 5087-5099

O'Regan, B. C.; Barnes, P. R. F.; Li, X.; Law, C.; Palomares, E.; Marin-Beloqui, J. M.

"High photocurrent in oligo-thienylenevinylene-based small molecule solar cells with 4.9% solar-to-electrical energy conversion"

J. Mater. Chem. A (**2015**), 3, 11340-11348

Montcada, N. F.; Dominguez, R.; Pelado, B.; Cruz, P. d. I.; Palomares, E.; Viterisi, A.; Langa, F.

"Indoline as electron donor unit in "Push-Pull" organic small molecules for solution processed organic solar cells: Effect of the molecular π -bridge on device efficiency"

Org. Electron. (**2015**), 20, 15-23

Montcada, N. F.; Cabau, L.; Kumar, C. V.; Cambarau, W.; Palomares, E.

"The influence of the mesoporous TiO₂ scaffold on the performance of methyl ammonium lead iodide (MAPI) perovskite solar cells: charge injection, charge recombination and solar cell efficiency relationship"

J. Mater. Chem. A (**2015**), 3, 22154-22161

Matas Adams, A.; Marin-Beloqui, J. M.; Stoica, G.; Palomares, E.

"Influence of the Molecular Weight and Size Dispersion of the Electroluminescent Polymer on the Performance of Air-Stable Hybrid Light-Emitting Diodes. ACS Appl. Mater."

Interfaces (**2015**), 7, 1078-1086.

Martinez-Ferrero, E.; Grigorian, S.; Ryan, J. W.; Cambarau, W.; Palomares, E.

"Solvent Annealing Control of Bulk Heterojunction Organic Solar Cells with 6.6% Efficiency Based on a Benzodithiophene Donor Core and Dicyano Acceptor Units"

J. Phys. Chem. C (**2015**), 119, 20871-20879

Kumar, C. V.; Cabau, L.; Viterisi, A.; Biswas, S.; Sharma, G. D.; Palomares, E.

"Solution processed organic solar cells based on A-D-D'-D-A small molecule with benzo[1,2-b:4,5-b']dithiophene donor (D') unit, cyclopentadithiophene donor (D) and ethylrhodanine acceptor unit having 6% light to energy conversion efficiency"

J. Mater. Chem. A (**2015**), 3, 4892-4902

Kumar, C. V.; Cabau, L.; Koukaras, E. N.; Viterisi, A.; Sharma, G. D.; Palomares, E.

"Efficient solution processed D1-A-D2-A-D1 small molecules bulk heterojunction solar cells based on alkoxy triphenylamine and benzo[1,2-b:4,5-b']thiophene units"

Org. Electron. (**2015**), 26, 36-47

Kumar, C. V.; Cabau, L.; Koukaras, E. N.; Sharma, G. D.; Palomares, E.

"A- π -D- π -A based porphyrin for solution processed small molecule bulk heterojunction solar cells"

J. Mater. Chem. A (**2015**), 3, 16287-16301

Kumar, C. V.; Cabau, L.; Koukaras, E. N.; Sharma, A.; Sharma, G. D.; Palomares, E.

2015 Annual Scientific Report

"Metal-free organic sensitizers with narrow absorption in the visible for solar cells exceeding 10% efficiency"

Energy Environ. Sci. (2015), 8, 2010-2018

Joly, D.; Pelleja, L.; Narbey, S.; Oswald, F.; Meyer, T.; Kervella, Y.; Maldivi, P.; Clifford, J. N.; Palomares, E.; Demadrille, R.

"H₂ generation and sulfide to sulfoxide oxidation with H₂O and sunlight with a model photoelectrosynthesis cell"

Coord. Chem. Rev. (2015), 304-305, 202-208

Farras, P.; Di Giovanni, C.; Clifford, J. N.; Palomares, E.; Llobet, A.

"Increased short circuit current in an azafullerene-based organic solar cell"

Chem. Commun. (Cambridge, U. K.) (2015), 51, 1128-1130

Cambarau, W.; Fritze, U. F.; Viterisi, A.; Palomares, E.; von Delius, M.

"A single atom change "switches-on" the solar-to-energy conversion efficiency of Zn-porphyrin based dye sensitized solar cells to 10.5%"

Energy Environ. Sci. (2015), 8, 1368-1375

Cabau, L.; Vijay Kumar, C.; Moncho, A.; Clifford, J. N.; Lopez, N.; Palomares, E.

"Diaryl amino-substituted tetraarylethene (TAE) as an efficient and robust hole transport material for 11% methyl ammonium lead iodide perovskite solar cells"

Chem. Commun. (Cambridge, U. K.) (2015), 51, 13980-13982

Cabau, L.; Garcia-Benito, I.; Molina-Ontoria, A.; Montcada, N. F.; Martin, N.; Vidal-Ferran, A.; Palomares, E.

"Design, fabrication and charge recombination analysis of an interdigitated heterojunction nanomorphology in P3HT/PC70BM solar cells"

Nanoscale (2015), 7, 13848-13859.

Balderrama, V. S.; Albero, J.; Granero, P.; Ferre-Borrull, J.; Pallares, J.; Palomares, E.; Marsal, L. F.