Research Institute of Advanced Materials

Biannual report 2016 - 2017

Understanding and creating materials for a better future

inam
Institute of Advanced Materials
UJI Castelló

UNIVERSITAT JAUME I

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Contents

1. Introduction

The Research Institute of Advanced Materials at the University Jaume I (Institute of Advanced Materials, INAM) is a centre of interdisciplinary science and technology in the fields of physics, chemistry, and related fareas, applied to advanced materials, with vocation towards the progress of the socioeconomic environment and scientific excellence with international influence and impact.

Our vision is *Achieving a world class research center on the understanding and creation of materials, bringing scientific insight and producing advanced applications for a better future.*

To reach this goal we work on physical chemical understanding of advanced materials properties and operation, from molecules and interfaces to bulk compounds, connecting matter and light, to create new knowledge that bridges the gap between materials and devices. We pave the role for new functional materials that generate applications in clean energy supply and storage, lighting, and the creation of chemicals of high added value.

The Institute was formally created by Generalitat Valenciana on May, 4th 2015. This report presents the structure and results of the Institute in the first biennial period 2016-2017. We summarize the main scientific areas, the planning of activities and resources, and the main results in terms of publications, the scientific impact at the international level, and outreach activities.

Juan Bisquert
Director

2. Human resources and governance

The scientific and technological activities at INAM are organized by separate Research Divisions (RD), each one headed by experienced group leader (Principal Investigator, PI) with recognized scientific careers of great international impact. Interdisciplinary collaboration among researchers from different areas provides the ability to address novel research areas, thus allowing the emergence of innovative ideas and high-impact discoveries. Currently INAM is organized into 9 RD as follows

Research Division	Staff	Postdoc	Predoc-toral	Starting researcher	Admin	Total
Administration					2	2
Prof. Juan Bisquert	2	2	1			7
Prof. Eduardo Peris	1	1	4			6
Prof. Germà Garcia-Belmonte	2		2			4
Dr. Francisco Fabregat-Santiago	1		3			4
Dr. Jose Mata	1	1	1	2		5
Dr. Ivan Mora-Seró	1	1	3			5
Dr. Beatriz Julián	1		2	1		4
Dr. Sixto Giménez	1	1	1	2		5
Dr. Macarena Poyatos	1	1	2			4
Total	11	6	19	5	2	44

RD Bisquert includes Senior Researchers: Eva Barea, Antonio Guerrero and Elena Mas

The management of the Institute is established by a General Assembly that includes all members (according to membership rules established in the bylaws). The Governing Board is formed by the following members of the Institute

Director: Juan Bisquert
Deputy Director: Eduardo Peris
Secretary: Germà Garcia Belmonte

The Governing Board is assisted in routine decisions by a smaller assembly formed by all the Principal Investigators at the Institute denoted the *Junta Permanent*.

The directions of research at INAM are established by 4 years plans that indicate the purpose and direction of research objectives for the period. The activities of the Institute are evaluated from the perspective of the quadrennial plan by the Scientific Advisory Board of the INAM, that is the regular organ for control and advise of the scientific activities of the Institute. The composition of the Advisory Board at present is

Prof. Miquel A. Pericàs, Director, Institute of Chemical Research of Catalonia, Tarragona, Spain

James Durrant, Professor of Photochemistry, Imperial College, London, UK

Thuc-Quyen Nguyen, Professor of Chemistry and Biochemistry, University of California, Santa Barbara, CA, USA

