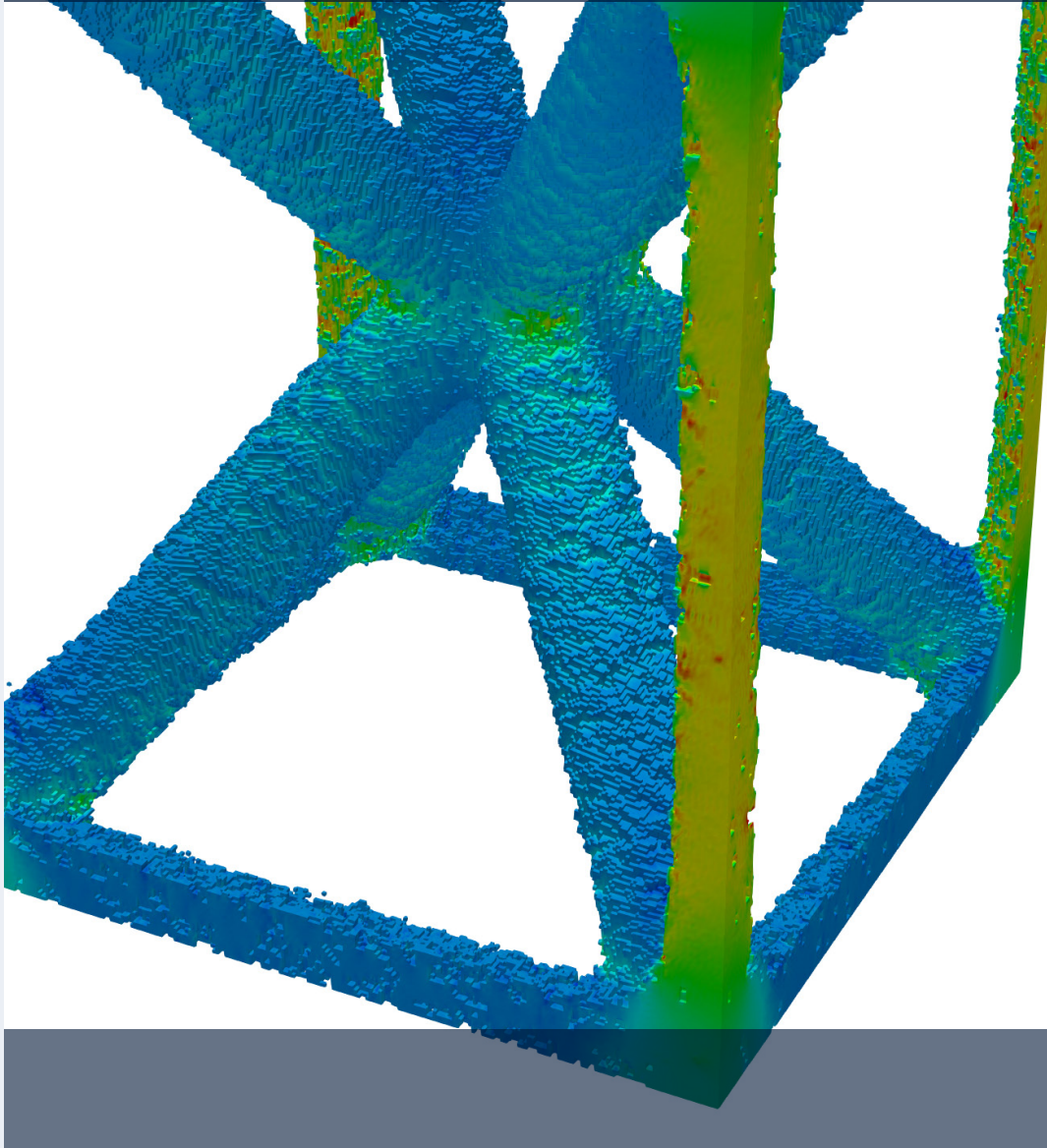


# encompassing research of excellence and technology transfer

imdea materials institute





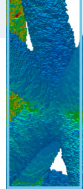
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研究生学习以及马德里生活介绍

1

**institute  
profile**

研究所简介



IMDEA Materials Institute has an **established international reputation in the areas of design, processing, characterization, modelling and simulation of advanced materials** for applications in different industrial sectors with particular emphasis in transport, energy and healthcare.

IMDEA Materials Institute, one of seven Madrid Institutes for Advanced Studies (IMDEA), is a public research centre founded in 2007 by Madrid's regional government. The goal of the Institute is to do research at the forefront of Materials Science and Engineering, attracting talent from all around the globe, and collaborating with companies in an effort to transfer fundamental and applied knowledge into valuable technology.

**mission**

We do research of excellence in Materials Science, contributing to tackle the challenges of society and fostering the sustainable development of the region of Madrid.

**vision**

Our vision for the future is that IMDEA Materials becomes a leading research institute, internationally recognized for its excellence in materials science and its contributions to the transformation of society.

**The mission and vision of the IMDEA Materials Institute is based in three main pillars:**



**excellence** in materials **science** and engineering research

science



**attraction of talented** researchers from all over the world to work in Madrid in an international and interdisciplinary environment

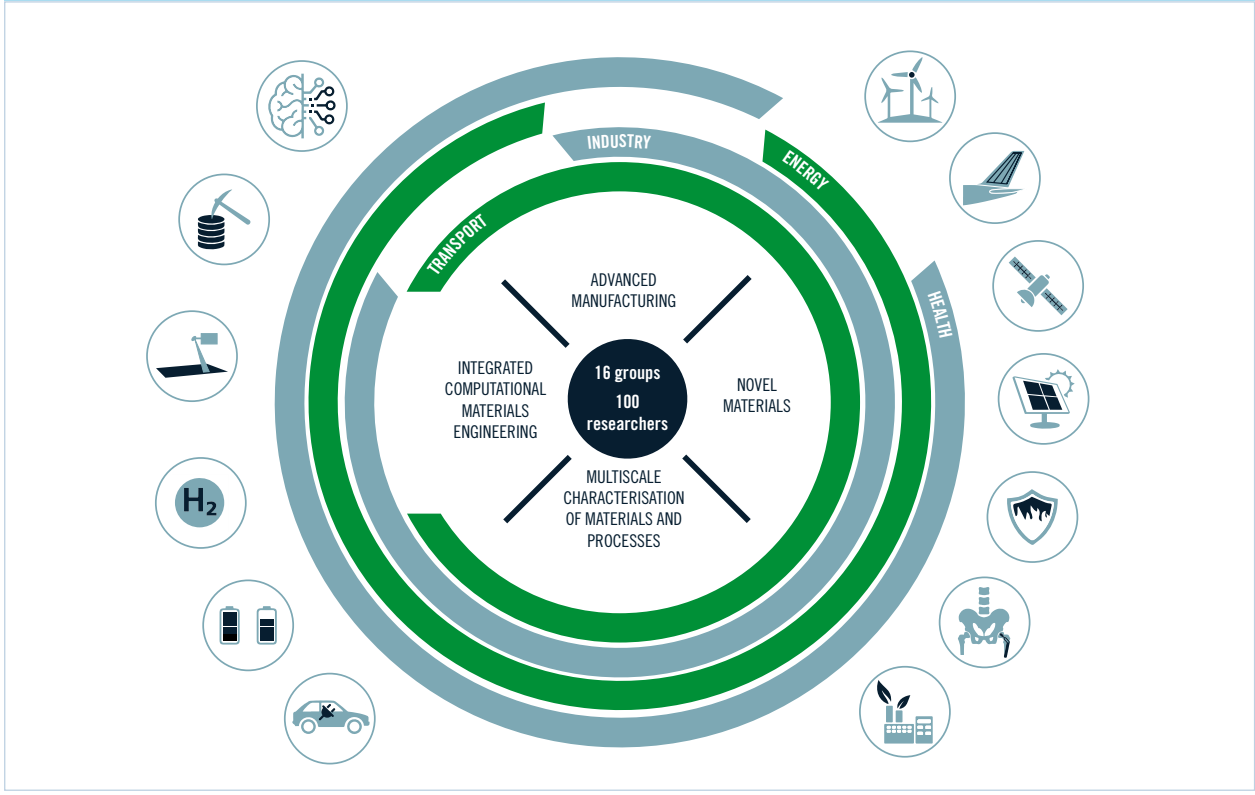
talent

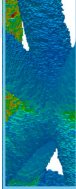


technology **transfer** to industry to increase competitiveness and maintain technological leadership

transfer

**SECTORS AND AREAS OF APPLICATION**





## RESEARCH PROGRAMMES



**Novel  
Materials**



**Advanced  
Manufacturing**



**Integrated Computational  
Materials Engineering**



**Multiscale Characterisation  
of Materials and Processes**



The core strength of the Institute is its international research team, consisting of talented researchers from 23 different nationalities, which carries out new scientific discoveries in Materials Science, and fosters the development of emerging technologies

**100** researchers, **23** nationalities,  
**37%** PhDs, **56%** foreign researchers  
**16** research groups



State-of-the-art laboratories to **manufacture, characterise and simulate advanced materials and nanomaterials**, including their integration in **lab scale prototypes and devices**.

