Two Phd fellowships funded by the Department of Materials Science on

Materials for Energy

The student can choose for his Phd thesis among the following topics

- Materials and devices for photovoltaic and thermoelectric applications
- Electrochemical devices for energy storage
- Materials and devices for polymeric fuel cells
- Materials for hydrogen photoproduction and for CO_2 reduction
- Nanoporous materials for gas storage and purification

Further information can be found at

https://www.mater.unimib.it/en/research/flexilab-project/work-packages

ISTITUTO ITALIANO DI TECNOLOGIA

Phd fellowship funded by Istituto Italiano di Tecnologia (IIT)

Machine Learning and Molecular Dynamics

Supervisor: Prof. Michele Parrinello (IIT)

Molecular dynamics based atomistic simulations are one of the pillars of contemporary material science. They provide invaluable insight, replace difficult or impossible experiments, explain and direct the experiments. However, in spite of the unrelenting increase in computer power, the accuracy of these calculations fall short of what would be needed to tackle many problems. Our group has developed a large variety of methods that have allowed pushing forward the frontier of this discipline. In particular we have focused our attention extending the time scales of these simulations so as to bridge the gap between the microscopic time scale of the simulations and the macroscopic time scale of many physical phenomena. The impetuous development of machine learning methodologies offers a new powerful tool for tackling this problem. During her/his PhD will be asked to participate to this effort having in mind applications to material science problems like that of crystallization and crystal growth.

Further information can be obtained from

Michele Parrinello (Michele.Parrinello@iit.it)

Phd fellowship funded by STMicroelectronics

Atomistic simulations of Ge-rich alloys for non-volatile phase change memories

University Tutor: Prof. Marco Bernasconi (University of Milano-Bicocca)

Among the variety of so-called emerging non-volatile electronic memories, phase change memories represent the most mature technology and the first to reach volume production. Phase change memories exploit a fast and reversible transformation between the amorphous and crystalline phases of chalcogenide alloys induced by Joule heating. The two phases of the active alloy have a large contrast in electronic resistivity and correspond to the two logical states of the memory.

In this project, the student will investigate the structural and functional properties of Ge-rich GeSbTe alloys of interest for high temperature applications of phase change memories. To this end, the student will perform atomistic simulations based on electronic structure calculations within Density Functional Theory and large-scale molecular dynamics simulations employing interatomic potentials generated by machine learning methods.

The Consortium Corimav in collaboration with Pirelli Tyre

finances 3 fellowships for the

Phd Program in Materials Science and Nanotechnology

on the projects

1) **Study of nanoparticles effect on multiphase rubber systems**

2) **Design and synthesis of supramolecular structures by self-assembling of tailored organic units for advanced polymeric materials**

3) **Design of environmental-friendly rubber composites driven by biodegradability assessment**

The projects will be carried out both in the University labs of the Department of Materials Science and in the laboratories of Pirelli Tyre under the joint supervision of University and company tutors.

For information please contact

- Dr. Barbara di Credico, Università Milano-Bicocca (barbara.dicredico@unimib.it).
- Dr. Raffaella Donetti, PIRELLI TYRE (raffaella.donetti@pirelli.com).

A description of the three projects is given below.

Study of nanoparticles effect on multiphase rubber systems

University tutor: Dr. Barbara Di Credico (barbara.dicredico@unimib.it)

Tyre materials are complex multiphase rubber systems containing different polymers, resins, anti-degradants, curatives, processing aids and reinforcing fillers. The miscibility of polymer blends and the diffusion of compound ingredients are recognized as important factors to define the structure and morphology of rubber nanocomposites which are in turn, the key factors for the overall materials properties. However, the natural immiscibility of most polymers often produces phase-separated morphologies, depending on both the single-phase properties and the compounding processing, which affect the mutual interactions between the different fluid and solid phases, downgrading the mechanical and thermal properties of the composites.

In this context, fillers choice and chemistry have great influence in preventing domain coarsening or stabilizing suitable morphologies. However, most of the proposed investigations for the physical mechanisms which control the nanoparticle-induced morphological modifications are controversial and mainly related to a specific polymer system. Thus, further endeavors are needed to understand the effect of filler on the overall polymer blends.

The proposed PhD program aims to study the influence of nanofillers on the behavior of the different polymer phases, to gain information on their potential effect on structural and morphological modifications of multiphase rubber systems. This will enable also to shed light on how the evolution of the polymer blend impacts on the filler organization in the composite.

In detail, since the internal system structure is strictly related to the interactions established among the various constituents, the mechanisms that govern the microstructural evolutions of polymers in the presence of fillers before, after, and during vulcanization will be evaluated respect to the filler properties (type, source, amount, size, shape, surface chemistry) and the compounding processes, by combining thermal and viscoelastic, and morphological analyses.

The acquired know-how will be exploited to design of sustainable tailor-made materials for advanced rubber applications.

Design and synthesis of supramolecular structures by self-assembling of tailored organic units for advanced polymeric materials

University tutor: Prof. Antonio Papagni (antonio.papagni@unimib.it)

Supramolecularly arranged organic systems are a modern tool in the development of new materials for advanced technological applications. Exploiting peculiar interactions able to promote self-assembling processes, interesting and important effects on rheological and viscoelastic properties and/or on self-healing capability were recently observed in polymeric materials.

The proposed research activity is focused on the design, synthesis and study of organic compounds bearing both self-assembling units and thermally activated reactive species to be employed in the modification of mechanical and elastomeric properties of polymers of potential interest in tyre applications. The thermal activated reactive species are thought to react with suitable functionalities present in the polymeric matrix while the self-assembling units are exploited for introducing intra and inter polymeric chain interactions with the aim of modulating rheological and viscoelastic parameters important in defining the mechanical properties of the polymeric material.

Design of environmental-friendly rubber composites driven by biodegradability assessment

University tutor: Prof. Paola Branduardi (paola.branduardi@unimib.it)

Sustainability is the main technological challenge of the foreseeable future – also in the field of rubber composites, legislation and market forces are aligning in the request to improve the environmental footprint of materials and products while keeping their technical performances. The final target is to embed this production chain in the model of “Circular Economy”, where renewable resources are transformed into products that at the end of their life either fully return to Nature or can be further used as raw materials for new products.

Very little is known today about the end of life of state-of-the-art rubber compounds. The proposed research activity is focused i) on the assessment of biodegradability of rubber compounds as a function of their formulation, morphology, process and aging, ii) paving the way to the rational design of more environmentally friendly rubber composites of potential interest in tyre applications.

In respect to the first aim, the project will optimize a protocol for mimicking the chemical-physical parameters of degradation in the environment and in a controlled composter for rubber compounds. This will constitute a benchmark to develop novel compounds. Both for novel formulation as well as for accelerating biodegradability, the project will see a convergence of topics related to material science as well as to biological macromolecules and bio-based processes.

The research activity will include biochemical and compounding activity to formulate rubber-based compounds and laboratory work to characterize mechanically such compounds and assess their biodegradability following standard methods or originally adapting them as needed.