

excellence  
as our technological key

imdea materials institute

annual report

2015

[www.materials.imdea.org](http://www.materials.imdea.org)

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**imdea**  
materials

f o r e w o r d

# foreword



**Javier Llorca**

Director, IMDEA Materials Institute

March 2017

annual report  
2016

Materials Science and Engineering has been at the root of new technological developments because they are always supported by a material substrate. Thus, materials research is sometimes driven by applications and sometimes by the materials themselves. In the latter case, research lines run parallel to the different families of materials: metals, polymers, ceramics and, more recently, biomaterials, composites as well as nanomaterials. During the first ten years, IMDEA Materials Institute has developed an expertise in the processing, characterisation and modelling of these types of materials, which was then applied –in collaboration with our industrial partners– to different sectors in the areas of transport, information technology and manufacturing, as well as in the exploration of emerging materials and processes for sustainable development. However, the Institute is aware of the societal challenges that lay ahead in the fields of energy and health care and has decided to attract expertise in these two fields in the following years. Two new research lines were opened during 2016 in electrochemistry and in solar energy harvesting and luminescence to widen the activities of IMDEA Materials Institute in energy. Together with the current activities in the development of structural materials for energy harvesting and storage –supported by the European Research Council–, IMDEA Materials is now ready to develop new materials designed to support the energy challenges of the society.

While the research output of an academic institution is usually measured by the quality and impact of the publications, patents and industrial applications of the knowledge developed, funding –particularly in competitive calls– is also a measure of success. It provides the means to carry out the research and indicates the capability of the Institute to articulate credible research goals that go beyond the state of the art. Since the beginning of its activities in 2007, IMDEA Materials Institute has been able to attract over 26 millions of euros from external funding sources. 50% of the funding was obtained from competitive calls of the European Union while 23% came from research contracts with industrial companies. In particular, IMDEA Materials Institute has been very successful in the highly competitive calls of the pillar of excellence (European Research Council, Marie-Slodowska Curie actions, etc.) of the Horizon 2020 program with 5.7 million euros in research grants during the period 2014-2016.

The outcome of the research activities performed during 2016 is summarized in the following pages. The personnel, current research projects, research infrastructures as well as dissemination activities (publications, conferences and seminars, patents, theses, etc.) can be found in this annual report together with a few scientific highlights on advanced materials for multifunctional applications, additive manufacturing, and the development of an open source library of material models.

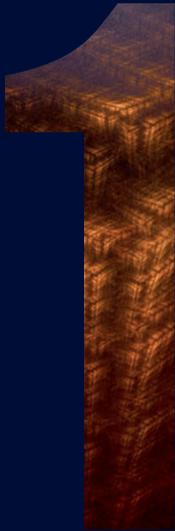
t a b l e o f  
c o n t e n t s

# table of contents

annual report  
2016

1. Introduction [6]
2. Research [11]
3. People [23]
4. Research Infrastructure [45]
5. Current Research Projects [60]
6. Dissemination of Results [86]
7. Scientific Highlights [115]

# i n t r o d u c t i o n



- 1.1. **About IMDEA Materials Institute [7]**
- 1.2. **Organizational chart [8]**
- 1.3. **Appointments to the Board of Trustees and Scientific Council [8]**
- 1.4. **Governing bodies [9]**
  - 1.4.1. Members of the Board of Trustees [9]
  - 1.4.2. Members of the Scientific Council [10]

annual report  
2016

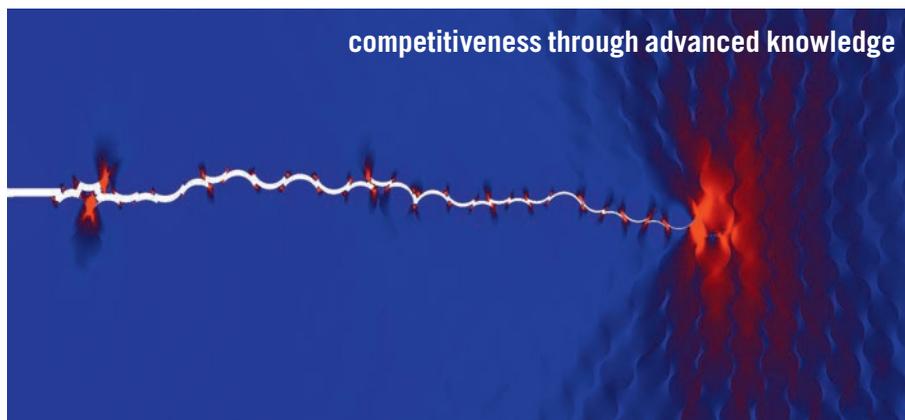
## 1.1. About IMDEA Materials Institute

The IMDEA Materials Institute (Madrid Institute for Advanced Studies of Materials) is a non-profit independent research organization promoted by the Madrid regional government (Comunidad de Madrid) to perform research in Materials Science and Engineering. IMDEA Materials Institute belongs to the Madrid Institute for Advanced Studies network, an institutional framework created in 2007 to **foster social and economic growth in the region of Madrid by promoting excellence in research and technology transfer to industry** in a number of strategic areas (water, food, energy, materials, nanoscience, networks and software).

IMDEA Materials Institute is committed to three main goals: **excellence in Materials Science and Engineering research, technology transfer to industry to increase competitiveness and maintain technological leadership**, and **attraction of talented researchers from all over the world** to work in Madrid in an international and interdisciplinary environment.

IMDEA Materials Institute has built an international reputation in the areas of **design, processing, characterisation and modelling of advanced materials** for applications in different industrial sectors with particular emphasis in transport, energy and manufacturing. The core strength of the Institute is its international research team, consisting of talented researchers from 14 different nationalities, that carry out new scientific discoveries in materials science, and foster the development of emerging technologies.

The IMDEA Materials Institute combines **oriented fundamental research with applied research** addressing the scientific and technological challenges that drive innovation in Materials Science and Engineering. This combination provides the institute the ability to address technological challenges in collaboration with companies to **create value in their products and processes through novel knowledge** that will be transformed into **technological innovations**.



## 1.2. Organizational chart

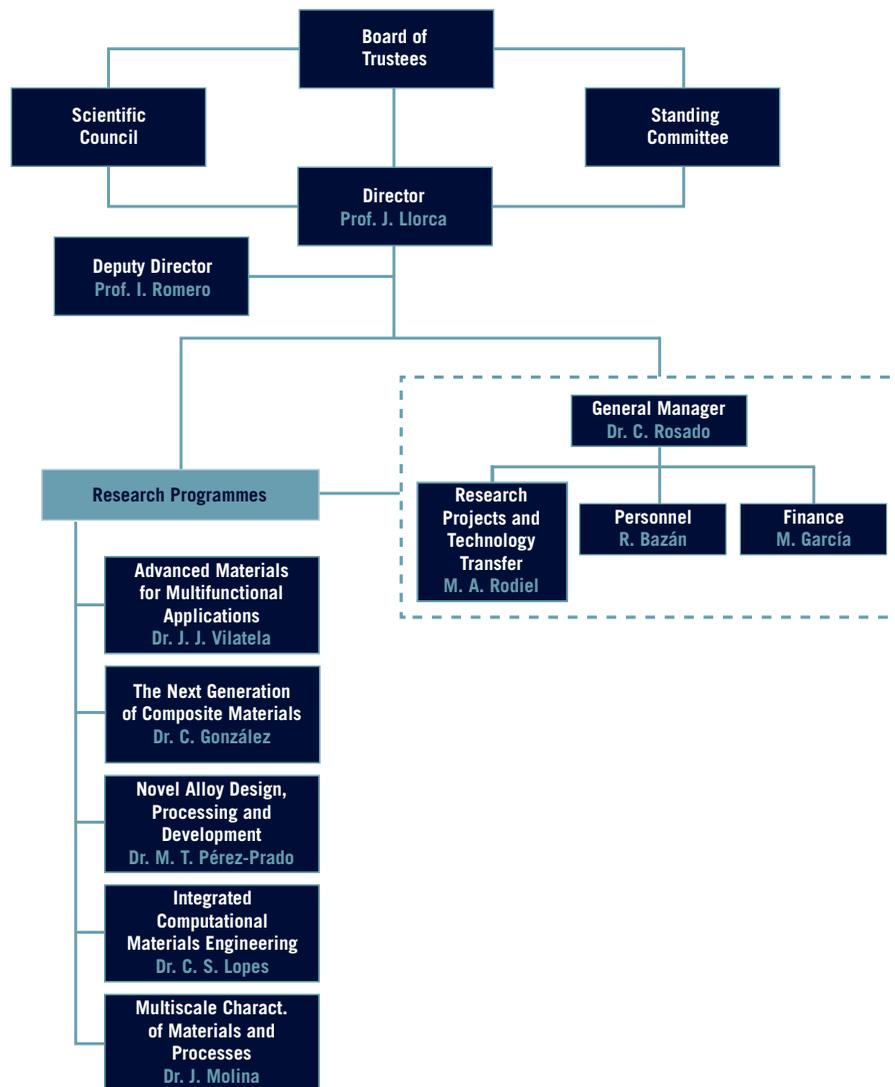


Figure 1. Organizational chart of IMDEA Materials Institute.

## 1.3. Appointments to the Board of Trustees and Scientific Council

Prof. Manuel Doblaré, Scientific Director, has resigned as trustee in representation of Abengoa Research S.L.

Prof. Andrew I. Cooper, Director of the Materials Innovation Factory, University of Liverpool, has been appointed to the Scientific Council.

The current members of the Board of Trustees and of the Scientific Council of the Institute are listed in the Governing Bodies section.



## 1.4. Governing bodies

### 1.4.1. Members of the Board of Trustees

#### CHAIRMAN OF THE FOUNDATION

---

**Prof. Juan Manuel Rojo**

*Emmeritus Professor  
Complutense University of Madrid,  
Spain*

#### VICE-CHAIRMAN OF THE FOUNDATION

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**Excmo. Sr. D. Rafael van Grieken  
Salvador**

*Counsellor of Education, Youth and  
Sports  
Madrid Regional Government*

#### PERMANENT TRUSTEES (REGIONAL GOVERNMENT)

---

**Excmo. Sr. D. Rafael van Grieken  
Salvador**

*Counsellor of Education, Youth and  
Sports  
Madrid Regional Government*

**Ilmo. Sr. D. José Manuel Torralba  
Castelló**

*General Director for Universities and  
Research  
Madrid Regional Government*

**Dr. Rafael A. García Muñoz**

*Deputy General Director for  
Research  
Madrid Regional Government*

**Mr. José de la Sota Rius**

*Coordinator of the Area of Reseach,  
Development and Innovation  
Fundación para el Conocimiento  
(Madri+d)*

#### UNIVERSITIES AND PUBLIC RESEARCH INSTITUTIONS

---

**Prof. Antonio Hernando**

*Professor  
Complutense University of Madrid,  
Spain*

**Prof. Manuel Ocaña**

*Professor  
Materials Science Institute of  
Seville (CSIC), Spain*

**Prof. Manuel Laso**

*Professor  
Technical University of Madrid,  
Spain*

**Prof. Francisco Javier Prieto**

*Vice-President for Research  
Carlos III University of Madrid,  
Spain*

#### SCIENTIFIC TRUSTEES

---

**Prof. Peter Gumbsch**

*Director, Fraunhofer Institute for  
Mechanics of Materials  
Professor University of Karlsruhe,  
Germany*

**Prof. Andreas Mortensen**

*Vice-provost for Research  
Professor  
Ecole Federale Polytechnique of  
Lausanne, Switzerland*

**Prof. Trevor William Clyne**

*Professor  
Cambridge University, UK*

**Prof. Dierk Raabe**

*Director, Max-Planck Institute for  
Iron Research  
Professor  
RWTH Aachen University, Germany*

**Prof. Juan Manuel Rojo**

*Emmeritus Professor  
Complutense University of Madrid,  
Spain*

#### EXPERT TRUSTEES

---

**Mr. Pedro Escudero**

*Managing Director  
European Value Advisors*

#### COMPANIES TRUSTEES

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**AIRBUS OPERATIONS S.L.**

*Dr. José Sánchez Gómez. Head of  
Composite Materials  
Getafe, Madrid, Spain*

**ABENGOA RESEARCH S.L.**

*Seville, Spain*

**GRUPO ANTOLIN S.A.**

*Mr. Javier Villacampa, Corporate  
Innovation Director  
Burgos, Spain*

**INDUSTRIA DE**

**TURBOPROPULSORES S.A.**

*Dr. José Ignacio Ulizar. Director of  
Technology  
San Fernando de Henares, Madrid,  
Spain*

#### SECRETARY

---

**Mr. Alejandro Blázquez**

## 1.4.2. Members of the Scientific Council

### **Prof. John E. Allison**

*Professor  
University of Michigan, USA*

### **Prof. Brian Cantor**

*Vice-chancellor  
University of Bradford, UK*

### **Prof. Trevor W. Clyne**

*Professor  
Cambridge University, UK*

### **Prof. Dr. Andrew I. Cooper**

*Director, Materials Innovation Factory  
Professor  
University of Liverpool, UK*

### **Prof. William A. Curtin**

*Director, Institute of Mechanical  
Engineering  
Professor  
Ecole Federale Polytechnique of  
Lausanne, Switzerland*

### **Prof. Peter Gumbsch**

*Director, Fraunhofer Institute for  
Mechanics of Materials  
Professor  
University of Karlsruhe, Germany*

### **Prof. Yiu-Wing Mai**

*Director, Centre for Advanced Materials  
Technology  
Professor  
University of Sydney, Australia*

### **Prof. Andreas Mortensen**

*Vice-provost for Research  
Professor  
École Fédérale Polytechnique of  
Lausanne, Switzerland*

### **Prof. Pedro Muñoz-Esquer**

*Independent consultant*

### **Prof. Eugenio Oñate**

*Director, International Centre for  
Numerical Methods in Engineering  
Professor  
Polytechnic University of Catalonia,  
Spain*

### **Prof. Dr. Dierk Raabe**

*Director, Max-Planck Institute for Iron  
Research  
Professor  
RWTH Aachen University, Germany*

### **Prof. Juan Manuel Rojo**

*Emmeritus Professor  
Complutense University of Madrid, Spain*

### **Prof. Mauricio Terrones**

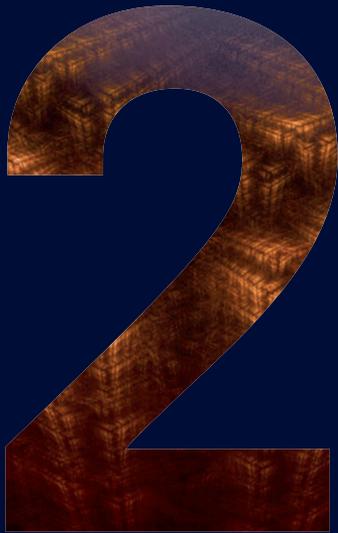
*Professor  
The Pennsylvania State University, USA*

### **Prof. John R. Willis**

*Professor  
Cambridge University, UK*



# r e s e a r c h



## 2.1. Research Programmes [12]

- 2.1.1. Advanced Materials for Multifunctional Applications [13]
- 2.1.2. The Next Generation of Composite Materials [15]
- 2.1.3. Novel Alloy Design, Processing and Development [17]
- 2.1.4. Integrated Computational Materials Engineering [19]
- 2.1.5. Multiscale Characterisation of Materials and Processes [21]

annual report  
2016

## 2.1. Research Programmes

The research activities of IMDEA Materials Institute are organised in five research programmes devoted to:

- Advanced materials for multifunctional applications
- The next generation of composite materials
- Alloy design, processing and development
- Integrated computational materials engineering
- Multiscale characterisation of materials and processes

These programmes are focused on the development of advanced materials mainly in the sectors of transport, energy and manufacturing as well as on the exploration of emerging materials and processes for sustainable development.

Each research programme combines the expertise of different research groups (processing, characterisation and simulation) leading to a multidisciplinary effort to achieve results beyond the state-of-the-art. Moreover, knowledge transfer between different research programmes is promoted by the fact that different research groups are often involved in two or more programmes.

Driven by the talent of the researchers, research programmes combine cutting-edge fundamental oriented research in topics at the frontiers of knowledge with applied research encompassing the midterm interest of our industrial partners to provide long-term technological leadership.



Figure 2. Research programmes and strategic partners of IMDEA Materials Institute



## Advanced Materials for Multifunctional Applications

The Programme on *Advanced Materials for Multifunctional Applications* at IMDEA Materials Institute combines expertise in design and synthesis of nano and molecular building blocks and their integration into macroscopic materials and devices. The guiding objective is to simultaneously realise various functions, including fire safety, high-performance mechanical properties and efficient energy management, amongst other properties. 34 researchers in the programme combine expertise spanning from *in silico* molecular design to fabrication of large energy storing devices. The following are the main research lines of the programme:

- **Synthesis, emerging technologies and integration of carbon-based nanomaterials (graphene, nanotubes, nanofibres and hybrids):**
  - Nanomaterials integration towards devices and energy managing devices: synthesis of nanocarbon/semiconductor hybrids for photo and electrocatalysis, interaction of nanocarbons with liquid molecules, polyelectrolytes and inorganic salts.
  - Sensors: chemical, piezoresistive, piezoelectric.
  - Hierarchical materials: materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity.
  - Size effects in the mechanical behaviour of multifunctional materials: study of structure-property relations in macroscopic ensembles of nanobuilding blocks, and development of mechanical models for hierarchical materials and their interfaces.
- **Synthesis and properties of polymer-based multifunctional nanocomposites:**
  - Sustainable materials: bio-based nanocarriers, novel guest-host nanomaterials, nano-cross linkers, functional dye-sensitized solar cells, multifunctional polymer nanocomposites, etc.
  - Fire retardant materials through nanodesign: multifunctional nanomaterials to increase fire retardancy: layered double hydroxides, sepiolite, molybdenum disulphide ( $\text{MoS}_2$ ), nanocarbon, nano metal hydroxide, novel functional nanomaterials, nanocoatings, etc.
- **Computational and data-driven Materials Discovery**
  - Discovery of porous materials for energy applications ( $\text{CO}_2$  capture, methane storage).
  - Design of ionic liquids.
  - Characterisation of nanoparticles and others.

- **Electrochemical Energy storage**

- Tailored designing of nanostructured electrode materials, interfaces and electrolyte compositions.
- Spectroscopic/microscopic studies and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O<sub>2</sub>.

[Link to relevant research projects](#)



**Research groups involved:**



**Multifunctional Nanocomposites**

Dr. J. J. Vilatela  
*Programme leader*



**High Performance Polymer Nanocomposites**

Dr. D.-Y. Wang



**Computational and Data-Driven Materials Discovery**

Dr. M. Haranczyk



**Electrochemical Energy Storage, Nanomaterials**

Dr. V. Etacheri



**Nano-architectures and Materials Design**

Dr. R. Guzmán de Villoria



## The Next Generation of Composite Materials



The *The Next Generation of Composite Materials* Programme aims at developing solutions for high performance structural composites with enhanced multifunctional capabilities such as thermal, electrical and fire resistance. The programme is focused on key aspects of material science and engineering including manufacturing, optimisation of material performance (damage tolerance and impact resistance), material characterisation at different length scales (nanoindentation, X-ray tomography) and development of modelling tools for both virtual processing and virtual testing. Manufacturing of composites by injection/infusion/pultrusion or prepreg consolidation is assisted by advanced sensors that support the use of smart manufacturing techniques toward process optimisation. Multiscale physically-based simulation tools are envisaged to predict the mechanical performance of structural composites as a function of their structure allowing a significant reduction of costly experimental campaigns. The main research lines of the programme are shown below.

- **Processing of high performance composites:**
  - Optimisation of out-of-autoclave processing (injection/infusion/pultrusion or prepreg consolidation) and other manufacturing strategies (semicured products). Hot-forming. Non-conventional curing strategies.
  - Smart manufacturing processes based on advanced simulations and sensors.
- **Recycling and repair of structural composites:**
  - Green (recyclable) epoxies. Electric current-assisted curing for bondings and repairs. Effect of ageing on composite performance.
- **New frontiers of structural performance:**
  - High temperature properties. Behaviour under impact. Self-healing, self-sensing and smart materials, Composites with non-conventional lay-up configuration.
- **Composites with multifunctional capabilities:**
  - Fire resistance. Electrical and thermal conductivity. Energy management. Sensing. Barrier properties. Non-destructive evaluation and health monitoring.

- **Micromechanics of composites:**
  - In situ measurement of matrix, fibre and interface properties. Micromechanical-based failure criteria. Computational-design of composites with optimised properties (non circular fibres, thin plies, novel fibre architectures, etc.)
- **Virtual testing of composites:**
  - Multiscale strategies for design and optimisation of composite materials and structures. Behaviour of composite materials and structures under high velocity impact (ice, metallic fragment or blade). Crash-worthiness and failure of composite structures. Effects of defects.
- **Virtual processing of composites:**
  - Smart manufacturing. Multiphysics models of autoclave and out-of-autoclave curing. Porosity nucleation and growth during curing.

[Link to relevant research projects](#)



**Research groups involved:**



**Structural Composites**  
Dr. C. González  
*Programme leader*



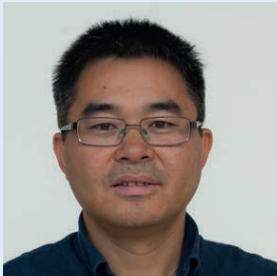
**Design & Simulation of Composite Structures**  
Dr. C. López



**Multifunctional Nanocomposites**  
Dr. J. J. Vilatela



**Nano-architectures and Materials Design**  
Dr. R. Guzmán de Villoria



**High Performance Polymer Nanocomposites**  
Dr. D.-Y. Wang



**Nanomechanics**  
Dr. J. M. Molina-Aldareguía



**X-ray Characterisation of Materials**  
Dr. F. Sket



the power of talent



## Novel Alloy Design, Processing and Development

The programme, integrated by experts in physical simulation, solidification and casting, physical metallurgy, solid state processing and computational materials engineering, aims to explore the processing-structure-property relationships in bulk metals, with special emphasis on the role of microstructure on plasticity at all length scales. This interdisciplinary pool of researchers is formed by physicists, chemists, and engineers (materials, mechanical and aeronautical) carrying out fundamental research and also working in close collaboration with companies in the transport, aerospace, energy and biomedical sectors. Research facilities include state-of-the-art equipment for processing at a lab scale (casting, wrought processing, Gleeble technology, atomization), microstructural characterisation (electron microscopy, X-ray diffraction, nanotomography) and mechanical property testing at a wide range of temperatures and strain rates. The main research lines of the programme are listed below.

- **Metallic alloys for high temperature structural applications:**
  - Ni/Co-based superalloys for aeroengine components: NiAl and TiAl based alloys for the next generation of turbine blades. FeAl alloys for steam turbines.
- **Lightweight (Mg, Al, Ti) alloys and their composites:**
  - Development of advanced medical implants from pure Ti. The next generation electrical conductors from Al alloys. Mg alloys and nanocomposites for green transport.
- **High strength steels:**
  - Development of novel thermo-mechanical processing routes for the fabrication of quenched and partitioned steels with superior mechanical properties. Analysis of processing-microstructure-properties relationship on macro- and microscales with emphasis on their strength, ductility, fatigue and fracture resistance.
- **Solid state processing:**
  - Development of new alloys by thermo-mechanical approaches and by powder manufacturing via mechanical alloying and gas atomization in non-oxidation conditions. Consolidation by field-assisted sintering and conventional press and sintering.
  - Design of metallic powders for additive manufacturing.

- **Solidification and Casting:**
  - Optimisation of casting processes and solidification-microstructure relationships using traditional (vacuum induction melting, vacuum arc melting, gravity and tilt casting, directional solidification) and advanced techniques (centrifugal and suction casting, vacuum melt atomization).
- **Physical simulation of metallurgical processes:**
  - Development of novel thermo-mechanical processing routes for the fabrication of metallic materials with superior properties. Design and optimisation of metallurgical processes (rolling, forging, extrusion, welding, casting, etc.)
- **High throughput screening of materials:**
  - Rapid screening of phases, crystal structures, properties, microstructure and kinetics in bulk materials by the Kinetic Diffusion Multiple Technique. Manufacturing of bulk materials libraries for the fast assessment of mechanical properties.

[Link to relevant research projects](#)



**Research groups involved:**



**Physical Metallurgy**  
Dr. T. Pérez-Prado  
*Programme leader*



**Solid State Processing**  
Dr. A. García-Junceda



**Solidification Processing and Engineering**  
S. Milenkovic



**Physical Simulation**  
Dr. I. Sabirov



**Multiscale Materials Modelling**  
Dr. J. Segurado



**Computational Alloy Design**  
Dr. Y. Cui



**X-ray characterisation of materials**  
Dr. F. Sket



**Mechanics of Materials**  
Prof. J. LLorca

- **Model-based materials design:**
  - Integration of modelling tools (atomistic, computational thermodynamics and kinetics, phase field) to simulate the microstructural development of materials during processing.
- **Simulation of the mechanical behaviour:**
  - Development and calibration of microstructural-based constitutive models to predict the mechanical behaviour of single crystals and polycrystals. Implementation of the constitutive models in finite element codes to simulate the mechanical behaviour of structural components.



## Integrated Computational Materials Engineering

The research program on Integrated Computational Materials Engineering (ICME) is aimed at integrating all the available simulation tools into multiscale modelling strategies capable of simulating processing, microstructure, properties and performance of engineering materials, so new materials can be designed, tested and optimized before they are actually manufactured in the laboratory. The focus of the program is on materials engineering, i.e. understanding how the microstructure of materials develops during processing (virtual processing), the relationship between microstructure and properties (virtual testing) and how to optimize materials for a given application (virtual design). Moreover, experiments are also an integral part of the research program for the calibration and validation of the models at different length and time scales.

The expertise of the researchers in the program covers a wide range of simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum) and is supported by a high performance computer cluster.

The following are the main ICME research lines at IMDEA Materials Institute.

- **Virtual materials design, including virtual processing and virtual testing:**
  - Light (Al, Mg and Ti) metallic alloys and their composites. Ni-based superalloys. Multifunctional composite materials and structures. Materials for energy generation and storage.

- **Materials modelling at different length and time scales:**
  - First principles calculations. Molecular mechanics and molecular dynamics. Dislocation dynamics. Object and lattice Kinetic Monte Carlo. Computational thermodynamics and kinetics. Phase field. Numerical methods for solids (finite elements and other approximations for solid mechanics). Computational micro-mechanics. Computational mechanics. Material informatics for analysis of large material datasets. Data-driven materials design.
  
- **Multiscale materials modelling:**
  - Bottom-up approaches (scale bridging). Development of modular multi-scale tools. High throughput screening integration. Concurrent models. Homogenization theory. Modelling and simulation of multiscale transport phenomena (application to advanced materials for batteries).

[Link to relevant research projects](#)



**Research groups involved:**



**Design & Simulation  
of Composite Structures**  
Dr. C. Lópes  
*Programme Leader*



**Mechanics of Materials**  
Prof. J. LLorca



**Multiscale Materials  
Modelling**  
Dr. J. Segurado



**Computational Alloy Design**  
Dr. Y. Cui



**Computational Solid  
Mechanics**  
Prof. I. Romero



**Computational and Data-  
Driven Materials Discovery**  
Dr. M.j Haranczyk

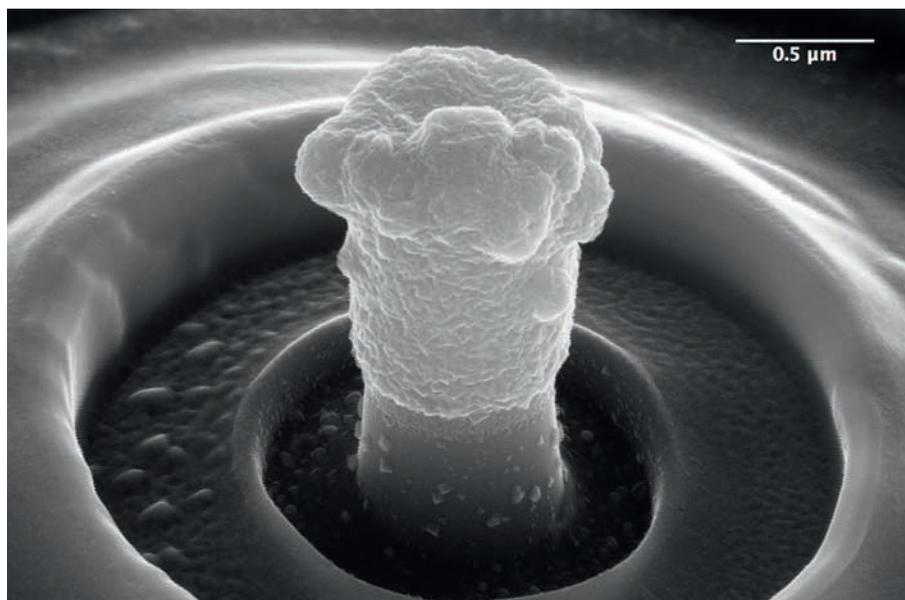


## Multiscale Characterisation of Materials and Processes



Progress in the development of new materials and processing methods can only come from a thorough understanding of microstructure evolution, either during processing or during service operation. Since the microstructural features that determine the material behaviour usually span several length scales (for instance, from the macroscopic defect distribution to the nanometer scale precipitates in the case of metallic alloys), this understanding can only come from advanced 4D characterisation techniques, capable of determining the evolution of the 3-dimensional microstructure over time at different length scales (hence the name 4D). This is precisely the objective of this programme, i.e., to understand microstructure/defect evolution in advanced materials during processing and service using advanced characterisation techniques, such as:

- **3D Characterisation of materials**, including microstructural, chemical and crystallographic information across several scales:
  - X-ray tomography and diffraction.
  - Scanning electron microscopy and focus ion beam, including 3D energy-dispersive X-ray microanalysis and electron back-scatter diffraction.
  - Transmission electron microscopy, including 3D energy-dispersive X-ray microanalysis and tomography.
  - Multiscale correlative tomography studies, i.e. tomography across multiple scales by combining insights from different techniques.



- **In-situ characterisation of processes across multiple scales (4D characterisation):**
  - Mechanical testing across several length scales: tension, compression, fatigue, creep, etc in the scanning electron microscope and X-ray tomography scanner. Properties and deformation mechanisms of small volumes by nanomechanical testing in the scanning and transmission electron microscopes: properties of metallic phases, interfaces, nanoparticles, carbon based nanomaterials (carbon nanotubes, graphene, ...).
  - Elevated temperature nanomechanical testing.
  - 4D characterisation of forming processes by X-ray tomography: Infiltration and resin flow in composites. Solidification of metallic alloys.
- **Cross-correlation between experiments and multiscale simulations** (molecular dynamics, dislocation dynamics, crystal plasticity, finite elements, ...).