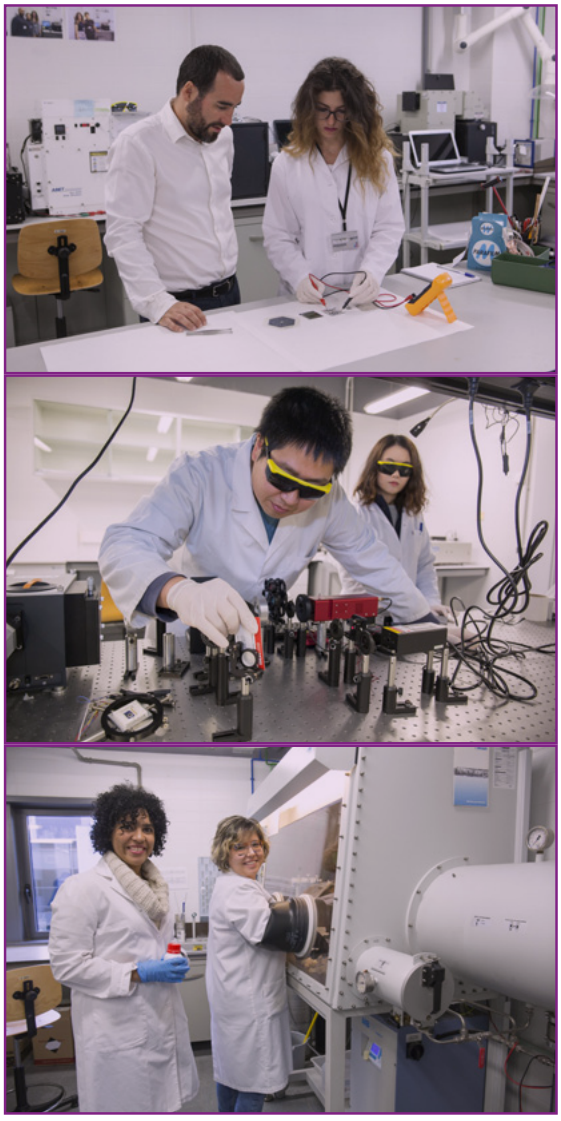
Prof. Luis A. Oro, Instituto de Síntesis Química y Catálisis Homogénea, Dep. Inorganic Chemistry, University of Zaragoza-CSIC, Zaragoza, Spain.

3. Research objectives

The general scientific aim of INAM is focused on the development of scientific research lines based on Advanced Materials for three main areas:

-energy,
-optoelectronics, and
-catalysis.

Currently the scientific activities are organized by the guidelines of the strategic plan of INAM for 2016-2019, that includes the following lines of action.



Thematic lines of research

A1. Advanced materials for energy conversion
A2. Advanced materials for catalysis
A3. Advanced materials for light emission
A4. Advanced materials for energy storage
A5. Advanced materials for sensors
A6. Other topics.

The first three areas account for the vast majority of research activities of the teams, along the following lines

- **Advanced materials for energy conversion** focuses on the development of materials for photovoltaic conversion in which the absorbed light is transformed into electricity or chemical fuel efficiently. The use of organic and inorganic materials will be studied and hybrids beyond the materials present in the current photovoltaic market in order to reduce costs and improve efficiencies. Special attention to the physical processes that allow this energy conversion will be paid as the special properties of each family of materials affect this conversion.

- **Advanced materials for catalysis:** This line includes activities related to the synthesis and characterization of molecular and solid materials with catalytic applications, for the production of organic molecules with high added value. This research front fulfills the requirements for the chemical industry from waste products or from raw chemical without any value.

- **Advanced materials for light emission** includes the study of materials with luminescent properties, both photoluminescence and electroluminescence. A special interest in

the light emission is to tune over a wide range of wavelengths from ultraviolet to infrared, visible through all be provided. The combination of materials for white light emission will also be studied.

In addition, there are also interesting related studies of materials and devices in the topics A4 and A5. For example, the pioneering implementation of hybrid perovskites as battery cathodes, which were the first papers on this topic worldwide:

Vicente, N.; Garcia-Belmonte, G. Methylammonium Lead Bromide Perovskite Battery Anodes Reversibly Host High Li-Ion Concentrations. Journal of Physical Chemistry Letters, 2017, 8, 1371-1374.

This is an important example of innovative multidisciplinary research results obtained uniquely at INAM.

