

# institute Materials

### Encompassing Research of Excellence and Technology Transfer



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#### Research Projects Offered 2015 可申请研究项目和方向

**1.** Development of new strengthened Co alloy base on Co-Al-W system by PM route

新型 Co-Al-W 基高温合金的粉末冶金制备技术 Supervisor: Prof. Jose Manuel Torralba

2. Analysis of slip and twinning in lightweight magnesium alloys by in-situ testing and 3D-EBSD

先进轻质镁合金中滑移和孪晶的原位分析及 3D-EBSD 研究 Supervisor: Dr. María Teresa Perez-Prado

**3. Physical simulation of welding of metallic materials** 金属材料焊接过程的物理模拟 Supervisor: **Dr. Ilchat Sabirov** 

 Atomistic simulation of the recrystallization processes for photovoltaic applications
光伏材料中再结晶过程的原子尺度模拟
Supervisor: Dr. Ignacio Martin-Bragado

5. Multiscale simulation of epitaxial processes in semiconductors for microelectronic applications 微电子半导体材料中外延生长过程的多尺度模拟 Supervisor: Dr. Ignacio Martin-Bragado

6. New generation high performance bio-base polymeric material: From molecular design to application 新一代高性能生物基聚合物材料:从分子设计到应用 Supervisor: Dr. De-Yi Wang

**7. Multifunctional nanomaterial: a new way to fabricate high performance ecofriendly fire retardant polymer nanocomposites** 多功能纳米材料:研究高性能环境友好型阻燃聚合物材料的新方法 Supervisor: **Dr. De-Yi Wang** 

8. Mesoscale model of microstructure during solid state phase transformation 固态相变过程中材料微观组织的计算机模拟 Supervisor: Dr. Yuwen Cui

9. Integrated Computational Materials Engineering (ICME) for exploration of advanced materials

集成计算材料工程在先进材料的设计中的应用 Supervisor: **Dr. Yuwen Cui** 



### 1. Development of new strengthened Co alloy base on Co-Al-W system by PM route

**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. José M. Torralba Head of Solid State Processing Group and Full Professor of Carlos III University of Madrid

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#### **Project description**

The aim of this project is to develop new strengthened Co alloys, on the base of the Co-Al-W system. The in situ development of different precipitates, such as  $\gamma'$ , carbides and carbonitrides are allowed thank to the alloying elements and processing conditions. For promoting an optimum dispersion, it is necessary to select properly consolidation thermal cycle and atmosphere during sintering. Further heat treatments after different noel processing routes as Field Assisted Sintering, can assess the final microstructure. The goal is to develop materials with a high level of wear performance combined with a good corrosion resistance and good level of mechanical properties at high temperature designing a typical ODS microstructure. The work will include phase diagram constitution and phase equilibrium studies; powder development; solid state processing of alloys; characterization of mechanical properties at room and elevated temperature; microstructural analysis.

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

The student will be introduced to and trained to work with the following techniques: ternary and quaternary phase diagram constitution, diffusion couples, mechanical alloying, press and sintering, metallographic techniques sample preparation, microstructure analysis using optical, scanning and transmission electron microscopy, EBSD and mechanical testing.

#### Skills required for CSC student/scholar

Solid background in phase diagrams, metallography and mechanical behaviour of metallic materials; good spoken and written English.

#### Remarks

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### 2. Analysis of slip and twinning in lightweight magnesium alloys by in-situ testing and 3D-EBSD

### **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. María Teresa Pérez Prado, Senior Researcher Physical Metallurgy Group Head of the Alloy Design, Processing and Development Programme

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#### **Project description**

The project aims to investigate the effect of grain size, composition and grain boundaries on slip and twinning in pure Mg and several Mg alloys. The ultimate goal is to better understand the plasticity of these materials in order to design stronger and more isotropic microstructures, thus increasing their attractiveness for the green transport industry.

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

This is a unique opportunity for an enthusiastic young scientist to gain expertise in state of the art-characterization techniques, such as in-situ testing in an SEM, slip trace analysis and 3D-EBSD as well as in processing, microstructural design and mechanical properties of metallic materials. The student will have the opportunity to establish a solid network of contacts within the metallurgy research community.