[Link to relevant research projects](#)



**Research groups involved:**



**Nanomechanics**  
Dr. J. M. Molina-Aldareguía  
*Programme Leader*



**X-Ray Characterization of Materials**  
Dr. F. Sket



**Multifunctional Nanocomposites**  
Dr. J. J. Vilatela



**Structural Composites**  
Dr. C. González



**Physical Metallurgy**  
Dr. T. Pérez-Prado



**Multiscale Materials Modelling**  
Dr. J. Segurado



**Mechanics of Materials**  
Prof. J. LLorca

people

3

- 3.1. Senior Researchers [24]
- 3.2. Researchers [29]
- 3.3. Visiting Scientists [30]
- 3.4. Postdoctoral Research Associates [31]
- 3.5. Research Assistants [36]
- 3.6. Laboratory Technicians [42]
- 3.7. General Management [43]
- 3.8. International Project Office [44]

annual report  
2016

IMDEA Materials Institute is committed to attract talented researchers from all over the world to Madrid to work in an international and interdisciplinary environment. The Institute currently consists of 16 staff researchers, 3 visiting researchers, 29 post-doctoral researchers and 59 doctoral students from 14 different nationalities plus approximately 20 master students. It should be noted that 40% of the researchers are foreign nationals while 50% of the PhD were granted by foreign universities. This international team with multidisciplinary expertise is contributing to establish IMDEA Materials Institute as an international reference in Materials Science and Engineering. The researchers are supported by eight Laboratory Technicians and the Management and Administrative staff, including an international Project Office.

IMDEA Materials Institute endorsed in 2007 the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers that set out the rules and obligations of researchers, their employers and funders, as well as transparent and fair recruitment procedures. The Institute received the 'Human Resources Excellence in Research' award from the European Commission in 2015.

# senior researchers



**Prof. Javier Llorca**  
Director, Mechanics  
of Materials

Ph.D. in Materials Science from Technical University of Madrid, Spain

Professor of Materials Science, Technical University of Madrid

#### Research Interests

Development of novel multiscale simulation strategies to carry out virtual design, virtual processing and virtual testing of engineering materials for structural applications; experimental characterisation techniques to measure the mechanical properties of materials under extreme conditions at microscopic and macroscopic levels; analysis of the relationship between microstructure and mechanical properties in advanced structural materials.

**Prof. Ignacio Romero**  
Deputy Director,  
Computational Solid  
Mechanics

Ph.D. in Civil Engineering, from University of California Berkeley, USA

Professor of Mechanics, Technical University of Madrid

#### Research Interests

Numerical methods for nonlinear mechanics of solids, fluids, and structures. Development of time integration methods for Hamiltonian and coupled problems, models and numerical methods for nonlinear beams and shells, improved finite elements for solid mechanics, error estimators in nonlinear dynamics and multiscale methods for material modelling.





**Dr. Carlos González**

Senior Researcher, Structural Composites

Ph.D. in Materials Science from Technical University of Madrid. Spain

Associate Professor of Materials Science, Technical University of Madrid

**Research Interests**

Processing, characterisation and modelling (theoretical and numerical) of the mechanical performance of advanced structural materials, with special emphasis in metal- and polymeric-matrix composites; and development of physically-based, micromechanical models of the deformation and fracture (multi-scale models to design novel virtual testing strategies).



**Dr. Claudio Saul Lopes**

Senior Researcher, Design & Simulation of Composite Structures

Ph.D. in Aerospace Engineering from Delft University of Technology. The Netherlands

**Research Interests**

Design and simulation of composite structures; design of advanced composites with non-conventional architectures and by non-conventional methods, such as fibre-steered composite panels manufactured by means of Advanced Fibre Placement; numerical analysis and computational simulation of damage and failure of composite structures; impact and damage tolerance analysis of composite structures.

**Dr. Maciej Haranczyk**

Senior Researcher, Computational and Data-Driven Materials Discovery

Ph.D. in Chemistry from University of Gdansk, Poland

**Research Interests**

Computational and data-driven materials discovery and design. His work effectively combines novel materials informatics approaches with traditional computational material science techniques such as electronic structure calculations and/or molecular simulations. Moreover, his work often requires leveraging on the recent developments in applied mathematics and computer science.





**Dr. Jon M. Molina-Aldareguía**

Senior Researcher,  
Micromechanics and  
Nanomechanics

Ph.D. in Materials Engineering from  
Cambridge University. UK

**Research Interests**

Micromechanics and nanomechanics of multifunctional materials; microstructural and mechanical characterisation of thin-films, multiphase materials using nanoindentation and advanced focus-ion beam and electron microscopy analysis, mechanical testing inside the scanning and transmission electron microscopes.

**Dr. Srdjan Milenkovic**

Senior Researcher,  
Solidification Processing &  
Engineering

Ph.D. in Materials Engineering  
from State University of Campinas. Brazil

**Research Interests**

Processing, solidification behaviour, mechanical and microstructural characterisation, as well as processing-structure-property relationships of Ni-based superalloys, intermetallic compounds and eutectic alloys for high-temperature applications; nanotechnology in general, and more specifically, synthesis and characterisation of metallic nanowires through directional solidification and electrochemical treatment of eutectic alloys.



**Dr. María Teresa Pérez-Prado**

Senior Researcher, Metal  
Physics

Ph.D. in Materials Science from  
Complutense University of Madrid.  
Spain

**Research Interests**

Applied and fundamental work on the processing, characterisation and mechanical behaviour of advanced metallic materials for automotive, energy and biomedical applications; study of the mechanical response of bulk and porous magnesium alloys, as well as the *in situ* investigation of the deformation and recrystallization mechanisms of TiAl alloys; and fabrication of novel metallic phases with improved mechanical and functional properties by severe plastic deformation involving compression and shear.





### Dr. Ilchat Sabirov

Senior Researcher, Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

#### Research Interests

Deformation processing of metallic materials and its effect on the microstructure and properties, physical simulation of metallurgical processes. Development of unique thermo-mechanical processing routes that optimise performance of metallic materials.

### Dr. Javier Segurado

Senior Researcher, Multiscale Materials Modelling

Ph.D. in Materials Engineering from Technical University of Madrid. Spain

Associate Professor of Materials Science, Technical University of Madrid

#### Research Interests

Multiscale modelling of structural materials; physically-based models to simulate the mechanical behaviour of metals at different length scales: molecular dynamics, discrete dislocation dynamics and single-crystal plasticity models; computational homogenization models and concurrent multiscale techniques for polycrystalline materials; and development of computational micromechanics strategies to simulate the mechanical behaviour until failure of both particle- and fibre-reinforced composites.



### Dr. Juan José Vilatela

Senior Researcher, Multifunctional Nanocomposites

Ph.D. in Materials Science from University of Cambridge. UK

#### Research Interests

His group's work is largely focused on the development of macroscopic materials made up of nanobuilding blocks in a way that the unique properties at the nanoscale are preserved through the assembly process and a new generation of high-performance engineering materials is produced. Central to this work is a process to make continuous macroscopic fibres made up of CNTs. The group works actively in studying their hierarchical structures by advanced X-ray techniques, reinforcement at multiple length-scales and the electrochemical interactions of CNT fibres with liquids and polymers. This research has helped establish the unique combination of properties of CNT fibres, and is enabling the fabrication of multifunctional composites that can store energy or have sensing functions.





**Dr. De-Yi Wang**

Senior Researcher, High Performance Nanocomposites

Ph.D. in Polymer Chemistry and Physics from Sichuan University, China

**Research Interests**

Application-oriented fundamental problems and novel technologies in multifunctional nanomaterials, eco-benign fire retardants, high performance environment-friendly polymers and nanocomposites (bio-based and/or petro-based); synthesis and modification of novel multifunctional nanostructured materials, design and processing of high performance polymers and their nanocomposites, with particular emphasis in structural properties and behaviour under fire.



**Dr. Yuwen Cui**

Senior Researcher, Computational Alloy Design

Ph.D. in Materials Science from Central South University, China

**Research Interests**

Computational thermodynamics (i.e. CALPHAD) and kinetics; high throughput diffusion research and diffusion modelling; microstructural simulation by using the Landau theory and phase field model; development of commercial thermodynamics databases and computational alloy design of Pb-free micro-solders, Ni-base superalloys and the new generation of Co-based high temperature alloys; development of lightweight interstitial alloys for hydrogen storage.



# researchers



**Dr. Vinodkumar Etacheri**  
(New incorporation)

Researcher, Electrochemical Energy Storage, Nanomaterials

Ph.D. in Materials Chemistry from Dublin Institute of Technology, Ireland

#### Research Interests

Tailored designing of nanostructured electrode materials, interfaces and electrolyte compositions, their spectroscopic/microscopic study and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O<sub>2</sub> batteries.



**Dr. Roberto Guzmán de Villoria**

Researcher, Nano-Architectures and Materials Design

Ph.D. in Mechanical Engineering from the University of Zaragoza, Spain

#### Research Interests

Nano-architectures; design and development of new materials and structures with tailored mechanical and functional properties; manufacturing new nano-engineered materials, bio-inspired materials and mechanomutable structures for transportation, energy and biomedical applications.



**Dr. Federico Sket**

Researcher, X-ray characterisation of materials

Ph.D. in Materials Engineering from Max-Planck Institute for Iron Research, Germany

#### Research Interests

Microstructural evolution of metal alloys and fibre-reinforced composites for engineering applications using advanced laboratory and synchrotron X-ray tomography as well as X-ray diffraction; processing of composite materials and relationship between processing conditions and microstructural evolution; mechanical deformation of materials and evolution of mechanical and microstructural properties; development of in-situ devices (based on in-situ X-ray microtomography and X-ray diffraction) for testing mechanical properties and processing using X-rays; and incorporation of experimental results to the development of physically-based models for optimisation of material processing and properties.

# visiting scientists



**Dr. Rigoberto Burgueño**  
 Visiting Scientist, Structural Engineering

Ph.D. in Engineering Sciences from the University of California, San Diego. USA

Professor of Structural Engineering. Michigan State University. USA

**Research Interests**

Multiscale assessment and design of tailored materials, devices and structures. Development of mechanical metamaterials using elastic instabilities; hybrid nano- and micro-structured material systems; multiscale modelling and simulation; design optimisation of materials and structures; solid and structural mechanics; hybrid structural systems; experimental characterisation of materials and structures; soft-computing methods for structural integrity assessment; inelastic response of concrete structures; and earthquake engineering.



**Prof. Shibin Nie**  
 Visiting Scientist, Bio-based fire retardant materials

Ph.D. in Polymeric Chemistry from University of Science and Technology. China

Associate Professor. Energy Resources and Safety, Anhui University of Science and Technology. China

**Research Interests**

Thermal and flame retardant properties of polymer nanocomposites; synergistic effect of metal compounds with intumescent flame retardants, such as metals, metal oxides, metal salts, metal chelates; catalyzing carbonization of polymer nanocomposites; thermal and flame retardant properties of semibiocomposites or biocomposites based on starch and lignin.



**Dr. Arnaud Weck**  
 Visiting Scientist, Fracture at the Microscale

Ph.D. in Materials Science and Engineering from McMaster University, Ontario, Canada

Associate Professor of Mechanical Engineering. University of Ottawa. Canada

**Research Interests**

Relationship between microstructure and mechanical properties of materials with particular emphasis on the mechanisms leading to material fracture; strength and fracture response of materials using ultrafast lasers to induce artificial defects in materials. The growth of these defects is then studied in-situ under optical and electron microscopes or using high resolution X-ray tomography; and advanced finite element simulations combined with crystal plasticity and nonlocal damage models to predict the deformation and fracture of complex materials.

# postdoctoral research associates



**Dr. Belén Aleman**  
Postdoctoral Research Associate

Ph.D. in Physics from Complutense University of Madrid. Spain

#### Research Interests

Synthesis of continuous macroscopic fibres made up with carbon nanotubes with molecular control to fix the final macroscopic properties of the material; chemical and structural analysis by X-ray synchrotron radiation based diffraction and XPS microscopy; and vacuum systems development for gas phase simulation experiments under UV radiation and plasma.



**Dr. Juan Pablo Balbuena**  
Postdoctoral Research Associate

Ph.D. in Physics from Autonomous University of Barcelona. Spain

#### Research Interests

Kinetic Monte Carlo (KMC) simulation of diffusion and activation/deactivation of dopants, impurities and radiation-induced defects in silicon and germanium-based materials; lattice KMC modelling of epitaxial processes in Si, Ge and III-V semiconductors; ensemble Monte Carlo simulation of bulk properties in semiconductors; drift-diffusion approximation model for charge carriers transport in semiconductor devices; and hybrid CPU-GPU parallel C++ programming algorithms.

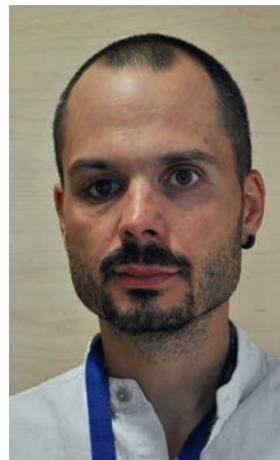


**Dr. Juan Ignacio Beltrán**  
Postdoctoral Research Associate

Ph.D. in Physics from Autonomous University of Madrid. Spain

#### Research Interests

Ab-initio based modelling of interfaces to rationalise the relation between atomistic and electronic structure for designing materials with application in electronics, multiferroics and/or magnetism.



**Dr. Marco Bernabei**  
Postdoctoral Research Associate

Ph.D. in Physics from University of the Basque Country University. Spain

#### Research Interests

Atomistic modelling and computer simulation techniques for the design and characterisation of new porous materials in crystalline and/or amorphous solid state.



**Dr. Laura Cabana**  
Postdoctoral Research Associate

Ph.D. in Materials Science from Autonomous University of Barcelona. Spain

**Research Interests**

Growth of nanostructures with multifunctional properties; investigation of strategies for the scaling up production of nanomaterials at the macroscale; optimisation of the production method to obtain a highly pure material; modification of nanostructure properties after purification treatments; and effects of the purification when forming nanocomposite materials for different applications.

**Dr. Aitor Cruzado**  
Postdoctoral Research Associate

Ph.D. in Industrial Engineering from Mondragon University. Spain

**Research Interests**

Fatigue and fracture modelling, multiscale modelling (crystal plasticity and finite element method), modelling of fretting and wear, structural integrity.



**Dr. Carmen Cepeda**  
Postdoctoral Research Associate

Ph.D. in Chemistry from University of Alicante. Spain

**Research Interests**

Relationship between microstructure and mechanical properties of advanced metallic alloys, thermo-mechanical processes based on severe plastic deformation, processing and characterisation of multilayer materials with high damage tolerance based on high-strength aluminium alloys for aerospace applications.

**Dr. Soundes Djaziri**  
Postdoctoral Research Associate

Ph.D. in Materials Physics from University of Poitiers. France

**Research Interests**

Structure-property connections for functional materials; crystal structure characterisation and stress measurements using X-ray diffraction methods (laboratory and synchrotron sources); In-situ studies under extreme environments (physical or thermo-mechanical) of composite materials by X-ray diffraction, radiography or electron microscopy.



**Dr. Daniel Cintora**  
Postdoctoral Research Associate

Ph.D. in Materials and Energy from University of Córdoba. Spain

**Research Interests**

Synthesis, characterisation and application of materials for energy storage and conversion; electrochemistry of inorganic materials, conducting polymers, polymer electrolytes, hybrid materials, composite electrodes, and their application in devices such as batteries and fuel cells.

**Dr. Olben Falcó**  
Postdoctoral Research Associate

Ph.D. in Mechanical Engineering from University of Girona. Spain

**Research Interests**

Design of advanced composites laminates with non-conventional architectures manufactured by means of advanced fibre placement; numerical analysis and simulation of progressive damage and failure in variable stiffness composite panels experimental studies of “tow-drop” defects under in-plane and impact loading; and damage resistance and damage tolerance analysis in variable stiffness composite panels.



**Dr. Carmine Coluccini**  
Postdoctoral Research Associate

Ph.D. in Chemical Science from Università di Bologna. Italy.

**Research Interests**

Organic synthesis, design and synthesis of organic and organometallic dyes for dye-sensitized solar cells (DSSC), and organometallic complexes as electrolytes for DSSC; aromatic fluorescent polymers, supramolecular chemistry.

**Dr. Juan Pedro Fernández**  
Postdoctoral Research Associate

Ph.D. in Chemistry from the Complutense University of Madrid. Spain

**Research Interests**

Processing and characterisation of polymer-based nanocomposites; study of the effect of the nanocompounds on the structure and properties of polymer matrices.





**Dr. Bin Gan**

Postdoctoral Research Associate

Ph.D. in Materials Science and Engineering from Illinois Institute of Technology. USA

**Research Interests**

Superalloys, intermetallics, structural materials, semiconductors, thin films and hard coatings; high temperature nanomechanics and micromechanics; grain boundary engineering and electron backscatter diffraction techniques.



**Dr. Andrea García-Junceda**

Postdoctoral Research Associate

Ph.D. in Materials Science and Technology from Complutense University of Madrid. Spain

**Research Interests**

Materials characterisation, optimisation of the mechanical properties of metallic alloys by modification of their processing route; optimisation of novel structural materials for energy generation plants; and fabrication of oxide-dispersion strengthened alloys by powder metallurgy and optimisation of their properties.



**Dr. Diego Garijo**

Postdoctoral Research Associate

Ph.D. in Aerospace Engineering from Technical University of Madrid. Spain

**Research Interests**

Computational mechanics (finite element, spectral and meshless methods); composite materials, fracture mechanics, structural health monitoring and optimisation.

**Dr. Sandip Haldar**

Postdoctoral Research Associate

Ph.D. in Mechanics and Materials at the University of Maryland, College Park. USA

**Research Interests**

Solid mechanics; composite materials; and experimental mechanics.

**Dr. Sarra Haouala**

Postdoctoral Research Associate

Ph.D. in Engineering Sciences at the Université Catholique de Louvain. Belgium

**Research Interests**

Computational mechanics of materials; and multi-scale modelling of heterogeneous materials.

**Dr. Vignesh Babu Heeralal**

Postdoctoral Research Associate

Ph.D. in Chemistry from University of Hyderabad. India

**Research Interests**

High performance flame retardant polymer composite and/or nanocomposites; polymer composites processing and manufacture; and environmentally friendly thermoset polymers from renewable feed-backs.





**Dr. Anna Hynowska**

Postdoctoral Research Associate

Ph.D. in Materials Science from Autonomous University of Madrid. Spain

**Research Interests**

Complex shaped Fe-Al intermetallic parts development by reactive infiltration method.



**Dr. Hong Liu**

Postdoctoral Research Associate

Ph.D. in Materials Science and Engineering from University of Monash. Australia

**Research Interests**

Study of microstructure evolution and deformation mechanisms of light alloys (e.g. Mg and Al based alloys) and their microstructural characterisation by means of phase field method.



**Dr. Amitava Moitra**

Postdoctoral Research Associate

Ph.D. in Engineering (Applied) Physics from Mississippi State University. USA

**Research Interests**

Integrated computational materials engineering; density functional theory; large scale atomistic simulations, molecular dynamics, semiempirical potential generation (EAM/MEAM); and deformation mechanisms in HCP materials.

**Dr. Miguel Monclús**

Postdoctoral Research Associate

Ph.D. in Thin Film Technology from Dublin City University. Ireland

**Research Interests**

Characterisation and performance of coatings, multilayers and nanostructured materials by means of nanoindentation, atomic force microscopy and other advanced techniques and instruments.

**Dr. Joseba Múgica**

Postdoctoral Research Associate

Ph.D. in Mechanics and Manufacturing from Mondragón University. Spain

**Research Interests**

Characterisation of the mechanical behaviour of composite materials and fibre metal laminates; computational micro and mesomechanics of composite materials; and impact and damage tolerance analysis of composite structures.

**Dr. David Portillo**

Visiting Postdoctoral Research Associate

Ph.D. in Nuclear Fusion from Polytechnic University of Madrid. Spain

**Research Interests**

Numerical methods for solid and fluid mechanics; simulation of laboratory plasma physics experiments; and inertial confinement fusion.





**Dr. Andrey Sarikov**  
Postdoctoral Research Associate

Ph.D. in Solid State Physics from V. Lashkarev Institute of Semiconductor Physics. NAS Ukraine. Ukraine

**Research Interests**

Thermodynamics and kinetics of phase separation in nonstoichiometric silicon oxide films; thermodynamics and kinetics of metal induced crystallisation of amorphous and disordered Si; and Monte Carlo modelling of the formation and transformation of semiconductor structures.

**Dr. Xin Wen**  
Postdoctoral Research Associate

Ph.D. in Chemistry and Physics of Polymers at Changchun Institute of Applied Chemistry. China.

**Research Interests**

Synthesis and application of carbon materials; and high-performance (nano) composites of polymers



**Dr. Jintao Wan**  
Postdoctoral Research Associate

Ph.D. in Chemical Engineering from Zhejiang University. China.

**Research Interests**

Thermal analysis of polymer materials; environmentally friendly thermosetting polymers from renewable feedbacks; polymer reaction engineering and polymer product engineering; and high performance, flame retardant and low smoke polymer composites.

**Dr. Jian Xu**  
Postdoctoral Research Associate

Ph.D. in Computational Science in Engineering from University of Leuven. Belgium

**Research Interests**

Quasi-static and fatigue damage modelling/experiment; multiscale modelling impact and damage tolerance analysis of composite structures.



**Dr. Xin Wang**  
Postdoctoral Research Associate

Ph.D. in Safety Science and Engineering from University of Science and Technology of China. China.

**Research Interests**

Flame retardant polymer-based nanocomposites; synthesis of halogen-free flame retardants; and UV-curing flame retardant coatings.



# research assistants



**Pablo Acuña**

MSc: Autonomous University of Barcelona. Spain  
Research: High performance polymers



**Ángel Alvaredo**

BEng: Salamanca University. Spain  
Research: Composite materials



**Cecilia Andradas**

BSc: Autonomous University of Madrid. Spain  
Research: In silico synthesis of new materials



**Eva Andrés**

MSc: Technical University of Madrid. Spain  
Research: Coupled thermomechanics



**Bárbara Bellón**

MEng: Castilla la Mancha University. Spain  
Research: Design, processing and modelling of cast metallic alloys



**Marta Cartón**

MSc: Carlos III University of Madrid. Spain  
Research: Co-based superalloys for high temperature applications



**Almudena Casado**

MSc: Carlos III University of Madrid. Spain  
Research: Solidification and casting



**Jaime Castro**

MSc: Technical University of Madrid. Spain  
Research: Vacuum-assisted infiltration and microfluid flow



**Marcos Cejuela**

MSc: University of Valencia, Spain  
Research: Developing on novel magnets



**Yi Chen**

MEng: Northwestern Polytechnical University, China  
Research: Thermo-kinetic study of near beta Ti alloys



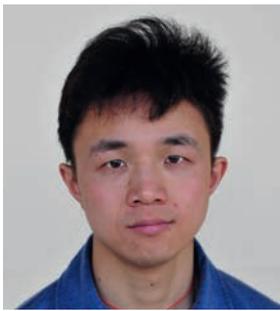
**Miguel Cristobal**

MEng: Technical University of Madrid, Spain  
Research: Steel development



**Daniel del Pozo**

MEng: Technical University of Madrid, Spain  
Research: Modelling of ice impact on jet turbines



**Xiangxing Deng**

MSc: Hunan Institute of Engineering, China  
Research: Development of innovative materials for cutting tools



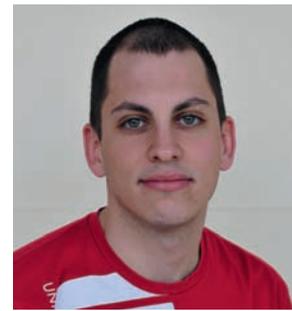
**Ignacio Dopico**

MEng: Autonomous University of Madrid-CIEMAT, Spain  
Research: Atomistic materials modelling



**Gustavo Esteban**

MEng: Technical University of Madrid, Spain  
Research: Multiscale simulation of plasticity in metals



**Juan Carlos Fernández**

MSc: Carlos III University of Madrid, Spain  
Research: Electric curing of carbon nanotubes/epoxy resins



**Andrea Fernández**

MSc: Carlos III University of Madrid, Spain  
Research: Recycling composite materials



**Can Fu**

MSc: Wuhan University of Technology, China  
Research: Eco-friendly fire retardant coating



**Alejandro García**

MEng: Carlos III University of Madrid, Spain  
Research: High energy impact on aeronautical composite structures



**Pablo García-Chao**

MSc: University of Manchester, UK  
Research: Development of advanced high-strength steels



**Ismael Gómez**

MSc: Autonomous University of Madrid. Spain  
 Research: Development of software tools for materials discovery



**Miguel Herráez**

MEng: Carlos III University of Madrid. Spain  
 Research: Nano-architectures and materials design



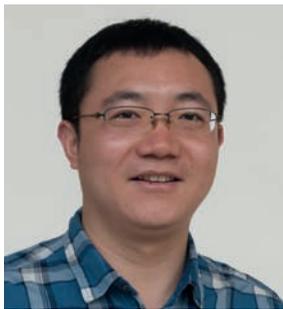
**Luis Carlos Herrera Ramírez**

MEng: Carlos III University of Madrid. Spain  
 Research: Impact in composite materials



**Marcos Jiménez**

MEng: Carlos III University of Madrid. Spain  
 Research: Micromechanics of Ni superalloys



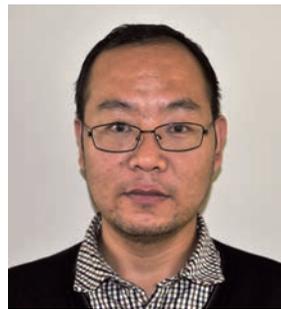
**Zhi Li**

MSc: Shanghai Jiang Tong University. China  
 Research: New generation fire retardant materials



**Na Li**

MEng: Beihang University. China  
 Research: Kinetics of Magnesium Alloys



**Jifeng Li**

MEng: Academy of Engineering Physics. China  
 Research: Multiscale Materials Modelling



**Yang Lingwei**

MEng: Central South University. China  
 Research: Nanoscale metal-ceramic multilayers



**Sergio Lucarini**

MEng: Polytechnic University of Bilbao. Spain  
 Research: Multiscale Plasticity



**Rudi Maça**

MSc: Technical University of Munich. Germany  
 Research: Electrochemical energy storage



**Francisca Martínez**

MEng: Carlos III University of Madrid. Spain  
 Research: Numerical simulation of composites under Impact



**Mohammad Marvi-Mashhadi**

MSc: Ferdowsi University of Mashhad. Iran  
 Research: Multiscale modelling of polyurethane foams



**Bartolomé Mas**

MEng Technical University of Madrid. Spain  
Research: Multifunctional composites based on CNT fibres



**Alfonso Monreal**

MEng Technical University of Madrid. Spain  
Research: Production and properties of thermoset nanocomposites



**Hugo Mora**

MEng: Carlos III University of Madrid. Spain  
Research: Development of coating on nanostructured Ti for biomedical applications



**Alicia Moya**

MSc: Complutense University of Madrid. Spain  
Research: Nanohybrids for photocatalysis



**Fernando Naya**

MEng: Polytechnic University of Madrid. Spain  
Research: Multiscale simulation of composites



**Yunfu Ou**

MSc: Hunan University. China  
Research: Multi-functional CNT fibre Composite Materials



**Cemre Ozmenci**

MEng: Koç University. Turkey  
Research: Multiscale mechanical characterisation and modelling of cast metallic alloys



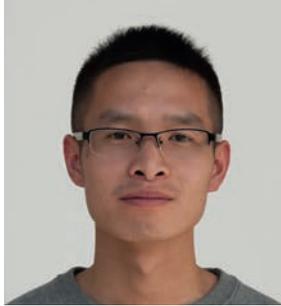
**Alberto Jesús Palomares**

MEng: University of Extremadura. Spain  
Research: Micromechanics of inter-metallic materials



**Yetang Pan**

MSc: Harbin Institute of Technology. China  
Research: Fire retardant polymeric materials



**Xia Peikang**

MSc: Shanghai University, China  
 Research: High strain rate mechanical behaviour of advanced high strength steels



**Nerea Pérez**

BEng: University of Almería, Spain  
 Research: Polymer nanocomposites



**Daniel Rodriguez**

MEng: Technical University of Madrid, Spain  
 Research: Multiscale plasticity



**Pablo Romero**

MEng: Technical University of Madrid, Spain  
 Research: Nano-architectures and materials design



**Raúl Sánchez**

MEng: University of Cantabria, Spain  
 Research: Nanoindentation of light alloys



**Raquel Sanguine (visiting)**

MEng: Pontifical Catholic University of Rio Grande do Sul, Brasil  
 Research: Solidification processing and properties of Zn-Al hypoeutectic alloys



**Jose Antonio Santiago**

MSc: Polytechnic University of Madrid, Spain  
 Research: Synthesis and nanomechanical characterisation of DLC coatings



**Rodrigo Santos**

MSc: Delft University of Technology, Netherlands  
 Research: Dislocation dynamics simulations of strengthening in metallic alloys



**Evgeny Senokos**

MEng: Lomonosov Moscow University, Russia  
 Research: Nanostructured supercapacitors



**Juan José Torres**

MEng: University of Navarre. Spain  
Research: Voids in out-of-autoclave prepregs



**Miguel A. Valdés**

MEng: Technical University of Madrid. Spain  
Research: High-strength steels



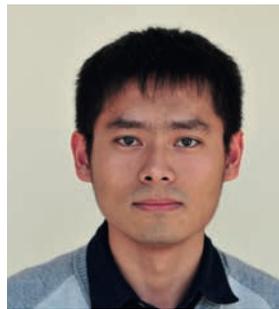
**Arcadio Varona**

MEng: Rey Juan Carlos University. Spain  
Research: Advanced NiAl-based eutectic alloys



**Jingya Wang**

MSc: Shanghai University. China  
Research: Computational Thermodynamics of Magnesium Alloys



**Chuanyun Wang**

MSc: Northwestern Polytechnical University. China  
Research: High throughput diffusion and phase transformation



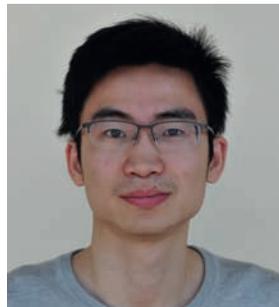
**Guanglong Xu**

MEng: Central South University. China  
Research: Computational alloy design



**Jing Zhang**

MEng: University of Manchester. UK  
Research: Multifunctional nanomaterials based polymer nanocomposites