The physics areas are mainly devoted to topics A1 and A3, while chemistry areas develop most activity in A2.

Regarding the methods and techniques, the present strategic plan includes the following lines of activities:

Advanced research methods and tools

B1. New methods of synthesis and preparation of advanced materials and molecules

B2. Models and simulation of materials and devices.

B3. Design and optimization of interfaces, morphologies, nanostructures.

B4. Structural characterization of materials, interfaces and devices.

B5. Optoelectronic characterization of materials, interfaces and devices.

B6. Other developments.

- **New methods of synthesis and preparation of advanced materials and molecules.** One of the main activities of the institute is the preparation of materials using original synthesis or deposition methods, in the form of molecules, thin films and others.

- **Models and simulation of materials and devices.** Studies will be carried out from first principles to establish the physical properties of materials and interfaces. Moreover, modeling and simulation of processes involved in the function of the devices will be addressed: optical absorption, freight, cargo transfer, electrochemical reactions, etc.

- **Design and optimization of interfaces, morphologies, nanostructures** consists of the combination and morphologies of materials that can lead to the desired functionality. Study encompasses deposition methods and compatibility, contact formation, the study of load transfer interfaces, forming porous structures to increase the specific area, the functionalization and / or nanostructures sensitivization.

- **Structural characterization of materials, interfaces and devices** will allow a complete structural

characterization of materials and interfaces. This characterization allows us to relate the parameters of these processes with the methods of synthesis. Includes the extensive application of microscopies.

- **Optoelectronic characterization of materials, interfaces and devices** will develop a complete electrical, optical and physical-chemical characterization of materials and devices. This characterization is twofold, to understand the physico-chemical, photonic and electronic processes occurring in materials and devices.

4. Summary of scientific results

Research highlights

- Impact of the research of INAM members may be summarized by the fact that in the 2013-2017 period INAM accumulated 4500 citations.
- This is a significant proportion (30%) of the total citations of our University Jaume I. UJI is the first University in Chemistry classifications by normalized impact and excellence in Spain (CYD 2016 report).
- The extraordinary impact of INAM research can be gauged by production in this period of more than 300 papers in journals indexed in the Clarivate Web of Science.
- In the period 2016-2017 100 papers were published and 30% of them were high quality papers in journals with impact factor larger than 9.
- An outstanding proportion larger than 10% of these papers were qualified as Highly Cited Papers. This classification includes just 1% of most cited papers are included in this category.
- Owing to the high impact of our work, researcher Juan Bisquert became **Highly Cited Researcher 2014, 2015, 2016 and 2017** in Clarivate Web of Science list. This list identifies 3000 authors ranking among the top 1% most cited for their subject field between 2002 and 2012.
- In 2016 and 2017 researcher Ivan Mora Seró has been also elected to this list due to major work on quantum dot and perovskite solar cells.
- Iván Mora Seró has achieved the ERC Consolidator Grant (2017).
- These achievements have been a key step for Universitat Jaume I to enter the prestigious University ranking of Shangai, thanks to a total of 3 Highly Cited scientists in the University.
- Eduardo Peris is among the 25 most-cited Spanish researchers in the field of Chemistry.
- Peris is the President of the Organometallic Chemistry Division from the RSEQ, which holds more than 600 members, thus being the strongest division in the Spanish Chemistry Community.

Journal Impact Factor	Nº publications 2016-2017	Percentage
>9	33	31
[3..9]	55	52
<3	18	17
Total	106	100

Publications by journal impact factor

A. Thematic lines of research	Nº publications 2016-2017	Percentage
A1. Advanced materials for energy conversion	68	64
A2. Advanced materials for catalysis	18	17
A3. Advanced materials for light emission	7	7
A4. Advanced materials for energy storage	4	4
A5. Advanced materials for sensors	9	8
Total	106	100

