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Research Projects Offer 2016
2016 年可申请研究项目和方向

1. Multiscale modeling and experimental validation of strengthening mechanisms in engineering alloys
工程合金中的强化机理的多尺度模拟与实验验证
Supervisor: **Prof. Javier LLorca**

2. Quasicontinuum simulation of transport processes at finite temperature
有限温度下传输过程准静态连续尺度模拟
Supervisor: **Dr. Ignacio Romero**

3. High temperature mechanical behavior of metal-ceramic nanolaminates
金属-陶瓷纳米多层膜的高温力学行为研究
Supervisor: **Dr. Jon Molina-Aldareguia**

4. Bio-inspired hierarchical composites
仿生多层次复合材料研究
Supervisor: **Dr. Roberto Guzman de Villoria**

5. New generation fire safety polymer composites： molecular design and structural properties relationship
新一代阻燃聚合物基复合材料：分子设计及结构与性能关系
Supervisor: **Dr. De-Yi Wang**

6. Study on the fire behaviors during the combustion of polymeric materials
聚合物基材料的火行为研究
Supervisor: **Dr. De-Yi Wang**

7. Computer-aided synthesis of zeolite materials
计算机辅助沸石材料的合成
Supervisor: **Dr. Maciej Haranczyk**

8. Computational discovery of porous molecular materials
多孔分子材料的计算
Supervisor: **Dr. Maciej Haranczyk**

9. Development of β-solidifying multiphase γ-TiAl alloys
β 凝固型多相 γ - TiAl 合金研究
Supervisor: **Dr. Srdjan Milenkovic**

10. High-throughput discovery of High Entropy Alloys (HEA)
高熵合金的高通量研究
Supervisor: **Dr. Srdjan Milenkovic**

11. Development of ductile and creep resistant Fe-Al-X alloys
具有韧性和抗蠕变性能 Fe-Al-X 合金的研究
Supervisor: **Dr. Srdjan Milenkovic**

institute imdea materials

1. Multiscale modeling and experimental validation of strengthening mechanisms in engineering alloys

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Prof. Dr. Javier LLorca, Director
Head of the Mechanics of Materials Group

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Project description

The aim of the project is to develop a multiscale modeling strategy to quantify the contribution of different factors (solute concentration, precipitate distribution, size and shape, grain boundaries) to the strength of engineering alloys. This will be accomplished by a bottom-up modeling approach using DFT, molecular dynamics, dislocation dynamics and continuum models. The contribution of each mechanism will be experimentally measured by means of nanomechanical tests (in situ TEM and SEM nanoindentation, micropillar compression, etc) at different length scales (from nm to µm) in single crystals and polycrystals of alloys with different composition and microstructure manufactured to this purpose. This information will be used to validate the strengthening predicted by the multiscale models for each mechanism.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

The students working in this project will participate in the development and experimental validation of state-of-the-art modeling tools to carry out virtual tests of engineering alloys. This topic is at the core of the Materials Genome Initiatives in Europe, USA and China and is expected to lead to scientific advances with a large industrial impact. In addition, the student will benefit from the multicultural environment of the institute and of the interdisciplinary nature of the research.

Skills required for CSC students/scholars

A solid background in physical metallurgical is required as well as fluent English (oral and written). Experience in computational materials science (including molecular dynamics, crystal plasticity, finite elements) will be valued for the modeling position.

Remarks

The project may host 2 PhD students, one of them focused in the development of the multiscale modeling approach and another in the experimental validation. This investigation is funded by an Advanced Grant of the European Research Council on the topic “Virtual design, virtual processing and virtual testing of metallic materials”.

2. Quasicontinuum simulation of transport processes at finite temperature

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Ignacio Romero, Senior Researcher
Computational Solid Mechanics Group

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Project description

This project aims to develop and implement time and space multiscale methods for slow transport problems in crystalline solids, including heat and mass diffusion. The student will implement the Quasicontinuum method in IRIS, a simulation code developed in our group, and add new formulations for the integration of the fast transients in the atomic motions.

Project outcomes the student achieves through CSC and IMDEA

The student will gain an understanding of multiscale modelling, non-equilibrium thermomechanics, and computational material science. The methods developed will be applied to the study of silicon lithiation, a phenomenon in material science that is crucial for the development of high-energy rechargeable batteries. The work will be published in scientific journals and presented in international conferences.

Skills required for CSC student/scholar

Solid background in material science, math, and C or C++. Strong motivation for simulation techniques. Good spoken and written English.