**Lu Zhang**

MEng: Central South University. China  
Research: Polymer composites and nanocomposites



**Xiaomin Zhao**

MEng: Shanghai Jiao Tong University. China  
Research: Polymer nanocomposites

# laboratory technicians



**Vanesa Martínez**

MEng: University of Valencia. Spain



**Dr. Miguel Castillo**

PhD: University of Sevilla. Spain



**Marcos Angulo**

V.T.: Specialist Technician. Spain



**Miguel de la Cruz**

V.T.: Specialist Technician. Spain



**José Luis Jiménez**

V.T.: Specialist Technician. Spain



**Dr. Jose Sánchez del Río**

PhD: Autonomous University of Madrid. Spain



**Victor Reguero**

MEng: University of Valladolid. Spain



**Fernando Fernández**

V.T.: Specialist Technician. Spain

# general management



**Dr. Covadonga Rosado**  
General Manager



**Rosa Bazán**  
Personnel Manager



**Mar García**  
Finance Manager



**Vanessa Hernán-Gómez**  
Accounting Specialist



**Sofía Buendía**  
Executive Assistant



**Mariana Huerta**  
Public Relations and Events  
Assistant

# international project office



**Miguel Ángel Rodiel**  
Technology Director & Head  
of Project Office



**Dr. Germán Infante**  
R&D Project Manager



**Fernando Gómez**  
R&D Project Manager

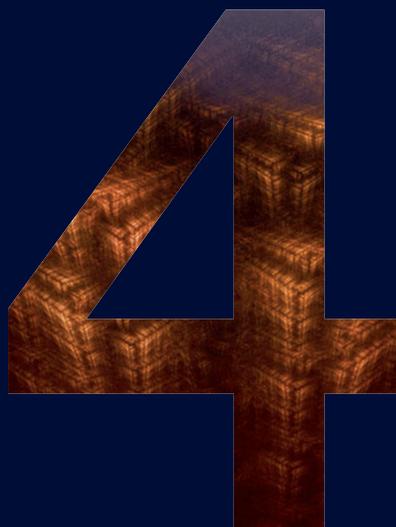


**Dr. Eduardo Troche**  
R&D Project Manager



**Mª José Pérez**  
R&D Project Management  
Assistant

# research infrastructure



- 4.1. **Synthesis, processing and integration of materials [46]**
- 4.2. **Microstructural and chemical characterisation [50]**
- 4.3. **Mechanical properties [52]**
- 4.4. **Functional properties [54]**
- 4.5. **Simulation [57]**

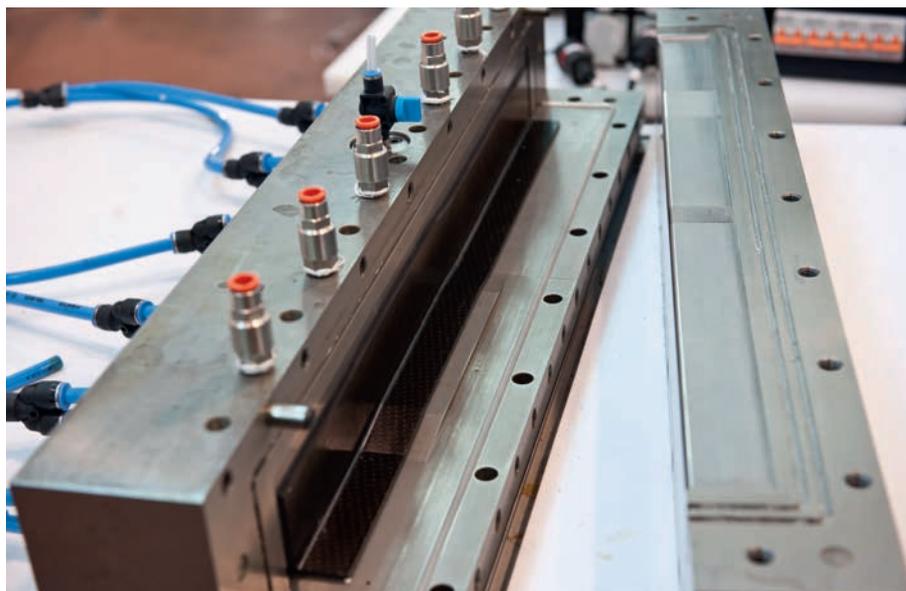
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2016

## 4.1. Synthesis, processing and integration of materials

### Metallic alloys

- **Arc Melting and Casting Furnace** (Arc 200, Arcast Inc.) for melting, alloying, casting, rapid solidification and atomization of reactive and high melting point elements and alloys up to 3500°C using a clean ceramic free cold crucible process. The furnace offers many options including: tilt casting, centrifugal casting, suction casting, zone melting and gas atomization under inert atmosphere or high vacuum.
- **Vacuum Induction Melting and Casting System** (VSG 002 DS, PVA TePla) to melt a wide range of metals, alloys or special materials under high vacuum, fine vacuum or different gas atmospheres with subsequent casting into moulds or forms. In addition, it is equipped with a directional solidification device, which enables the growth of single crystals and aligned columnar structures.
- **Physical Simulation of Processing** (Gleeble 3800, Dynamic Systems Inc.) to perform laboratory scale simulation of casting, welding, diffusion bonding and hot deformation processing (rolling, forging, extrusion) of a wide range of metallic alloys (steels, Ni-based superalloys, Ti, Al and Mg alloys, etc), as well as their thermo-mechanical characterisation.
- **High Temperature Furnace** (Nabertherm, RHTH 120/600/16) to carry out heat treatments up to 1600°C in vacuum or inert atmosphere.
- **Planetary Mills** (FRITSCH PULVERISETTE 6 classic & 7 premium) for the finest rapid, batchwise comminution of hard to soft grinding material, dry or in suspension, down to colloidal or nanometer fineness. Maximum sample quantity: 225 ml (model 6 classic), 70 ml (model 7 premium). Rotational speed of main disk up to 1000 rpm (model 7 premium).





### Polymer based composites and nanocomposites

- **Pultrusion Line** (design in-house, IMDEA Materials Institute) to manufacture continuous composite profiles of thermoset matrices reinforced with carbon, glass, aramid, and other advanced fibres. Fibre fabrics or roving are pulled off reels, guided through a resin bath or resin impregnation system and subsequently into a series of heated metallic dies to eliminate the excess of resin, obtain the correct shape and cure the resin. The pultruded continuous profile is extracted from the dies by means of hydraulic grips.
- **Resin Transfer Moulding** (Megaject MkV, Magnus Venus Plastech) to manufacture composite components with excellent surface finish, dimensional stability, and mechanical properties by low-pressure injection of thermoset polymers into a metallic mould containing the fibre preform.
- **Hot-Plate Press** (LabPro 400, Fontijne Presses) to consolidate laminate panels from pre-impregnated sheets of fibre-reinforced composites or nanocomposites by simultaneous application of pressure (up to 400 kN) and heat (up to 400°C). Both thermoset and thermoplastic matrix composites can be processed.
- **Micro compounder** (MC 15, Xplore) for compounding thermoplastic based materials or polymeric materials with minute amounts of costly synthesized materials and additives. It has a base capacity of 15 ml. and a maximum torque value is 9000 Nm. Equipped with co-rotating and counter-rotating screws.



- **Extruder** (KETSE 20/40 EC, Brabender) co-rotating twin screw extruder which offers a variety of thermoplastic polymers processing possibilities. It has an integrated drive with a power of 11 kW and reaches speed up to max. 1200 rpm. Output is 0.5 - 9 kg/h.
- **Injection Molding Machine** (Arburg 320 C) to carry out high pressure injection of the raw material into a mold which shapes the polymer into the desired shape. Injection molding can be performed with commonly thermoplastic polymers and is widely used for manufacturing a variety of parts.
- **Three-Roll Mill** (Exakt 80 E, Exact Technologies) to disperse fillers and additives in viscous matrix. The shearing forces to break agglomerate are generated by three hardchrome-plated rollers that rotate at different angular velocities and where gap (minimum 5 mm) and speed setting are controlled electronically. The machine is equipped with a cooling-heating unit which allows the temperature control on roller surface in a range of -10 – 100°C.
- **Chemical Synthesis Laboratory** (built in-house, IMDEA Materials Institute) to carry out chemical synthesis, including organic, inorganic and nanomaterial synthesis, aiming at creating and functionalizing new materials.

## Nanomaterials

- **Carbon Nanotube Fibre Spinning Reactor** (built in-house, IMDEA Materials Institute) to produce continuous macroscopic fibres made out of CNTs directly spun from the gas-phase during chemical vapour deposition. It can produce kilometres of fibre per day, at rates between 10 – 50 m/min.
- **Horizontal Chemical Vapour Deposition Reactor** (built in-house, IMDEA Materials Institute) to carry out nano-structure synthesis, such as vertically aligned carbon nanotubes, nanorods or graphene. The system has been automatized to control all the synthesis parameters ( $T_{max}=1200\text{ }^{\circ}\text{C}$ ).
- **Electrospinning Unit** (NANON-01A, MECC) to produce non-woven nanofibrous mats as well as aligned bundles of nanofibres based on various polymers, ceramics and composites. Nanofibres of different shape (smooth and porous surfaces, beaded, core-sheath) and orientations (non-woven cloth, aligned, and aligned multi-layer) can be manufactured.



## Batteries

- **Ar-Filled Glove Box** (Vigor Sci-Lab) that can achieve high-purity (99.999%) Ar-atmosphere required for fabricating rechargeable batteries (Li, Na, K-ion, Li/Na-S, Li-O<sub>2</sub> systems). The system is equipped with oxygen and moisture sensors and absorbers. Oxygen and moisture levels less than 1 ppm can be achieved in this glove box system. **(New equipment)**
- **Coin cell battery fabricator** (MTI) to fabricate various types of 2032-type coin batteries for electrochemical testing. This system can be also employed for opening the coin cells after electrochemical testing to perform postcycling microscopic/spectroscopic analysis. **(New equipment)**
- **Hydrothermal System** (Parr Instruments) to synthesis metal oxide and carbon based materials for functional applications including electrochemical energy storage. Temperature can be adjusted upto 300 °C and the total volume of the reactor is 200 mL. **(New equipment)**
- **Tube Furnace** (MTI) to synthesize materials through reduction and oxidation reactions depending up on the working gas selected. Temperatures up to 1200 °C can be achieved in Ar, N<sub>2</sub>, Air, NH<sub>3</sub> and H<sub>2</sub> atmospheres. Outlet of the tube furnace is connected to a water trap to remove byproducts produced during the material synthesis. **(New equipment)**
- **Planetary Mixer** (Thinky SR-500) to homogenise the electrochemically active material with conductive carbon additive and binder in a suitable solvent. The slurry obtained can be uniformly coated on Cu or Al foils to prepare electrodes for rechargeable batteries. **(New equipment)**
- **Vacuum Oven** (Thermo Scientific) to remove solvents and drying the electrode materials for rechargeable batteries. A maximum operating temperature of 250 °C and vacuum of 10 mbar can be achieved. **(New equipment)**

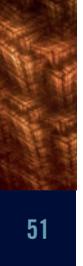


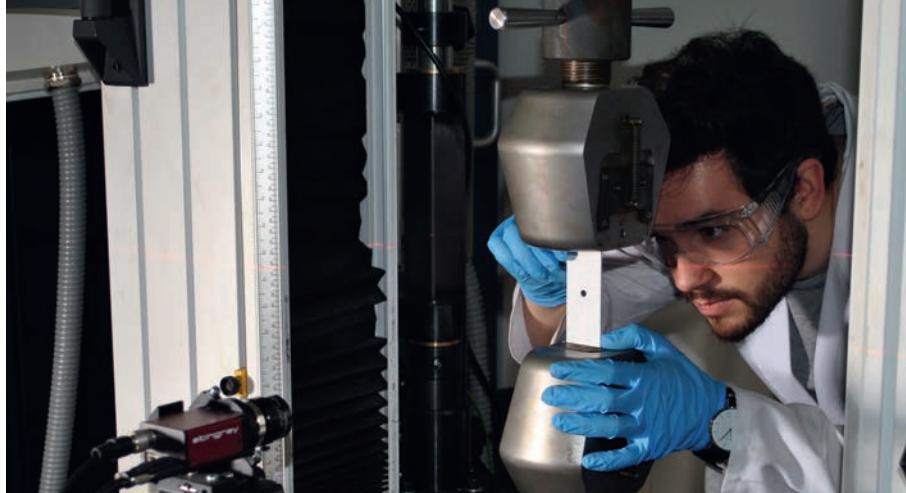
## 4.2. Microstructural and chemical characterisation

- **Field-Emission Transmission Electron Microscope** (Talos F200X, FEI) combines outstanding high-resolution S/TEM and TEM imaging with an energy dispersive X-ray spectroscopy integrated system fully compatible with high-resolution 3D tomography. It is also equipped with a PicoIndenter platform to perform *in situ* tests. This equipment is available to external users through the webpage of the institute (<http://materials.imdea.org/research-infrastructure/services-rates/external-use-of-tem/>)
- **Dual-Beam Focus Ion Beam-Field Emission Scanning Electron Microscope** (Helios NanoLab 600i, FEI) fully equipped with STEM detector, X-Ray microanalysis (EDS) and electron backscatter diffraction (EBSD) for 3-D microstructural, chemical and crystallographic orientation analysis. The system is also suited for site-specific TEM sample preparation, micro machining and patterning by ion-beam milling.
- **Scanning Electron Microscope** (EVO MA15, Zeiss) with chemical microanalysis (EDS Oxford INCA 350) and automated pressure regulation from 10 to 400 Pa to work with non-metallic samples without the need of metalizing.
- **Atomic Force Microscope** (Park XE150, Park Systems) to carry out nanoscale characterisation of materials, including non-contact and contact atomic force microscopy. Additional features include magnetic microscopy, thermal microscopy, nanolithography and a high temperature stage to carry out measurements up to 250°C.



- **Ram Micro spectroscopy system** (Renishaw, PLC) for obtaining the vibrational spectra of the molecular bonds. It is fully equipped with a Leica DM2700 microscope with 5x, 20x, 50x, 100x objectives, a 532nm Nd:YAG laser (50 mW at 532 nm) and a diffraction grating of 1800 l/mm. It is also equipped with a scanning stage for advanced mapping with 112x76x20 mm range and 100 nm resolution.
- **X-ray Computer-assisted 3D Nanotomography Scanner** (Nanotom, Phoenix) for three-dimensional visualization and quantitative analysis of microstructural features in a wide variety of materials ranging from metal powders and minerals to polymers and biomaterials. The scanner combines a 160 KV X-ray source to study highly absorbing materials together with a nanofocus tube to provide high resolution (0.2-0.3  $\mu\text{m}$  detail detectability).
- **X-ray Diffractometer** (Empyrean, PANalytical) for phase analysis, texture, and residual stress determination, as well as reflectometry. It is equipped with a state-of-the-art X-ray platform for the analysis of powders, thin films, nanomaterials and solid samples. The device is furnished with exchangeable tubes of Cu and Cr radiation, with three sample stages (standard, reflection-transmission spinner and Chi-Phi-x-y-z), an automated sample changer, and a linear detector (PIXcel 1D).
- **Gel Permeation Chromatographer** (2414, Waters) that includes a Waters 2414 refractive index detector, a Waters 2489 UV/Visible detector, a Waters 1500 column heater, and a series of Waters polystyrene GPC columns. It is used to determine molecular weight and molecular weight distribution of soluble polymers or oligomers. It can detect effective molecular range of 100-600,000 Da, with THF or DMF as the mobile phase and an upper limiting temperature of 60  $^{\circ}\text{C}$ .
- **Ultrasound non-Destructive Inspection System, C-Scan** (Triton 1500, Tecnitest) to detect and evaluate defects by non-destructive ultrasounds technique. The system finds and determines the size and position of the typical defects in composite materials (voids, delaminations, cracks, etc).
- **Sample Preparation Laboratory** furnished with the following equipment: i) two cutting machines that allow for both precision slicing as well as cutting of large sample, ii) a wire cutting saw, iii) three polishing wheels (one manual, two automatic), including one for the preparation or large, planar sample, and iv) two electrolytic polishing machines, one for double-sided samples, suitable for TEM disk finishing, and one for one-side surface finishing of bulk samples.





### 4.3. Mechanical properties

#### Mechanical characterisation

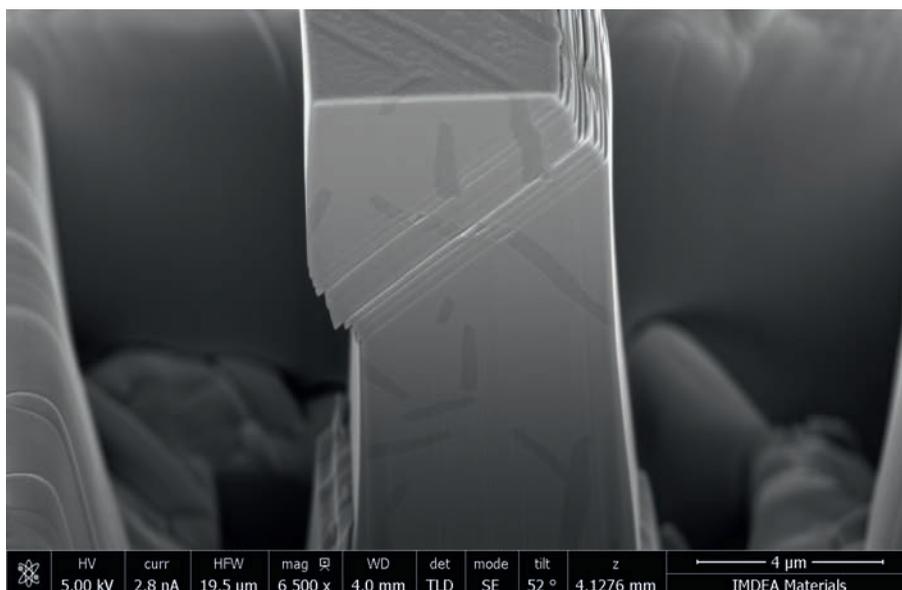
- **Dual Column Universal Testing System** (INSTRON 5966) to perform mechanical tests (including tension and compression, shear, flexure, peel, tear, cyclic and bending). The INSTRON 5966 model has 10 kN of capacity and 1756 mm of vertical test space.
- **Universal Electromechanical testing machine** (Instron 3384) to characterize the mechanical properties of materials, include fixtures for different tests (tension, compression, bending, fracture), load cells (10 kN, 30 kN and 150 kN), and extensometers.
- **Fatigue Testing System** (INSTRON 8802). Servo-hydraulic mechanical testing machine (maximum load of 250 kN) with precision-aligned, high-stiffness load frames to carry out a broad range of static and dynamic tests from small coupons to large components. It is equipped with an environmental chamber for mechanical tests between -150°C and 350°C.
- **Drop Weight Impact Test System** (INSTRON CEAST 9350) designed to deliver impact energies in the range 0.6 to 757 J. This instrument can be used to test any type of materials from composites to finished products, and is suitable for a range of impact applications including tensile impact.
- **Fibre Mechanical Testing Machine** (FAVIMAT+) to characterize fibre mechanical properties, as well as linear density and crimp. Measurement of the mechanical properties in a liquid medium is also possible.
- **Dynamic Mechanical Analysis** (Q800, TA Instruments) to determine the elastic-viscous behaviour of materials, mainly polymers. The machine works in the temperature range of -150 – 600°C, frequency range of 0.01 – 200 Hz and the maximum force is 18 N. Clamps for dual/single cantilever, 3 point bend, and tension are available.



- **Digital Image Correlation System** (Vic-3D, Correlated Solutions) to perform non-contact full-field displacement mapping by means of images acquired by an optical system of stereographic cameras. The images obtained are compared to images in the reference configuration and used by the expert system to obtain the full 3D displacement field and the corresponding strains.
- **Rheometer** (AR2000EX, TA Instruments) to determine the rheological behaviour and viscoelastic properties of fluids, polymer melts, solids and reactive materials (resins) in the temperature range 25°C to 400°C.

### Nanomechanics

- **High Temperature Nanoindentation System** (Nanotest Vantage, Micro Materials) to perform instrumented nanoindentation at temperatures up to 750°C in air and inert environments. The instrument uses both tip and sample heating, ensuring stability for long duration testing, including creep tests. This is the first dedicated high temperature nanoindentation instrument in Spain.
- **Nanoindentation System** (TI950, Hysitron) to perform instrumented nanoindentation, as well as other nanomechanical testing studies, such as micropillar compression in a range of materials, including test at temperatures up to 500°C. The capabilities include nanoindentation with several loading heads tailored for different applications (maximum load resolution, 1 nN), dynamic measurements, scratch and wear testing and SPM imaging and modulus mapping performed with the same indenter tip.



- **In-situ Nanoindenter** (PI87, Hysitron) to carry out elevated temperature mechanical testing inside a scanning electron microscope for the in-situ observation of the deformation mechanisms. The stage allows the simultaneous acquisition of the load-displacement record and of the SEM images during mechanical testing (nanoindentation, micro-compression, micro-bending, micro-tension) of micrometer and sub-micrometer size volumes, including elevated temperature testing.
- **Mechanical Stage for in-situ Testing in X-ray Tomography** ( $\mu$ TM, built in-house, IMDEA Materials Institute) to carry out in-situ mechanical tests under X-ray radiation in computer assisted tomography systems. The stage, designed and developed in-house, can be used both at synchrotron radiation facilities and inside laboratory tomography systems, for the investigation of the damage initiation and propagation in a wide variety of materials.
- **Micromechanical Testing**, focused ion-beam, scanning ultrasonic, or atomic force microscopy. Two stages for tension/compression testing (Kammrath and Weiss) to observe the specimen surface upon loading under light, scanning electron compression and fibre tensile testing are available, with maximum loads of 10 kN and 1 N, respectively. A heating unit allows to carry out tests up to 700°C.
- **Nanoindenter Stage** (PI87, Hysitron) to carry out mechanical tests inside a scanning electron microscope (SEM) for the in-situ observation of the deformation mechanisms. The stage allows the simultaneous acquisition of the load-displacement record and the SEM images during mechanical testing (nanoindentation, micro-compression, micro-bending, micro-tension) of micrometer and sub-micrometer size volumes, including elevated temperature testing.

#### 4.4. Functional properties

##### Thermal

- **Thermal Conductivity Analyser** (TPS 2500 S Hot Disk) to measure the thermal conductivity of samples based on a transient method technique. The equipment can be used to measure a wide variety of samples, from insulators to metals, as well as to determine thermal diffusivity in anisotropic materials.
- **Differential Scanning Calorimeter** (Q200, TA Instruments) to analyse thermal properties/ phase transitions of different materials up to 725°C. Equipped with Tzero technology, it provides highly reproducible baselines, superior sensitivity and resolution. It is coupled with a cooling system to operate over a temperature range of  $-40^{\circ}\text{C}$  to  $400^{\circ}\text{C}$  and high cooling rates of  $\sim 50^{\circ}\text{C}/\text{min}$ . This DSC equipment is also coupled



with a **FTIR Spectrometer** (Nicolet iS50) to measure infrared spectra of absorption, emission, photoconductivity or Raman scattering of a solid, liquid or gas from far-infrared to visible light.

- **Thermogravimetric Analyser** (Q50, TA Instruments) to understand the thermal stability and composition up to 1000°C by analysing the weight changes in a material as a function of temperature (or time) in a controlled atmosphere.
- **Horizontal Pushrod Dilatometer (New equipment)** (DIL 402 Expedis Supreme, NETZSCH) for the measurement of dimensional changes as a function of temperature on the basis of DIN EN 821, DIN 51045, ASTM E831 or ASTM E288 standards. The measurements can be carried out in vacuum, inert or oxidizing gas atmosphere. The dilatometer is equipped with a, novel “NanoEye” optoelectronic sensor with unmatched resolution over the entire measuring range, which allows direct sequential measurement of samples of different lengths and with different expansion behaviour at maximum precision.

### Fire resistance

- **Micro-scale Combustion Calorimeter** (Fire Testing Technology) to carry out laboratory scale tests of the flammability of materials with milligram quantities. The tests provide the peak heat release rate, the total heat released, the time to the peak heat release rate and the heat release capacity of the material. The samples are tested according to ASTM standard D7309-07.
- **Dual Cone Calorimeter** (Fire Testing Technology) to study the forced combustion behaviour of polymers simulating real fire conditions; fire relevant properties including time-to-ignition, critical ignition flux heat release rates (HRR), peak of HRR, mass loss rates, smoke production, CO<sub>2</sub> and CO yields, effective heat of combustion,



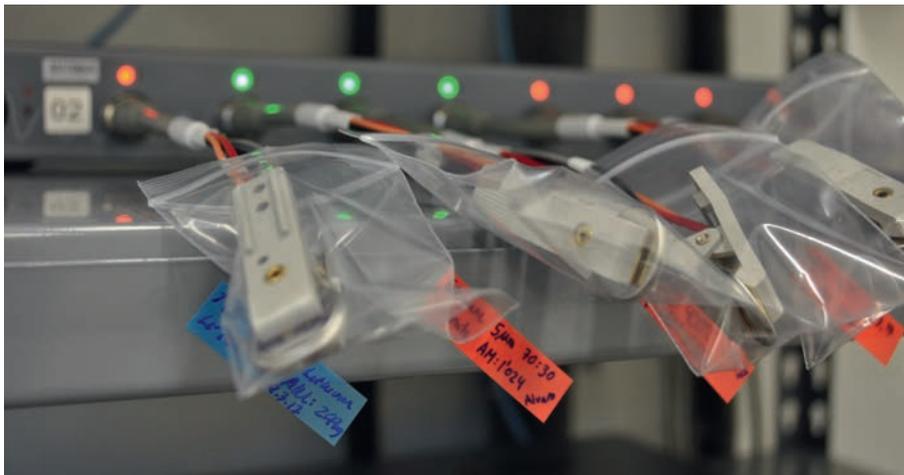
and specific extinction areas are directly measured according to ASTM/ISO standards.

- **UL94 Horizontal/Vertical Flame Chamber** (Fire Testing Technology), a widely used flame testing methodology, for selecting materials to be used as enclosures for electronic equipment and other consumer applications. Tests performed include horizontal burning test (UL94 HB), vertical burning test (UL94 V-0, V-1, or V-2), vertical burning test (5VA or 5VB), thin material vertical burning test (VTM-0, VTM-1 or VTM-2), and horizontal burning foamed material test (HF-1, HF-2 or HBF).
- **(Limiting) Oxygen Index** (Fire Testing Technology) to measure the relative flammability of a material by evaluating the minimum concentration of oxygen in precisely controlled oxygen-nitrogen mixture that will just support flaming combustion of a specimen.



## Electrochemical

- **Battery tester** (Neware BTS 4000, Neware) to perform the evaluation of secondary batteries through galvanostatic charge discharge tests. Each channel can handle 0 to 10 mA current and 0 to  $\pm 5$ V potential. One unit can simultaneously test 8 different batteries and different current densities. Charge-discharge measurements can also be performed at elevated temperature. **(New equipment)**
- **Electrochemical Workstation** (Zive SP1) to perform a wide range of electrochemical tests (Including galvanostatic, potentiostatic and electrochemical impedance spectroscopy) for characterizing batteries, supercapacitors as well as corrosion protection coatings. Current and voltage ranges are 1A and 10 V, respectively. Built in frequency generator can produce AC waves of up to 1MHz frequency. **(New equipment)**



- **Karl Fischer Moisture Analyser** (TOB Energy) to measure moisture content in various solvents up to 1 ppm level. This ensures the preparation of moisture free electrolytes for rechargeable batteries. **(New equipment)**
- **Conductivity Meter** (TOB Energy) to measure the ionic conductivity of electrolyte solutions. The equipment is capable of temperature compensation (-20 to 100 °C) during the conductivity measurement. **(New equipment)**
- **Two-channel Potentiostat** (ECLab SP200, BioLogic) with EIS and nano-current modules to carry out electrochemical studies. **(New equipment)**

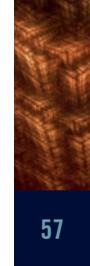
### Electrical and optical

- **Source-meter unit** (2450 Keithley) for electrical characterisation of devices and measurement of nanocurrents. **(New equipment)**
- **150W Xe lamp** (67001, Newport) and **Electrochemical Cell** for photoelectrocatalytic studies. **(New equipment)**
- **Microprobe Station** for electrical characterisation of optoelectronic devices. **(New equipment)**

## 4.5. Simulation

### High performance computing

- High Performance Computer cluster with 600+ Intel Xeon CPU cores and NVIDIA GPU acceleration leading to a computational power of 90 Tflops
- Access to CeSViMa (Madrid Centre for Supercomputing and Visualization) super-computing facilities.
- Commercial and open source software tools for modelling and simulation in Materials Science and Engineering (CALPHAD, DICTRA, Micress, Abaqus, LS-Dyna, PamCrash, LAMMPS, etc.).



## Simulation tools

### IRIS ©

IRIS is an object oriented, general purpose, parallel code for computational mechanics in solid, fluid, and structural applications. It has finite element and meshless capabilities, a wide range of material models, and solvers for linear and nonlinear, stationary and transient simulations. Currently, it can be applied in problems of linear and nonlinear solid mechanics, beams, shells, membranes, compressible and incompressible flows, thermal analysis and thermomechanical problems.



### CAPSUL ©

CAPSUL is a suite of crystal plasticity and polycrystalline homogenization simulation tools. The suite includes:

- A crystal plasticity constitutive model, aimed at predicting the elasto-plastic behaviour at the crystal level. The model incorporates physically-based and phenomenological implementations and both slip and twinning mechanisms are considered. Both monotonic response and cyclic behaviour are considered by the combination of different laws for isotropic hardening, kinematic hardening and cyclic softening. The model has already been successfully applied to simulate the mechanical performance of FCC (Al and Ni-based superalloys) and HCP alloys (Mg and Ti), including stress-strain curves and texture evolution under monotonic loading as well as crack initiation and fatigue life under cyclic loading. The model is programmed as a UMAT subroutine for Abaqus.
- A tool to generate finite element models representative of the actual alloy microstructure (grain size, shape and orientation distribution) using as input statistical data obtained from microscopy images.
- An inverse optimisation tool to obtain the crystal plasticity model parameters from the result of a set of mechanical tests (both microtests or tests on polycrystals)
- A set of python scripts to generate cyclic loading conditions and to postprocess the results to obtain fatigue indicator parameters and other measures from microfields.





## VIPER ©

VIPER (VIRtual Ply propERty) is a simulation tool developed within the framework of computational micromechanics by IMDEA Materials to predict ply properties of fibre-reinforced composite materials from the properties and spatial distribution of the different phases and interfaces in the composite. The tool is also able to generate composite microstructures with arbitrary fibre geometries as well as hybrid microstructures hence allowing for in-silico ply property design and optimisation.