Publications per research line

B. Advanced research methods and tools	Nº publications 2016-2017	Percentage
B1. New methods of synthesis and preparation of advanced materials and molecules	33	31
B2. Models and simulation of materials and devices	7	7
B3. Design and optimization of interfaces, morphologies, nanostructures	31	29
B4. Structural-compositional characterization of materials, interfaces and devices	6	6
B5. Optoelectronic characterization of materials, interfaces and devices	27	25
B6. Other developments	2	2
Total	106	100

Publications per methods line

Research Division	Nº publications 2016-2017	Percentage*
Prof. Juan Bisquert	53	50
Prof. Eduardo Peris	16	15
Prof. Germà Garcia-Belmonte	20	19
Dr. Francisco Fabregat-Santiago	13	12
Dr. Jose Mata	6	6
Dr. Ivan Mora-Seró	21	20
Dr. Beatriz Julián	5	5
Dr. Sixto Giménez	9	8
Dr. Macarena Poyatos	8	8
Total	151	142

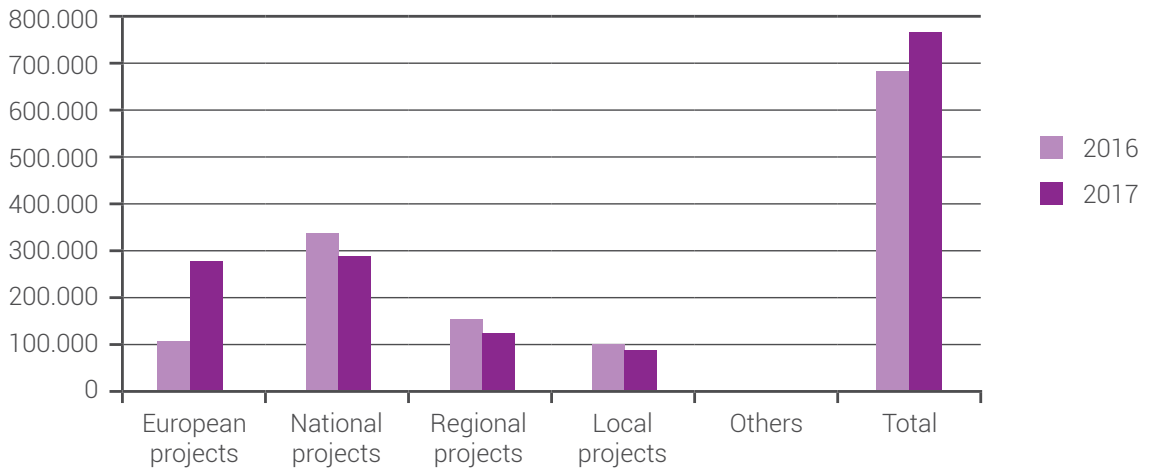
Publications per research division

*includes shared papers

5. Financial Report

	2016	2017
European projects	103.845	272.196
National projects	327.235	280.540
Regional projects	150.900	120.400
Local projects	89.634	83.752
Others		
Total	**671.614**	**756.888**

Distribution of funding by sources



6. Interaction with socioeconomic environment

Activity	2016	2017
Primary/Secondary school training day	3	3
Conference and workshop for non-specialists audience	1	3
Information in newspapers and newsletter magazines	0	4
Open doors day	2	0
Total	6	10

Outreach activities

Sample of outreach activities

- 2016 Members from INAM developed a school-kit to for practical work in introductory aspects related to electricity and solar energy. Concepts such voltage, current, energy, power, solar cells energy production and consumption are treated in a practical, fun and accessible manner. The kit which is portable and allows 8 groups of students working at the same time. During academicyear 15/16, the Kit was used at

- CEIP BernatArtola, Castelló (two 2-hour lab sessions) for 6th year primary school students. Press new:
- CEIP El Pinar, Grau de Castello (two 2-hour lab sessions) for 6th year primary school students
- IES VallD'alba, VallD'alba(Castelló), (four 2-hour lab sessions) for 2nd year secondary School students.