### The facilities of IMDEA Materials Institute

The building and laboratories of IMDEA Materials Institute are located at the Scientific and Technological Park of the Technical University of Madrid in Technoetafe, Madrid.

**2.640 m<sup>2</sup>** of research labs

Auditorium (200 people) and networking space for international Conferences and Workshops.

Metals, composites, polymers, 3D printing, multiscale modelling and artificial intelligence, nanostructured materials, multiscale characterisation of materials and processes, fire resistance, electrochemistry and biomaterials and cell culture.



2

**research  
programmes**

研究课题

# research



**talent**



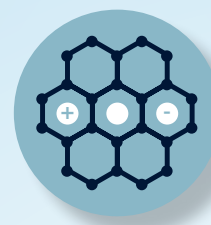
**science**



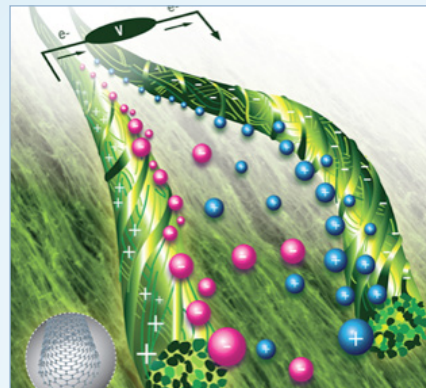
**transfer**

The Institute is currently organised into sixteen **research groups** focused on different areas in the field of Materials Science and Engineering. Each of these groups is led by one staff researcher, who is in charge of coordinating and supervising a research team of post and predoctoral researchers. The research groups, as key units of the Institute, develop research projects and collaborations to drive the frontier of science of their field forward and transfer knowledge into valuable technology.

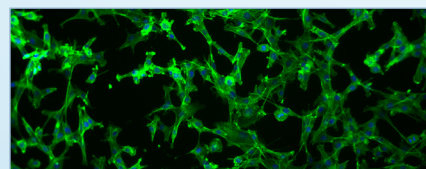
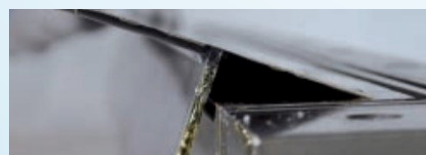
As a result of a high degree of internal collaboration, each research group at the IMDEA Materials Institute participates in several of our **research programmes**. Driven by the talent of the researchers, the research programmes combine cutting-edge fundamental oriented research in topics at the frontiers of knowledge with applied research encompassing the midterm interest of our industrial partners to provide long-term technological leadership.



**Novel Materials**



- Synthesis and integration of nanomaterials
- Synthesis and properties of polymer-based multifunctional nanocomposites
- Materials for hydrogen economy
- Metallic materials
- Materials for extreme conditions
- Materials for Lithium-Ion Batteries (LIBs)
- Materials for post LIBs
- Lightweight materials
- Green materials approaches
- Regenerative engineering
- Medical treatments



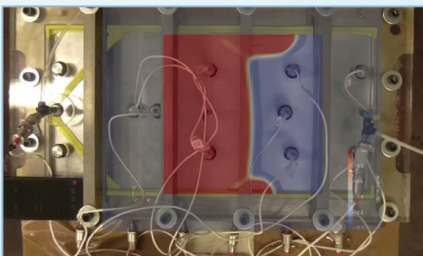
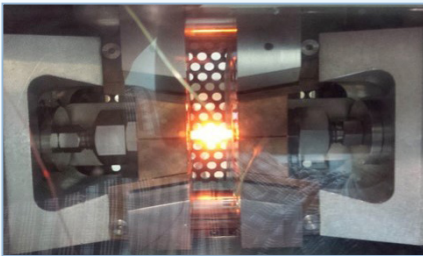




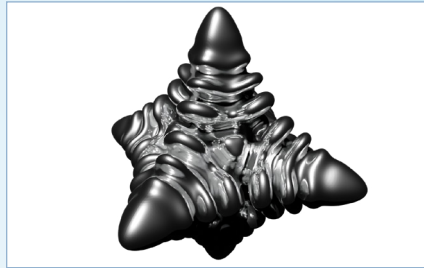
## Advanced Manufacturing



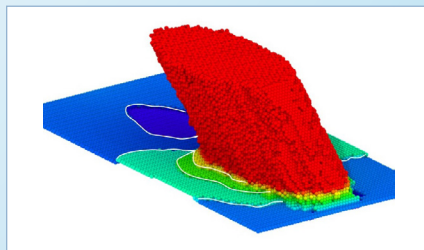
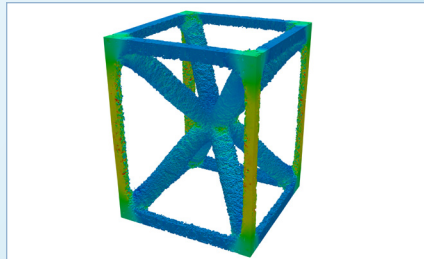
- Industry 4.0
- Bulk nanostructured materials
- Liquid and solid-state processing
- 3D printing



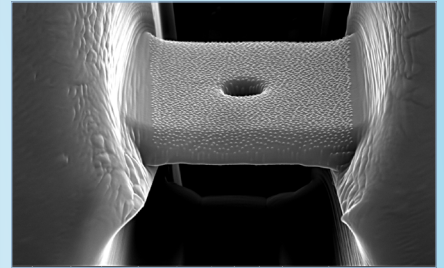
## Integrated Computational Materials Engineering



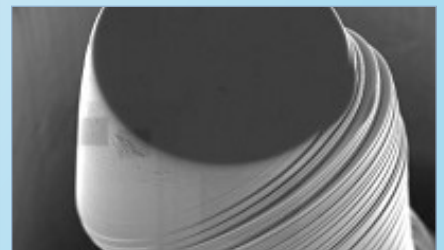
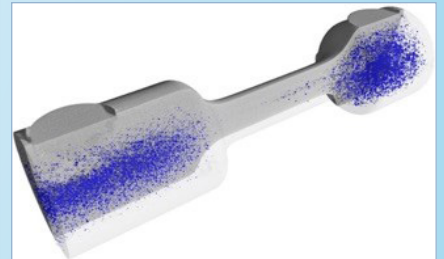
- Virtual materials design, including virtual processing and virtual testing
- Materials modelling at different length and time scales
- Multiscale materials modelling
- Modelling and simulation strategies for different applications
- Computational and data-driven materials discovery



## Multiscale Characterisation of Materials and Processes



- Advanced material characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques
- 4D characterisation: in-situ multiscale characterisation of processes
- Correlation between experiments and multiscale simulations (molecular dynamics, dislocation dynamics, crystal plasticity, finite elements,...)



# facilities



talent



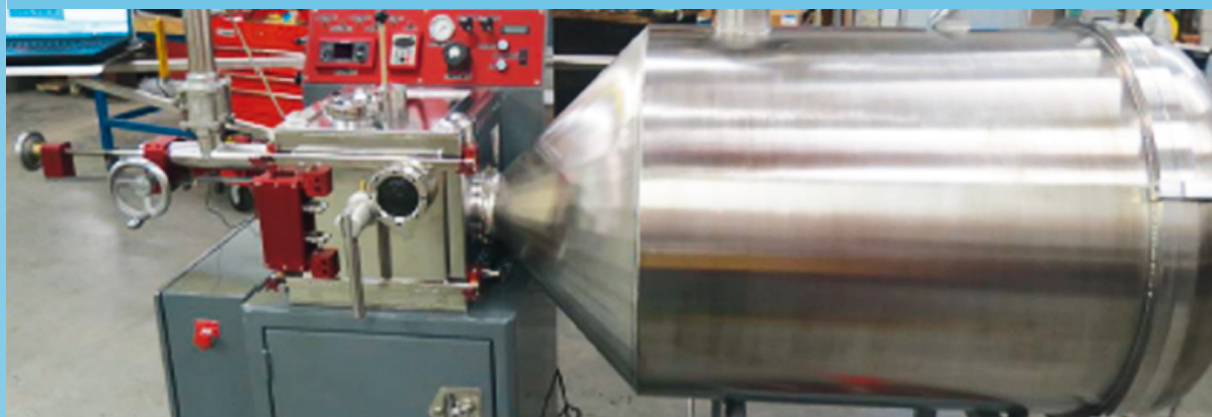
science



transfer

IMDEA Materials Institute has **state-of-the-art laboratories to manufacture, characterise and simulate** advanced materials and nanomaterials, including their integration in **lab scale prototypes and devices**.

## Synthesis, processing and integration of materials



### Metallic alloys

- Bulk processing techniques: casting by induction and arc melting, GLEEBLE 3800 thermo-mechanical simulator equipped with tools for physical simulation of casting, rolling, forging, welding, sintering, and controlled heat treatments.
- Powders manufactured by gas atomisation and mechanical milling. Selective laser melting technology for additive manufacturing of metals.