#### Skills required for CSC student/scholar

Background in Materials Science and Engineering/Physics/Metallurgy and expertise in microstructure characterization and/or mechanical behavior of metallic materials is desirable. Excellent academic credentials as well as fluent spoken and written English will be highly regarded.

#### Remarks

#### 3. Physical simulation of welding of metallic 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. Ilchat Sabirov, Senior Researcher Head of the Physical Simulation Group

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#### **Project description**

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Welding is the most widely used technique by manufacturers to join metals and alloys efficiently and to add value to their products. Welding is crucial to improving the life-cycle costs, quality, and reliability of manufactured goods. The future growth of welding depends largely on the adoption of modern welding processes and tools for selection of optimal welding parameters.

The main objective of the present project is to develop physical simulation tools to study the effect of welding on microstructure and properties of metallic materials. Significant attention will be paid to cracking susceptibility of welds. The work will be carried out in collaboration with industrial company(ies).

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

Apart of mastering state of the art techniques for physical simulation, microstructural and mechanical characterization, the PhD student will gain a fundamental knowledge on the effect of welding on microstructure and properties of metallic materials. 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 metals science or metallurgy; fluency in English language.

Remarks

The project can host 1 PhD student

### **4.** Atomistic simulation of the recrystallization processes for photovoltaic applications

**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 Martin-Bragado, Researcher Atomistic Materials Modeling Group Head of the Integrated Computational Materials Engineering Programme

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#### **Project description**

This project focuses on the Molecular dynamics and Lattice Kinetic Monte Carlo simulation of recrystallization of molten silicon for Photovoltaic Applications. The goal is to better understand the physical processes during such transition, in particular at the point where grain boundaries incorporate new material from the molten phase. The final objective is the simulation of the regrowth rates, facets, and the formation of defects during this process.

#### Project outcomes the student achieves through CSC and IMDEA

The student will get a deep understanding of two particular atomistic techniques (Molecular Dynamics and Lattice Kinetic Monte Carlo). He/she will also learn how photovoltaic cells are produced and will achieve an extremely deep knowledge about recrystallization processes. The student will be working in an international team. The student will also get introduced into the development of scientific software and the use of simulation tools and atomistic data generation and visualization. His/her work will not only be published in high impact scientific journals, but also will be disseminated through the incorporation into an Open Source initiative to produce a Kinetic Monte Carlo simulator. Contact with interested companies is expected.

#### Skills required for CSC student/scholar

Solid background in solid state physics or similar. Some background in electronic processing. Familiarity with GNU/Linux systems and/or programming languages. Strong interest in working in simulation techniques. Some autonomy in doing research. Good spoken and written English.

#### Remarks

This project can host 1 PhD student

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### 5. Multiscale simulation of epitaxial processes in semiconductors for microelectronic applications

**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 Martin-Bragado, Researcher Atomistic Materials Modeling Group Head of the Integrated Computational Materials Engineering Programme

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#### **Project description**

This project will work on the multiscale simulation, using Molecular Dynamics with empirical potentials, and Lattice and Object Kinetic Monte Carlo (KMC), and Finite Element Methods (FEM), of epitaxial processes of interest for the fabrication of novel semiconductor devices in SiGe, Ge and III-V materials. Both the Solid Phase Epitaxial Regrowth and a Solid-Gas Epitaxial Growth will be researched. The project will extract useful atomistic information using Molecular Dynamics that will be incorporated into a KMC simulator. A FEM module will also be used to compute mechanical properties to be fed back into the KMC simulator. The final objective of this project is to a) gain deep understanding on the physical mechanisms of epitaxy b) develop predictive models, and c) research on the improvement of semiconductor devices fabricated using these technologies.