-2016 INAM Open doors day for companies. Organize USE, UJI, Program: Programa de visites a la UJI 25 aniversari. Participants: Torrecid, Al-Farben, BECSA, Ferro Spain, Fundació Dávalos-Fletcher.

-2016 INAM Open doors day for primary school students. Organize INAM, Physics Department, UJI. Participants: CEIP Bernat Artola.

- 2017. As a member of the expert committee of the Príncipe Felipe Science Museum, Professor Eduardo Peris organized a series of scientific outreach workshops at the Valencia Science Museum. This initiative brought the science held at the Universitat Jaume I to more than 200 students from secondary schools in the Region of Valencia.

- 2017 Professor Macarena Poyatos was highlighted in the magazine 'Talento' of Castellón, as one of the most relevant and influential scientists in the province of Castellón.

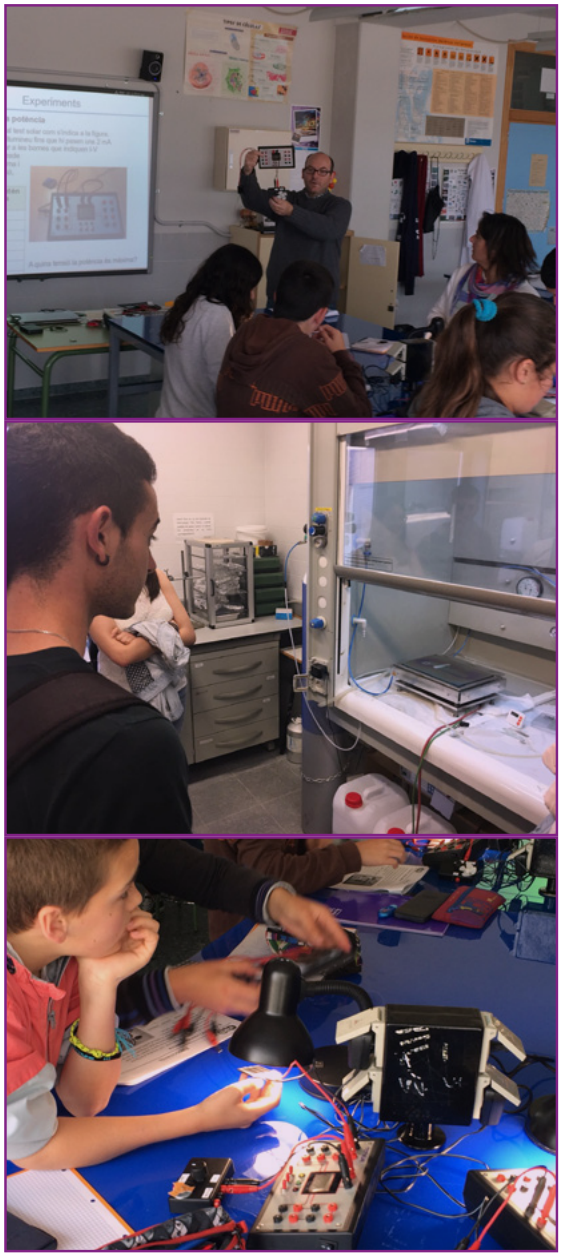
- 2017 Jornadas 17CA77IN010 - Ciencias, tecnología y arte: STEM+. Organizers CEFIRE, Servicio Formación del profesorado Generalitat Valenciana. Contribution: "Herramientas para la enseñanza de conceptos de electricidad y de energia"

-2017 FirUjiCiencia. Activity Type: Fair of workshops for students from kinder garden to secondary schools. Organizers: UJI and CEFIRE. Contribution: "Energia solar"

2017 Conference by Juan Bisquert "Energías renovables del futuro: fotovoltaica y fuel solar" at Ciudad de las Artes y de las Ciencias de Valencia in the cycle of conferences "Una Comunitat amb ciència".