### Polymer based composites and nanocomposites

- Liquid moulding processing: RTM resin transfer moulding, VI vacuum infusion, RFI resin film infusion and pultrusion.
- Prepreg lamination using vacuum bagging of autoclave and out-of-autoclave prepregs (OoA) or laminate hot-press moulding (<math><400^{\circ}\text{C}</math>).
- Semi-industrial equipment for compounding and injection moulding of thermoplastics.
- Integration of advanced nano-fillers.
- Filament maker for 3D printing (3dvo).
- Melt flow index.

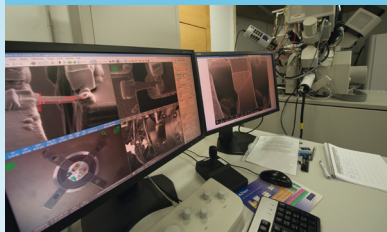
### Nanomaterials

- Synthesis and chemical modification of nanocarbons, inorganic materials, nanoporous semiconductors, thin films, zeolites and other nanomaterials.
- Evaporation equipment in controlled atmospheres, high-pressure reactors and in-house chemical vapour deposition systems.

### Energy storage and conversion devices

- Synthesis and characterisation of nanostructured electrode materials for energy storage applications. Fabrication of composite electrodes and integration in various types of rechargeable batteries (Li-ion, Li-S, Li-O<sub>2</sub>, Na-ion, and hybrid batteries etc.).
- Fabrication and testing of nanocarbon-based electrodes and their integration with liquid and solid electrolytes to form large-area (> 100 cm<sup>2</sup>) flexible supercapacitors.
- Integration of energy-storage functions in structural composites
- Fabrication (solvent-based deposition, physical vapour deposition, high temperature sintering ovens and hot plates) and characterization (solar simulators, incident photon-to-current conversion, electrochemical impedance spectroscopy and intensity-modulated photovoltage spectroscopy) of hybrid solar cells and thin-film organic solar cells.

## Microstructural and chemical characterisation



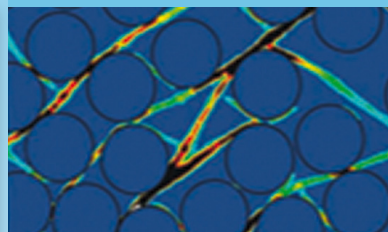
- 3D microscopy at different length-scales, including X-ray tomography, X-ray diffraction, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB, and 3D-TEM and 3D-EDS in the TEM.
- In-situ thermos-mechanical testing of miniaturised samples in the X-ray tomography system, as well as in the SEM and TEM.
- In-situ processing studies in the X-ray tomography system, such as casting, infiltration and curing of polymer based materials.
- Raman spectrophotometer.
- Gel permeation chromatography.
- Particle size analyser.
- Freeze dryer.
- In-situ thermal studies of polymers in the X-ray diffractometer

## Mechanical properties



- Mechanical testing of a wide range of materials, using electromechanical and hydraulic machines (quasi-static, dynamic, fracture and fatigue testing in a wide range of temperatures).
- Characterisation of mechanical properties at multiple length scales, including nanoindentation, micropillar compression, microtensile testing and fracture micromechanics.
- Tests can be carried out both ex-situ and in-situ in SEM, TEM and X-ray tomography including measurements at elevated temperature.

## Simulation



- Simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum) to design or improve materials and components by means of virtual testing and virtual processing.
- High-performance computer cluster (600+ Intel Xeon CPU cores and NVIDIA GPU acceleration leading to a computational power of 90 Tflops).
- In-house developed simulation tools.
- Commercial and open source software tools for modelling and simulation in Materials Science and Engineering (CALPHAD, DICTRA, Micress, Abaqus, LS-Dyna, PamCrash, LAMMPS, VASP, etc.).

## Functional properties



### Fire resistance

- Rapid laboratory scale tests for screening (micro-scale combustion calorimetry and oxygen index).
- Dual cone calorimetry and UL94 Horizontal/Vertical Flame Chamber.

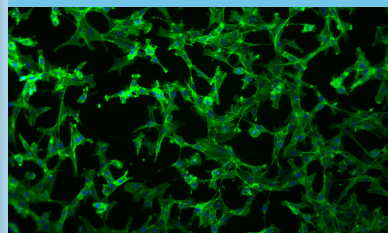
### Thermal

- DSC, TGA and Hot Disk Thermal Conductivity analyser. Thermal behaviour of mechanical properties, DMA and rheology.
- Pushrod Dilatometer for the measurement of dimensional changes.

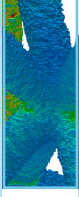
### Electrochemical

- Electrochemical characterisation of energy storage devices (Li-ion, Li-S, Li-O<sub>2</sub>, Na-ion, and hybrid batteries). Simultaneous testing of 100 batteries can be performed using multichannel battery testers.
- Galvanostatic/potentiostatic cycling at various current densities.
- Single channel Zive SP1 electrochemical workstation is used for cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) study of batteries.
- LCR equipment to quantify dielectric properties in composites.

## Biomaterials and cell culture



- Confocal, fluorescence and inverted microscopes
- PCR instrument
- Multi-mode plate reader (absorbance, fluorescence, luminescence)
- Ultrasonic processor
- Autoclave
- Protein gel electrophoresis and blotting system
- Liquid nitrogen tank for cell storage and -80 °C freezer
- Prusa mini 3D printer
- Biosafety cabinets
- Benchtop and CO<sub>2</sub> incubators
- Centrifuge and microcentrifuge, vortex mixers, hot plate stirrer, dry block heater, UV lamp, and thermostatic water baths

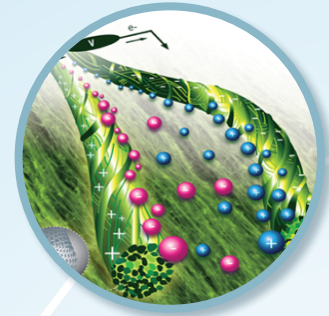


# programme

# Novel Materials

## Goal and vision

The programme on Novel Materials combines expertise in design and synthesis of nano and molecular building blocks with their integration into macroscopic materials and devices, in developing solutions for high-performance structural composites with enhanced multifunctional capabilities such as thermal, electrical and fire resistance, and in exploring the processing-structure-property relationship with special emphasis on the role of microstructure on the mechanical response at all length scales. This interdisciplinary pool of researchers is formed by chemists, physicists, and engineers (chemistry, materials, mechanical and aeronautical) carrying out both fundamental and applied research via close collaboration with companies in the transport, aerospace, energy, safety, and biomedical sectors. Research facilities include state-of-the-art equipment for synthesis, processing, manufacturing, structural/materials characterization and material properties.



**Multifunctional  
Nanocomposites**



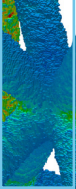
**Computat  
Mat**



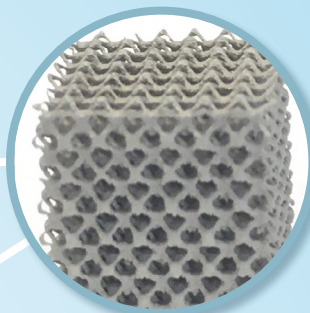
**Physical Simulation**



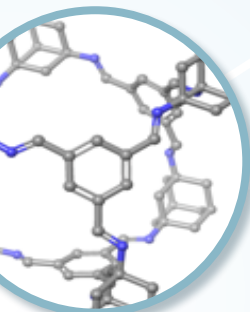
**S  
P**



**High Performance  
Polymer  
Nanocomposites**



**Bio/Chemo/Mechanics  
of Materials**



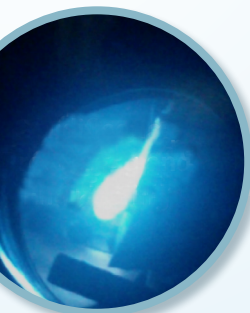
**Computational and Data-Driven  
Materials Discovery**



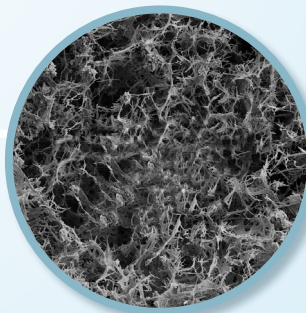
**Nanomechanics and  
Micromechanics**



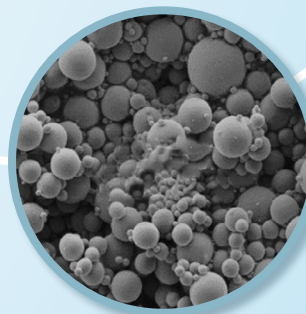
**Structural  
composites**



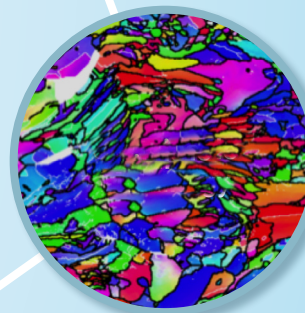
**Solidification  
Processing &  
Engineering**



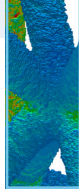
**Biomaterials and  
Regenerative Medicine**



**Sustainable  
Powder  
Metallurgy**



**Sustainable  
Metallurgy**



## Main research lines

### Synthesis and integration of nanomaterials (nanotubes, nanofibers, MXene, quantum dots, graphene, and hybrids)

- Synthesis of nanocarbon/semiconductor hybrids for photo and electrocatalysis, interaction of nanocarbons with liquid molecules, polyelectrolytes and inorganic salts.
- Synthesis of inorganic nanowires and assembly as macroscopic yarns and fabrics.
- Sensors: triboelectric, thermoresistive chemical, piezoresistive, piezoelectric.
- Hierarchical materials: materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity.
- Electrospinning for polymeric nano-membranes.