Remarks

This project can host 1 PhD student

3. High temperature mechanical behavior of metal-ceramic nanolaminates

Duration of project and time-length for hosting CSC student/scholar
4 years

Name of the project leader/supervisor, and contact info including webpage link
Dr. Jon Molina-Aldareguia, Senior Researcher
Head of Micro and Nanomechanics of advanced materials

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Project description
Multilayered materials at the nanoscale exhibit exciting possibilities for extremely high strength, fatigue resistance, thermal resistance, wear resistance, and biocompatibility. The scholar will join a collaborative research program between IMDEA Materials and Arizona State University in order to study the high temperature nanoindentation and micropillar compression behavior of Al/SiC nanolaminates

Project outcomes that CSC student/scholar could expect to achieve via working in IMDEA
The student will gain expertise in advanced microstructural characterization techniques, such as SEM, FIB, TEM and EBSD, including 3D-characterization, and mechanical testing, including nanomechanical testing (nanoindentation, microtensile and microcompresion testing) inside the SEM and TEM. He will work in close collaboration with researchers carrying out multiscale simulation of the mechanical behavior of materials.

Skills required for CSC student/scholar
Background in Materials Science and Engineering/Physics/Metallurgy and expertise in microstructural characterization and/or mechanical behavior of metallic materials is desirable. Excellent academic credentials as well as fluent spoken and written English are necessary.

Remarks
The project can host 1 PhD student

4. Bio-inspired hierarchical composites

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Roberto Guzman de Villoria, Researcher
Head of the Nano-Architectures and Materials Design Group

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Project description

Fiber-reinforced polymers (FRP's) have excellent strength and stiffness to weight ratio required for driven structural applications such as aircraft, aerospace, etc. However, several materials improvements are required for the next aircraft generation such as highly tough and damage tolerance resistance composites and material improvements for functional properties such as electrical and thermal conductivity. Natural materials have unusual properties unmatched by engineered materials-their high mineral content makes them stiff and strong, but they're also very tough because of microscopic features that hinder crack propagation. Recent attempts to replicate some of these strategies in man-made materials are also shown to illustrate the variety of unusual properties that can be achieved through the proposed bioinspired approach.

Here, we will study a different approach using novel bioinspired hierarchical composite materials. Inspired on biological composites, different nano/microstructures will be designed to enhance the mechanical and also the multifunctional (electrical, thermal, etc) properties of the composite in the through-the-thickness direction.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

The PhD student will gain a deep knowledge on composite fabrication and novel fabrication techniques adapted to composites (3D printing, nanocomposite fabrication). A deep mastering in mechanical testing will also be reached. The results of this investigation will be published in high impact international peer-reviewed journals.

Skills required for CSC student/scholar

A solid background in mechanical engineering and composite materials; fluency in English language.

Remarks

The project can host 1 PhD student

5. New generation fire safety polymer composites: molecular design and structural properties relationship

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. De-Yi Wang, Senior Researcher
Head of the High Performance Polymer Nanocomposites (HPPN) Group
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www.materials.imdea.org

Project description

More and more polymer-based materials have been used in the industry and society due to the ease of processing ability, lightweight and high performance. However, most of polymers are flammable and lead to high fire risk. This project would focus on the development of new generation fire safety polymer composites and understanding the structural properties relationship. A combination of innovative molecular design and chemistry synthesis, nanotechnology, advanced polymer processing, etc, will be used in the project. In particular, a series of novel bio-based materials and reinforced materials will be studied, aiming at preparing high performance sustainable fire retardant polymer composites. This is a unique opportunity for an enthusiastic young scientist to join an excellent international lab located at an excellent research environment with all the start-of-the-art core facilities and apply innovative approaches to design new polymeric materials with multifunctional and tuneable properties.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

By implementing the project, student will master the knowledge on design and development of high performance fire safety polymer-based materials and will be trained in advanced characterization techniques from molecular to the further application. It is expected to establish wide contact with both of European academia and industry during the study. The student would be working in a really international environment and performing research at a high international standard and in the knowledge frontier of material science and technology.

Skills required for CSC student/scholar

A solid background in polymer materials, polymer chemistry, chemical engineering, or related disciplines; good spoken and written English; excellent team cooperation personality.

Remarks

The project may host 1 PhD student/scholar. High Performance Polymer Nanocomposites (HPPN) Group in IMDEA Materials Institute has set up close collaboration with some top-level research institutions from Germany, UK, Italy, New Zealand, France, etc. Consequently the student will be involved in an environment with many potentialities and the perfect expertise for the fulfillment of the project.