Moreover, IMDEA Materials Institute has developed other in-house codes for modelling and simulation of thermodynamic properties and phase diagrams as well as mechanical behaviour and damage evolution of engineering materials.



## Muesli ©

MUESLI is an Open Source library of material models for general numerical methods of continuum mechanics problems. It includes common models for elastic and inelastic solids in small and large strain regimes (elastic, J2 plastic, viscoelastic, Ogden, Neo-hookean, Mooney-Rivlin, ...) as well as the standard fluid materials (Newtonian and non-newtonian). Written in C++, it has been designed for easy integration with existing research codes and extensibility. In addition, an interface with LS-Dyna and Abaqus is provided so that the implemented material models can be used, without modification, in these commercial finite element codes.



## MMonCa ©

MMONCA is an Open Source Kinetic Monte Carlo simulator developed by the Atomistic Modelling of Materials group and collaborators. It contains a Lattice KMC module, used mainly for simulation of epitaxy, and an off-lattice Object KMC module for simulation of damage irradiation in simple elements (Si, Ge, Fe, Cu...), binary compounds (SiC, GaAs) and alloys (FeCr, SiGe). The Kinetic Monte Carlo simulator is coupled to a finite element code to include the effect of mechanical stresses, and to an Ion Implant Simulator.

For more information about IMDEA Materials Institute's codes, please visit:

<http://materials.imdea.org/research/simulation-tools/>

c u r r e n t  
r e s e a r c h  
p r o j e c t s

5

annual report  
2016



**The Institute has participated in 65 research projects in 2016. 14 of these projects started during the year.** Although the number of projects has decreased as compared to 2015, the total project funding in 2016 was 23% higher than in 2015. In particular, project funding coming from European and national/regional competitive calls increased by 39% and 66%, respectively, compared to year 2015, whereas funding coming from industrial contracts decreased by 15% year-on-year.

The project portfolio is divided into three main groups: 32 projects were obtained in international competitive calls, out of which 20 were funded by the European Union and 12 by the Chinese Scholarship Council. In addition, 13 projects were supported by research programmes sponsored by the Spanish Ministry of Economy, Industry and Competitiveness and two by the Regional Government of Madrid, while 18 projects were directly funded through industrial contracts. Several of these industrial contracts are supported by the Spanish Centre for the Development of Industrial Technology (CDTI).

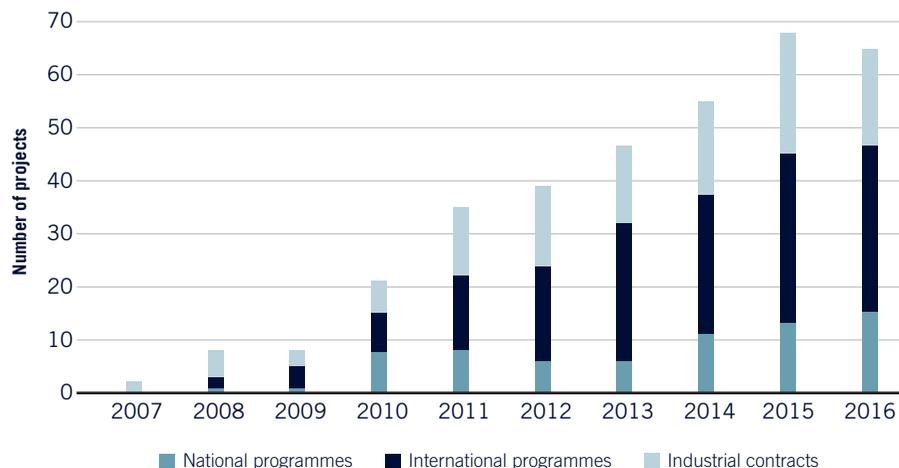


Figure 3. Number of active research projects per year by funding source

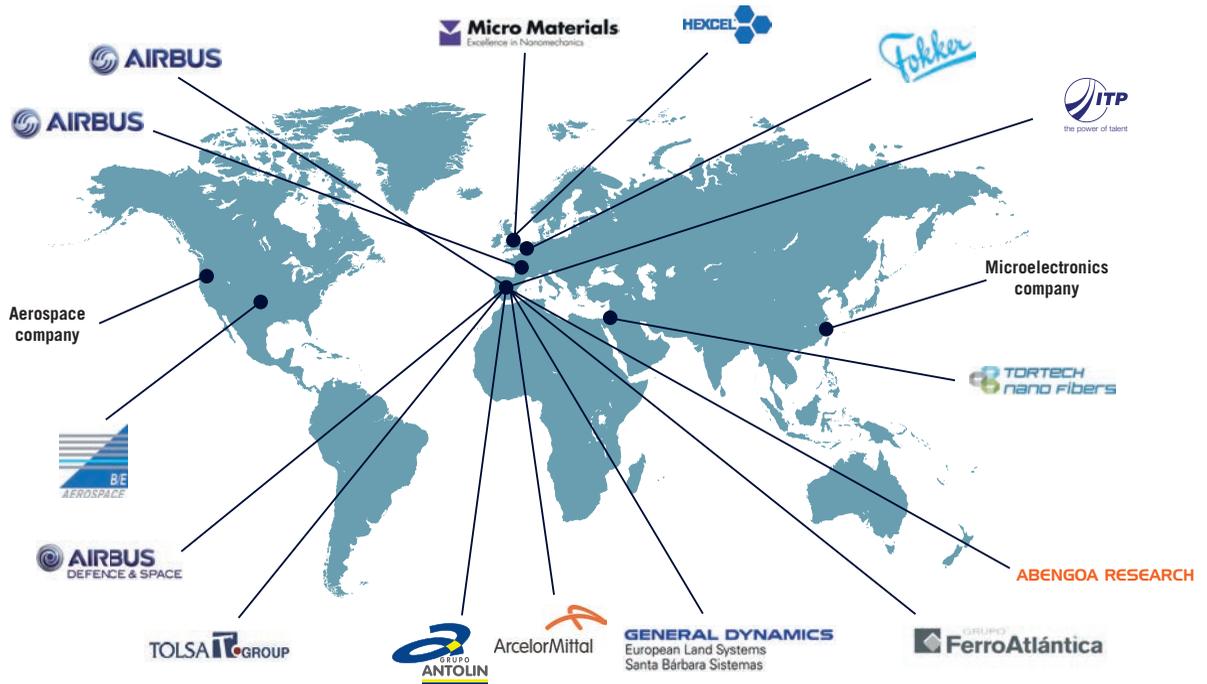


Figure 4. Active strategic industrial partnerships of IMDEA Materials Institute

A brief description of the projects started in 2016 is provided below:

## STEM

“Structural energy harvesting composite materials”

**Funding:** European Research Council, Starting Grant, European Union-Horizon 2020 Programme

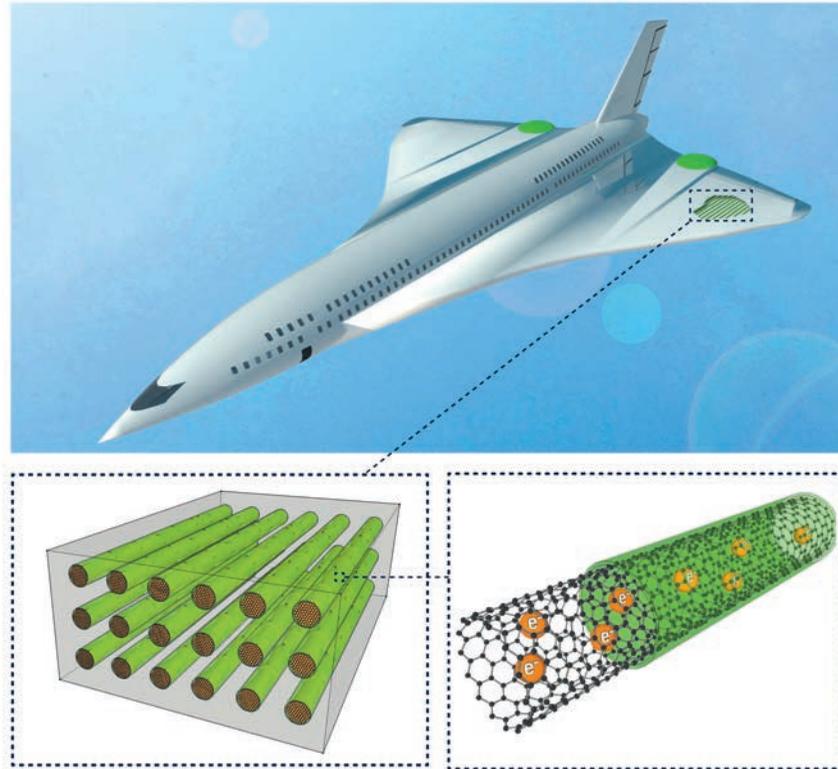
**Duration:** 2016-2021

**Principal Investigator:** Dr. J. J. Vilatela



The purpose of this project is the development of new multifunctional structural composite materials that combine high performance mechanical properties and the possibility to harvest energy. The multifunctional composites are based on a continuous macroscopic fibre made up of highly aligned carbon nanotubes that has bulk mechanical, electrical and thermal properties already similar to carbon fibre and the mesoporosity and chemical resistance of an activated carbon; which will be combined with nanostructured semiconductors that can transfer charge/energy when subjected to external stimuli and integrated in a polymer matrix to form composite structures. The project comprises a detailed multiscale study of materials synthesis and properties, including in-situ spec-

trosopy, electron microscopy and synchrotron XRD during mechanical testing, and basic optoelectronic measurements.



## DYNACOMP

“Dynamic behaviour of composite materials for next generation aeroengines”

**Funding:** Marie Skłodowska-Curie-ITN-EID, Horizon 2020 Programme, European Union-Horizon 2020 Programme

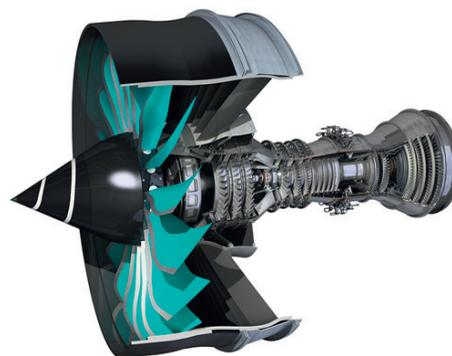
**Partners:** IMDEA Materials Institute (Project Coordinator), HEXCEL, Micro Materials, Technical University of Madrid and Madri+d foundation

**Duration:** 2016-2020

**Principal Investigator:** Dr. J. Molina

DYNACOMP is an European Industrial Doctorate (EID) programme focused on the design of the next generation of structural composite materials for high strain rate applications. This goal will be achieved by the development of a consistent, physically based multiscale simulation strategy informed by the dynamic properties of the constituents (fibre, matrix and fibre/matrix interface) measured with a novel micromechanical testing

methodology. The technological focus is put into the introduction of new composite components into the next generation of aeronautical engines, but the implications are numerous in other sectors where composite materials have been identified as a key enabling technology, such as in transport, energy generation and biomedical applications. To accomplish this, the programme brings together one research institution (IMDEA Materials Institute), two industrial partners (HEXCEL and Micro Materials), one academic institution (The Technical University of Madrid) and a non-profit organization (Madri+d).



The joint academic and industrial training programme offered by this EID will ensure that the innovative aspects of the research work find a quick industrial integration and will provide the ESRs with a truly interdisciplinary and intersectoral training, enhancing their employability and career perspectives.

IMDEA Materials Institute coordinates the DYNACOMP project and will lead the scientific direction of the programme.

## ACERCOM

“Fibre metal laminates for application in marine renewable energy”

**Funding:** Challenges-Collaboration Programme, Spanish Ministry of Economy, Industry and Competitiveness

**Partners:** ArcelorMittal (Project Coordinator), Technical University of Madrid and IMDEA Materials Institute (Technical Coordinator)

**Duration:** 2016-2019

**Principal Investigator:** Dr. C. González

Marine wind energy is playing a key role in the development of renewable energy. The marine wind resource is greater and of better quality than the land one and this makes possible to install more efficient powerful windmills. Moreover, the environmental impact of those off-shore structures is less than the one created by land wind mills. It can be said that generally speaking, marine wind energy has a great potential both at European and Spanish level. However, the installation and maintenance costs of marine windmills has to be reduced in order to allow an increase of the installed power. The development of novel materials is paramount in order to decrease the installation and maintenance costs of marine windmills since they will allow the manufacture of lighter, more efficient designs. Structural steel has traditionally been the material employed for building windmill towers. However, steel has a series of drawbacks (those associated to its weight, fatigue behaviour and corrosion resistance). The weight reduction in windmill towers





will be achieved by the partial substitution of steel by a lighter, more resistant composite material. These materials are manufactured by intercalating sheets of steel and composites, which are known as fibre metal laminates.

The ACERCOM project will incorporate all the structural and functional requirements needed for the design of a novel fibre metal laminate valid for application in marine renewable energy. The ACERCOM project will analyse valid combinations of composite materials and their manufacturing routes via infusion or via pre-impregnated composites. Those materials will be fully characterized with regards to their mechanical properties, resistance to extreme environments and fire behaviour. The conditions for industrial upscaling (machining, joining, conformability, ...) will be also analysed within the project. Within the framework of this ambitious collaborative project, coordinated by ArcelorMittal, IMDEA Materials Institute will mainly carry out the modelling, fabrication and characterisation of fibre metal laminates for application in marine wind energy.



## OPTIQPAP

“Optimisation of quenched and partitioned steels designed for industrial applications”

**Funding:** Research Fund for Coal and Steel, European Union-Horizon 2020 Programme

**Partners:** IMDEA Materials Institute (project coordinator), Fundació CTM Centre Tecnològic, ThyssenKrupp Steel Europe AG, Universiteit Gent, Centro Sviluppo Materiali, Technische Universiteit Delft and TATA steel Nederland Technology.

**Duration:** 2016-2019

**Principal Investigator:** Dr. I. Sabirov



Despite significant research on microstructure, strength, ductility and strain hardening of advanced high strength steels processed via Quenching and Partitioning (Q&P) in the current literature, their application related performance has not yet been studied. The OptiQPAP project focuses on the intelligent microstructural design in the high strength Q&P steels for simultaneous improvement of various mechanical properties, which are required for their commercialization. Special attention will be paid to fatigue and fracture behaviour, wear resistance, weldability, ductile-brittle transition temperature, high strain rate behaviour and energy absorption, along with the formability and bendability of Q&P steels.

IMDEA Materials coordinates the OptiQPAP project. The main activities of IMDEA Materials in this project include the analysis of microstructure, fatigue and wear mechanisms, the determination of tensile properties, the study of impact behaviour and the investigation of the low cycle fatigue behaviour. Properties of individual phases will be also analysed.

## EMULATE

“Multiscale approach for the simulation of thermomechanical problems under severe conditions: application to machining”

**Funding:** National R&D Programme for Societal Challenges), Spanish Ministry of Economy, Industry and Competitiveness

**Partners:** Mondragón University, Technical University of Madrid and IMDEA Materials Institute (Project Coordinator)

**Duration:** 2016-2018

**Principal Investigator:** Prof. I. Romero

Machining of metals is a crucial manufacturing process whose market is estimated to be of the order of 5% of GDP in developed countries. Despite its relevance, the physics of the problem are not well understood and the precise selection of operation parameters has to be tuned by trial and error in many cases (e.g., to ensure the proper tool life or surface integrity conditions in machined components). The next generation of airplane engines, those that can provide increased thrust with reduced environmental impact, require improved machining technologies that can only come from significant advances in the understanding of this process.

EMULATE proposes a multidisciplinary approach to enhance the comprehension of metal machining. For that, three topics will be analysed in order to improve this technology: 1) the development of accurate material models that incorporate the mechanisms of plasticity at the crystal level, as well as the effect of temperature over them; 2) the implementation of robust numerical methods that can upscale the former material models to the macro scale, and remain accurate despite the large deformations in the workpiece; 3) the validation of all material and numerical models with reliable experimental data coming from machining benchmarks, including temperature and microstructure measurements. IMDEA



Materials' team will be responsible for the formulation, analysis, implementation, and integration of numerical methods for simulation thermomechanical problems. The expected outcomes of the project are of two types: on the one hand, fundamental contributions to material modelling and simulation of thermomechanical processes under severe conditions; on the other, technological improvements in simulation tools and predictive capabilities in machining processes.



## EQUINOX

**“A novel process for manufacturing complex shaped Fe-Al intermetallic parts resistant to extreme environments”**

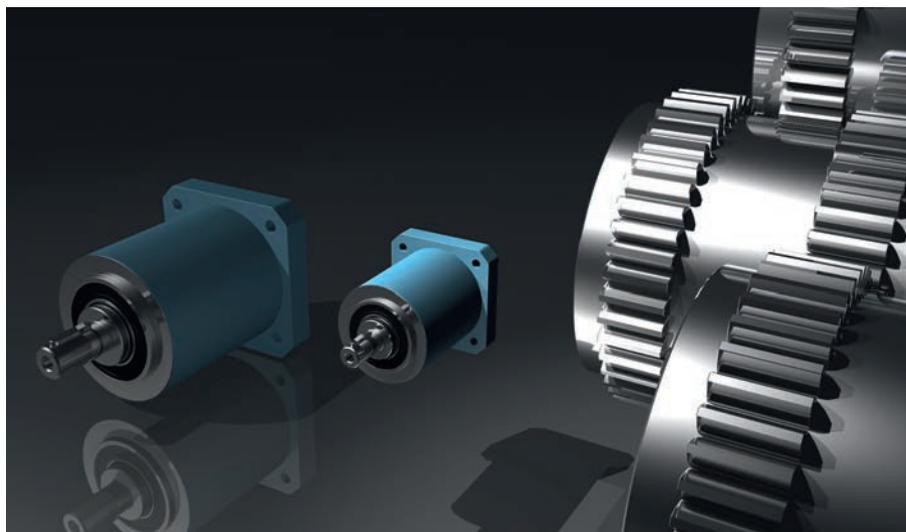
**Funding:** Climate action, environment, resource efficiency and raw materials, European Union-Horizon 2020 Programme

**Partners:** National Technical University of Athens (Project Coordinator), Elastotec GmbH Elastomertechniken, Kochanek Entwicklungsgesellschaft, IMDEA Materials Institute, Technica Univerzita V Liberci, Access e.V., Open Source Management Limited, CES Operations AS, Freni BREMBO Spa, and Yunzhnoye Design Office named after Mikhail Yangel

**Duration:** 2016-2019

**Principal Investigator:** Dr. S. Milenkovic

There is a need to find solutions to replace critical raw materials such as chromium, nickel, molybdenum and vanadium in high volume end consumer products. Steels and superalloys with considerable amounts of these materials are widely used in many industrial applications, particularly under extreme conditions where corrosion and wear resistance are needed. It is generally accepted that intermetallics in particular low cost FeAl offer outstanding material properties. Unfortunately, it is difficult to translate their properties to real products, as intermetallics suffer from low ductility at ambient temperature and poor machinability. The main objective of EQUINOX is to develop a novel process that allows to substitute Cr/Ni based (stainless) steel parts used in high volume end consumer products such as in the lock industry, electronics, process industry



and automotive industry with a novel near net shape production technology for a new class of highly advanced ductile Fe-Al based intermetallics. Ductility at low to medium temperatures, while maintaining good tensile strength and optimum level of residual stress will be based on a radical new production process that use abundant raw material  $\text{Fe}_3\text{O}_4$  and  $\text{Al}_2\text{O}_3$ .

IMDEA Materials Institute's main role in EQUINOX will be to develop a reactive infiltration process with and without the application of pressure. Pressureless infiltration will be performed by drop casting and immersion method. Pressure assisted methods will include suction and centrifugal casting.

## HYDTCOMP

**“Intralaminar hybridization, use of scraps and analysis of their effects. characterisation and modelling”**

**Funding:** National R&D Programme for Societal Challenges), Spanish Ministry of Economy, Industry and Competitiveness

**Partners:** University of Girona (UdG), Project Coordinator) and IMDEA Materials Institute

**Duration:** 2016-2018

**Principal Investigators:** Dr. R. Guzmán de Villoria and Dr. C. S. Lopes

Dimensioning transport structures with civil responsibility (e.g. aircraft) accounting for the materials fragility is the main reason to not take full advantage of the excellent elastic properties of carbon fibre composites. Increasing the energy dissipation in fracture events, expand the strain range at which it occurs and, therefore, reduce their brittleness, would directly result in a weight reduction of the component. It is in this context that a stream of research in the international community focused on providing composite materials with pseudo-ductility, through the intelligent use of different concepts of mixture of constituents, which is called hybridization, emerges.

This project concerns the development of technologies for local hybridization in cases where it is necessary (e.g. hybridization during tow spreading). New techniques will be used as the tow spreading, hybrid unidirectional tapes or laminates combining layers of different thickness (thin and traditional thickness) and / or different nature (carbon-glass, carbon-metal). Also a task will be devoted to the use of scraps of automated carbon fibre manufacturing processes to obtain hybrid laminates. The project will include the development of analytical models, advanced simulations (using high performance computing) and microstructural inspection to acquire a physical understanding of the synergistic effects of the hybridization (not yet reached by the



scientific community). Hybrid panels will be manufactured and the mechanical properties experimentally determined. Constitutive models for these materials will be developed as specific tools for design. IMDEA Materials team will develop the techniques of hybridization at (thin) ply level and hybridization by the use of materials scraps at laminate level. Furthermore, IMDEA Materials subproject will play a key role on characterisation and simulation of hybrid composite materials at micro level leading to an insight on the hybridization effects beyond the state of the art.



ADVANCED MATERIALS AND NANOMATERIALS  
SPANISH TECHNOLOGICAL PLATFORM

**materplat**

## MATERPLAT

“Advanced materials and nanomaterials spanish technological Platform”

**Funding:** Technological Platforms Programme, Spanish Ministry of Economy, Industry and Competitiveness

**Duration:** 2016-2018

**Project Coordinator:** M. A. Rodiel

Driven by the Spanish Ministry of Economy, Industry and Competitiveness, Technological Platforms are public-private team-work structures led by the industry, in which all the stakeholders of the Science-Technology-Innovation Spanish system interested in a given technological field, work together in a coordinated fashion in order to identify and prioritize medium and long term technological, research and innovation needs. Their main goal is the consecution of the scientific and technological advances that ensure the competitiveness, sustainability and growth of our business network, aligning the strategies of the different stakeholders and focusing R&D&I efforts.

The IMDEA Materials Institute is currently the coordinator, holding the Technical Secretariat since the end of 2016, of the Advanced Materials and Nanomaterials Spanish Technological Platform (MATERPLAT). The platform MATERPLAT, is currently presided by AIRBUS and counts on 170 Spanish associated entities, of which 42% are companies, interested in fostering research, development and the application of Advanced Materials and Nanomaterials. The Management Board of the Platform is formed by AIRBUS, ArcelorMittal, Repsol, B/S/H/, Keraben, CEINNMAT, Regemat3D, Aernnova, Acciona, ITP, AMES, AIMPLAS, Ciber-bbn, Ciemat, ITC, Tecnalía, Sernauto, PTE HPC, MEIC, CDTI and of course, the IMDEA Materials Institute.

## NANOFIRE

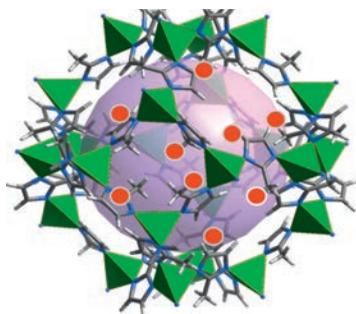
“Nanomaterials via host-guest interaction as multifunctional fire retardants to polymers”

Funding: **China Scholarship Council**

Duration: **2016-2020**

Principal Researchers: **Dr. D. Y. Wang**

The project deals with the development of new generation nanomaterials via host-guest interaction as multifunctional fire retardants for polymers. The aim of this work is not only to improve the flame retardancy and mechanical properties of conventional polymers, but also to transfer properties to the polymers, such as UV resistance, thermal conductivity, etc.



## MULTICOMP

“Multi-Functional Nano-Carbon Composite Materials Network”

Funding: **COST Action, European Union-Horizon 2020 Programme**

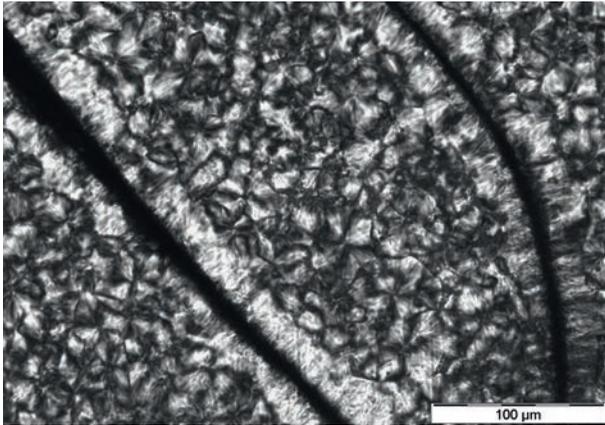
Partners: 31 participating countries, chaired by the Karlsruhe Institute of Technology. IMDEA Materials Institute is one of the representatives of Spain.

Duration: **2016-2020**

Principal Investigator: **Dr. J. P. Fernandez**

MultiComp is a COST Action designed to bring together theorists, experimentalists and industrialists in the field of nano-carbon materials technology. Although carbon nanotubes, graphene and few-layer graphene have been used to improve the properties of composite materials, two main problems remain to be solved before these composite materials can realize their full potential: (1) adequate dispersion of the nano-carbon reinforcement material, and (2) strong enough interfacial bonding between the nano-carbon reinforcement elements and the composite matrix. In addition to making modified Multi Walled Carbon Nanotubes (MWNTs) such as branched-MWNTs, the





Action will explore other possibilities of strengthening composites by integrating few-layer graphene; theoretical modelling of these nano-carbons and composites; development of new composite materials with electronic and multi-functional properties. This Action will provide an ideal platform, especially via short-term scientific exchanges, for permanent established researchers, post-doctoral workers and early-career investigators to enhance their research-related skills as well as their innovation and enterprise skills in this international network involving both academic and business enterprises.



## LIGHTIMP

### “X-ray computed tomography assessment of CNT-based CFRP damaged by impact lightning”

Funding: **Tortech Nano Fibres**

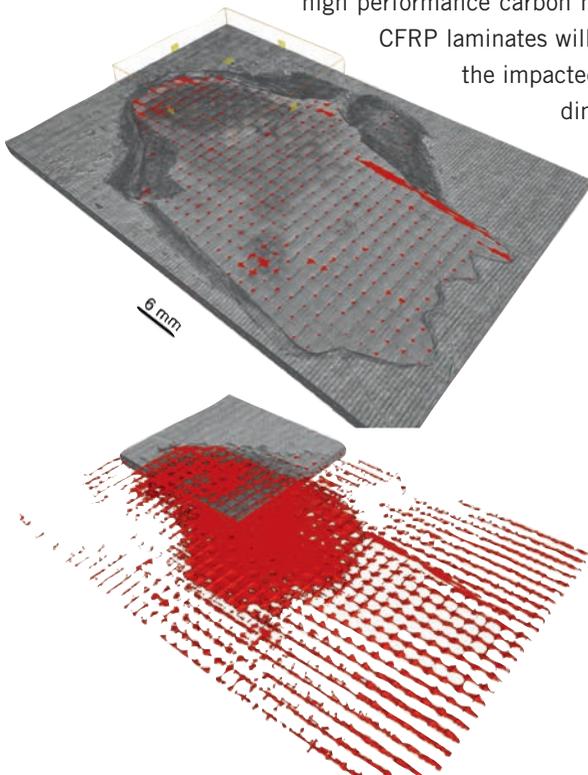
Duration: **2016**

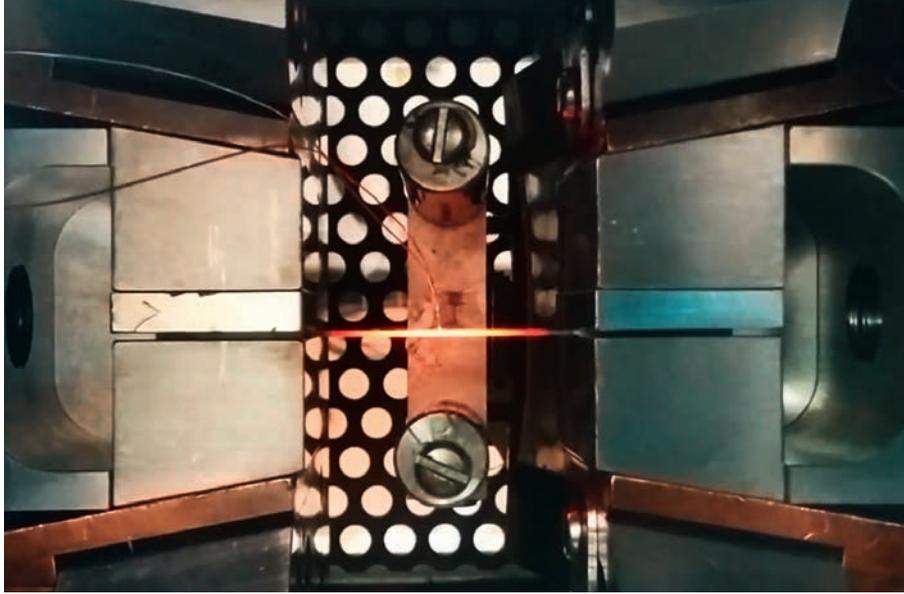
Principal Researchers: **Dr. F. Sket**

The main goal of LIGHTIMP is to analyse, by means of X-ray computed tomography (XCT), the damage generated by lightning impact on carbon fibre reinforced polymers (CFRP) laminates. The laminates’ surfaces will be protected by different amounts of high performance carbon nanotubes (CNT) veils and the typical copper mesh. The

CFRP laminates will be first subjected to lab controlled lightning impact and the impacted laminates inspected by XCT. This non-destructive three-

dimensional technique allowed observing and quantifying the damage generated at the surface and in the interior of the laminates and quantitatively compare the damage generated in the different laminate configurations.





## HIGHRATE

“Mechanical behaviour of advanced high strength steels at high strain rates”

Funding: **China Scholarship Council**

Duration: **2016-2020**

Principal Researchers: **Dr. I. Sabirov**

This main objective of this project is to study high strain rate mechanical behaviour of novel Advanced High Strength Steels (AHSS). The results of these investigations will greatly contribute to understanding of mechanical behaviour of the AHSS and help to reduce the dimensions of the AHSS components used in the automotive industry, and subsequently to reduce the weight of the cars while maintaining or improving their safety.