### Synthesis and properties of polymer-based multifunctional nanocomposites

- Sustainable materials: bio-based nanocarriers, novel guest-host nanomaterials, nano-cross linkers, multifunctional polymer nanocomposites, renewable and recyclable polymeric materials, biodegradable polymers, carbon fiber reinforcement, etc.
- Fire retardant materials through nanodesign: multifunctional nanomaterials to increase fire retardancy: layered double hydroxides, Metal-Organic Framework, sepiolite, molybdenum disulphide, nanocarbon, nano metal hydroxide, graphene, cellulose nanocrystal, etc.
- Energy storage and energy saving materials.
- Phase-change materials for thermal management.

### Materials for hydrogen economy

- High-throughput design and synthesis (magnetron sputtering) of novel catalysts for green hydrogen production and energy generation from hydrogen by means of elastic strain engineering.

### Metallic materials

- Advanced high strength steels showing combination of enhanced mechanical and in use properties.
- High alloy steels, superalloys and high entropy alloys.
- Analysis of chemistry-processing-microstructure-properties relationship on macro- and microscales with emphasis on their strength, ductility, fatigue and fracture resistance.
- Study of 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).
- Rapid screening of phases, crystal structures, properties, microstructure and kinetics in bulk materials by the Kinetic Diffusion Multiple Technique.
- Deposition of multiscale functional coating layer by employing methods such as blade casting, spin coating, spray coating, electrospinning, etc.

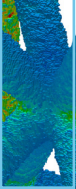
### Materials for extreme conditions

- Impact, high temperature, mechanical, fire, predictive simulation.
- Prediction and prevention strategy for metal, polymer based composite materials under simultaneously extreme conditions such as high temperature behavior under structural loading.

### Materials for Lithium-Ion Batteries (LIBs)

- Nanostructured silicon anodes.
- Carbon nanotube fabrics for hybrid electrodes and metal-free current collectors.
- Defect-engineered electrodes.
- Fire-retardant electrolytes.
- Flame resistant all solid-state polymer electrolytes.
- Electrolyte composition optimisation accelerated by Artificial Intelligence.
- Flexible and structural batteries.





### Materials for post LIBs

- Fire-retardant electrolytes.
- Electrolyte composition optimisation accelerated by AI.
- New electrodes and interfacial strategies for Zinc-ion batteries

### Lightweight materials

- Composite materials.
- Alloys.
- Hybrids.
- Sandwich-structured fire retardants.
- Porous polymers and polymer-based aerogel.
- Reversible crosslinking.

### Green materials approaches

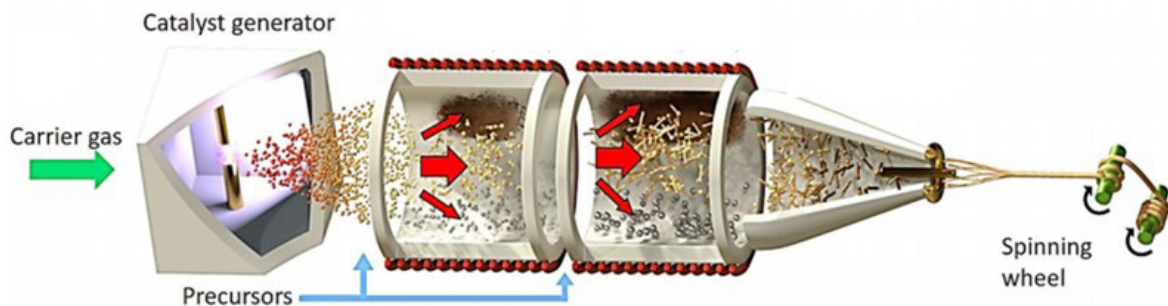
- Bio-based polymers fibres and additives.
- Reprocessable composites.
- Valorization of by-products in hydrogen production.
- Biobased thermal energy storage/phase change materials

### Regenerative engineering

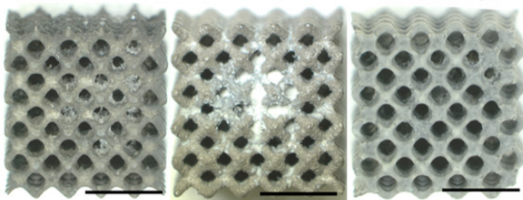
- Bioresorbable 3D printed metallic and composite scaffolds for bone regeneration.
- New materials for tissue engineering and regenerative medicine.
- Biodegradable cardiovascular metallic stents via 3D printing.

### Medical treatments

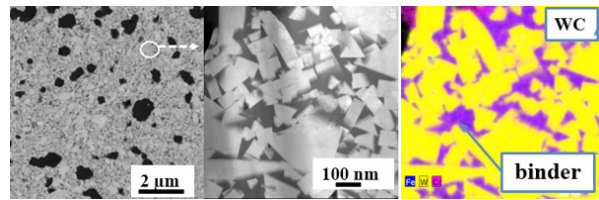
- Degradable metal nanoparticles for biomedical applications (anticancer or antibacterial activity).
- Biofunctionalization and surface modification on materials with molecules to improve their performance.
- Mechanotransduction.



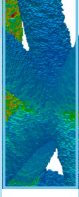
Schematic of the synthesis of 1D nanomaterials via a floating catalyst.



3D printed Mg scaffolds for bioresorbable bone implants



New cemented carbides Cr-Fe based nano-reinforced



# programme

# Advanced Manufacturing

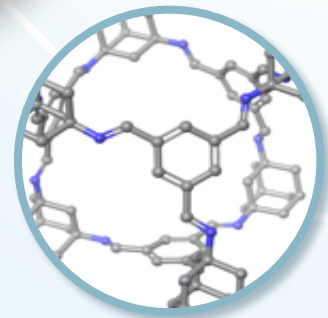
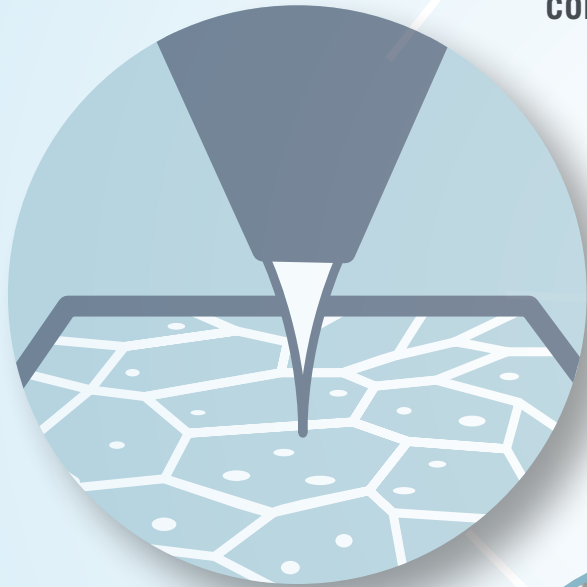
## Goal and vision

The programme on Advanced Manufacturing is highly interdisciplinary in nature spanning the fields of alloys, biomaterials, polymers, composites, energy materials, and involving both experimental and computational efforts. The objective of this programme is to improve quality, productivity, cost efficiency and sustainability in current manufacturing paradigms, as well as conceive and develop novel hybrid manufacturing techniques to enable the commercial realization of emerging products in the aerospace, biomedical, energy, automotive and other industrial sectors.

Effective unit-process innovation and development derives from an understanding of the physical and chemical phenomena influencing manufacturing processes. Therefore, a key part of this programme involves the creation and development of models based on Artificial Intelligence (AI) to predict the optimum manufacturing routes and quality of the manufactured products, as well as the modelling and understanding of tool-material interactions. This fundamental knowledge is supplemented by state-of-the-art characterization techniques needed to monitor the quality of manufactured products including their (micro)structure and mechanical and functional properties.