6. Study on the fire behaviors during the combustion of polymeric materials

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. De-Yi Wang, Senior Researcher
Head of the High Performance Polymer Nanocomposites (HPPN) Group
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www.materials.imdea.org

Project description

This research aims at studying the fire behaviors during the combustion of polymeric materials including both experimental research and computational study via collaboration with the top research center. Series fire behaviors, such as dripping behaviors, flame spread behaviors, etc, will be investigated. By carrying out this research, it is very important to predict the fire safety of polymer-based materials. The topic will offer an excellent opportunity for an enthusiastic young scientist to join top excellent international labs located at excellent research environments with all the start-of-the-art core facilities.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

During the project, student will learn the knowledge on study the fire behaviors via both experimental and computational methods. The results will be expected to be published on high impact international journals. By implementing this research, it is expected to establish wide contact with both of European academia and industry during the study. The student would be working in two top research labs at really international environment and performing research at high international standard and in the frontier of material science and technology.

Skills required for CSC student/scholar

A solid background in fire safety, fire engineering, polymer materials, chemistry, or related disciplines; good spoken and written English; excellent team cooperation personality

Remarks

The research will host 1 PhD student/scholar. High Performance Polymer Nanocomposites (HPPN) Group in IMDEA Materials Institute has set up close collaboration with some top-level research institutions from Germany, UK, Italy, Spain, France, etc. Consequently the student will be involved in an environment with many potentialities and the perfect expertise for the fulfillment of the project.

7. Computer-aided synthesis of zeolite materials

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Maciej Haranczyk, Senior Researcher
Computational and Data-Driven Materials Discovery Group
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Project description

Zeolites are the most commonly used class of crystalline porous materials. They are applied across many industries as sorbents, membranes and catalysts. The scale of their use is enormous as their commercial impact reaches hundreds of billions of dollars annually. Nevertheless, there are only about 200 zeolite materials known experimentally while the number of predicted structures reaches millions. The large discrepancy between the numbers of known and predicted materials comes from major synthetic difficulties. This projects aims at facilitating synthesis of (new) zeolites by applications of hybrid computational techniques. In particular, the goal of this project is to design of zeolite-specific structure directing agents – organic molecules that aid formation of desired pore morphology during synthesis – via applications of molecular simulation and chemoinformatics techniques.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

The student will get a solid training in chemoinformatics techniques. He/she will learn concepts behind reaction design, similarity searching and docking. He/she will work with large material databases, computational high-throughput screening approaches and molecular modelling techniques. The student will also have a chance to learn scientific programming. The student will also be working in an international team.

Skills required for CSC student/scholar

Solid background in computational chemistry, material science or a related field. Familiarity with Mac/Linux systems. Strong interest in data-driven research. Good spoken and written English.
Previous research experience and programming experience is desired though not necessary.

Remarks

This project can host 1 PhD student. Computational and Data-Driven Materials Discovery Group at IMDEA Materials Institute has set up close collaborations with a number of top-notch research institutions from USA, UK and Switzerland etc. Consequently the student will be involved in such international collaboration and will have a chance to explore further career opportunities in the collaborating institutions.

8. Computational discovery of porous molecular materials

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Maciej Haranczyk, Senior Researcher
Computational and Data-Driven Materials Discovery Group
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Project description

This project focuses on applications of material informatics and molecular simulations techniques to the discovery of novel porous molecular materials. Porous molecular materials offer many advantages over other classes of porous materials such as zeolites and metal organic frameworks. Their structure is highly tuneable while their synthesis is relatively easy and cheap. They can be applied as sorbents in many industrial separations. The goal of this project is to develop and apply an efficient computational technique to custom-design new materials for use in specific separations.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

The student will get a solid training in chemo- and material informatics techniques. He/she will learn how to work with large material databases and perform tasks such as structure enumeration, characterization and high-throughput screening. The latter will involve off-the-shelve simulation packages as well as in-house GPU-based codes. He/she will also have a chance to apply various machine learning methodologies to accelerate materials discovery. The student will also be introduced to the development of scientific software. The student will also be working in an international team.

Skills required for CSC student/scholar

Solid background in computational chemistry, material science or a related field. Familiarity with Mac/Linux systems and/or programming languages. Strong interest in data-driven research. Good spoken and written English.
Previous research experience is desired though not necessary.

Remarks

This project can host 1 PhD student. Computational and Data-Driven Materials Discovery Group at IMDEA Materials Institute has set up close collaborations with a number of top-notch research institutions from USA, UK and Switzerland etc. Consequently the student will be involved in such international collaboration and will have a chance to explore further career opportunities in the collaborating institutions.