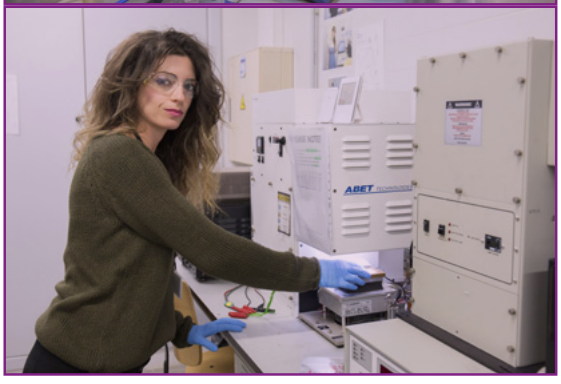
2017 Ivan Mora Seró conference in Valencia, El Mundo de los Nanomateriales" in the cycle of conferences Fundació Valenciana d'Estudis Avançats "

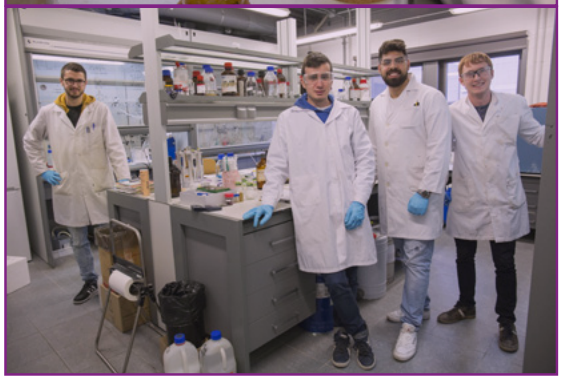
2017 Researchers at INAM Juan Bisquert, Francisco Fabregat and Sixyo Gimenz, in cooperation with the Department of Phycis, organize the Course of preparation for the Physics Olimpics, were about 40 students from secondary school get introduced to physics and problema solving.



7. Gender Balance

	Men	Women	Total
Staff	7	4	11
Postdoctoral	4	2	6
Predoctoral	11	8	19
Starting Research	2	3	5
Admin		2	2
Total	**24**	**19**	**43**





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9. Publications-Books

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Bisquert, J. Nanostructured Energy Devices: Foundations of Carrier Transport, CRC Press, 2017

Bisquert, J. The Physics of Solar Cells – Perovskites, Organics, and Fundamentals of Photovoltaics, CRC Press, 2017

10. Publications-Book chapters

Bisquert, J.; Garcia-Belmonte, G.; Mora-Sero, I. "Characterization of Capacitance, Transport and Recombination Parameters in Hybrid Perovskite and Organic Solar Cells". In *Unconventional Thin Film Photovoltaics*, Como, E. D., Angelis, F. D., Snaith, H., Walker, A., Eds.; Royal Society of Chemistry, 2016.

Bisquert, J.; Garcia-Belmonte, G.; Guerrero, A. "Impedance Characteristics of Hybrid Organometal Halide Perovskite Solar Cells." In *Organic-Inorganic Halide Perovskite Photovoltaics: From Fundamentals to Device Architectures*; Park, N.-G., Grätzel, M., Miyasaka, T., Eds.; Springer, 2016.

Fabregat-Santiago, F, Barea, E. M., Giménez, S. Bisquert, J. Impedance Spectroscopy in Molecular Devices in *Molecular Devices for Solar Energy Conversion and Storage*, Tian, Haining, Boschloo, Gerrit, Hagfeldt, Anders Eds., Springer, 2017, pp. 353-384.