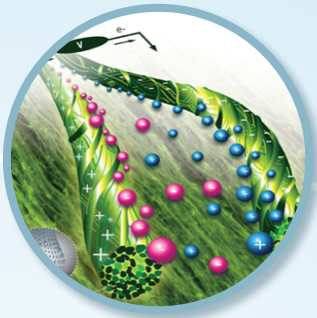


**Structural  
composites**

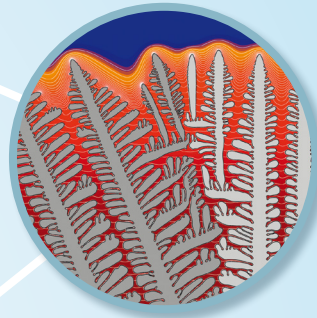


**Computational and  
Data-Driven Materials  
Discovery**





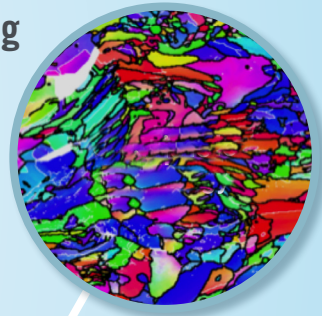
**Multifunctional  
Nanocomposites**



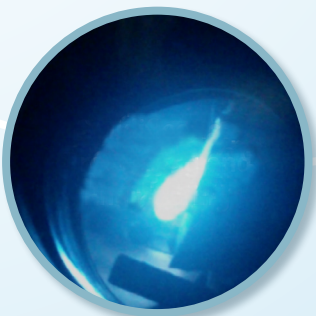
**Modelling and  
Simulation of  
Materials Processing**



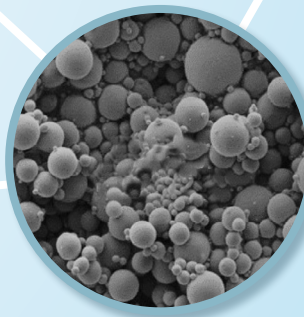
**Physical Simulation**



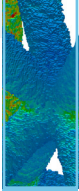
**Sustainable  
Metallurgy**



**Solidification  
Processing & Engineering**



**Sustainable Powder Metallurgy**



## Main research lines

### Industry 4.0

- Virtual testing of structural composites. Analysis of the effect of manufacturing defects on structural performance.
- Virtual processing of structural composites including hot-forming and out-of-autoclave (injection, infusion, compression moulding). Surrogate and reduced order models for manufacturing based on multiphysics simulations.
- AI techniques applied to manufacturing. Digital twins for manufacturing processes. Smart detection of defects by sensors including the active control of manufacturing systems.
- Structural health monitoring (SHM) with carbon nanotube yarns integrated sensors. Automated damage detection models based on AI.

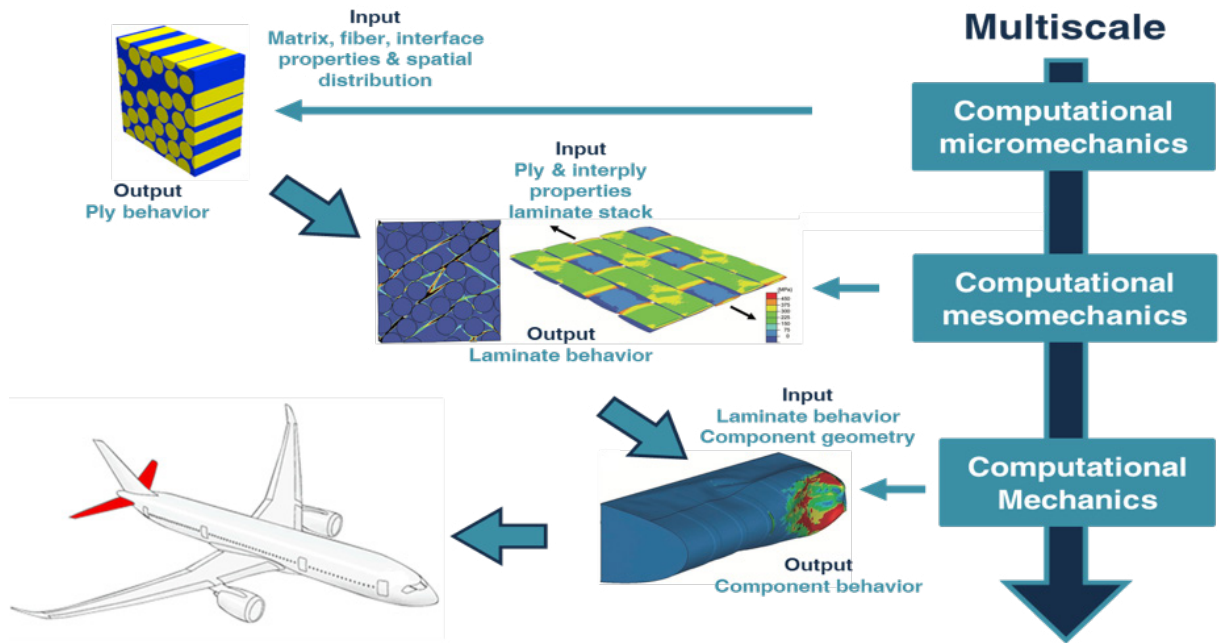
- AI-guided materials design and chemical process.
- Electric current-assisted curing for bondings and repairs.
- Multifunctional composites for structural and energy storage applications.

### Bulk nanostructured materials

- Gas-phase assembly of continuous fabrics and fibres of carbon nanotubes and inorganic nanowires (Si, SiC).
- Integration of these nanostructured fabrics into electrochemical devices and composite materials.

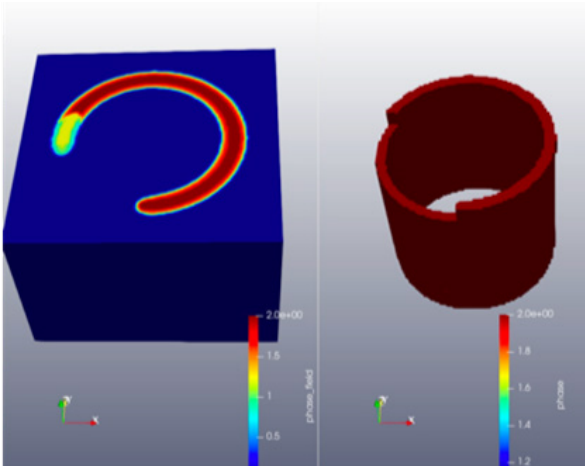
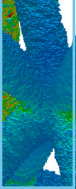
### Liquid and solid-state processing

- Rapid alloy prototyping and manufacturing of bulk alloy libraries for the fast assessment of properties.
- Optimisation of casting processes.

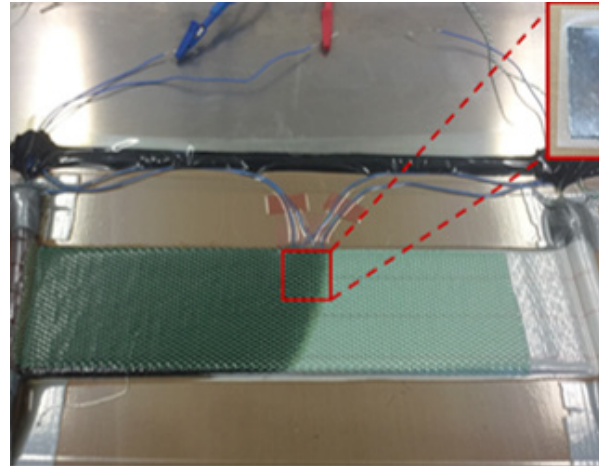


Virtual testing strategy for composites (static and dynamic properties)

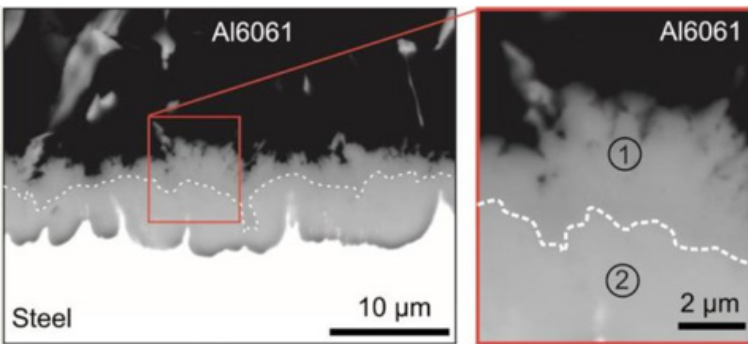




Finite element modelling of selective laser melting processing. Temperature (left) and layer-by-layer addition of materials by selective melting (right)

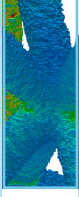


Structural supercapacitor produced by stamping a carbon nanotube fibre-based electric double-layer capacitor (EDLC) interleaf, embedding it between carbon fibre plies and infusion/curing of epoxy resin



Physical simulation of joining of dissimilar materials, steel and aluminium) to predict the interface and its properties.