## CRASHING II

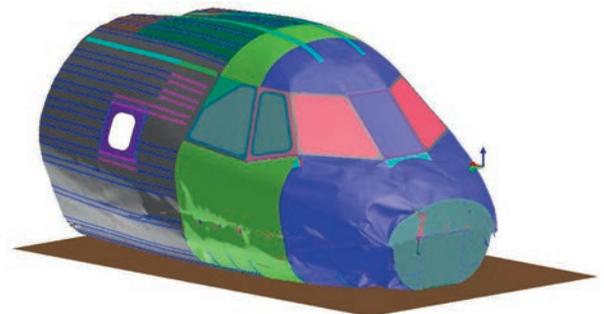
“Front fuselage crashworthiness modelling”

Funding: **Airbus Defense & Sapace**

Duration: **2016-2017**

Principal Researchers: **Dr. C. S. Lopes**

The CRASHING II project is the follow up of the Clean-sky CRASHING project and is focused on the modelling and simulation of the crashworthiness of an aircraft front fuselage using numerical composite material models developed in the initial project. The cabin model will be simulated in different crashing scenarios to evaluate its safety performance and provide design guidelines for future configurations.





## NABISCO

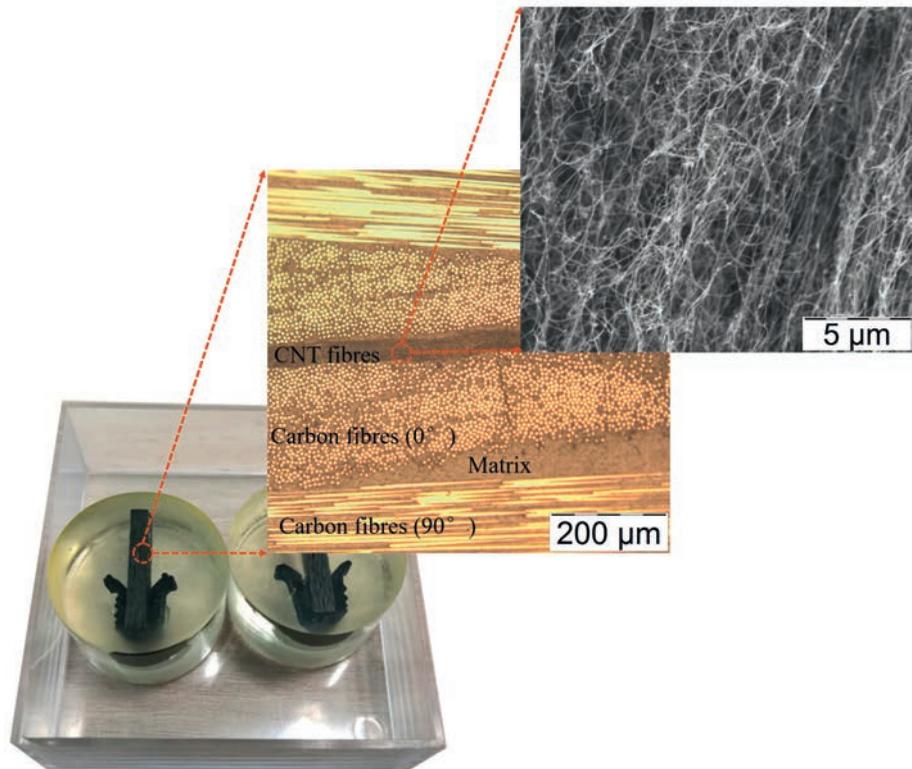
“Integration of carbon nanotubes fibres in structural composites”

Funding: **China Scholarship Council**

Duration: **2016-2020**

Principal Researchers: **Dr. J. J. Vilatela**

The main goal of NABISCO project is the development of strategies to integrate macroscopic fibres and films of CNTs into structural laminate composites. The aim is to improve the mechanical properties of traditional fibre-reinforced polymer composites, while providing them with new functions derived from the unique yarn-like structure of CNT fibres and the low dimensionality of their constituents.



Other ongoing research projects in 2016 at IMDEA Materials Institute were:

### VIRMETAL “Virtual design, processing and testing of advanced metallic alloys for engineering applications”

**Funding:** European Research Council, Advanced Grant, European Union-Horizon 2020 Programme

**Duration:** 2015-2020

**Principal Investigator:** Prof. J. Llorca



### COMETAD “Development of computational and experimental techniques for analysis and design of fire retardant polymers”

**Funding:** National programme for the promotion of excellence in scientific and technical research, Spanish Ministry of Innovation and Competitiveness

**Partners:** International Centre for Numerical Methods in Engineering (CIMNE), Project Coordinator) and IMDEA Materials Institute

**Duration:** 2015-2017

**Principal Investigator:** Dr. D. Y. Wang



### FUTUREALVE “Materials and advanced fabrication technologies for the new generation of high speed turbines”

**Funding:** Centre for Industrial Technological Development (CIEN programme), Spanish Ministry of Economy and Competitiveness and Industria de Turbo Propulsores S.A. (ITP)

**Partners:** National consortium led by ITP. IMDEA Materials Institute collaborates with ITP.

**Duration:** 2015-2016

**Principal Researchers:** Dr. J. Molina and Dr. I. Sabirov



### STEM “Structural energy harvesting composite materials”

**Funding:** Projects Europe Excellence, Spanish Ministry of Economy and Competitiveness

**Duration:** 2015-2016

**Principal Investigator:** Dr. J. J. Vilatela





### MICROFRAC “Visualization and modelling of fracture at the microscale”

Funding: Marie Skłodowska-Curie-IF, European Union-Horizon 2020 Programme

Duration: 2015-2016

Principal Investigator: Dr. A. Weck



### ADVANSEAT “Modular concept for removable advanced car seat”

Funding: Centre for Industrial Technological Development (CIEN programme), Spanish Ministry of Economy and Competitiveness and Grupo Antolin

Partners: National consortium led by Grupo Antolin. IMDEA Materials Institute collaborates with Grupo Antolin.

Duration: 2015-2017

Principal Researchers: Dr. C. González and Dr. C. S. Lopes



### NEOADFOAM “Innovative additives for foams with improved thermal insulation and fire resistance”

Funding: Challenges - Collaboration, Spanish Ministry of Innovation and Competitiveness

Partners: TOLSA S.A. (Project Coordinator), Cellmat group (University of Valladolid) and IMDEA Materials Institute

Duration: 2015-2017

Principal Investigator: Dr. D. Y. Wang



### HIPREP “High Performance Reinforced Fire-retardant Polymers”

Funding: China Scholarship Council

Duration: 2015-2019

Principal Researchers: Dr. D. Y. Wang



### TK-Cobalt “High Throughput Diffusion Experimentation and Computational Thermo-Kinetics for Advanced Co-base High Temperature Alloys”

Funding: China Scholarship Council

Duration: 2015-2019

Principal Researchers: Dr. Y. Cui

## MICROTEST “Correlation study of mechanical properties / microstructure / fracture behaviour of industrial parts and standardized tensile specimens”



Funding: **European Powder Metallurgy Association (EPMA)**

Duration: **2015-2016**

Principal Researchers: **Dr. M. T. Pérez-Prado**

## NearBetaTi “Structural phase transformation under shear and composition gradient in Ti alloys”

Funding: **China Scholarship Council**

Duration: **2015-2019**

Principal Researchers: **Dr. Y. Cui and Dr. J. Molina**



## CRIRCEM “Development of innovative materials for the cutting tool industry”

Funding: **China Scholarship Council**

Duration: **2015-2019**

Principal Researchers: **Dr. A. García-Junceda**



## CRISTAL “Corrosion resistant Zn-Al hypoeutectic alloys”

Funding: **CAPES Foundation, Brazil**

Duration: **2015 - 2016**

Principal Researchers: **Dr. S. Milenkovic**



## EXTRECP “Crystal Plasticity modelling under extreme conditions”

Funding: **China Scholarship Council**

Duration: **2015-2019**

Principal Researchers: **Dr. J. Segurado and Prof. I. Romero**



## FIREINF “Fire retardant epoxy infusion resin composites”

**Funding:** Foundation for the Research Development and Application of Composite Materials (FIDAMC)

**Partners:** Foundation for the Research Development and Application of Composite Materials (FIDAMC) and IMDEA Materials

**Duration:** 2015-2016

**Principal Researchers:** Dr. D. Y. Wang



## CRASHING “Characterisation of structural behaviour for high frequency phenomena”

**Funding:** Clean Sky Joint Undertaking, European Union-7th Framework Programme

**Partners:** IMDEA Materials Institute (Coordinator) and Carlos III University of Madrid

**Duration:** 2014-2016

**Principal Investigator:** Dr. C. S. Lopes

## DESMAN “New structural materials for energy harvesting and storage”

**Funding:** B/E Aerospace Inc (USA)

**Partners:** IMDEA Energy Institute

**Duration:** 2014-2017

**Principal Investigator:** Dr. J. J. Vilatela



## MODENA “Modelling of morphology development of micro- and nano structures”

**Funding:** NMP, European Union-7th Framework Programme

**Partners:** Norwegian University of Science and Technology (Coordinator, Norway), University of Trieste (Italy), BASF SE (Germany), Politecnico di Torino (Italy), Wikki Ltd. (UK), Eindhoven University of Technology (Netherlands), IMDEA Materials Institute (Spain), University of Stuttgart (Germany), Vysolka Skola Chemicko-Technologica (Czech Republic), Deutsches Institut für Normung (Germany)

**Duration:** 2013-2016

**Principal Investigator:** Prof. J. LLorca

## AROOA “Study of the factors influencing air removal in out-of-autoclave processing of composites”

Funding: **Hexcel Composites Limited (UK)**

Duration: **2014-2017**

Principal Investigators: **Dr. F. Sket and Dr. C. González**



## SIMUFOING “Development and validation of simulation methods for ice and bird ingestion in plane engines”

Funding: **Industria de Turbo Propulsores S.A. (ITP)**

Duration: **2014-2017**

Principal Investigator: **Dr. I. Romero**



## NEW EPOXY “New generation high-performance fire retardant epoxy nanocomposites: structure-property relationship”

Funding: **Marie Curie Action - IIF, European Union-7th Framework Programme**

Duration: **2014-2016**

Principal Investigator: **Dr. Jin Tao Wan and Dr. D. Y. Wang**



## SICASOL “Solar-grade silicon: purification in high vacuum furnace”

Funding: **Silicio Ferrosolar S.L (FerroAtlántica Group) and Spanish Centre for Industrial Technological Development (CDTI)**

Duration: **2014-2015**

Principal Investigators: **Prof. J. M. Torralba and Dr. Milenkovic**



## VIRTEST “Multiscale virtual testing of CFRP samples”

Funding: **Fokker Aerostructures B.V.**

Duration: **2014-2017**

Principal Investigator: **Dr. C. S. Lopes**





### EPISIM “Simulation of epitaxial growth”

Area: **Asia / Pacific**  
Duration: **2014-2016**  
Principal Investigator: **Dr. J. P. Balbuena**



### ONLINE-RTM “Online NDT RTM inspection in composites”



Funding: **Centre for Industrial Technological Development (ESTENEA CIEN programme), Spanish Ministry of Economy and Competitiveness and Airbus Operations S.L.**  
Duration: **2014-2016**  
Principal Investigator: **Dr. C. Gonzalez**



**Comunidad de Madrid**



**EUROPEAN UNION**  
STRUCTURAL FUNDS

### DIMMAT “Multiscale design of advanced materials”

Funding: **Regional Government of Madrid**  
Partners: **IMDEA Materials Institute (Coordinator), National Centre for Metals Research (CSIC), Institute for Materials Science (CSIC), Institute for Nuclear Fusion of the Technical University of Madrid (UPM), Department of Materials Science, Technical University of Madrid (UPM), Carlos III University of Madrid and Complutense University of Madrid.**  
Duration: **2014-2018**  
Principal Investigator: **Dr. M. T. Perez-Prado**



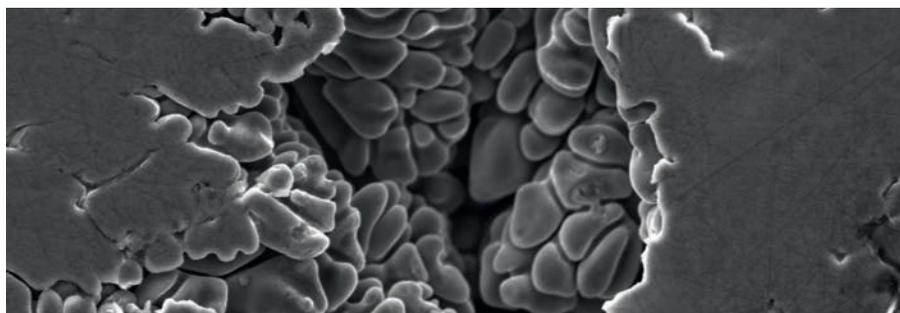
**Comunidad de Madrid**



**EUROPEAN UNION**  
STRUCTURAL FUNDS

### MAD2D “Fundamental properties and applications of graphene and other bidimensional materials”

Funding: **Regional Government of Madrid**  
Partners: **Institute of Materials Science of Madrid (CSIC) (Coordinator), IMDEA Nanoscience Institute, IMDEA Materials Institute, IMDEA Energy and Autonomous University of Madrid.**  
Duration: **2014-2018**  
Principal Investigators: **Dr. J. J. Vilatela and Dr. J. Molina**



## FERROGENESYS “Heat resistant Fe-base alloys for application in generation energy systems”

**Funding:** Spanish Ministry of Economy and Competitiveness

**Partners:** National Centre for Metals Research (CSIC) (Coordinator), Centre for Energy Research (CIEMAT), IMDEA Materials Institute, Centre of Technical Studies and Research and Carlos III University of Madrid.

**Duration:** 2014-2017

**Principal Investigator:** Dr. M. Monclús



## SEPIFIRE “Study of sepiolite-based fire retardant systems”

**Funding:** Spanish Ministry of Economy and Competitiveness

**Partners:** TOLSA S.A. and Institute of Materials Science of Madrid (CSIC)

**Duration:** 2014-2017

**Principal Investigator:** Dr. D.-Y. Wang



## GAS “Glasses and stability Excellence Network”

**Funding:** Spanish Ministry of Economy and Competitiveness

**Partners:** Nanomaterials and Microdevices group from the Autonomous University of Barcelona (Coordinator), Characterisation of Materials group from the Polytechnic University of Catalonia (UPC), Polymer and Soft Materials group from Joint Centre University of the Basque Country University and the Spanish National Research Council, Laboratory of Low temperatures from the Autonomous University of Madrid, Brillouin Spectroscopy Laboratory from the Institute of Materials Science of Madrid and IMDEA Materials Institute.

**Duration:** 2014-2016

**Principal Investigator:** Prof. J. LLorca



## FOTOFUEL “Solar fuels production challenges Excellence Network”

**Funding:** Spanish Ministry of Economy and Competitiveness

**Partners:** IMDEA Energy Institute (Coordinator), Institute of Catalysis and Petrochemistry, Institute of Chemical Research of Catalonia, IMDEA Materials Institute, ALBA, University of Barcelona, Jaume I University, Solar Platform of Almeria, MATGAS.

**Duration:** 2014-2016

**Principal Investigator:** Dr. J. J. Vilatela





### SCREENDM “Screening of kinetic/microstructural information for Ti-alloys by diffusion multiple technique”

Funding: **China Scholarship Council**

Duration: **2014-2018**

Principal Investigator: **Dr. Y. Cui**



### MICROMECH “Microstructure based material mechanical models for superalloys”

Funding: **Clean Sky Joint Undertaking, EU Seventh Framework Programme for Research (FP7)**

Partners: IMDEA Materials Institute

Duration: **2013-2016**

Principal Researcher: **Dr. J. Segurado**



### PilotManu “Pilot manufacturing line for production of highly innovative materials”

Funding: **NMP, European Union-7th Framework Programme**

Partners: MBN Nanomaterialia (Coordinator, Italy), IMDEA Materials Institute (Spain), +90 (Turkey), Putzier (Germany), INOP (Poland), Manudirect (Italy), Centre for Process Innovation (United Kingdom), IMPACT INNOVATIONS GmbH (Germany), Matres (Italy) and Diam Edil SA (Switzerland)

Duration: **2013-2017**

Principal Investigator: **Prof. J. M. Torralba**



### COMPOSE3 “Compound semiconductors for 3D integration”

Funding: **ICT, European Union-7th Framework Programme**

Partners: IBM Research GmbH (Coordinator, Switzerland), STMicroelectronics-Crolles (France), Commissariat a l'Energie Atomique - Leti (France), University of Glasgow (United Kingdom), Tyndall National Institute (Ireland), Centre National de la Recherche Scientifique (France), DTF Technology GmbH (Germany) and IMDEA Materials Institute (Spain)

Duration: **2013-2016**

Principal Investigator: **Dr. A. Sarikov**

## ECURE “Electrically-curable resin for bonding/repair”

Funding: **AIRBUS OPERATIONS S.L. (Spain)**

Duration: **2013-2016**

Principal Investigator: **Dr. J. J. Vilatela and Dr. J. P. Fernández**



## ICMEG “Integrative computational materials engineering expert group”

Funding: **NMP, European Union-7th Framework Programme**

Partners: ACCESS e.V. (Germany), K&S GmbH Projektmanagement (Germany), e-Xtream engineering S.A. (Belgium), IMDEA Materials Institute (Spain), Thermo-Cal Software AB (Sweden), Stichting Materials Innovation Institute (Netherlands), Czech Technical University in Prague (Czech Republic), RWTH Aachen Technical University (Germany), Centre for Numerical Methods in Engineering (Spain), simufact engineering GmbH (Germany) and Kungliga Tekniska Högskolan (Sweden)

Duration: **2013-2016**

Principal Investigator: **Dr. Y. Cui**

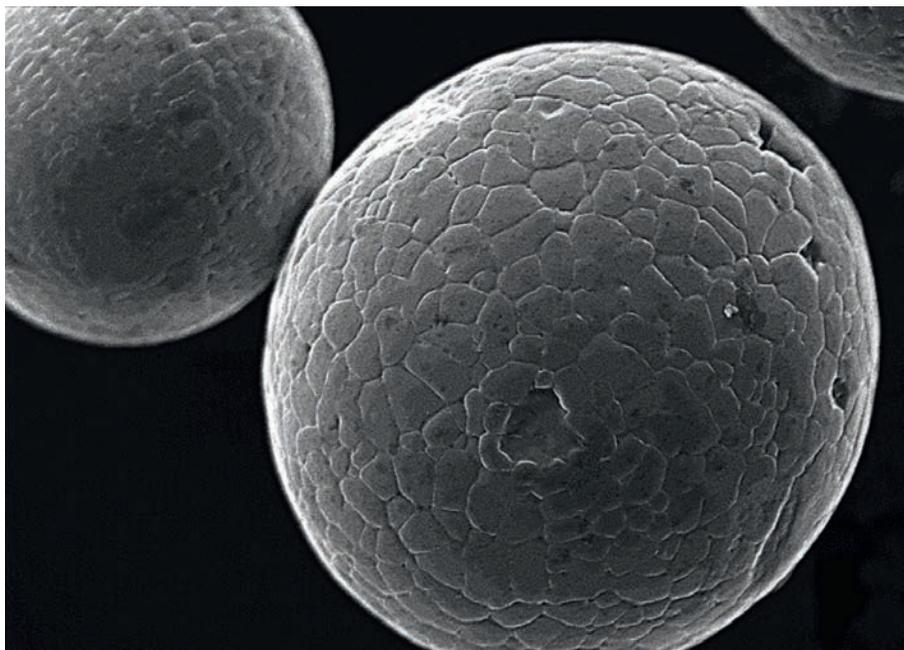


## NFRP “Nano-engineered fibre-reinforced polymers”

Funding: **Marie Curie Action- CIG, European Union-7th Framework Programme**

Duration: **2013-2017**

Principal Investigator: **Dr. R. Guzmán de Villoria**





## ECOPVC “Eco-friendly fire retardant PVC nanocomposites”

Funding: **China Scholarship Council**

Duration: **2013-2017**

Principal Investigator: **Dr. D.-Y. Wang**



## HOTNANOMECH “Nanomechanical testing of strong solids at high temperatures”

Funding: **Spanish Ministry of Economy and Competitiveness**

Duration: **2013-2016**

Principal Investigator: **Dr. J. M. Molina-Aldareguía**



## MUDATCOM “Multifunctional and damage tolerant composites: Integration of advanced carbon nanofillers and non-conventional laminates”

Funding: **Spanish Ministry of Economy and Competitiveness**

Partners: Technical University of Madrid (Coordinator, Spain), IMDEA Materials Institute (Spain) and University of Girona (Spain)

Duration: **2013-2016**

Principal Investigator: **Dr. J. J. Vilatela**



## EXOMET “Physical processing of molten light alloys under the influence of external fields”

Funding: **NMP, European Union-7th Framework Programme**

Partners: Consortium of 26 European partners coordinated by the European Space Agency (France)

Duration: **2012-2016**

Principal Investigators: **Dr. J. M. Molina-Aldareguía and Dr. M. T. Pérez-Prado**



## MUFIN “Multifunctional fibre nanocomposites”

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**

Duration: **2012-2016**

Principal Investigator: **Dr. J. J. Vilatela**



## SIMSCREEN (“Simulation for screening properties of materials”)

Funding: **AIRBUS OPERATIONS S.A.S. (France)**

Duration: **2012-2016**

Principal Investigator: **Dr. C. González**



## ECOFIRENANO “New generation of eco-benign multifunctional layered double hydroxide (LDH)-based fire retardant and nanocomposites”

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**

Duration: **2012-2016**

Principal Investigator: **Dr. D.-Y. Wang**



## ITER PCR “Mechanical analysis ITER Pre-Compression Rings”

Funding: **EADS CASA Espacio (Spain)**

Duration: **2012-2016**

Principal Investigator: **Dr. C. González**



## NECTAR “New generation of NiAl-based eutectic composites with tuneable properties”

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**

Duration: **2012-2016**

Principal Investigator: **Dr. S. Milenkovic**



## VMD (“Virtual Materials Design”)

Funding: **Abengoa Research S. L. (Spain)**

Duration: **2012-2016**

Principal Investigator: **Prof. J. LLorca**





## SIMET “Numerical simulation for metallic fragments impact on composite solutions”

Funding: **AIRBUS OPERATIONS S.L. (Spain)**

Duration: **2015-2016**

Principal Investigators: **Dr. C. González**



## HIFIRE “High performance environmentally friendly fire retardant epoxy nanocomposites”

Funding: **China Scholarship Council (China)**

Duration: **2012-2016**

Principal Investigators: **Dr. D.-Y. Wang and Prof. J. LLorca**



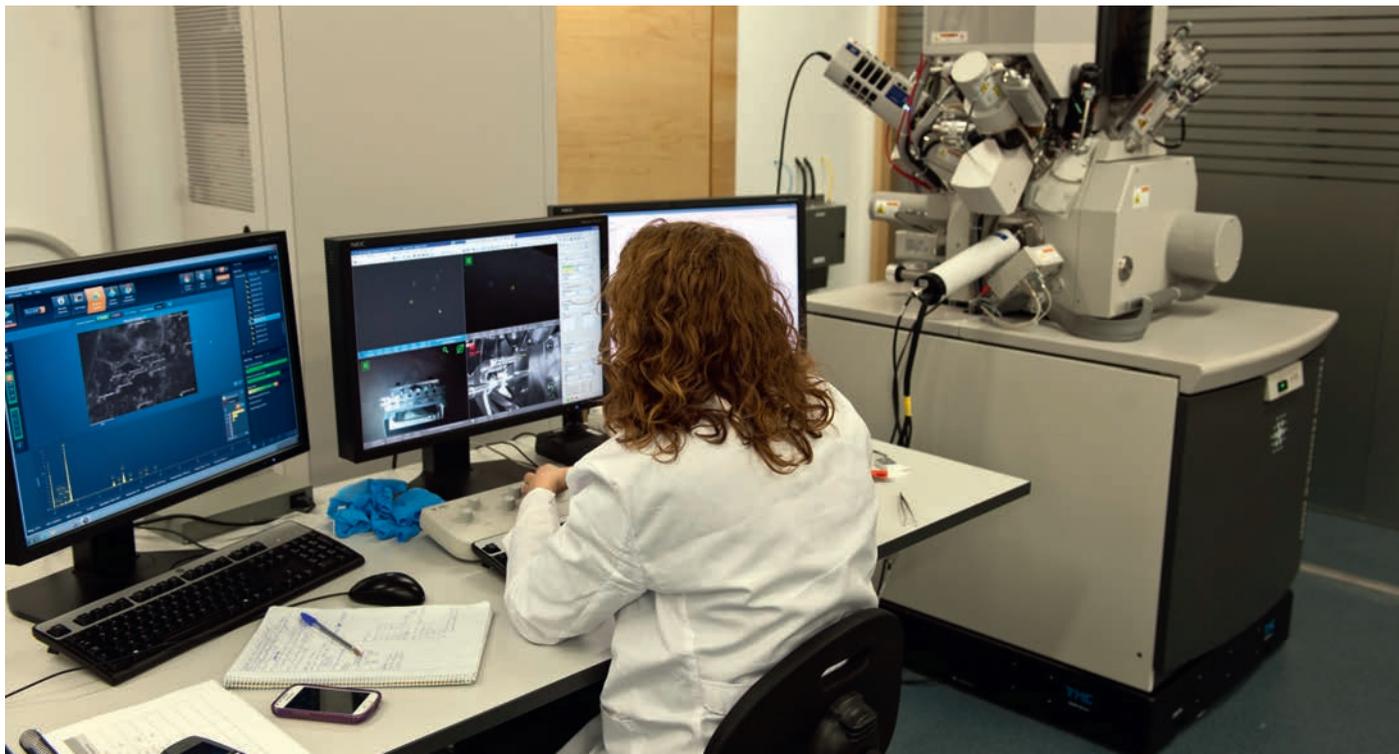
## MAAXIMUS “More affordable aircraft structure lifecycle through extended, integrated, & mature numerical sizing”

Funding: **Transport, European Union-7th Framework Programme**

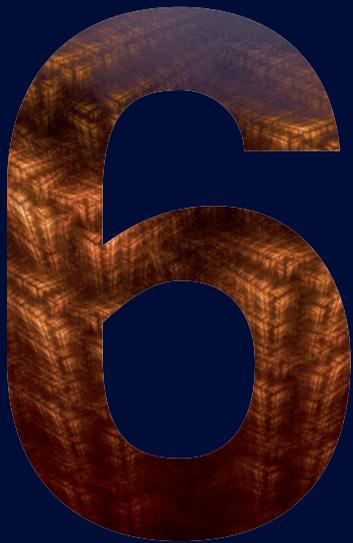
Partners: Consortium of 57 European partners from 18 countries coordinated by AIRBUS OPERATIONS GmbH

Duration: **2008-2016**

Principal Investigator: **Prof. J. LLorca**



# dissemination of results



- 6.1. **Publications [87]**
- 6.2. **Book Chapters [95]**
- 6.3. **International Conferences [95]**
  - 6.3.1. Invited and Plenary talks [95]
  - 6.3.2. Regular contributions [97]
  - 6.3.3. Membership in Organising Committees [101]
- 6.4. **Hosting and organisation of international Conferences and Workshops [102]**
- 6.5. **Invited Seminars and Lectures [103]**
- 6.6. **Seminars [105]**
- 6.7. **Fellowships [106]**
- 6.8. **Awards [107]**
- 6.9. **Institutional Activities [107]**
- 6.10. **Outreach [108]**
- 6.11. **Theses [108]**
  - 6.11.1. PhD Theses [108]
  - 6.11.2. Master/Bachelor Theses [109]
- 6.12. **Internships / Visiting students [110]**
- 6.13. **Courses [114]**

annual report  
2016

## 6.1. Publications

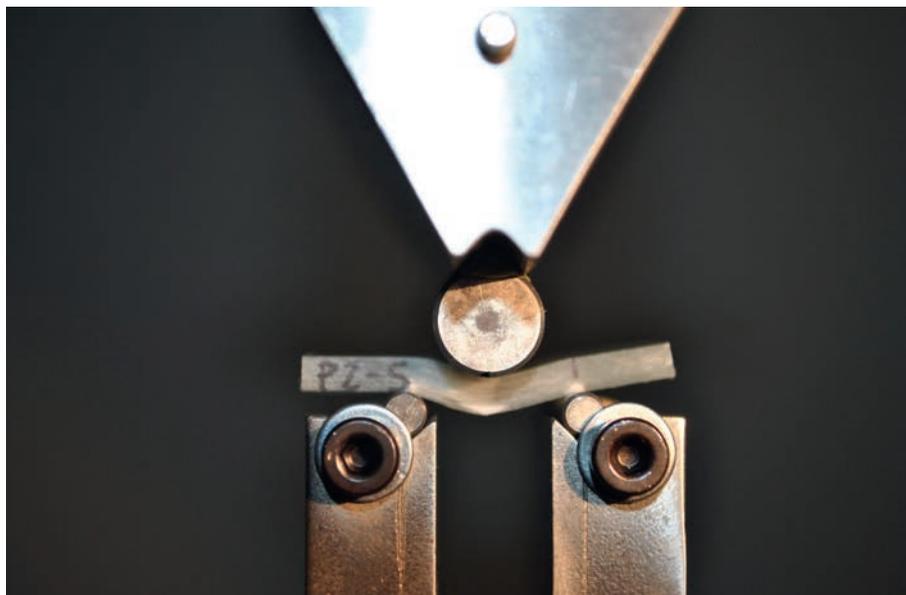
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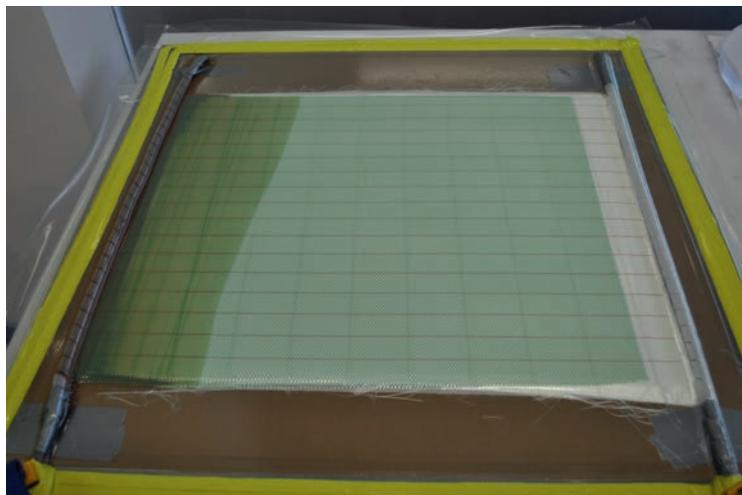
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98. J. S. Moya, A. Martínez, R. López-Píriz, F. Guitián, L. A. Díaz, L. Esteban-Tejeda, B. Cabal, F. Sket, E. Fernández-García, A. P. Tomsia, R. Torrecillas. *Histological response of soda-lime*

*glass-ceramic bactericidal rods implanted in the jaws of beagle dogs.* **Scientific Reports** **6**, 31478, 2016.