11. Research Projects

International funding

Title: No-Limit - Boosting Photovoltaic Performance By The Synergistic Interaction Of Halide Perovskites And Semiconductor Quantum Dots
Acronym of the project: NO LIMIT
Funding entity: ERC- European Research Council
Modality: ERC consolidator
Entity code: ERC-2016-COG/ERC-2016-COG-724424
Principal researchers: Iván Mora-Seró
Dates: 2017-2022
Total amount: 2.000.000 €

Title: An Artificial Leaf: a photo-electro-catalytic cell from earth-abundant materials for sustainable solar production of CO2-based chemicals and fuels
Acronym of the project: ALEAF
Funding entity: European Commission
Modality: Collaborative project H2020-FETPROACT
Entity code: 732840
Principal researchers: Juan Bisquert, Sixto Giménez
Dates: 2017-2020
Total amount: 443.770 €

Title: Making Perovskites Truly Exploitable
Acronym of the project: MAESTRO
Funding entity: European Union
Modality: European Training Networks (MSCA-ITN-ETN)
Entity code: 764787
Principal researchers: Francisco Fabregat-Santiago
Dates: 2017-2021
Total amount: 3.852.446,00 €

Title: Internew - Innovate Interfaces for Energy-Related Applications
Acronym of the project: INTERNEW
Funding entity: European Union
Modality: ITN: Marie Curie initial training networks
Entity code: 5341/2012
Principal researchers: Iván Mora-Seró
Dates: 2014-2017
Total amount: 109.200,00 €

National projects

Title: Perovskitafotovoltaicas de alto rendimento
Acronym of the project: PEREST
Funding entity: Ministerio de Economía y Competitividad
Modality: Programa Estatal de I+D+i Orientada a los Retos de la Sociedad
Entity code: MAT2016-76892-C3-1-R
Principal researchers: Juan Bisquert, Germà Garcia-Belmonte
Dates: 2016-2019
Total amount: 200.000 €

Title: RYC Antonio Guerrero
Acronym of the project:RYC-2014-16809
Funding entity: Ministerio de Economía y Competitividad
Modality: Ramon y Cajal
Entity code: RYC-2014-16809
Principal researchers: Antonio Guerrero
Dates: 2015-2020
Total amount: 40.000 €

Title: Ayudas Juan de la Cierva-Incorporación
Acronym of theproject: JdC
Fundingentity: Ministerio de Economía y Competitividad
Modality: Formación Del Subprograma Estatal de Incorporación del Programa Estatal de Promoción Del Talento y Su Empleabilidad.
Entity code: IJCI-2015-23407
Principal researchers: Eduardo Peris
Dates: 2017-2019
Total amount: 64.000 €

Title: Catalytic applications of organometallic complexes immobilized on the surface of graphenes.
Acronym of the project: GRAPHCAT
Funding entity: Ministerio de Economía y Competitividad
Modality: Programa Estatal de I+D+I Orientada a losRetos de la Sociedad
Entity code: CTQ2015-69153-C2-2-R
Principal researchers: Jose Mata
Dates: 2016-2018
Total amount: 55.000,00€

Title: Ligandos Poliaromáticos Para El Diseño De Catalizadores Mejorados
Acronym of theproject: POLCAT
Fundingentity: Ministerio de Economía y Competitividad
Modality: Convocatoria De Ayudas Correspondientes Al Programa Estatal Fomento De La Investigación Científica Y Técnica De Excelencia
Entitycode: CTQ2014-51999-P
Principal researchers: Eduardo Peris, Macarena Poyatos
Dates: 2015-2017
Total amount: 138.000,00€

Title: Perovskitas para células solares tandem y caracterización optoelectrónica de los dispositivos tamdem
Acronym of theproject: NASCENT
Fundingentity: Ministerio de Economía y Competitividad
Modality: Programa Estatal de I+D+i Orientada a los Retos de la Sociedad
Entitycode: ENE2014-56237-C4-3-R
Principal researchers: Francisco Fabregat-Santiago, Elena Mas Marzá
Dates: 2015- 2017
Total amount: 174.240 €

Title: Tecnologías Fotovoltaicas Emergentes
Acronym of theproject: TFE
Fundingentity: Ministerio de Economía y Competitividad
Modality: Ayuda Estatal Fomento de la Excelencia
Principal researchers: Juan Bisquert
Dates: 2015-2017
Total amount: 30.000,00€