- Development of novel thermo-mechanical processes and powder metallurgy routes via mechanical alloying and gas atomization in non-oxidation conditions.
  - Consolidation by field-assisted sintering and conventional press and sintering.
  - Development of functional thermoplastic filaments (flame retardant, thermal conductive, biodegradable, reinforced, electrically conductive, etc) for 3D printing.
  - Data-driven design of 3D printed metamaterials.
  - Custom made implants using new biocompatible alloys.
  - Stereolithography, including resin synthesis and characterization.
  - Extrusion-based 3D printing of biomaterials and bioprinting.
  - Predictive simulation.
  - In-situ monitoring.
- 3D printing**
- Metallic materials, including powder design, fabrication and characterization.
  - Composites, polymers, recycled fibers and hybrids.
  - PLA composite materials reinforced with Mg, Zn or CaPs nanoparticles and continuous metallic wires.



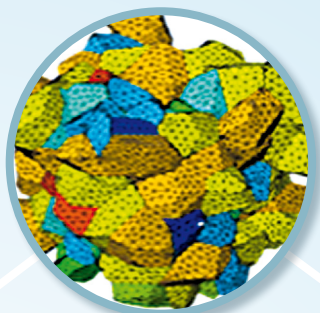
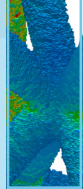
## programme

# Integrated Computational Materials Engineering

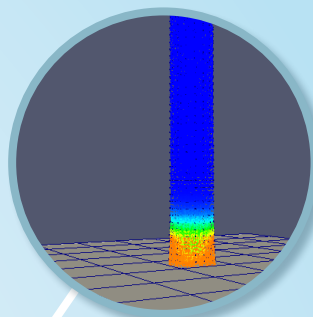
### Goal and vision

The research programme on Integrated Computational Materials Engineering (ICME) is aimed at integrating all the available simulation tools into multi-scale 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 programme 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 optimise materials for a given application (virtual design). Moreover, experiments are also an integral part of the research programme for the calibration and validation of the models at different length and time scales. The expertise of the researchers in the programme covers a wide range of simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum) and is supported by a high-performance computer cluster.

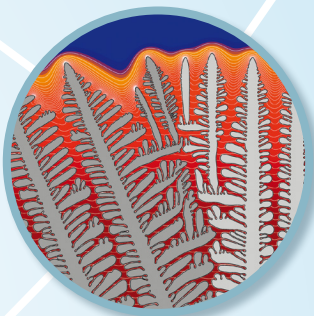




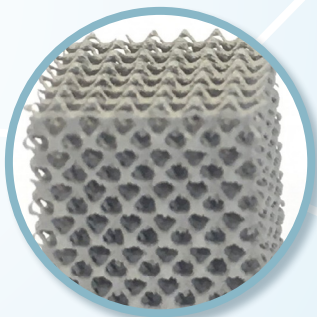
**Multiscale Materials  
Modelling**



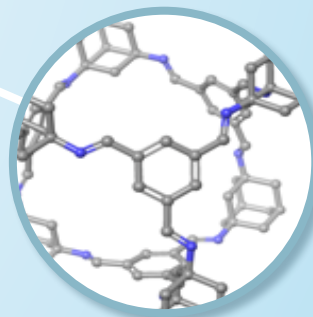
**Computational  
Solid Mechanics**



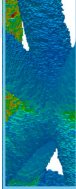
**Modelling and  
Simulation of  
Materials Processing**



**Bio/Chemo/Mechanics  
of Materials**



**Computational and Data-Driven  
Materials Discovery**



## Main research lines

### Virtual materials design, including virtual processing and virtual testing

- Virtual material discovery for functional applications, through the use of DFT, cluster expansion and atomistic approaches combined with AI.
- Virtual processing: Integration of modelling tools (atomistic, computational thermodynamics and kinetics, phase-field) to simulate the microstructural development of materials during processing.
- Virtual testing of metallic alloys: Development, calibration and numerical implementation of microstructural-based constitutive models to predict the mechanical behaviour of single crystals. Simulation of the mechanical response of polycrystalline metals by means of FFT and FEM based polycrystalline homogenization.
- Virtual testing of composites: Implementation of the constitutive models in finite element codes to simulate the mechanical behaviour of structural components.
- Smart manufacturing: multiphysics models of autoclave and out-of-autoclave curing of composite materials accounting for porosity evolution during the process. Simulation-based smart manufacturing processes. Sensing and process control.
- These approaches are applied to several materials, in particular
  - Light (Al, Mg and Ti) metallic alloys and their composites.

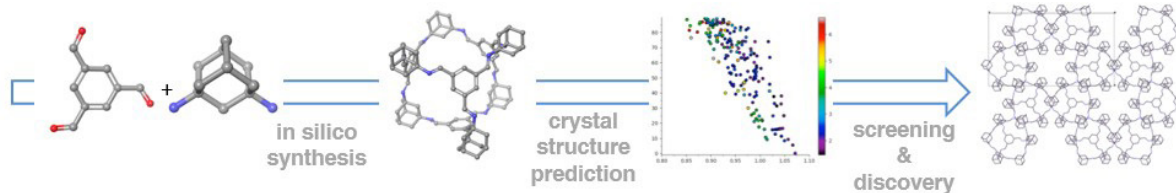
- Ni-based superalloys.
- Multifunctional composite materials and structures.
- Materials for catalysis.

### 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.
- Finite Element solvers for multiphysics problems.
- Fast Fourier based solvers for computational homogenization.

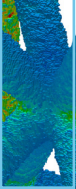
### Multiscale materials modelling

- Bottom-up approaches (scale bridging).
- Development of modular multi-scale tools.
- High throughput screening integration.
- Concurrent models.
- Mean-field homogenisation
- Computational homogenization including FEM and Fast Fourier Transform –FFT–based solvers
- Modelling and simulation of multiscale transport phenomena (application to advanced materials for batteries).



Computational, data-driven materials discovery





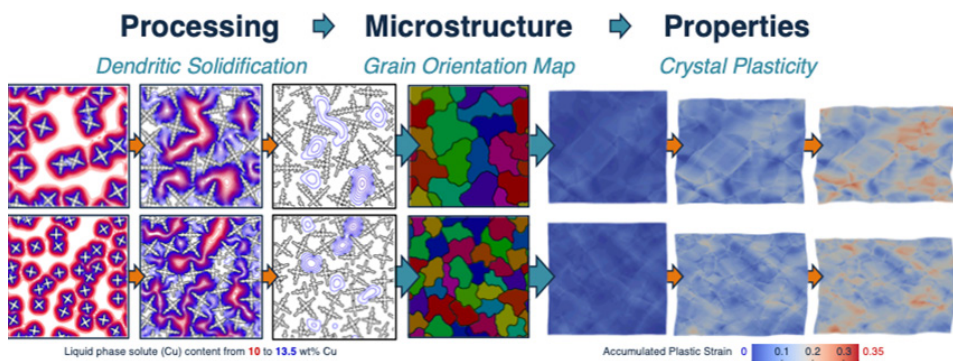
## Modelling and simulation strategies for different applications

- Multiscale modelling of dendritic growth (dendritic needle network approach).
- Numerical methods for solids (finite elements and FFT approaches).
- Computational mechanics and micromechanics.
- Material informatics for analysis of large material datasets.
- Modelling and simulation of H<sub>2</sub> embrittlement in metallic tanks and pipes.
- Study of H<sub>2</sub> diffusion mechanisms in metals.
- Discovery of new catalysts for H<sub>2</sub> production and fuel cells.
- Discovery of new catalysts for CO<sub>2</sub> reduction reaction.
- Virtual design and testing of mechanical metamaterials.

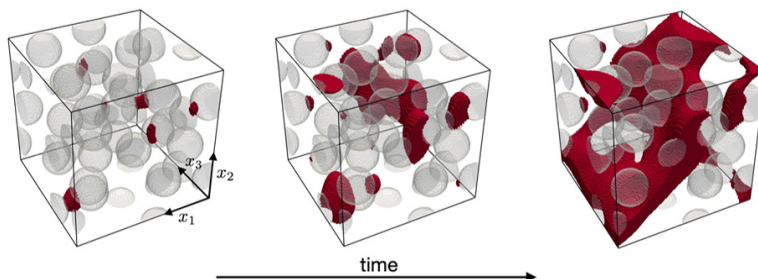
- Simulation of the additive manufacturing process in metals including macroscopic simulation of the thermo-mechanical process by multiphysics finite element models, microstructure evolution through phase-field and prediction of mechanical response using computational polycrystalline homogenization.

## Computational and data-driven materials discovery

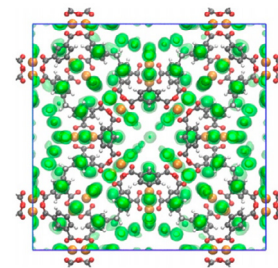
- Discovery of porous materials for energy applications (CO<sub>2</sub> capture, methane storage).
- Design of ionic liquids.
- Materials discovery: structures with high H<sub>2</sub> working capacity and H<sub>2</sub> adsorption-desorption performance.
- Porous material design for capture and storage of CO<sub>2</sub>.
- Design of Metal-Organic Frameworks (MOFs) for separation of gases for anaesthesia (Xe/Kr).