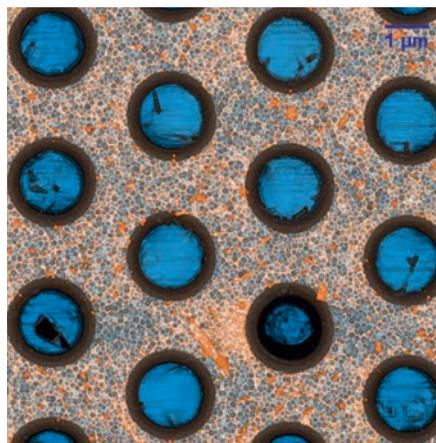
99. W. Guo, B. Gan, J. M. Molina-Aldareguia, J. D. Poplawsky, D. Raabe. *Structure and dynamics of shear bands in amorphous-crystalline nanolaminates.* **Scripta Materialia** **110**, 28-32, 2016.

100. C. M. Cepeda-Jiménez, A. Hernando, J. M. Barandiarán, M. T. Pérez-Prado. *Onset of room temperature ferromagnetism by plastic deformation in three paramagnetic pure metals.* **Scripta Materialia** **118**, 41-45, 2016.

101. A. Sarikov. *Kinetic model of precipitate growth during phase separation in metastable binary solid solutions.* **Solid State Phenomena** **242**, 196-202, 2016.

102. M. Amati, B. Aleman, B. Bozzini, L. Gregoratti, H. Sezen, M. Kiskinova. *Characterization of catalytic materials with scanning photoelectron microscopy: Present and future.* **Surface Science** **652**, 20-25, 2016.

103. C. Li, Z. Ma, X. Zhang, H. Fan, J. Wan. *Silicone-modified phenolic resin: Relationships between molecular structure and curing behavior.* **Thermochimica Acta** **639**, 53-65, 2016.



## 6.2. Book Chapters

1. D. Y. Wang (Editor), **Novel Fire Retardant Polymers and Composite Materials**, Elsevier, 2016.
2. I. Romero, *High Frequency Dissipative Integration Schemes for Linear and Nonlinear Elastodynamics in Structure-preserving Integrators in Nonlinear Structural Dynamics and Flexible Multi-body Dynamics*, Volume 565, Springer, 2016.
3. A. Sarikov, *Thermodynamic study of the phase separation mechanisms in nonstoichiometric Si oxide films during high temperature annealing in Nanomaterials and Nanotechnology*, One Central Press, 2016.
4. J. P. Fernández-Blázquez, *Structure and Dynamics of Main-Chain Liquid Crystalline Polymers with Biphenyl Mesogens in Liquid Crystalline Polymers. Volume 1–Structure and Chemistry*, Springer, 2016

## 6.3. International Conferences

### 6.3.1. Invited and Plenary talks

1. “Multiscale micromechanical model of needle-punched nonwoven fabrics”, F. Martínez-Hergueta, A. Ridruejo, C. González, J. LLorca, **15<sup>th</sup> Gesellschaft für Angewandte Mathematik und Mechanik Seminar on Microstructures**, Paris, France, January 2016.
2. “A multiscale modeling strategy for virtual processing and virtual testing of cast metallic components”, J. LLorca, **Industrial Workshop on Multi-scale and Multi-physics Materials Modeling for Advanced Industries**, Madrid, Spain, January 2016.
3. “Computational micromechanics of composites: a mature discipline?”, C. González, **Multi-scale Modelling of the Structural Integrity of**

**Composite Materials**, Newport Pagnell, United Kingdom, January 2016.

4. “Layer thickness effects on the strength and deformation mechanisms in Al/SiC nanolaminates”, J. M. Molina-Aldareguia, L. Yang, C. Mayer, J. LLorca, N. Chawla, **TMS 145<sup>th</sup> Annual Meeting & Exhibition**. Tennessee, USA, February 2016.
5. “Nanotechnology VS Flammability”, D. Y. Wang, **COST MP1105 Training School on Strategies to study fire behaviours and fire retardant mechanisms**, Barcelona, Spain, February 2016.
6. “Some ideas on new generation flame retardants for polymers”, D. Y Wang, **First International Conference on ECO-friendly Flame Retardant Additives and Materials (ECOFRAM)**, Mons, Belgium, March 2016.
7. “Crystal Plasticity simulations of the mechanical behavior of Mg alloys”, J. Segurado, V. Herrera, R. Sánchez, J. Molina, J. LLorca, **Mach Conference 2016**, Annapolis, USA, April 2016.

8. “Ballistic performance of needle-punched nonwoven fabrics: experiments and modelling”, F. Martínez-Hergueta, A. Ridruejo, C. González, J. LLorca, **Multiscale Modeling of Fibrous and Textile Materials. EuroMech colloquium 569**, Paris, France, April 2016.

9. “CAPSUL: a tool for computational homogenization of polycrystals”, A. Cruzado, B. Bellón, J. Segurado, J. LLorca, **Second International Workshop on Software Solutions for Integrated Computational Materials Engineering**, Barcelona, Spain, April 2016.

10. “A roadmap for virtual processing and virtual testing of cast metallic materials”, J. LLorca, **Second International Workshop on Software Solutions for Integrated Computational Materials Engineering**, Barcelona, Spain, April 2016.

11. "Coupled Nonlinear Ginzburg-Landau and Mechanics Model for Martensitic Transformations in Polycrystals", G. Xu, Y. Cui, **Second International Workshop on Software Solutions for Integrated Computational Materials Engineering**, Barcelona, Spain, April 2016.
12. "ICME – Integrated Computational Materials Engineering for Rare Metallic Materials", Y. Cui, **The 16<sup>th</sup> National Conference on Titanium of China**, Xi'an, China, April 2016.
13. "New approaches to impart flame retardancy to polymers", D. Y. Wang, **Plastic are Future Seminar, AIMPLAS**, Valencia, Spain, April 2016.
14. "Understanding grain size effects in pure Mg polycrystals", C. M. Cepeda-Jiménez, J. M. Molina-Aldareguia, M. T. Pérez-Prado, **International Conference on Processing & Manufacturing of Advanced Materials (THERMEC 2016)**, Graz, Austria, June 2016.
15. "Multifunctional Composites with Macroscopic CNT Fibres", J. J. Vilatela, **Albert Cardon Lecture, 17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, München, Germany, June 2016.
16. "Recent Advances in Nano Fire Retardants", D. Y. Wang, **4<sup>th</sup> International Symposium on Flame-Retardant Materials & Technologies (ISFRMT2016)**, Changchun, China, June 2016.
17. "Role of temperature in the strength of nanolaminates: is smaller always stronger?", J. M. Molina-Aldareguia, **Junior EUROMAT**, Laussane, Switzerland, July 2016.
18. "Advanced characterization of slip and twinning: application to gain basic understanding of plasticity of pure Mg and Mg alloys", C. M. Cepeda-Jiménez, J. M. Molina-Aldareguia, M. T. Pérez-Prado, **International Materials Research Congress (IMRC 2016)**, Cancún, Mexico, July 2016.
19. "A model for the multiscale simulation of thermo-chemo-mechanical problems", I. Romero, **40<sup>th</sup> Solid Mechanics Conference**, Warsaw, Poland, August 2016.
20. "Multiscale computational mechanics of structural materials: composites & metals", J. LLorca, **Biomedical Engineering and Regenerative Medicine Summer School, National University of Ireland**, Galway, Ireland, August 2016.
21. "Microstructure based simulation of fatigue of superalloy inconel 718", J. Segurado, A. Cruzado, S. Lucarini, J. LLorca, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.
22. "Microscale mechanical characterization of fiber, matrix and interfaces in fiber-reinforced composites", J. LLorca, **4<sup>th</sup> International Conference on Nanomechanics and Nanocomposites**, Vicenza, Italy, September 2016.
23. "Exploiting diffusion multiples for efficient alloy design", M. T. Pérez-Prado, C. Wang, Y. Cui, **DARE Annual Workshop 2016**, UK, September 2016.
24. "Effect of microstructure on fatigue behavior of advanced high strength steels produced by quenching and partitioning and the role of retained austenite", I. De Diego-Calderon, A. Lara, J. M. Molina-Aldareguia, R. Petrov, D. De Knif, I. Sabirov, **Materials Science and Engineering 2016 (MSE)**, Darmstadt, Germany, September 2016.
25. "High Throughput Characterization of Microstructure & Micro-Nano Mechanical Properties", Y. Cui, **International Forum of Advanced Materials**, Nanjing, China, September 2016.
26. "Development of a new CrFe-WC cemented carbide processed by field-assisted sintering techniques", A. García-Junceda, I. Sáez, J. M. Torralba, **XXI KONTECH Conference**, Dobiegniew, Poland, September 2016.

invited and plenary talks

27. “Microstructure based simulation of fatigue of superalloy inconel 718”, J. Segurado, **8<sup>th</sup> Multiscale Materials Modeling Conference**, Dijon, France, October 2016.
28. “Retardants Functionalized Nanomaterials: A Promising Way to Improve Fire Safety of Polymers”, D. Y. Wang, **2016 International Seminar on Advanced Materials Research (2016 ISAMR)**, Kunming, China, October 2016.
29. “Microstructural Possibilities of Co-Al-W Alloys Processed by SPS: Effects of Al and W Contents”, M. Cartón-Cordero, R. Casas, M. Campos, J. M. Torralba, **Advances in Materials and Processing Technologies Conference 2016 (AMPT2016)**, Kuala Lumpur, Malaysia, November 2016.
30. “Optimum layer thickness for high temperature mechanical properties of ARB Cu/Nb nanoscale multilayers”, J. Snel, M. Monclús, I. J. Beyerlein, N. A. Mara, J. M. Molina-Aldareguia, J. LLorca, **2016 MRS Fall Meeting & Exhibit**, Boston, USA, November 2016.
31. “Tuning the magnetic properties of metals by severe straining”, C. M. Cepeda-Jiménez, A. Hernando, M. T. Pérez-Prado, **2016 MRS Fall Meeting & Exhibit**, Boston, USA, November 2016.
32. “Application of EBSD-assisted slip trace analysis to unravel the controversial plasticity of polycrystalline magnesium”, C. M. Cepeda-Jiménez, J. M. Molina-Aldareguia, M. T. Pérez-Prado, **4<sup>th</sup> International Conference on Advances in Materials & Materials Processing (iCAMMP-IV)**, Kharagpur, India, November 2016.
33. “Nano fire retardant to polymers: Where we are and where we go”, D. Y. Wang, **12<sup>th</sup> IPF Colloquium on Multifunctional Polymeric Materials: From functional nanofillers to bioinspired materials and smart surfaces**, Dresden, Germany, November 2016.

## 6.3.2. Regular contributions

1. “Anisotropy, size, and aspect ratio effects in micropillar compression of Al-SiC nanolaminate composites”, C. Mayer, Y. Lingwei, S. Singh, Y.-L. Shen, J. M. Molina-Aldareguia, J. LLorca, N. Chawla, **TMS 145<sup>th</sup> Annual Meeting & Exhibition**, Nashville, USA, February 2016.
2. “Un modelo micromecánico del comportamiento en fatiga de una superaleación de base Niquel”, J. Segurado, J. LLorca, A. Cruzado, S. Lucarini, **33 Encuentro del Grupo Español de Fractura**, San Sebastián, Spain, March 2016.
3. “Hardening effect of precipitates against slip and twinning in magnesium-rare earth alloys”, P. Hidalgo-Manrique, J. Robson, M. T. Pérez-Prado, **International Workshop on Mechanistic Behavior of hcp Alloys**, Oxford, United Kingdom, April 2016.
4. “Hierarchical nanoporous silica doped with tin as novel multifunctional hybrid material to flexible PVC”, Y. T. Pan, **COST Action MP1105 Workshop on Innovations in Flame Retardancy of Textiles and Related Materials**, Poznan, Poland, April 2016.
5. “Impact of a novel flame retardant on the properties of reinforced epoxy composites”, D. Y. Wang, **COST Action MP1105 workshop on Innovations in Flame Retardancy of Textiles and Related Materials**, Poznan, Poland, April 2016.
6. “Numerical methods for the solution of non-smooth elasto-visco-plasticity”, D. D. Pozo, I. Romero, **10<sup>th</sup> International Conference on Mechanics of Time Dependent Materials**, Paris, France, May 2016.
7. “Unconditionally energy and entropy stable integration methods for nonlinear models of dissipative solids”, I. Romero, D. Portillo, **IUTAM symposium on Dynamic Instabilities of Solids**, Madrid, Spain, May 2016.

8. "A micromechanical evaluation of the effect of fiber shape in carbon fiber composites", C. González, **5<sup>th</sup> International Carbon Composite Conference (IC3)**, Arcachon, France, May 2016.
9. "Coupled nonlinear Ginzburg-Landau and mechanics model for martensitic transformations in polycrystals", Y. Cui, G. Xu, **CALPHAD XLV**, Awaji Island, Japan, May 2016.
10. "MUESLI: a Material Universal Library", I. Romero, D. Portillo, D. D. Pozo, D. Rodriguez, J. Segurado, **VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2016)**, Crete, Greece, June 2016.
11. "A versatile multiscale framework for the mechanical simulation of nonwovens", A. Ridruejo, F. Martínez-Hergueta, C. González, J. LLorca, **VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2016)**, Crete, Greece, June 2016.
12. "Dual scale vacuum infiltration of fiber-reinforced composites: from in situ synchrotron experiments to numerical simulations", J. Vilá, F. Sket, C. González, J. LLorca, **17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, Munich, Germany, June 2016.
13. "On the effect of fibre shape in fiber reinforced polymers: strength and toughness", M. Herráez, C. González, C. S. Lopes, R. Guzmán de Villoria, J. LLorca, T. Varela, J. Sánchez-Gómez, **17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, Munich, Germany, June 2016.
14. "Mechanisms of air removal and void development in out-of-autoclave processing of hand lay-up laminates", J. J. Torres, F. Sket, C. González, **17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, Munich, Germany, June 2016.
15. "Experimental characterization of triaxial braided composites", A. García-Carpintero, J. W. Roelse, J. J. M. Knippenberg, J. Xu, C. S. Lopes, C. González, **17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, Munich, Germany, June 2016.
16. "Intralaminar fracture toughness characterization: a computational micromechanics perspective", M. Herráez, C. González, C. S. Lopes, **17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, Munich, Germany, June 2016.
17. "Computational micromechanics on polymer matrix composites under different environments: longitudinal, transverse and shear ply properties", F. Naya, C. S. Lopes, C. González, **17<sup>th</sup> European Conference on Composite Materials (ECCM17)**, Munich, Germany, June 2016.
18. "Multifunctional Hybrid Composites for Thermal Barrier and High Temperature Applications", L. C. Herrera-Ramírez, M. Cano, R. Guzman de Villoria, **17<sup>th</sup> European Conference on Composites Materials (ECCM17)**, Munich, Germany, June 2016.
19. "Graphene-based Hybrid Microstructures for Interlaminar Reinforcement of Fiber-reinforced Composites", L. C. Herrera, R. Guzmán de Villoria, **17<sup>th</sup> European Conference on Composites Materials (ECCM17)**, Munich, Germany, June 2016.
20. "Precipitation hardening against slip and twinning in magnesium alloys", P. Hidalgo-Manrique, M. T. Pérez-Prado, J. Robson, **International Conference on Processing & Manufacturing of Advanced Materials (THERMEC 2016)**, Graz, Austria, June 2016.
21. "Use of novel additive alloy melting route for the fabrication of AISI 304 stainless steel modified by Cu additions and subsequent characterization", M. Cristóbal, S. Milenkovic, D. San Martin, C. Capdevila, **XIV Congreso Nacional de Materiales**, Gijón, Spain, June 2016.
22. "Design and characterisation of novel duplex stainless steels processed by field-assisted hot pressing", A. García-Junceda, M. Rincón, J. M.





Torralba, **XIV Congreso Nacional de Materiales**, Gijón, Spain, June 2016.

23. "Effect of the Zr addition on the precipitates of a ferritic ODS steel (14Cr-3W-5Al)", E. Macía, A. García-Junceda, M. Campos, **XIV Congreso Nacional de Materiales**, Gijón, Spain, June 2016.

24. "Development of Co alloys by SPS", M. Cartón-Cordero, M. Campos, L. Antonio Díaz, J. M. Torralba, **XIV Congreso Nacional de Materiales**, Gijón, Spain, June 2016.

25. "Electrospun TiO<sub>2</sub> fibres and their hybridization with nanocarbons: from electronic properties to photocatalytic hydrogen production". A. Moya, A. Cherevan, P. Reñones, A. Molina, A. Castellanos-Gómez, V. A. de la Peña O'Shea, D. Eder, J. J. Vilatela. **ELEN2016- Electrospinning for Energy 2016**, Montpellier, France, June 2016.

26. "Bulk Heterojunction Electrodes Based on CNT fibre/ZnO Hybrids Produced by ALD". A. Monreal-Bernal, A. Moya, N. Kemnade, V. Reguero, B. Mas, E. Senokos, A. S. Cherevan, D. Eder, J. J. Vilatela, **Synchrotron Radiation to study Atomic Layer deposition (SR-ALD) Workshop**, Barcelone, Spain, June 2016.

27. "Synthesis of Kilometers of continuous macroscopic fibres using heterogeneous catalyst", V. Reguero, J. J. Vilatela, **II Young researcher meeting of the Catalytic Spanish Society (SECAT)**, Ciudad Real, Spain, June 2016.

28. "Impact of phenylphosphonate-based flame retardant on mechanical properties and flammability of epoxy and epoxy/glass fiber composite", X. Zhao, **4<sup>th</sup> International Symposium on Flame-Retardant Materials & Technologies (ISFRMT2016)**, Changchun, China, June 2016.

29. "A piezoresistive sensor based on CNT yarns", S. Frutos, J. C. Fernández-Toribio, B. Mas, A. Ridruejo, J. J. Vilatela, **8<sup>th</sup> European Workshop on Structural Health Monitoring (EWSHM 2016)**, Bilbao, Spain, July 2016.

30. "Wettability and infiltration of liquid silicon and aluminum on porous substrates", A. Casado, J. M. Torralba, S. Milenkovic, **6<sup>th</sup> International Congress on Ceramics**, Dresden, Germany, August 2016.

31. "Development of Multifunctional EDLC based on Macroscopic Fibres of CNTs", E. Senokos, V. Reguero, J. Palma, J. J. Vilatela, R. Marcilla, **The 67<sup>th</sup> Annual Meeting of the International Society of Electrochemistry**, The Hague, The Netherlands, August 2016.

32. "Fibre Steering for Composite Panels with Improved Structural Performance", C.S. Lopes, M. Jeliakov, **Brazilian Conference on Composite Materials (BCCM-3)**, Gramado, Brazil, August 2016.

33. "Entropy-Energy-Momentum integration schemes for non-smooth dissipative problems", D. Portillo, J. C. García Orden, I. Romero, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

34. "Temperature dependency of slip and twinning in pure mg studied by nanoindentation", R. Sánchez, J. M. Molina-Aldareguia, J. Segurado, M. T. Pérez-Prado, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

35. "Effect of microstructure on fatigue behavior of advanced high strength steels produced by quenching and partitioning and the role of retained austenite", I. de Diego-Calderón, P. Rodríguez-Calvillo, A. Lara, J. M. Molina-Aldareguia, R. Petrov, D. de Knijf, I. Sabirov, **Materials Science and Engineering 2016 (MSE)**. Darmstadt, Germany, September 2016.

36. "Competing deformation mechanisms in Cu/Nb nanolaminates as a function of layer thickness and temperature", J. LLorca, J. Snel, M. Monclús, J. M. Molina-Aldareguia, N. Mara, I. Beyerlein, **15<sup>th</sup> European Mechanics of Materials**

**Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

37. “Multiscale modelling of the mechanical behavior polyurethane foams”, M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

38. “Microstructure based simulation of fatigue of superalloy Inconel 718”, M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

39. “Implementation of periodic boundary conditions through a penalty method”, C. González, M. Herraes, C. S. Lopes, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

40. “Intralaminar fracture toughness characterization through computational micromechanics”, M. Herraes, S. Sádaba, C. González, C. S. Lopes, J. Segurado, F. Naya, **15<sup>th</sup> European Mechanics of Materials Conference (EMMC 2015)**, Brussels, Belgium, September 2016.

41. “CNT fiber-based multifunctional composites: the understanding the effect of the polymer infiltration on its mechanical and electrical properties”, B. Mas, A. Monreal-Bernal, J. J. Vilatela, **ICNN4 - 4<sup>th</sup> International Conference on Nanomechanics and Nanocomposites**, Vicenza, Italy, September 2016.

42. “Interlaminar and Intralaminar Fracture Behavior of Carbon Fiber Reinforced Polymer Composites”, S. Haldar, C. S. Lopes, C. Gonzalez, **15<sup>th</sup> International Conference on Fracture and Damage Mechanics**, Alicante, Spain, September 2016.

43. “Positive biocompatibility of nanocrystalline glass-like carbón thin films”, N. Rodriguez-Losada, P. Romero, R. Guzman de Villoria, J. A. Aguirre, **XXXVIII Congreso de la Sociedad Española**

**de Ciencias Fisiológicas (SECF)**, Zaragoza, Spain, September 2016.

44. “Multiscale modeling of IN718 superalloy based on micropillar compression and computational homogenization”, A. Cruzado, B. Gan, J. Segurado, J. M. Molina-Aldareguia, J. LLorca, **8<sup>th</sup> Multiscale Materials Modeling Conference**, Dijon, France, October 2016.

45. “Room temperature ferromagnetism in non-magnetic pure metals induced by severe plastic deformation”, C. M. Cepeda-Jiménez, A. Hernandez, M. T. Pérez-Prado, **2016 EMI International Conference**, Metz, France, October 2016.

46. “Enhanced multifunctional properties of UFG Aluminium alloys”, I. Sabirov, R. Z. Valiev, M. Yu. Murashkin, N. A. Enikeev, **2016 EMI International Conference**, Metz, France, October 2016.

47. “Wettability and infiltration of liquid silicon on graphite substrates”, A. Casado, J. M. Torralba, S. Milenkovic, **55<sup>th</sup> National Congress of the Spanish Society of Ceramics and Glass**, Seville, Spain, October 2016

48. “Interface study of nanocarbon/semiconductor hybrids: from photoelectrochemical properties to higher photocatalyst efficiencies”. A. Moya, A. Monreal-Bernal, N. Kemnade, A. Cherevan, D. Eder, J. J. Vilatela, **1<sup>st</sup> Fotofuel School & Conference**, Almería, Spain, October 2016.

49. “Novel WC hardmetal with Cr/Fe binder alloy sintered by SPS”, A. García-Junceda, I. Sáez, J. M. Torralba, **World PM2016 Congress**, Hamburg, Germany, October 2016.

50. “Characterisation of duplex stainless steels sintered by field-assisted hot pressing (FAHP)”, A. García-Junceda, M. Rincón, J. M. Torralba, **World PM2016 Congress**, Hamburg, Germany, October 2016.

51. “Mechanical Behaviour of Novel Sintered Co-Al-W Alloys at high Temperatures”, M. Cartón-Cordero, M. Campos, J. M. Torralba, S. Neumeier, L. Freund, M. Kolb, **World PM2016 Congress**, Hamburg, Germany, October 2016.
52. “Influence of Zirconium addition on the different precipitates of ODS ferritic steel”, E. Macía, A. García-Junceda, M. Campos, **World PM2016 Congress**, Hamburg, Germany, October 2016.
53. “PVDF transcrystallinity induced by Carbon Nanotube Fibres”, A. Monreal, J. J. Vilatela, J. P. Fernández-Blázquez, **Workshop on Multifunctional Nano-Carbon Composite Materials**, Crete, Greece, October 2016.
54. “Zr source on oxide dispersion in ferritic ODS steel with addition of group 4 elements (Y-Al-Ti-Zr)”, E. Macía, J. Cornide, A. García-Junceda, M. Campos, J. M. Torralba, **Advances in Materials and Processing Technologies Conference 2016 (AMPT2016)**, Kuala Lumpur, Malaysia, November 2016.
55. “Mechanical Properties of Metal-Ceramic Nanolaminates: Effect of Constrain and Temperature”, L. W. Yang, J. M. Molina-Aldareguia, C. Mayer, N. Chawla, N. Li, N. Mara, J. LLorca, **2016 MRS Fall Meeting & Exhibit**, Boston, USA, November 2016.
56. “In situ synchrotron experiments of crack nucleation and propagation in Ni-based superalloys: experimental results and crystal plasticity modelling”, D. González, M. Jiménez, J. M. Molina-Aldareguia, J. Segurado, J. LLorca, J. Kelleher, A. King, W. Ludwig, C. Lupton, J. Tong, T. Wigger, **2016 MRS Fall Meeting & Exhibit**, USA, November 2016.
2. **14<sup>th</sup> International Conference on Reliability and Stress-Related Phenomena in Nanoelectronics – Experiments and Simulations**. J. M. Molina-Aldareguia (Co-chair). Bad Schandau, Germany, May 2016.
3. **VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS)**. J. LLorca (Organizer of the International Symposium on Integrated Computational Materials Engineering). Crete, Greece, June 2016.
4. **17<sup>th</sup> European Conference on Composite Materials**. C. S. Lopes and C. González. (Co-Organizers of the sessions on Novel composite microstructures: design and/or prototyping, on Dynamic Loading - Impact, Crash, Blast and on Ground-Based Transportation). Munich, Germany, June 2016.
5. **17<sup>th</sup> European Conference on Composite Materials**. C. González. (Co-Organizer of the sessions on Fracture and Damage Micromechanics, and on Process Simulation I. Draping and LCM). Munich, Germany, June 2016.
6. **15<sup>th</sup> European Mechanics of Materials Conference 2016**. C. González (Organizer of the minisymposium on Mechanics of Composites: Experiments and models). Brussels, Belgium, June 2016.
7. **International Conference on Research, Innovation and Leadership at the Crossroads of Science, Engineering and Medicine**. J. LLorca (Co-organizer). Madrid, Spain, July 2016.
8. **International Forum of Advanced Materials**. Y. Cui. (Organizer of the symposium on the Materials Genome Initiative). Nanjing, China, September 2016.
9. **Thermodynamic of Alloys (TOFA2016)**. S. Milenkovic. (Member of the International Scientific Advisory Board). Santos, Brazil, September 2016.

### 6.3.3. Membership in Organising Committees

1. **COST MP1105 Training School on Strategies to study fire behaviours and fire retardant mechanisms**. D. Y. Wang (Co-organizer). Barcelona, Spain, February 2016.

#### 6.4. Hosting and organisation of international Conferences and Workshops

One international conference and two international workshops were organised by IMDEA Materials Institute in 2016. Those events were held at the institute, taking advantage of the facilities available in our building.

One of the conferences was an initiative of a group of friends and colleagues to honor **Prof. Subra Suresh** on occasion of his sixtieth birthday. Over 150 representatives of global research, gathered around Professor Subra Suresh, President of Carnegie Mellon University, to discuss about interdisciplinary of research in Materials, Mechanics, Engineering and Medicine.

**1. 7<sup>th</sup> International Conference on Composites Testing and Model Identification**, C. Gonzalez and C. S. Lopes (Chairmen), April 2015

**2. "Testing and Characterisation of Composite Materials" - Seminar and Demonstration INSTRON ELECTROPULS**, June 2016

**3. "Research, Innovation and Leadership at the Crossroads of Science, Engineering and Medicine"** honoring Prof. Subra Suresh on his sixtieth birthday, Javier Llorca, Ming Dao, Lei Lu and Upadrasta Ramamurty (Chairs), June 2016



**Research, Innovation and Leadership  
at the Crossroads of Science,  
Engineering and Medicine**

conferences  
and workshops

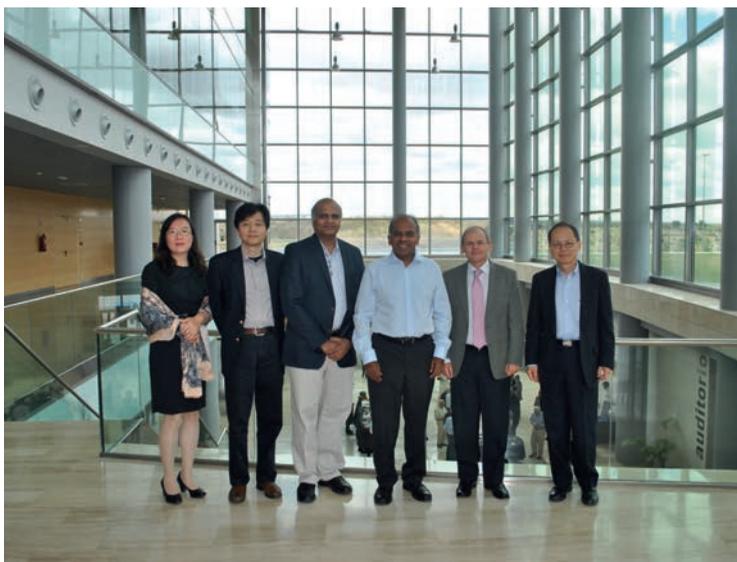
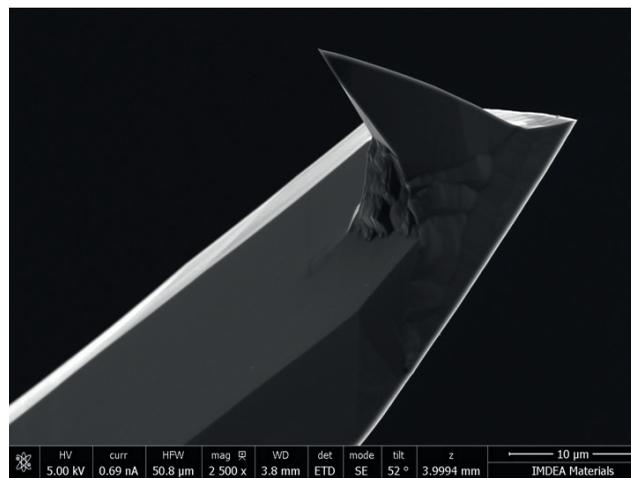


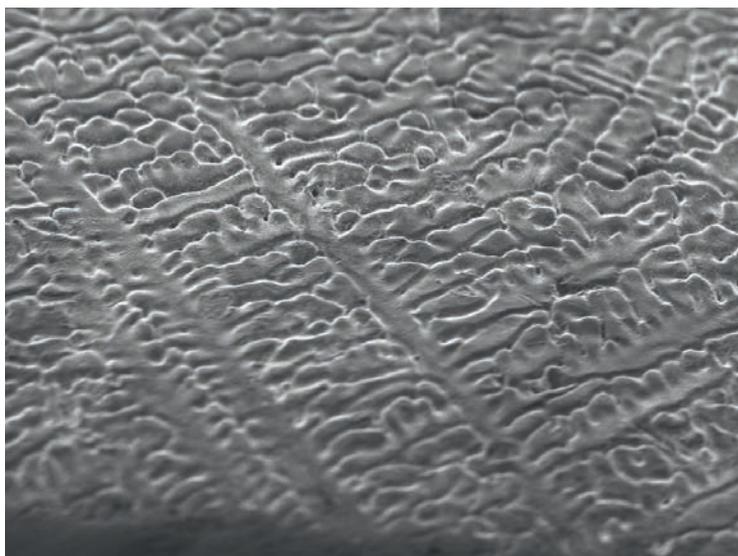
Figure 5. From left to right, Prof. Lei Lu, Prof. Ming Dao, Prof. Upadrasta Ramamurty, Prof. Subra Suresh, Prof. Javier Llorca and Prof. Jimmy Hsia during the Conference to honor Prof. Subra Suresh on his sixtieth birthday at IMDEA Materials Institute.