#### Project outcomes that CSC student/scholar could expected to achieve

The student will get a deep understanding of two particular atomistic techniques (Molecular Dynamics and Lattice Kinetic Monte Carlo). He/she will get an expert on the simulation of semiconductor processing for microelectronics fabrication using Technology Computer Aided Design (TCAD) tools. The student will be working in an international team. The student will also get introduced into the development of scientific software and the use of simulation tools and atomistic data generation and visualization. His/her work will not only be published in high impact scientific journals, but also will be disseminated through the incorporation into an Open Source initiative to produce a Kinetic Monte Carlo simulator. Contact with semiconductor foundries is possible.

#### Skills required for CSC student/scholar

Solid background in solid state physics or similar. Some background in electronic processing and/or semiconductor physics. Familiarity with GNU/Linux systems and/or programming languages. Strong interest in working in simulation techniques. Some autonomy in doing research. Good spoken and written English.

#### Remarks

This project can host 1 PhD student



**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 Tel:* +34 91 549 3422, +34 91 787 1888 (Direct) Link to ShortBio www.materials.imdea.org

#### **Project description**

This project would focus on the development of new generation s high performance biobase polymeric material. A combination of innovative molecular design and chemistry synthesis, advanced polymer processing, etc, will be used in the project. In particular, a series of novel bio-based functional monomers will be studied, aiming at preparing high performance bio-based polymers. 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 bio-based polymers and will be trained in advanced characterization techniques from molecular to the further application. It is expected to establish wide contact with European 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.

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### 7. Multifunctional nanomaterial: a new way to fabricate high performance eco friendly fire retardant polymer nanocomposites

**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 Tel:* +34 91 549 3422, +34 91 787 1888 (Direct) Link to ShortBio www.materials.imdea.org

#### **Project description**

This project would focus on the development of new generation sustainable fire safe polymer nanocomposites via multidisciplinary approach. The ground-breaking idea by a combination of innovative molecular design, chemistry synthesis, functionalization, advanced polymer processing and fire retarding technology will be used to develop new functional polymer nanocomposites. Advanced experimental analytical techniques will be employed to understand structure-property relationship. 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.

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

During the project, student will learn the knowledge on design of the functional nanomterial and development of high performance polymer nanocomposites and will be trained in advanced characterization techniques applied to new multifunctional nanomaterials and eco-benign fire retardant technology. The results of the investigation will be expected to be published on high impact international journals. The student would be working in a really international environment and performing research at a high international standard and in the frontier of material science and technology.

#### Skills required for CSC student/scholar

A solid background in polymer materials, chemistry, nanomaterials 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.

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#### 8. Mesoscale model of microstructure during solid state phase transformation

**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. Yuwen Cui, Researcher Head of Computational Alloy Design Group

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#### **Project description**

The research aims at developing the mesoscale Landau/Phase field model to simulate the microstructures resulting from solid state phase transformation in advanced materials, esp. steels and shape memory alloys.

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

The student will develop the Landau model and its code by applying the crystallography, group theory and continuum mechanics. He/she will understand the mechanisms of phase transformation in new novel alloys. The results of the investigation will be published in high impact international peer-reviewed journals.

#### Skills required for CSC student/scholar

A solid background in metallurgy or materials science degree; working knowledge of diffusion and kinetics theory; experience in mesoscale modeling will be considered an important advantage although is not required; good spoken and written English.

Remarks

**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. Yuwen Cui, Researcher Head of Computational Alloy Design Group

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#### **Project description**

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The project aims to perform integrated modelling for lightweight metals to develop fundamental understanding of phase transformation mechanism induced by the processing, and ultimately quantify the links between processing, microstructure/kinetics and mechanical property for designing new lightweight metallic materials including Mg, Al, and Ti alloys.

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

The student will develop an integrated model (e.g. Molecular Dynamics, Phase Field Crystal, Computational Thermodynamics, etc) and apply it to explore the phase transformation induced by severe deformation, and understand the advantages of the new microstructure towards improved mechanical properties. The results of the investigation will be published in high impact international peer-reviewed journals.

#### **Skills required for CSC student/scholar**

Experience in atomistic and multiscale modelling (e.g. first principle, MD, computational thermodynamics, etc); working knowledge of processing and characterization of materials will be considered an important advantage although is not required; good spoken and written English.

#### Remarks