9. Development of β-solidifying multiphase γ-TiAl alloys

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Srdjan Milenkovic, Researcher
Head of Solidification Processing and Engineering Group

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Project description

Advanced intermetallic multi-phase γ-TiAl based alloys are potential candidates to replace heavy Ni-base superalloys in the next generation of aircraft and automotive combustion engines. Aimed components are turbine blades and turbocharger turbine wheels. Concerning the cost factor arising during processing, new processing solutions regarding low-cost and highly reliable production processes are needed. This fundamental study targets the replacement of hot-working, i.e. forging, for the production of turbine blades. But without forging no grain refinement takes place by means of a recrystallization process because of the lack of stored lattice defects. Therefore, new heat treatment concepts have to be considered for obtaining final microstructures with balanced mechanical properties in respect to sufficient tensile ductility at room temperature as well as high creep strength at elevated temperatures. This project deals with the adjustment of microstructures in a cast and heat-treated alloys solely by exploiting effects of phase transformations and chemical driving forces due to phase imbalances between different heat treatment steps and compares the mechanical properties to those obtained for forged and heat-treated material.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

By implementing the project the student will be introduced to and trained to master several experimental techniques: casting, thermomechanical treatment, physical simulation of metallurgical processes, metallographic techniques, microstructure analysis using, optical, scanning and transmission electron microscopy, EBSD and mechanical testing. In addition, he/she will get deep knowledge on the processing-microstructure-properties relationships. The results of the investigation will be published in high impact international peer-reviewed journals.

Skills required for CSC student/scholar

Basic knowledge of phase diagrams, metallography and mechanical properties of materials

Remarks

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10. High-throughput discovery of High Entropy Alloys (HEA)

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Srdjan Milenkovic, Researcher
Head of Solidification Processing and Engineering Group

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Project description

High entropy alloys constitute a new class of materials, quite different from the traditional alloys, consisting of several principal elements intermixed in the crystal lattice. Although showing some attractive properties, an extensive work, both theoretical and experimental, is urgently needed to fully understand the microstructure-properties relationship of this novel family of metallic materials.

The aim of the proposal is to use systematic design approach for rapid screening and discovery of two-phase HEA alloys for structural applications at intermediate temperatures (600-800ºC). The vast composition space of HEA offers great potential for useful discoveries, but at the same time is also the biggest barrier to alloy discovery and development. Therefore, high-throughput methods will be used in several stages. In the first stage high-throughput computations of phase equilibria using the CALPHAD methodology will be applied. High-throughput method for creating macroscopic materials libraries with controlled composition gradients will be used in the second stage, and in the stage 3 high-throughput experiments will be performed on materials libraries with controlled microstructure gradients.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

During the project the student will be introduced to and trained to master several experimental techniques: casting and directional solidification, metallographic techniques, microstructure analysis using, optical, scanning and transmission electron microscopy, EBSD and nanomechanical testing (compression and nanoidentation). In addition, he/she will get deep knowledge of the thermodynamic calculations. The results of the investigation will be published in high impact international peer-reviewed journals.

Skills required for CSC student/scholar

Basic knowledge of thermodynamics, phase diagrams, metallography and casting.

Remarks

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11. Development of ductile and creep resistant Fe-Al-X alloys

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Srdjan Milenkovic, Researcher
Head of Solidification Processing and Engineering Group

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Project description

Fe_3Al based alloys have been studied extensively to exploit their high-temperature properties, in particular their high strength to weight ratio and excellent oxidation and sulfidation resistance. Therefore, they are considered as an alternative to high-alloyed steels for applications at elevated temperatures in corrosive environments such as steam turbines for energy generation. However, insufficient strength at high temperatures has been for long time their major drawback, which prevented their use in such applications.

The aim of this project is to develop ductile, tough and corrosion resistant alloy, by combining Laves phase strengthening and grain refinement by processing. The work will include:

- phase diagram constitution and phase equilibrium studies
- solidification processing of alloys
- characterization of mechanical and corrosion properties at room and elevated temperatures
- analysis of deformation mechanisms

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

By implementing the project the student will be introduced to and trained to master several experimental techniques: centrifugal and suction casting, thermomechanical treatment, physical simulation of metallurgical processes, metallographic techniques, microstructure analysis using, optical, scanning and transmission electron microscopy, EBSD and mechanical testing. In addition, he/she will get deep knowledge on the processing-microstructure-properties relationships. The results of the investigation will be published in high impact international peer-reviewed journals.

Skills required for CSC student/scholar

Basic knowledge of phase diagrams, metallography, casting and mechanical behaviour of metallic materials

Remarks

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