## 6.5. Invited Seminars and Lectures

1. “*Multiscale Modelling of Composites: Towards Virtual Testing and Design*”, C. S. Lopes, **University of Oxford**, Oxford, United Kingdom, February 2016.
2. “*Multiscale Virtual Analysis of Composites: from microscale to non-conventional structural designs*”, C. S. Lopes, **NASA Langley Research Centre (LaRC)**, Langley, USA, February 2016.
3. “*Multiscale Virtual Analysis of Composites: from microscale to non-conventional structural designs*”, C. S. Lopes, **University of South Carolina**, Columbia, USA, February 2016.
4. “*Multiscale modelling of structural materials: roadmaps for virtual testing of composites & metallic alloys*”, J. LLorca, Department of Mechanical Engineering, **National University of Singapore**, Singapore, Singapore, March 2016.
5. “*Advanced characterization of slip and twinning activity in pure Magnesium*”, M.T. Pérez-Prado, Department of Materials Science and Metallurgy, **University of Cambridge**, Cambridge, UK, April 2016.
6. “*Multiscale modelling of structural materials: roadmaps for virtual testing of composites & metallic alloys*”, J. LLorca, State Key Laboratory of High Performance Complex Manufacturing, College of Mechanical and Electrical Engineering, **Central South University**, Changsa, China, May 2016.
7. “*A multiscale modelling strategy for virtual design of composites metallic materials*”, J. LLorca, College of Materials Science and Engineering, **Central South University**, Changsa, China, May 2016.
8. “*A multiscale modelling strategy for virtual design of composites metallic materials: application to Ni-based superalloys*”, J. LLorca, School of Materials Science, **Northwestern Polytechnical University**, Xi’an, China, May 2016.
9. “*High temperature mechanical performance of metallic and metal-ceramic nanoscale multilayers*”, J. LLorca, State Key Laboratory for the Mechanical Behavior of Materials, **Xi’an Jiaotong University**, Xi’an, China, May 2016.
10. “*High temperature mechanical performance of metallic and metal-ceramic nanoscale multilayers*”, J. LLorca, Department of Mechanical and Civil Engineering, **California Institute of Technology**, Pasadena, Usa, May 2016.
11. “*New generation fire-retardant polymer nanocomposites*”, D. Y. Wang, **Shenyang University of Chemical and Technology**, Shenyang, China, June 2016.
12. “*Virtual testing of metallic materials: from nanomechanical testing to simulation of macroscopic properties*”, J. Segurado, J. LLorca, Interdisciplinary Centre for Advanced Materials Simulation, **Ruhr-Universität Bochum**, Bochum, Germany, July 2016.
13. “*Fire retardant polymers*”, D. Y. Wang, **Oriental YUHONG Company**, Beijin, China, July 2016.



14. "Molecular design VS Fire retardancy of polymers", D. Y. Wang, **Beijing Institute of Fashion Technology**, Beijing, China, July 2016.
15. "New approaches to impart flame retardancy to polymers", D. Y. Wang, **Xi'an Jiaotong University**, Xi'an, China, July 2016.
16. "Computational micromechanics of structural materials", J. LLorca, **CENAERO**, Charleroi, Belgium, September 2016.
17. "IMDEA Materials Institute and research activities on steels". I. Sabirov. **Arcelor Mittal Global R&D Auto**, Maizières lès Metz, France, October 2016.
18. "Multiscale Predictive Virtual Testing: a roadmap to efficient design and optimization of composites for structural integrity", C. S. Lopes, **United States Air Force Research Lab (AFRL)**, Wright-Patterson, USA, October 2016.
19. "Some ideas on fire retardancy of polymeric materials", D. Y. Wang, **Zhejiang University**, Hangzhou, China, October 2016.
20. "New generation eco-friendly fire retardant polymeric materials", D. Y. Wang, **South China University of Technology**, Guangdong Sheng, China, October 2016.
21. "Mechanical properties of metal-ceramic nanolaminates", J. M. Molina-Aldareguia, **Institute of Metals Research (IMR)**, Shenyang, China, November 2016.
22. "Using nanoindentation to assess slip and twinning activity in Mg between RT and 300 °C", J. M. Molina-Aldareguia, **Northwestern Polytechnic University**, Xi'an, China, November 2016.
23. "Micro and Nanomechanical testing oriented to fast material design", J. M. Molina-Aldareguia, **Central South University**, Changsa, China, November 2016.
24. "Mechanical properties of metal-ceramic nanolaminates", J. M. Molina-Aldareguia, **Xi'an Jiaotong University**, Xi'an, China, November 2016.
25. "A multiscale modelling strategy for virtual design of metallic alloys", J. LLorca, Department of Mechanical Engineering, **Stanford University**, Palo Alto, USA, November 2016.
26. "A multiscale modelling strategy for virtual design of metallic alloys", J. LLorca, **Los Alamos National Laboratory**, Los Alamos, USA, November 2016.
27. "High temperature mechanical performance of metallic and metal-ceramic nanoscale multilayers", J. LLorca, Department of Materials Science and Engineering, **University of Texas at Arlington**, Arlington, USA, November 2016.
28. "Computational micromechanics of structural materials", J. LLorca, School of Engineering and Applied Sciences, **Harvard University**, Cambridge, USA, November 2016.
29. "Innovative high-throughput methods for alloys fabrication in bulk form", S. Milenkovic, **ACCESS**, Aachen, Germany, December 2016



## 6.6. Seminars

1. "Nanoscale engineering and electrochemical approaches to next-generation energy storage" **Dr. Vinodkumar Etacheri** (from Purdue University). January 2016.
2. "Photonic devices based in III-V semiconductors", **Dr. Jose María Ulloa**, "AIN microcantilevers" **Dr. Gonzalo Fuentes**, "Graphene electronic devices" **Dr. Javier Martínez** (from Institute of Optoelectronics Systems and Microtechnology, Technical University of Madrid). January 2016.
3. "Laser spinning a new technique for nanofiber production", **Prof. Juan Pou** (from University of Vigo). January 2016.
4. "Simulations of composite reinforcement forming processes" **Prof. Philippe Boisse**, (from University of Lyon) February 2016.
5. "Ductile fracture studies using artificial microvoids in metals and polymers", **Prof. Arnaud Weck** (from University of Ottawa). February 2016.
6. "Tailoring microstructures and interfaces for improving functionalities in ceramics", **Prof. Victor Orera** (from Aragón Materials Science Institute) February 2016.
7. "Magnetorheological elastomers and elastoplastic metallic materials: from micro-deformation mechanisms to instabilities" **Dr. Kostas Danas** (from École Polytechnique, Palaiseau). February 2016.
8. "Industry perspective on ICME modelling approaches for superalloys", **Dr. Raghavendra Adharapurapu** (from General Electric India Technology Centre). February 2016.
9. "Challenges and expectations from modeling infusion-based processes for structural composites", **Prof. Sylvain Drapier** (from École des Mines de Saint-Etienne). February 2016.
10. "New developments for locking problems in Isogeometric Analysis: nearly-incompressibility and solid shells", **Dr. Pablo Antolín** (from University of Pavia). February 2016.
11. "Interdependent modeling and characterization to identify effects of slip transfer at grain boundaries in heterogeneous deformation", **Prof. Thomas R. Bieler** (from Michigan State University). March 2016.
12. "Integration of materials science and structural engineering for the design of advanced materials systems", **Prof. Rigoberto Burgueño** (from Michigan State University). March 2016.
13. "Surprise!... Size matters! Probing the fundamental size dependence of yield strength. – Continuum Mechanics R.I. P.", **Prof. Migel Jennet** (from Coventry University). March 2016.
14. "Fidelity simulation of brittle fracture problems with universal meshes", **Prof. Adrian J. Lew** (from Stanford University). March 2016.
15. "Composite materials, drivers for clean and cost-effective ground transport?", **Dr. Véronique Michaud** (from École Polytechnique fédérale de Lausanne). April 2016.
16. "Computer systems for materials processing technology design", **Dr. Maciej Pietrzyk** (from AGH University of Science and Technology). April 2016.
17. "High strength Copper-Niobium nanomaterials", **Dr. Sezer Özerinç** (from University of Illinois at Urbana-Champaign). May 2016.
18. "Ultrafast laser-matter interactions: mechanical properties and surface texturing", **Prof. Arnaud Weck** (from University of Ottawa). May 2016.
19. "Molecular engineering of materials for high performance and stable perovskite solar cells",

**Prof. Shahzada Ahmad** (from Abengoa Research). May 2016.

20. “Water Splitting: from molecular catalysis to functional devices”, **Mr. Sergi Grau** (from Institute of Chemical Research of Catalonia). May 2016

21. “Hybrid organic-inorganic materials for optoelectronic devices”, **Prof. Rubén D. Costa** (from Friedrich-Alexander-Universität Erlangen-Nürnberg). June 2016.

22. “Material research in the context of nuclear reactor safety” **Mr. Markus Niffenegger & Dr. Vicente Herrera** (from Paul Scherrer Institut). June 2016.

23. “Data-based vibration structural health monitoring methodology for composite laminated structures” **Dr. David García Cava**. (from University of Strathclyde). June 2016.

24. “Bulk nanostructured materials processed by severe plastic deformation. From fundamentals towards applications”, **Dr. Alexander Zhilyaev** (from Institute for Metals Superplasticity Problems of Russian Academy of Science). July 2016.

25. “An overview on the designing of high entropy alloys”, **Dr. Isaac Toda – Caraballo** (from University of Cambridge). September 2016.

26. “Charge and energy transfer processes: From biological photoreceptors to nanostructures”, **Dr. Pedro Brana-Coto** (from Friedrich-Alexander-Universität Erlangen-Nürnberg). September 2016.

27. “Gradient Effects in fracture and damage”, **Dr. Emilio Martínez Pañeda** (from Technical University of Denmark). October 2016.

28. “Fundamentals of creep of materials”, **Prof. Oscar Ruano** (from Spanish National Research Center for Metallurgy). December 2016.

## 6.7. Fellowships

1. AMAROUT EUROPE Programmes (I and II), Marie Curie Action (PEOPLE-COFUND), European Union, 7<sup>th</sup> Framework Programme

- Call 2016: **Dr. S. Djaziri, Dr. S. Haouala, Dr. X. Wen**
- Call 2015: **Dr. M. Haranczyk, Dr. A. Moitra**
- Call 2014: **Dr. V. Babu**

2. Ramon y Cajal Programme, Spanish Ministry of Economy and Competitiveness

- Call 2014: **Dr. J. J. Vilatela**
- Call 2013: **Dr. C. S. Lopes, Dr. M. Haranczyk**
- Call 2012: **Dr. D. Y. Wang**
- Call 2011: **Dr. I. Sabirov**

3. Postdoctoral Fellowship Programmes, Spanish Ministry of Economy and Competitiveness

- Call 2015: **Dr. V. Etacheri, Dr. A. Baluch**
- Call 2013: **Dr. F. Sket**

4. China Scholarship Council

- Call 2016: **C. Fu, Y. Ou, X. Peikang, J. Zhang**
- Call 2015: **J. Li, N. Li, X. Deng, L. Zhang, J. Wang**
- Call 2014: **C. Wang**
- Call 2013: **Y. Pang, Y. Lingwei**
- Call 2012: **Y. Chen, X. Zhao**

5. Training University Lecturers (FPU) Programme, Spanish Ministry of Education, Culture and Sport

- Call 2015: **B. Bellón**
- Call 2014: **L. C. Herrera**

6. Predoctoral Fellowships Programmes, Spanish Ministry of Economy and Competitiveness

- Call 2013: **A. Palomares**

7. Youth Employment Programme, Spanish Ministry of Economy and Competitiveness

- Call 2014: **C. Andradas, J. Castro, M. Cejuela, H. Mora**

8. Youth Employment Programme, Madrid Regional Government

- Call 2016: **A. Doñoro, A. Larrañaga, J. de la Vega, A. Martín**
- Call 2015: **F. Fernández, N. Pérez**

9. Youth Employment Programme – predoctoral researchers, Madrid Regional Government

- Call 2016: **S. Lucarini, C. Gutierrez**

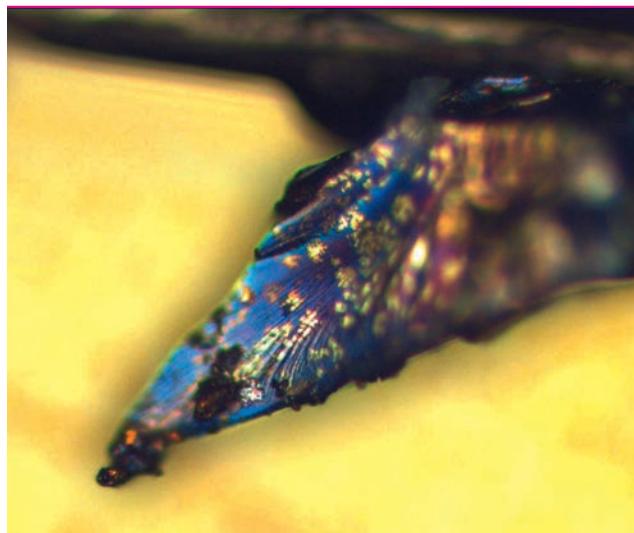
## 6.8. Awards

1. Fellow of the Royal Society of Chemistry  
· **Dr. D. Y. Wang**
2. Elected, Board of Directors of the Society of Engineering Science  
· **Prof. J. LLorca**
3. 2016 Thesis talk award, University Carlos III of Madrid  
· **Marcos Jiménez**
4. 2016 young investigator award, European Society of Composite Materials  
· **Dr. J. J. Vilatela**
5. Fellow of the Leibniz Institute of Polymer Research Dresden  
· **Dr. D. Y. Wang**

## 6.9. Institutional Activities

- Member of the *European Materials Modelling Council* (EMMC).
- Member of the *European Energy Research Alliance* (EERA AISBL).
- Member of the *Executive Committee of the Spanish Association for Numerical Methods in Engineering* (SEMNI).
- Council member of the *International Association for Computational Mechanics* (IACM).
- Member of the *Technical Committee of the M-Eranet* promoted and funded by the European Commission.
- Member of the *European Composites, Plastics and Polymer Processing Platform* (ECP4).
- Local Contact Point of the *EURAXESS* pan-European initiative.
- Technical Secretariat of the *Spanish Technological Platform of Advanced Materials and Nanomaterials* (MATERPLAT).
- Member of the *Board of Directors of the Spanish Association of Composite Materials* (AEMAC).
- Member of the *Spanish Aerospace Platform*.
- Member of the *Spanish Technological Platform for Advanced Manufacturing*.
- Member of the *Technological Clusters on Aerospace, Security and Renewable Energies* promoted by *Madrid Network*.
- Member of the *Network of Research Laboratories of Comunidad de Madrid* (REDLAB).

institutional  
activities



## 6.10. Outreach

- Participation in the Spanish National Radio (RNE) “24 horas”. J. J. Vilatela.
- Training on *Materials for aerospace applications*. Board of European Students of Technology (BEST).
- Collaboration with Formula Student UC3M team.
- Participation in the “XV Semana de la Ciencia”, promoted by *Fundación Madri+d*.
- Participation in the “*European Researchers’ night Madrid 2016*”, promoted by *Fundación Madri+d*.
- Organisation of primary and secondary school visits to IMDEA Materials Institute.

## 6.11. Theses

### 6.11.1. PhD Theses

*“Dual scale flow during vacuum infusion of composites: experiments and modelling”*

Student: Joaquim Vila

Technical University of Madrid

Advisor: Dr. C. González and Prof. J. LLorca

Date of defense: February 2016

*“Atomistic modeling of Ge damage accumulation, amorphization and solid phase epitaxial regrowth”*

Student: José Luis Gómez

Technical University of Madrid

Advisor: Dr. I. Martín-Bragado and Dr. J. Segurado

Date of defense: January 2016

*“Multiscale analysis of the mechanical behaviour of needle-punched nonwoven fabrics”*

Student: Francisca Martínez

Technical University of Madrid

Advisor: Prof. J. LLorca and Dr. C. González

Date of defense: February 2016

*“Multifunctional layered double hydroxide (LDH) based epoxy nanocomposites”*

Student: Ehsan Naderi Kalali

Carlos III University

Advisor: Dr. D. Y. Wang

Date of defense: January 2016

*“Coupled nonlinear Ginzburg-Landau and mechanics model for martensitic transformations in polycrystals”*

Student: Guanglong Xu

Technical University of Madrid

Advisor: Dr. Y. Cui and Prof. J. LLorca

Date of defense: February 2016

*“Assessment of the eutectic trough and properties of a multiphase alloy in the NiAl-Cr-W system”*

Student: Arcadio Varona

Carlos III University

Advisor: Dr. S. Milenkovic

Date of defense: September 2016

# outreach



## 6.11.2. Master/Bachelor Theses

*“Comportamiento mecánico de una aleación Al-Mg-Si de grano ultrafino”*

Student: Edurne Gomez  
Technical University of Madrid  
Advisor: Dr. I. Sabirov  
Date of defense: July 2016

*“Effect of grain refinement on mechanical behavior and biaxial stretching formability of Al 5083 alloy”*

Student: Miguel Angel Valdes  
Technical University of Madrid  
Advisor: Dr. I. Sabirov  
Date of defense: July 2016

*“Preparación de redes poliméricas inteligentes”*

Student: Luis Mario Martín  
Carlos III University  
Advisor: Dr. J. P. Fernández  
Date of defense: October 2016

*“Diseño y caracterización de aceros inoxidables dúplex consolidados mediante la técnica de compactación en caliente asistida por campo eléctrico”*

Student: Víctor Gómez  
Rey Juan Carlos University  
Advisor: Dr. A. García-Junceda  
Date of defense: July 2016

*“Estimación del efecto de las tierras raras en el comportamiento del magnesio mediante ensayos de indentación y modelos de plasticidad cristalina”*

Student: Javier Sánchez  
Technical University of Madrid  
Advisor: Dr. J. Segurado  
Date of defense: June 2016

*“Composite sensors based on CNT fibres”*

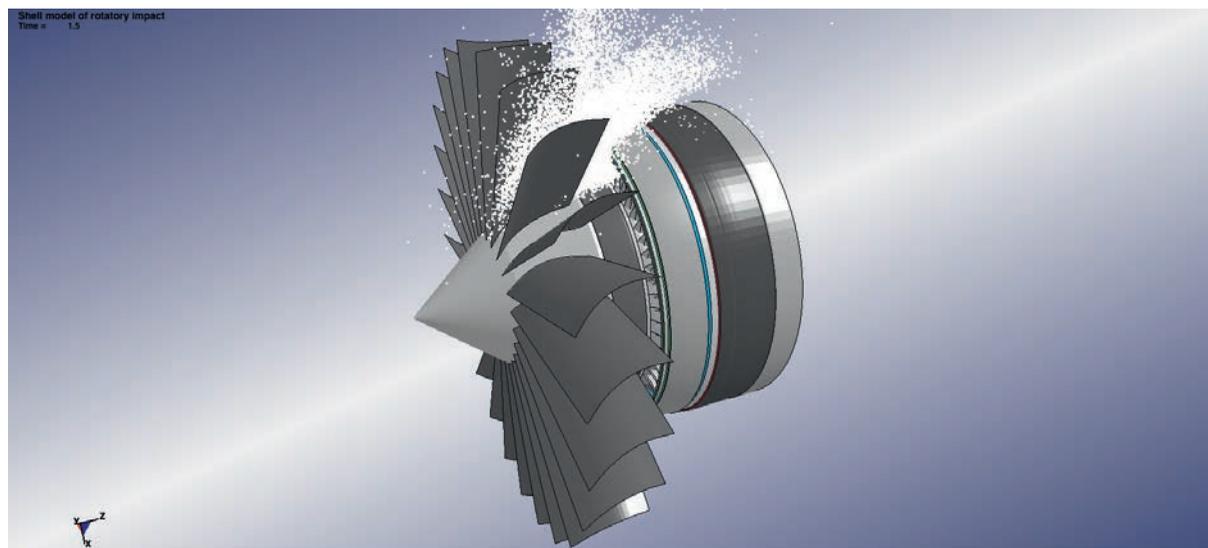
Student: Sergio Frutos  
Technical University of Madrid  
Advisor: Dr. J. J. Vilatela  
Date of defense: August 2016

*“High performance flame retardant polymer foms as new thermal insulators”*

Student: Jose Manuel Rodriguez  
Carlos III University  
Advisor: Dr. D. Y. Wang  
Date of defense: July 2016

*“Preparation and properties of hight performance halogen free flame retardant thermoplastics”*

Student: Javier Rosas  
Carlos III University  
Advisor: Dr. D. Y. Wang  
Date of defense: July 2016



## 6.12. Internships / Visiting students

*“Developing nanostructured TiO<sub>2</sub> electrodes for LI-ON batteries”*

Student: Leyre Maroto

Advisor: Dr. V. Etachery

Visiting student from: Rey Juan Carlos University

Period: August 2016-November 2016

*“In-plane characterization and fracture toughness of tri-axially braided composite materials”*

Student: Jeroen Knippenberg

Advisor: Dr. C. González, Dr. C. S. Lopes and A. García

Visiting student from: Eindhoven University of Technology

Period: February 2016-June 2016

*“Conductividad eléctrica a través del espesor en láminas delgadas de fibra de carbono con adición de nanotubos de carbono”*

Student: Héctor Bautista

Advisor: Dr. C. González and M. Herráez

Visiting student from: Technical University of Madrid

Period: February 2016-July 2016

*“Preparación de laminados híbridos mediante el esparcimiento de mechas. Fabricación de paneles”*

Student: Jonnathan Santos

Advisor: Dr. C. S. Lopes, Dr. C. González and M. Herráez

Visiting student from: University of Girona

Period: July 2016

*“Tomography of single ply tri-axially braided composite panels to obtain the mesh of the unit cell”*

Student: Bas Van Den Beuken

Advisor: Dr. C. S. Lopes, Dr. C. González and A. García

Visiting student from: University of Technology Eindhoven

Period: August 2016-December 2016

*“Micromechanical testing of interfaces of a new composite material for high temperature applications. Nanoindentation test for measuring the strength of interfaces of composite material at RT and different aging conditions”*

Student: Xiaochen Li

Advisor: Dr. C. S. Lopes and Dr. C. González

Visiting student from: University of Southern California

Period: September 2016 -December 2016

*“Nano-architecture and materials design”*

Student: Rubén Lebron

Advisor: Dr. R. Guzmán de Villoria

Visiting student from: Carlos III University

Period: February 2016- April 2016

*“Nano-architecture and materials design”*

Student: Mario Jañez

Advisor: Dr. R. Guzmán de Villoria

Visiting student from: Rey Juan Carlos University

Period: April 2016-June 2016

*“Nano-architecture and materials design”*

Student: Daniel Berlanga

Advisor: Dr. R. Guzmán de Villoria

Visiting student from: Technical University of Madrid

Period: June 2016- August 2016

*“Data-driven discovery of advanced materials. Towards the design of organic molecular-cages-based materials”*

Student: Raúl Pérez

Advisor: Dr. M. Haranczyk

Visiting student from: University of Granada

Period: June 2016-September 2016

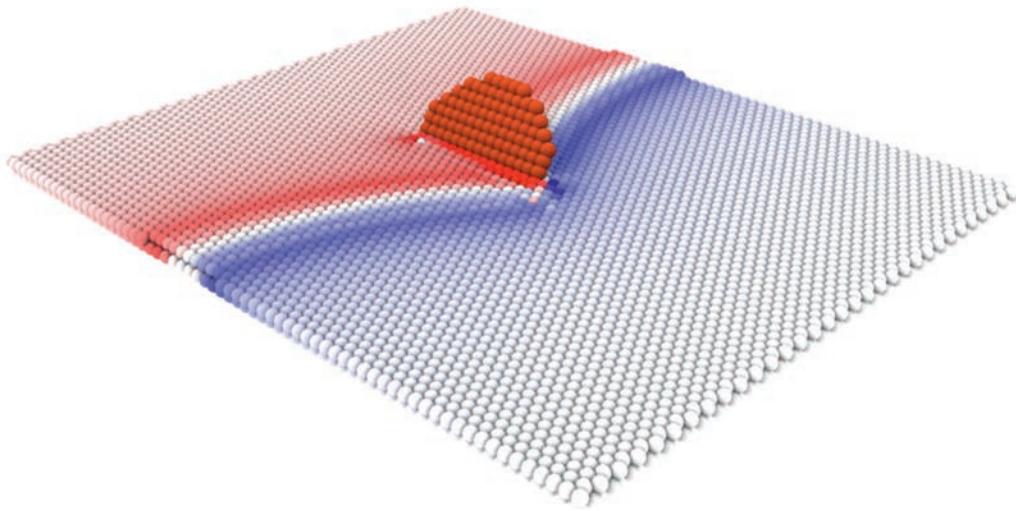
*“Characterization of micropillar behaviour during fracture”*

Student: Valerio Carollo

Advisor: Dr. J. Molina

Visiting student from: IMT School for Advanced Studies Lucca

Period: February 2016-August 2016



*“Life improvement of TiAl blades for new generation of aeroengines”*

Student: Cristina Gutierrez

Advisor: Dr. J. Molina

Visiting student from: University of Oviedo

Period: July 2016-September 2016

*“Study of deformation mechanism of Mn11 Magnesium alloy by slip trace analysis”*

Student: Cristina Prado

Advisor: Dr. M. T. Perez-Prado

Visiting student from: University of Varsovia

Period: June 2016-September 2016

*“Numerical methods for the simulation of explicit contact: application to ice impact”*

Student: Ignacio López

Advisor: Prof. I. Romero

Visiting student from: Technical University of Madrid

Period: June 2016-August 2016

*“Conformabilidad de aceros avanzados de alta resistencia (AHSS) obtenidos vía Q&P”*

Student: Alberto Cabo

Advisor: Dr. I. Sabirov

Visiting student from: Technical University of Madrid

Period: March 2016-June 2016

*“Desarrollo de un modelo micromecánico para la simulación de mecanismos de fluencia en Inconel 718”*

Student: Eva M<sup>a</sup> Andrés

Advisor: Dr. J. Segurado

Visiting student from: Technical University of Madrid

Period: April 2016-July 2016

*“Visualization of fracture at the microscale”*

Student: Sandra Colomina

Advisor: Dr. A. Weck

Visiting student from: Technical University of Madrid

Period: June 2016-July 2016

*“Fabricación de materiales compuestos y caracterización no destructiva por ultrasonidos y tomografía de rayos X”*

Student: Javier Bedmar

Advisor: Dr. F. Sket

Visiting student from: Rey Juan Carlos University

Period: June 2016-August 2016

*“Characterization of a piezoresistive carbon nanotube fiber based sensor for structural health monitoring”*

Student: Sergio Frutos

Advisor: Dr. J. J. Vilatela

Visiting student from: Technical University of Madrid

Period: July 2016- August 2016

*"Micromechanics of CNT fibres"*

Student: Hugo Solera

Advisor: Dr. J. J. Vilatela

Visiting student from: Universidad Iberoamericana

Period: May 2016-August 2016

*"Fabrication of flexible energy storage devices based on nanostructured carbon electrodes"*

Student: Silvia Caminero

Advisor: Dr. J. J. Vilatela, Dr. E. Vinod and Dr. V. Etacheri

Visiting student from: Autonomous University of Madrid

Period: June 2016-September 2016

*"Effect of phosphorus-containing flame retardant on RTM6/Carbon fiber composite: thermal stability, flammability and mechanical properties"*

Student: Juan Picón

Advisor: Dr. D. Y. Wang

Visiting student from: Technical University of Madrid

Period: January 2016-March 2016

*"From functional chemicals to high performance fire safety polymer-based composites"*

Student: Alejandro Jimenez

Advisor: Dr. D. Y. Wang

Visiting student from: Rey Juan Carlos University

Period: January 2016-June 2016

*"Novel Synthesis of hierarchical porous double-shelled hollow hybrid nanomaterials to reinforce multiple properties of flexible polyvinyl chloride film"*