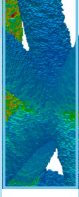
*Linking processing, microstructure, and properties by coupling multiscale models – here, dendritic needle network solidification model with crystal plasticity model*



*Ductile failure at the microscale using FFT and non-local models*



*Predicted distribution of Xe atoms in MOF*



## programme

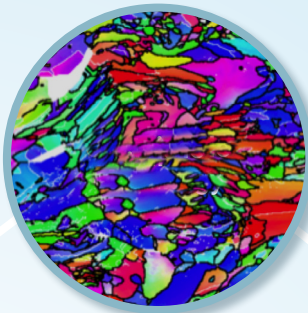
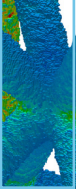
# Multiscale Characterisation of Materials and Processes

### Goal and vision

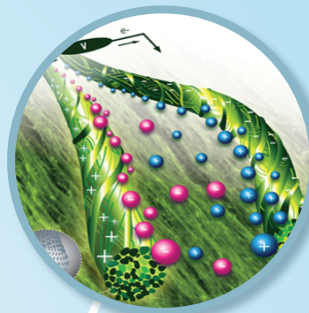
Progress in the development of new materials and processing methods can only come from a thorough understanding of the microstructure of the material in focus, its evolution during either processing or service operation, and its influence in the relevant properties for the purpose it was designed. Since 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 distribution and evolution in advanced materials during processing and service using advanced characterisation techniques.



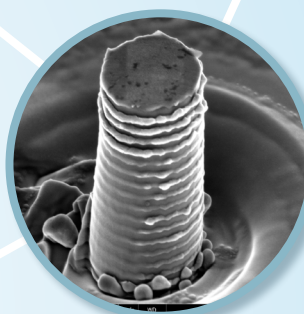




**Sustainable Metallurgy**



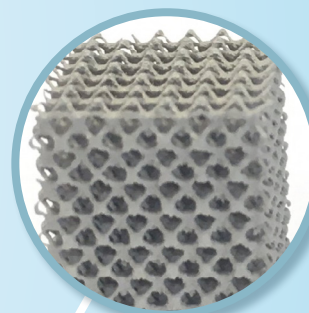
**Multifunctional Nanocomposites**



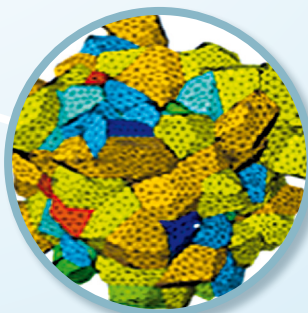
**Nanomechanics  
y Micromechanics**



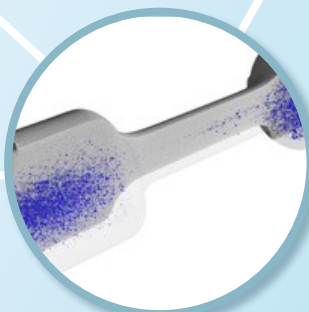
**Structural Composites**



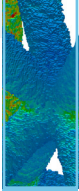
**Bio/Chemo/Mechanics  
of Materials**



**Multiscale Materials  
Modelling**



**X-Ray Characterisation  
of Materials**



## Main research lines

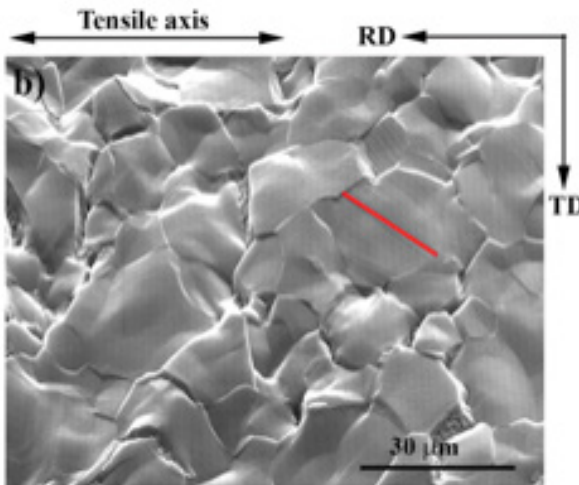
### Advanced material characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques

- Multiscale characterisation with optical and electron microscopy, X-rays, atom force microscopy, Raman spectroscopy, ultrasonic inspection. Some of the equipment we use for this are:
  - FIB-FEG-SEM, including 3D-EDS and 3D-EBSD. In-situ stages for thermomechanical testing
  - FEG-TEM including 3D-STEM and 3D-EDS with in situ stage for mechanical testing
  - X-Ray Tomograph (XCT) with in situ stage for thermomechanical testing, furnaces for thermal treatments and observation of chemical reactions, in situ composite curing, in situ composite infiltration
  - X-ray Diffractometer (XRD) equipped for residual stresses and texture determination, reflectometry analysis, Cu and Cr radiation, linear detector, in-situ furnace.

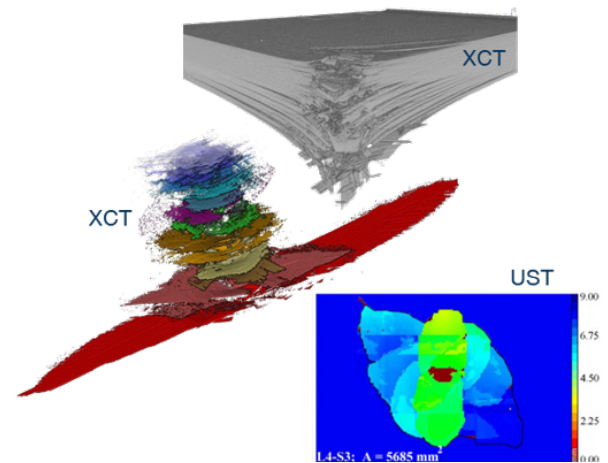
- Raman micro-spectrometer 5x, 20x, 50x, 100x microscope objectives, 532 nm Nd:YAG laser (50W) and diffraction grating of 1800 l/mm, 100 nm resolution.
- Characterisation of broad range of materials, e.g. biomaterials, plastics, metal matrix composites, fibre reinforced composites, metals, nanomaterials, etc.
- Use of large facilities such as neutron or synchrotron radiation facilities for characterisation
- Development of new methodologies (e.g. hardware for in situ testing and software tools) for material characterisation and analysis, also applying artificial intelligence methods.
- Spectroscopic/microscopic studies and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O<sub>2</sub>.

### 4D characterisation: in-situ multiscale characterisation of processes

- Thermo-mechanical testing across several length scales: tension, compression, fatigue, creep, etc. in the scanning electron microscope and X-ray tomograph.

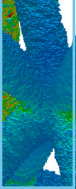


Deformation of polycrystals observed in SEM



Automatic damage extraction of 3D volumes by XCT and AI correlative techniques

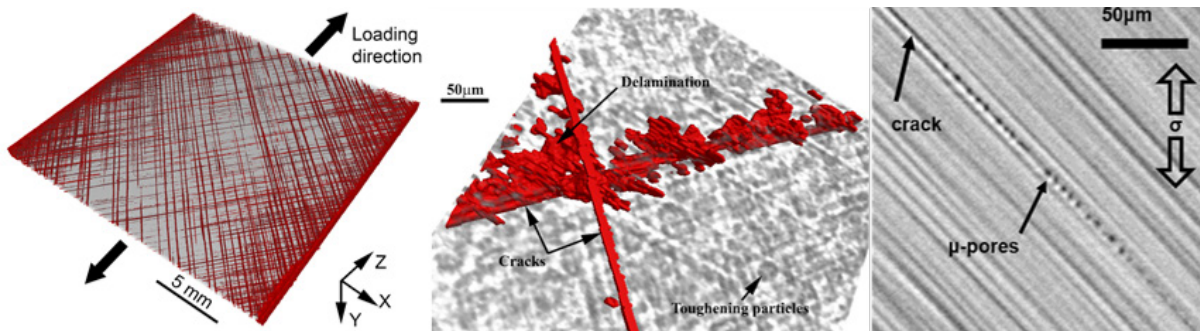




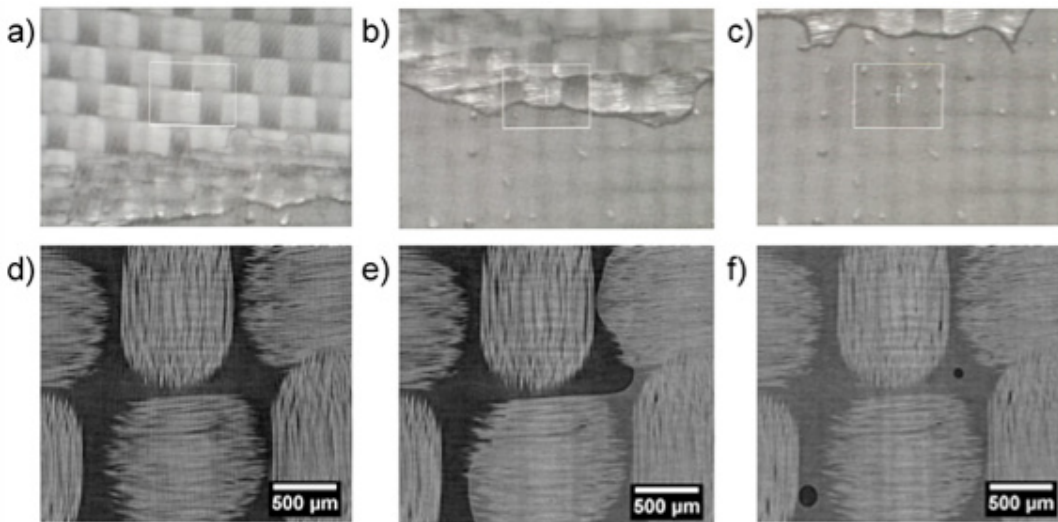
- Properties and deformation mechanisms of small volumes by nanomechanical testing in the scanning and transmission electron microscopes: properties of metallic phases, interfaces, nanoparticles, carbon-based nanomaterials (carbon nanotubes, graphene, etc).
- Elevated temperature nanomechanical testing.
- 4D characterisation of processes by X-ray tomography and X-ray diffraction: e.g. metallic alloy solidification, metallic alloy phase formation and chemical reactions, infiltration and resin flow in composites, composite curing, etc.