Title: Ramón y Cajal
Acronym of theproject: RYC Elena Más Marzá
Fundingentity: Ministerio de Economía y Competitividad
Modality: Ramon y Cajal
Entitycode: RYC-2011-07726 Elena Más Marzá
Principal researchers: Elena Mas Marzá
Dates: 2013-2017
Total amount: 125.644 €

Title: Desarrollo de emisores de luz policristalinos de bajo coste basados en perovskitas de haluro híbridas
Acronym of theproject: MAT2015-70611-ERC
Fundingentity: Ministerio de Economía y Competitividad
Modality: Ayuda Estatal Fomento de la Excelencia
Entitycode: MAT2015-70611-ERC
Principal researchers: Iván Mora-Seró
Dates: 2015-2016
Total amount: 60.000,00€

Title: Desarrollo de dispositivos orgánico-inorgánico de bajo coste con perovskitas para conversión de energía solar
Acronym of theproject: PESOL
Fundingentity: Ministerio de Economía y Competitividad
Modality: Convocatoria de ayudas 2013 del programa estatal de I+D+I orientada a los retos de la sociedad
Entitycode: MAT2013-47912-C3-1-R
Principal researchers: Juan Bisquert, Iván Mora-Seró
Dates: 2014-2016
Total amount: 271.138,78€

Title: Design of multifunctional materials based on graphene-metal complexes: applications in energy conversion and storage
Acronym of the project: AICO/GRAPH
Funding entity: GeneralitatValenciana
Modality: Solicitud de ayudas para grupos de investigaciónconsolidables AICO/2015
Entity code: AICO/2015/039
Principal researchers: Jose Mata
Dates: 2015-2016
Total amount: 40.000,00€

Title: Desarrollo integral de celulas solares mesoscopicas con semiconductores orgánicos e inorgánicos (disolar)
Acronym of theproject: PROMETEO-2009-058
Fundingentity: Generalitat Valenciana
Modality: Convocatoria de diferentes tipos de becas y ayudas para el fomento de la investigación cientifica y el desarrollo tecnológico de la C. Valenciana
Entitycode: PROMETEO/2009/058
Principal researchers: Juan Bisquert
Dates: 2009-2013
Total amount: 319.300 €

Regional projects

Title: Desarrollo integral de células solares mesoscópicas y producción de combustible solar (DISOLAR 2)
Acronym of theproject: PROMETEO DISOLARII
Fundingentity: Generalitat Valenciana
Modality: Programa Prometeo
Entitycode: PROMETEOII/2014/020
Principal researchers: Juan Bisquert
Dates: 2014-2017
Total amount: 223.270 €

Local projects from UJI

Title: Soluciones Inteligentes para la energia eléctrica basadas en dispositivos de celulas solares de perovskitas
Acronym of the project: SOLENPE
Fundingentity: Universitat Jaume I. UJI
Modality: Pla de Promoció de la Investigació UJI
Entitycode: UJI-B2016-05
Principal researchers: Eva Mª Barea
Dates: 2016-2019
Total amount: 30.000 €

Title: Development of hybrid nanomaterials based on graphene@organometallic complexes: Catalytic applications at the edge of homogeneous/heterogeneous processes.
Acronym of the project: GRAPH@ORG
Funding entity: UJI
Modality: Pla Propi d'Investigació UJI - Modalitat B) Grups consolidats investigador individuals
Principal researchers: Jose Mata
Dates: 2016-2018
Total amount: 20.000,00 €

Title: Desarrollo de ligandos poliaromáticos para la obtención de catalizadores con propiedades mejoradas
Acronym of theproject: CATAL
Funding entity: Universitat Jaume I. UJI
Modality: PLA PROPI INVESTIGACIÓ
Entity code: P11B2014-02
Principal researchers: Eduardo Peris
Dates: 2015-2017
Total amount: 40.000,00€

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