Student: Chengcheng Huang

Advisor: Dr. D. Y. Wang

Visiting student from: Technical University of Madrid

Period: January 2016-June 2016

*"Polymer nanocomposites"*

Student: Leijin Liu

Advisor: Dr. D. Y. Wang

Visiting student from: Technical University of Madrid

Period: February 2016-June 2016

*"Synthesis and polymer processing"*

Student: Xueyuan Gao

Advisor: Dr. D. Y. Wang

Visiting student from: Technical University of Madrid

Period: February 2016-July 2016

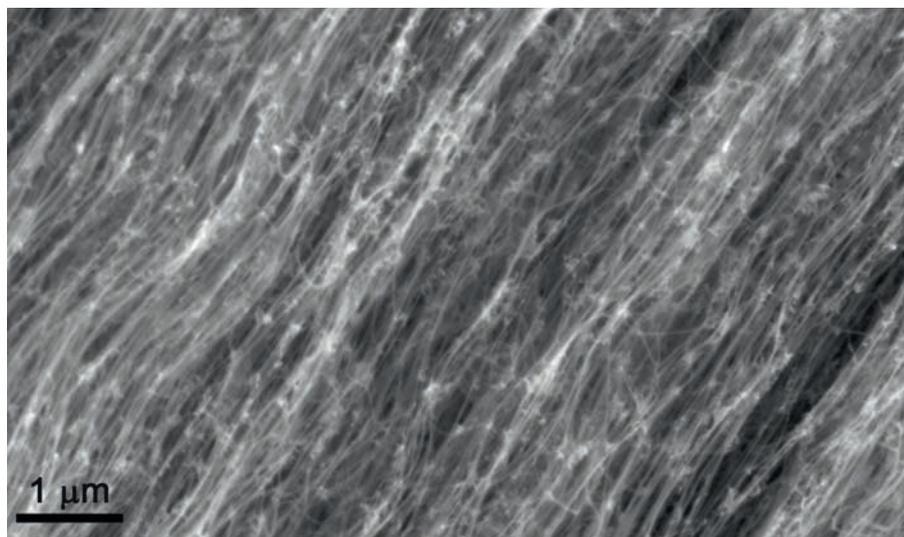
*"Preparation of PU foam"*

Student: Asunción Molina

Advisor: Dr. D. Y. Wang

Visiting student from: Complutense University of Madrid

Period: June 2016-August 2016



*"Functional LDH and its application in polymers"*

Student: Sara Montero

Advisor: Dr. D. Y. Wang

Visiting student from: Carlos III University

Period: June 2016-August 2016

*"Investigation of fire safety behaviors of chemical materials"*

Student: Daniel Fernández

Advisor: Dr. D. Y. Wang

Visiting student from: Rey Juan Carlos University

Period: June 2016-August 2016

*"Fire testing of polymers, preparation of polymer nano-composites and polymer blending"*

Student: Marina García Carrión

Advisor: Dr. D. Y. Wang

Visiting student from: Complutense University of Madrid

Period: July 2016-September 2016

*"Fiber reinforced PLA and its fire retardancy"*

Student: Adriana Pérez

Advisor: Dr. D. Y. Wang

Visiting student from: Autonomous University of Madrid

Period: September 2016-October 2016

*"Fire retardancy of P-containing based polymers"*

Student: Ceren Suer

Advisor: Dr. D. Y. Wang and N. Pérez

Visiting student from: Yildiz Technical University

Period: November 2016

*"Microstructural and in situ mechanical characterization of  $\gamma$ -TiAl alloy"*

Student: Raúl García

Advisor: A. Palomares and Dr. E. Ruiz Navas

Visiting student from: Carlos III University

Period: November 2015-September 2016

*"Damage tolerance of dispersed plies laminates under low impact velocity: Simulation and validation of an optimisation method"*

Student: Théophile Gaudin

Advisor: Dr. González and Dr. C. S. Lopes

Visiting student from: École Polytechnique fédérale de Lausanne

Date: September 2015-April 2016

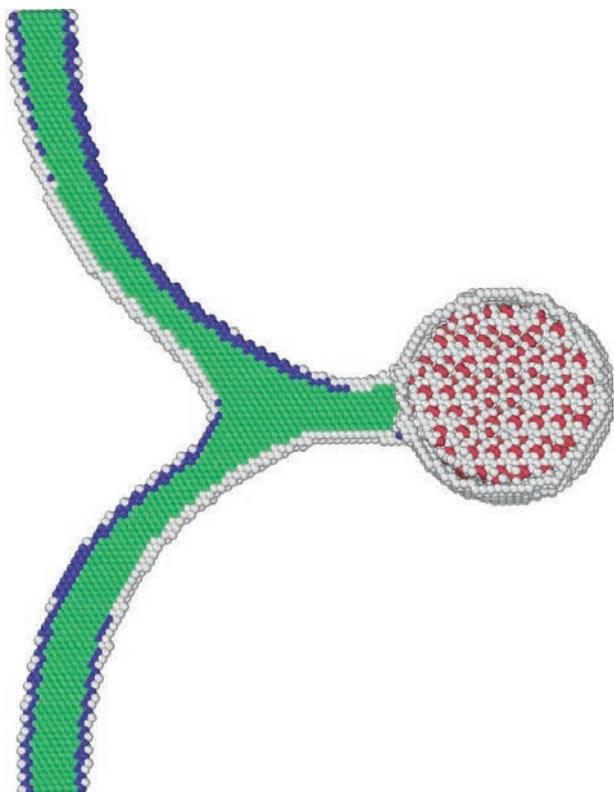
*"Novel duplex stainless steels processed by a powder metallurgy route involving field-assisted sintering technique"*

Student: Coral Henar Díaz

Advisor: Dr. A. García-Junceda

Visiting student from: Carlos III University

Date: November 2015-October 2016



## 6.13. Courses

### *"Hierarchical Composites"*

Master in Composite Materials, Technical University of Madrid and Airbus

Professor: Dr. J. J. Vilatela

### *"Non conventional Composites"*

Master in Composite Materials, Technical University of Madrid and Airbus

Professors: Prof. J. LLorca, Dr. J. J. Vilatela, Dr. R. Guzmán de Villoria, Dr. I. Sabirov

### *"Metal-matrix Composites"*

Master in Composite Materials, Technical University of Madrid and Airbus

Professor: Dr. I. Sabirov

### *"Simulation Techniques and Virtual Testing"*

Master in Composite Materials, Technical University of Madrid and Airbus

Professors: Dr. C. González, Dr. J. Segurado, Dr. C. S. Lopes, Dr. D. Garijo, Dr. J. Múgica

### *"Simulation in Materials Science and Engineering"*

Master in Materials Engineering, Technical University of Madrid

Professors: Prof. J. LLorca, Dr. C. S. Lopes, Dr. C. González, Dr. Y. Cui, Dr. M. Haranczyk

### *"Polymeric Materials for Advanced Applications"*

Master in Materials Engineering, Technical University of Madrid

Professor: Dr. D. Y. Wang

### *"Design and Fabrication of Advanced Composite Materials"*

Master in Materials Engineering, Technical University of Madrid

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### *"Advanced Strength of Materials"*

Master of Industrial Engineering, Technical University of Madrid

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### *"Mechanics of Composite Materials"*

Master in Mechanics, Saint Petersburg State University

Professor: Dr. I. Sabirov

### *"Thermal and Thermomechanical Testing of Materials"*

Master in Materials Science and Engineering, Carlos III University of Madrid

Professor: Dr. S. Milenkovic

### *"Nanomaterials"*

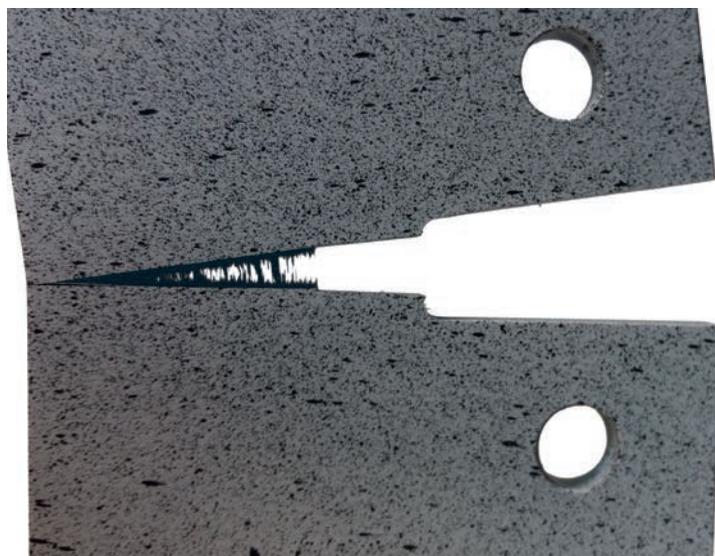
Master in Materials Science, Carlos III University of Madrid

Professor: Dr. J. J. Vilatela

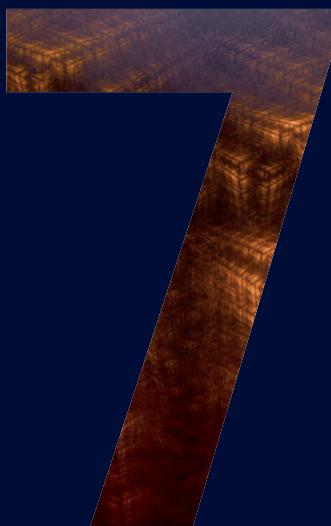
### *"Advanced Composite Materials"*

Master in Materials Science, Carlos III University of Madrid

Professors: Dr. C. S. Lopes, Dr. J. M. Molina



# scientific highlights



- 7.1. **Advanced materials for multifunctional applications [116]**
- 7.2. **Muesli: an open source library for the simulation of materials [120]**
- 7.3. **Design of metallic powders for additive manufacturing [122]**

annual report  
2016

# advanced materials

## Advanced materials for multifunctional applications

applications

### New challenges call for new materials and integration methods

Multifunctionality is a paradigm change in Materials Science and Engineering that aims at producing new materials and structures that can carry out multiple functions simultaneously. This quest is closely related to current technological trends, including the development of flexible optoelectronic devices, smart textiles, more efficient energy management and the electrification of transport. Electric vehicles, for example, require advanced energy storage solutions that are also safe, based on lightweight materials and compatible with mass-production methods. These challenges call for a new generation of advanced materials developed by multidisciplinary teams.

The 34 researchers in the Programme on Advanced Materials for Multifunctional Applications at IMDEA Materials Institute provide a wide expertise in design and synthesis of nanomaterials and their integration in devices and composites with combined fire-safety, high-performance mechanical properties and efficient energy management, amongst other properties.

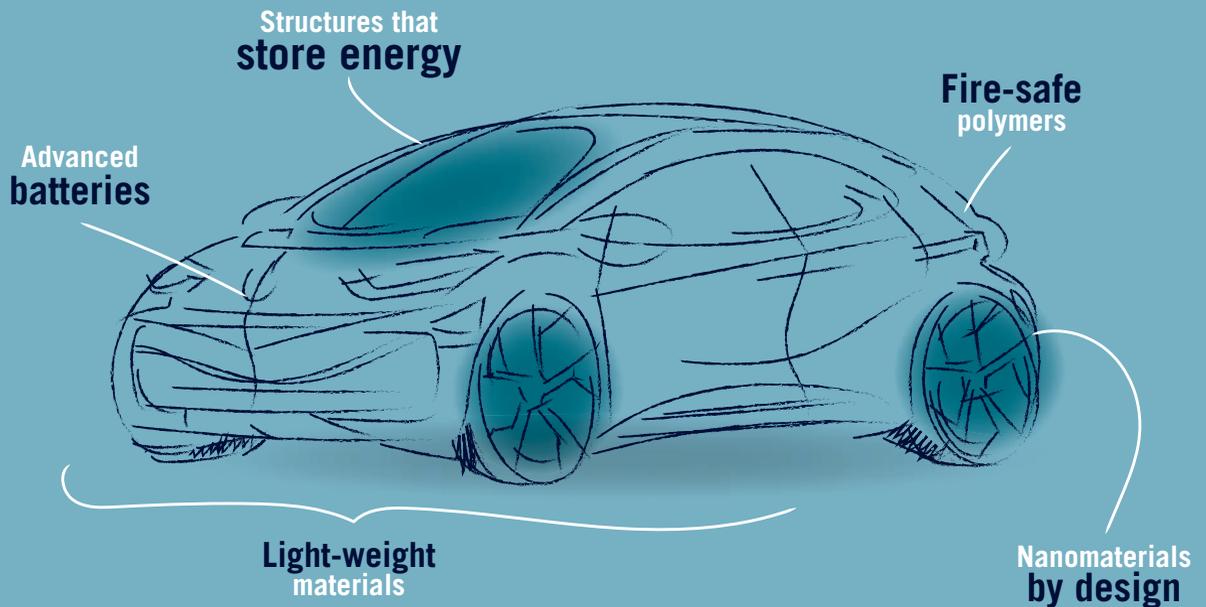


Figure 1. Multifunctional requirements envisaged in the next generation of electrical vehicles

# for multifunctional

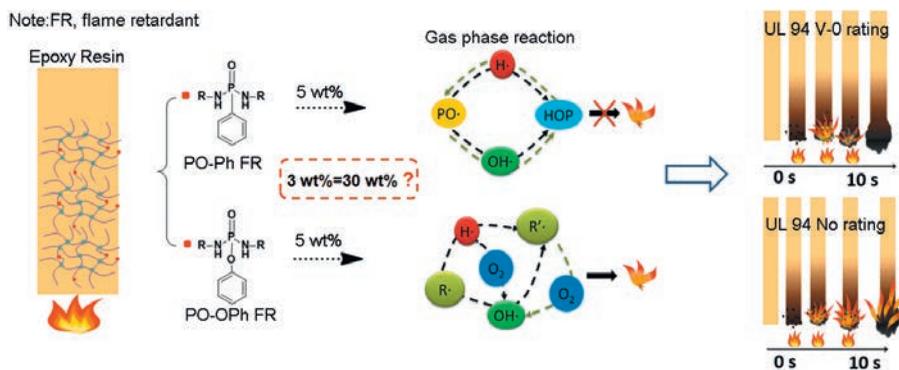


Figure 2. Impact of flame retardant's molecular design on the fire retardant efficiency of epoxy.

In the context of composite safety, the activities of the Programme include the development of eco-benign fire retardant materials and high performance environment-friendly polymers and composites using novel bio-based polymers and innovative synthetic chemistry and advanced processing methods. Our researchers have studied, for example, the synthesis, fire behaviour and mechanical properties of epoxies with halogen-free flame retardants [1].

Since mid-2016, researchers at IMDEA Materials Institute have also been active in the fabrication of new electrodes for ultrafast Li/Na ion storage based on new architectures combining advanced inorganic materials and porous nanocarbon scaffolds produced in-house (Figure 3 a-b), and using chemical methods to tailor interfaces for efficient charge storage and reduced fire hazard. There is rapid progress in the assembly and evaluation of batteries (Figure 3c) under operational conditions.

Nanocarbons are ideal elements in electrodes used for charge storage or charge transfer. Assembled as macroscopic fibres of long aligned CNTs, these materials combine very high electrical conductivity, chemical resistance and a large porosity to host other phases. Furthermore, their yarn-like network structure implies that they can simultaneously play the role of current collector and reinforcement in a composite. Work in the Programme aims at using CNT fibres in various structural energy managing composites. With reversible Li-ion intercalation (Figure 3d) capacity similar to commercial graphite anodes and toughness superior to that of Kevlar, the starting point for this work is encouraging [2].

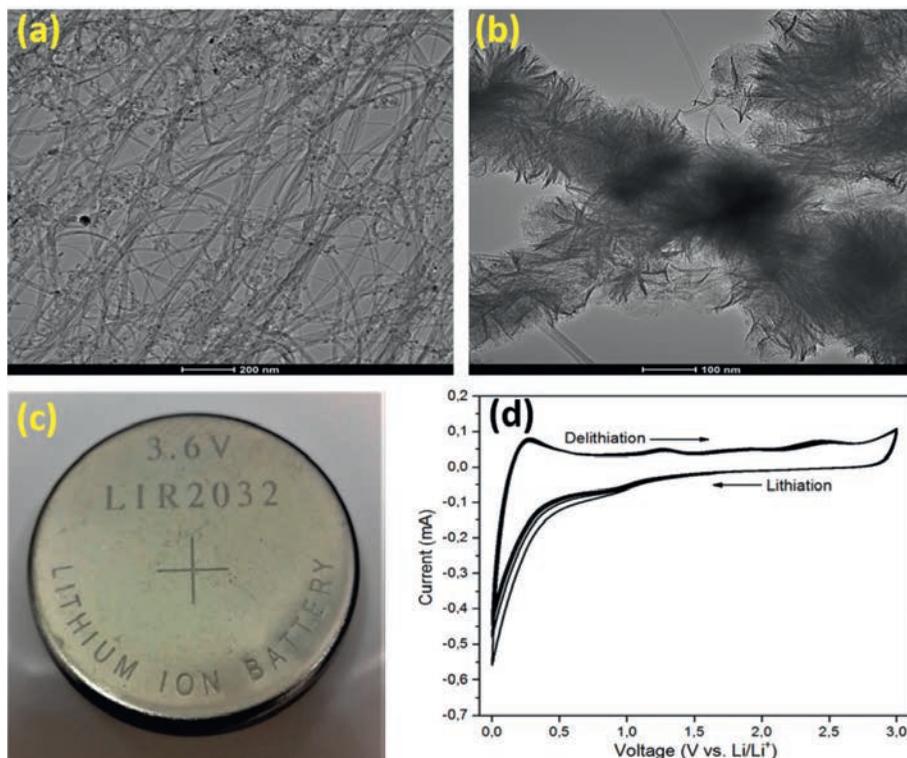


Figure 3. TEM images of (a) CNT and (b) TiO<sub>2</sub> nanosheet-CNT hybrid electrodes (c) photograph and (d) electrochemical performance of Li-ion battery containing CNT electrode.

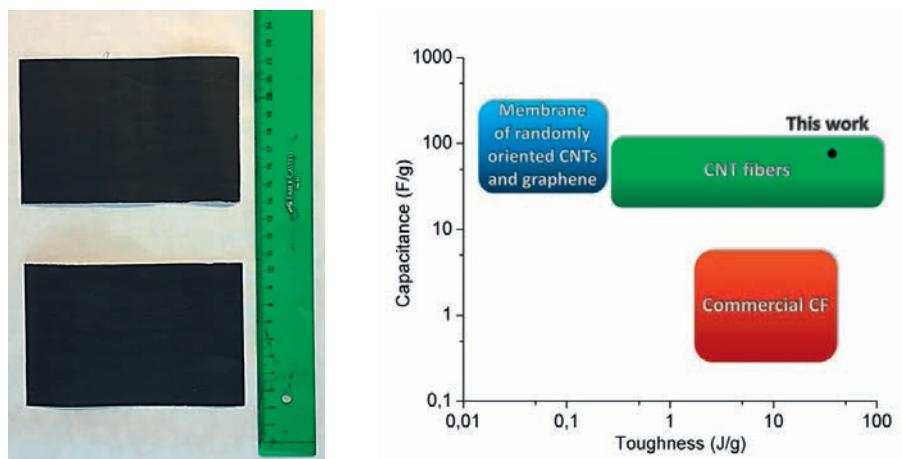


Figure 4. Multifunctional electrodes based on high performance carbon nanotubes fibres.

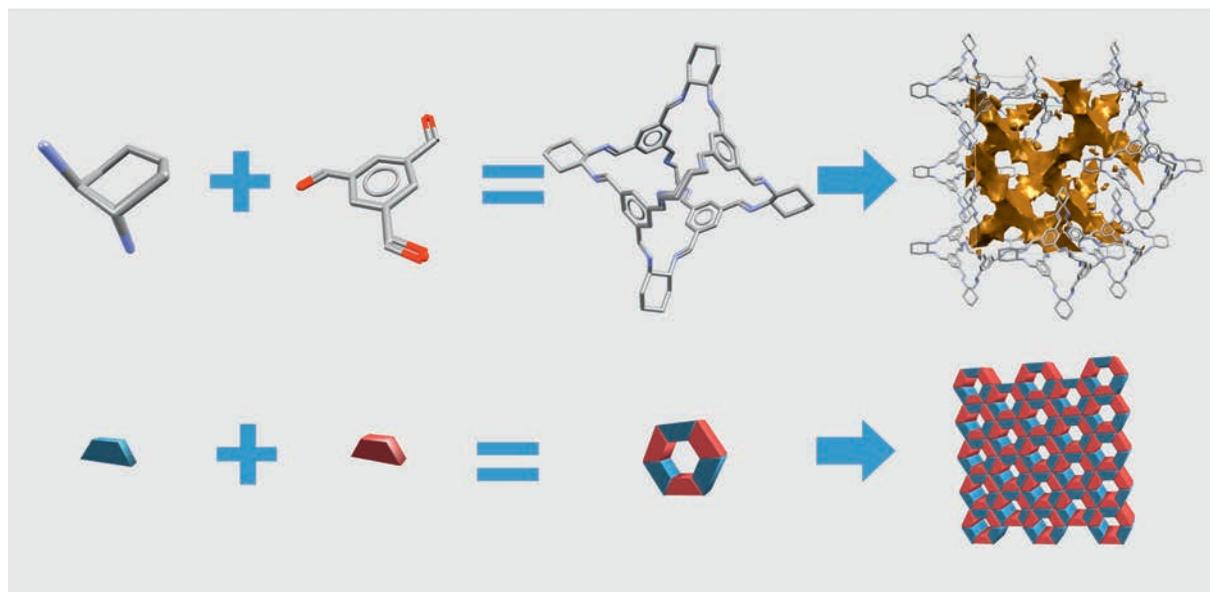


Figure 5. A sketch of an *in silico* porous molecular crystal structure prediction from a set of molecular fragments.

The growing list of required functions in applied materials and the ever-increasing library of molecular or nano building blocks point to the use of computational and data-driven materials discovery as another key element in the development of multifunctional materials. The research group at IMDEA Materials Institute dedicated to this topic develops strategies to enable *in silico* identification of the best molecules or materials for a given application at minimal computational costs. Their tools provide a) structure prediction and material database enumeration, b) high throughput structure characterization and property prediction and c) accelerated structure searchers using advanced algorithms. In the context of advanced porous materials, for example, these techniques have been used to discover high performing material for noble gas separations [3] while entirely new approaches are being developed to enable computer-aided design of tunable molecular materials.

## References

- [1] X. Zhao, H. V. Babu, J. LLorca, D. -Y. Wang. *Impact of halogen-free flame retardant with varied phosphorus chemical surrounding on the properties of diglycidyl ether of bisphenol-A type epoxy resin: synthesis, fire behaviour, flame-retardant mechanism and mechanical properties.* **RSC Adv** **6**, 59226-59236, 2016.
- [2] E. Senokos, V. Reguero, J. Palma, J. J. Vilatela, R. Marcilla. *Macroscopic fibres of CNTs as electrodes for multifunctional electric double layer capacitors: from quantum capacitance to device performance.* **Nanoscale** **8**, 3620-3628, 2016.
- [3] D. Banerjee, C. M. Simon, A. M. Plonka, R. K. Motkuri, J. Liu, X. Chen, B. Smit, J. B. Parise, M. Haranczyk, P. K. Thallapally. *Metal-Organic Framework with Optimal Adsorption, Separation, and Selectivity towards Xenon.* **Nature Communications** **7**, 11831, 2016.

# muesli: an open

## Muesli: an open source library for the simulation of materials

for the simulation  
of materials

Computational solid, fluid, and structural mechanics pivots on simulation codes that approximate the solution of (initial) boundary value problems whose equations are too complex to be solved analytically. These equations include balance laws, sometimes constraints and, invariably, material models. The latter consists of software implementations of the constitutive relations that describe the behaviour of materials under all possible loading paths.

Despite their presence in all simulation codes for mechanics, material models are currently not shared, and this slows down the progress of research. Each company and research institution involved in this area of research is thus forced to develop its own set of software routines for standard materials, debug, verify and test them, before they are linked to its own large scale code.

In addition, new computational material models presented in scientific publications are invariably limited to the use of the developers. This hinders its adoption by the international scientific community which should go again through the costly and repetitive process of implementing, debugging, verifying, and testing to use these models.

As yet another research centre that routinely goes through the aforementioned software development cycle, IMDEA Materials institute, and more precisely its Computational Solid Mechanics group, has analysed this problem and proposed a solution. MUESLI, a *Material Universal Library*, is an open source collection of material models at the continuum level launched in May 2016 and available in our web (<http://materials.imdea.org/research/simulation-tools/muesli/>). MUESLI encompasses continuum models for solid, fluid, and thermal mechanics in a C++, object oriented library designed for easy extension and flexible link with existing simulation codes. This library can be employed by research centres to explore new material models and by companies to implement their own specific material products.

MUESLI already includes the most commonly used continuum material models for solid, fluid, and thermal analyses. In particular, it has versions for small strain elastic, viscoelastic, elastoplastic, and viscoplastic materials, large strain hyperelastic and elastoplastic materials, Newtonian fluids, small strain strongly coupled materials, and Fourier type thermal conductors. Adding new material models is relatively simple because, in contrast with other implementations based on Fortran 77 or C, MUESLI makes use of high level

# source library

abstractions afforded by C++. As a result, the implementations in MUESLI resemble the symbolic expressions used in the mathematical description of the models implemented.

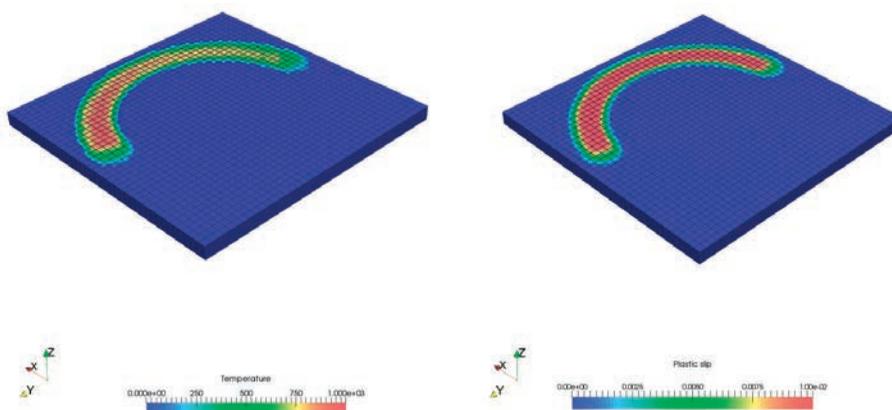
The material models implemented in MUESLI can be used in any simulation code, simply by developing a short interface. By doing so, and with a minimal amount of work, researchers can tap onto the large, and growing, database of material models implemented in the library. MUESLI can also be linked to commercial simulation codes and an interface is already available for Abaqus and LS-DYNA. Thus, the same material models can be employed in different research and commercial simulation programs, speeding up development time and technology transfer to companies.

MUESLI has some very useful features from the point of view of software design. In addition to a well-defined structure based on object oriented classes, and high-level syntax, the code includes several tools for self-testing. Thus, all material models in the library are verified for self consistency, and potential bugs can be easily found in complex implementations.

MUESLI has been created at the institute with the goal that researchers and companies which develop and use material models can share them. The library is distributed under a GPL 3.0 open source license, and includes documentation for the implemented models. True to its open source philosophy, the MUESLI project accepts external contributions, aiming to become a standard and useful tool for the material simulation community.

## References

- [1] Portillo, D. D. Pozo, D. Rodríguez-Galán, J. Segurado, I. Romero, I. *MUESLI: A material universal library. Advances in Engineering Software* 105, 1-8, 2017.



*Figure 1. Temperature and plastic deformation in a metallic plate during welding. The coupled thermomechanical behavior of the material is obtained with MUESLI.*

# design of metallic

## Design of metallic powders for additive manufacturing

Additive manufacturing (AM), often termed 3D printing of metals, is emerging as a new paradigm in the fabrication of metallic parts. Although still only a few parts made with this technology are being commercialized, it is envisioned that AM will impact significantly the fabrication of metallic components, allowing for more freedom in design, weight savings, waste reduction and added multifunctionalities. Applications where AM could replace existing manufacturing methods include, for example, metallic implants, which could be customized for each individual patient. Vast efforts are being made worldwide to explore further applications of this technology in all industrial sectors.

The Physical Metallurgy group at IMDEA Materials Institute has launched a new research line on the development of new feedstock for AM. In particular, a gas atomization process is currently being optimized to produce powders of pure metals and alloys with the right composition, morphology and size distribution that could then constitute the raw material for selected laser melting (SLM), electron beam melting (EBM) or laser metal deposition (LMD). Processing is carried out using a horizontal gas atomizer (Fig. 1), where bulk material is melted using an arc melting furnace and then atomized using a jet and cone nozzle type. Process optimization includes tailoring the melt temperature, melt flow, gas pressure and vacuum levels for each metal powder.



Figure 1. Gas atomizer unit available at IMDEA Materials.

# powders for additive

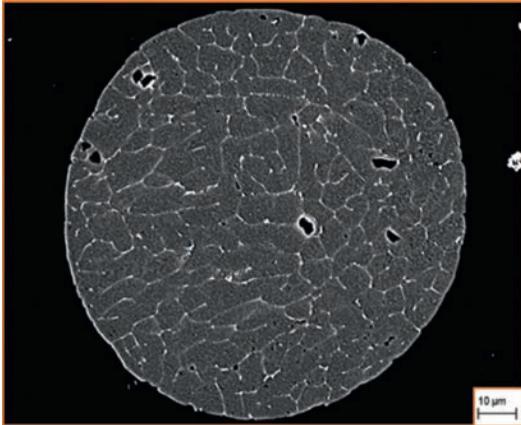


Figure 2. Scanning electron micrograph illustrating a cross sectional view of an Al 6082 powder particle.

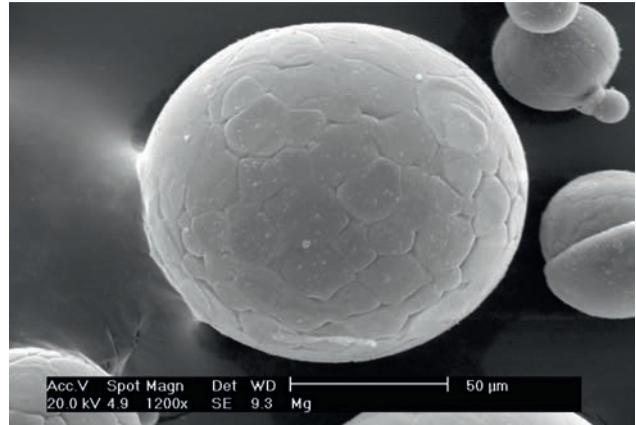


Figure 3. Spherical powder particles, of interest for AM applications.

The powders thus fabricated are characterized using a combination of techniques such as electron microscopy (Fig. 2), X-ray diffraction and various rheology methods. The main aim is to obtain particles with spherical morphology and with sizes smaller than about 100 microns, that are endowed with good flowability and packing density (Fig. 3). The ultimate goal of this research is to develop new alloy compositions that are specifically targeted for additive manufacturing applications and which can, ideally, exhibit unique properties beyond reach in conventionally fabricated metals.

The Physical Metallurgy group is currently partnering other international institutions in several EU-funded consortia aimed at optimizing additive manufacturing processes for the aerospace and biomedical sectors. In particular, funding has been obtained in the frame of the CleanSky2 and M-era.Net calls to fabricate, respectively, Al alloys and ultrafine Fe and Ti based eutectics in powder form for AM. The CleanSky2 consortium (Alforama) is led by Lortek (Spain) and integrated also by a group of KU Leuven (Belgium); the M-era.Net consortium (ELAM) is led by the DLR Institute for Materials Research (Germany) and other members including several companies (Access, Bosch-Mahle, P&G Manufacturing, all located in Germany) and research institutions such as Wigner RCP (Hungary) and the Fraunhofer Society (Germany).

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M-11630-2017





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