### Correlation between experiments and multiscale simulations (molecular dynamics, dislocation dynamics, crystal plasticity, finite elements, etc)

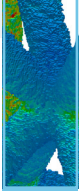
- Digital modelling from 3D structures.
- Integration of experimental statistical measurements into models.
- Experimental confirmation of modelling results.
- Experimental design based on models.



Multiscale & in-situ damage quantification of engineering materials



Resin Transfer Moulding (RTM) processing during XCT measurement



# Materials for Health Care

A new research line on Materials for Health Care became fully operational at the Institute in 2021. In February, Dr. Jennifer Patterson (PhD in Bioengineering from the University of Washington) joined us to lead a new research group on Biomaterials and Regenerative Medicine. She strongly reinforced our research groups already working in the field since 2018. By the end of the year, a fully equipped cell culture and biomaterials laboratory was running (see Figure 1 and the “facilities” section for more details).

This new research facility, co-funded by Madrid Regional Government and by the State Research Agency via the “María de Maeztu” program, allows us to analyse the response of living tissue to new tools, prostheses or devices for medical use that are also being investigated at the Institute (see ongoing projects below). The laboratory consists of a 33 m<sup>2</sup> Biological Safety Level-1 (BSL-1) room and a 29 m<sup>2</sup> BSL-2 area equipped with biosafety cabinets.

The following four research projects are currently running at our Institute in this area:

**1. BioImplant ITN - European Training Network to develop Improved Bioresorbable Materials for Orthopaedic and Vascular Implant Applications** (European Commission/ Horizon 2020 Programme – Marie Skłodowska-Curie actions - ITN - EID)

Combining polymer-, metal- and ceramic-based bio-absorbable materials, to deliver functionally superior bioabsorbable materials with enhanced mechanical behaviour and controllable degradation profiles.

**2. i-MPLANTS-CM - Metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants** (Regional Government of Madrid - Synergy projects)

Printing of metamaterials with shape memory alloys and functional gradients of properties. Development of intelligent implants, which will be implanted through minimally invasive procedures and will be able to evolve geometrically with the patients, shifting their shapes, according to the healing, growth and ageing processes.

**3. MAMAP-CM - Materials and models against pandemic** (Regional Government of Madrid - REACT-EU)

Materials design and development, device manufacturing, modelling and simulation to protect, fight and forecast pandemic expansion. Including the development of: i) biodegradable, biobased micro composites to deactivate viruses, ii) 3D in vitro models of airway tissues and iii) computational model of pandemic spread.

**4. BIOMET4D - Smart 4D biodegradable metallic shape-shifting implants for dynamic tissue restoration** (European Commission/Horizon Europe Programme – EIC pathfinder open)

Development of shape-shifting and load-bearing implants for dynamic tissue restoration and to introduce a revolutionary paradigm in how actuators can be implemented in biomedicine. Science-towards-technology breakthroughs will be demonstrated with new shape-morphing metamaterials, 4D smart metallic actuators and advanced multi-domain optimization tools.

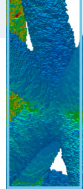
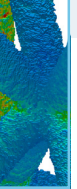


Figure 1. Cell culture and biomaterials laboratory at IMDEA Materials Institute.

# 3

## graduate study and life in madrid

研究生学习以及马德里生活介绍



## Why Madrid

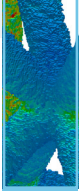
- Madrid is the capital of Spain.
- 6.5 million inhabitants in its Metropolitan Area and 3.3 million in the Capital. It is the third most populous city in the European Union.
- Capital of Spanish language and culture.
- Europe's third largest metropolitan area after Paris and London.
- Fourth richest city in Europe.
- Home to the 'Cortes Generales' - the Spanish Houses of Parliament - the Government of Spain, and the home of the Spanish Royal Family
- Average height above sea level: 667 m.
- Average temperature: 12 °C.
- Area: 605.77 km<sup>2</sup>.
- Income per capita in Madrid is \$40,000 and contributes 18% of the total national GDP.
- Barajas Airport, with annual passenger traffic of 50 millions, it is the fourth largest in Europe and tenth in the world. It is connected by metro and bus to the centre of the city.
- The Madrid metro is the second largest underground network in the world.
- There are five transport interchanges that connect the city bus network to the metro and railways.
- Madrid is linked by high-speed trains to the main Spanish cities.

Madrid is not just any city; it is a place full of energy and passion with a flavor of its own, rich in heritage to explore, full of spice and yet focused and highly sophisticated. In Madrid international students soon find themselves integrated into a multicultural environment to enjoy a city packed with creativity and fun where learning comes easy.

As the financial, political and cultural centre of Spain, Madrid is a modern, cosmopolitan city with a strong economy and a vibrant life. In recent years the growth and development of Madrid have placed it firmly within the network of global cities as the third great European metropolis and as the economic and cultural capital of the Spanish Speaking World.

The City of Madrid has a population of nearly three million people and is also the capital of the Madrid Region (Comunidad Autonoma de Madrid). This region is the economic powerhouse of Spain and also of Southern Europe; its six million inhabitants and their readiness to succeed make it possible every day... and night.

As a large metropolitan area, Madrid is tirelessly striving to attract productive investment, new technology businesses, scientific capability, creative talent, international institutions, a steady flow of tourists, and the staging of important events. Indeed, Madrid now stands out in many of these aspects over other major cities.



## Resource directory

### MADRID

Strategy and International Action Office  
Madrid Global  
<http://www.munimadrid.es/madridglobal>

Madrid City Council Official websites  
Resources for Culture and Leisure,  
Economy, Education, Environment,  
Immigration, Housing, Research, Sports  
and Youth  
<http://www.munimadrid.es/>

Entertainment and tourism  
<http://www.esmadrid.com/en>

Madrid Regional Government Official  
Website for Higher Education Information  
on Madrid Higher Education  
<http://www.emes.es/>

Madrid Regional Government Official  
Website for R&D Madri+d  
<http://www.madrimasd.org/empleo/default.asp>

The European Space for Higher  
Education  
European policy for Higher Education  
with Bologna process  
<http://www.eees.es/>

Chinese Students Association in Madrid  
[www.cn-es.org](http://www.cn-es.org)

## UNIVERSITIES

### Universidad Politécnica

[www.upm.es](http://www.upm.es)

Introduction (English)  
[www.dit.upm.es/aalvarez/UPM.Introduction.pdf](http://www.dit.upm.es/aalvarez/UPM.Introduction.pdf)

Introduction (Chinese)  
[www.dit.upm.es/aalvarez/MadeliGong.pdf](http://www.dit.upm.es/aalvarez/MadeliGong.pdf)

Practical Information for Students  
<http://www.upm.es/internacional/Students/>

### Universidad Autónoma

[www.uam.es](http://www.uam.es)

Orientation, Information and Employment  
<http://www.uam.es/estudiantes/coie.html>

Graduate Studies and Continuing  
Education  
<http://www.uam.es/estudios/doctorado/presentacion.html>

Scholarships  
<http://www.uam.es/estudiantes/becas.html>

Orientation and Student Support  
<http://www.uam.es/estudiantes/acceso/>

### Universidad Carlos III

[www.uc3m.es](http://www.uc3m.es)

English version:  
<http://www.uc3m.es/portal/page/portal/home>

Masters and PhD  
[http://www.uc3m.es/portal/page/portal/postgraduate\\_studies](http://www.uc3m.es/portal/page/portal/postgraduate_studies)

Living and Studying in Madrid  
[http://www.uc3m.es/portal/page/portal/get\\_know\\_us/living\\_studying\\_mad](http://www.uc3m.es/portal/page/portal/get_know_us/living_studying_mad)





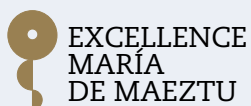




Comunidad  
de Madrid



EUROPEAN UNION  
STRUCTURAL FUNDS



EXCELLENCE  
MARÍA  
DE MAEZTU



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