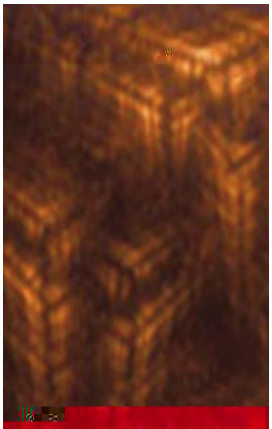

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Research Projects Offer 2016
2016

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

Supervisor: **Prof. Javier LLorca**

2. Quasicontinuum simulation of transport processes at finite temperature

Supervisor: **Dr. Ignacio Romero**

3. High temperature mechanical behavior of metal-ceramic nanolaminates

-

Supervisor: **Dr. Jon Molina-Aldareguia**

4. Bio-inspired hierarchical composites

Supervisor: **Dr. Roberto Guzman de Villoria**

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

Supervisor: **Dr. De-Yi Wang**

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

Supervisor: **Dr. De-Yi Wang**

7. Computer-aided synthesis of zeolite materials

Supervisor: **Dr. Maciej Haranczyk**

8. Computational discovery of porous molecular materials

Supervisor: **Dr. Maciej Haranczyk**

9. - -TiAl alloys
- TiAl

Supervisor: **Dr. Srdjan Milenkovic**

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

Supervisor: **Dr. Srdjan Milenkovic**

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

Supervisor: **Dr. Srdjan Milenkovic**

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

Email: *javier.llorca@imdea.org*
Tel: +34 91 549 3422
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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

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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www.materials.imdea.org/groups/csm
www.materials.imdea.org

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

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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Tel: +34 91 549 3422 (ext. 1044), +34 91 787 1888 (Direct)
http://nano-architectures.com/
www.materials.imdea.org

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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 enha mechanicfabricatio4(r)-6(e4(tu 1 378.79 455.59 Tm[-)]TJ45TBT

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
Email: *deyi.wang@imdea.org*
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http://www.materials.imdea.org/groups/hppn/
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

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

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

Group

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Tel: +34 91 549 3422
Link to short bio
www.materials.imdea.org

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.

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
Group
Email: maciej.haranczyk@imdea.org
Tel: +34 91 549 3422
Link to short bio
www.materials.imdea.org

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.

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 -solidifying multiphase -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

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

By implementing the project the student

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

Remarks

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

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

During the project the student

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

Remarks

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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Link to ShortBio
www.materials.imdea.org

Project description

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

By implementing the project the student

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

Remarks