



# PhD in INGEGNERIA DEI MATERIALI / MATERIALS ENGINEERING - 38th cycle

**INTERDISCIPLINARY Research Field: MACROMOLECULAR SIMULATIONS AND MACHINE  
LEARNING: A NOVEL TEMPORAL AND SPATIAL MULTI-SCALE APPROACH**

## Monthly net income of PhDscholarship (max 36 months)

**€ 1325.0**

In case of a change of the welfare rates or of changes of the scholarship minimum amount from the Ministry of University and Research, during the three-year period, the amount could be modified.

## Context of the research activity

### Motivation and objectives of the research in this field

Interdisciplinary PhD Grant  
The PhD research will be carried out in collaboration with research groups of the PhD programme in **"INFORMATION TECHNOLOGY"**.  
See <https://www.dottorato.polimi.it/?id=422&L=1> for further information.

### Methods and techniques that will be developed and used to carry out the research

The goal of the research is the study and development of novel machine learning techniques able to address the "reverse mapping" problem, i.e., the insertion of atomistic detail into coarse-grained models of high molecular weight amorphous polymers. The novelty of the proposed research activity resides in the ability to design new machine learning techniques (both in terms of architectures and training algorithms) to take into account and exploit the chemical-physical constraints characterizing the molecular simulation of polymeric materials. Such techniques will be able to encode the physical structures of polymeric materials by relying on deep learning models as well as dealing with transition manifolds able to support the long-time simulation of the system. By considering a series of "commodity polymers" (e.g., PE, a-PS, cis-PI, PDMS, PET), the two main outcomes of the research will be (a) a database of atomistic structures, from simulations on low molecular weight chains, and (b) novel machine-learning architectures and algorithms supporting the mapping of



	atomistic to coarse-grained models and back. For such purpose, deep learning solutions based on graph representations and learning-in-non-stationary frameworks will be considered and explored.
<b>Educational objectives</b>	The PhD candidate will learn the foundations of materials science, and of polymers in particular. He/she will also learn in depth about molecular simulations, and the high performance computational tools that are employed to carry them out. Finally, he/she will also learn about the analysis of large amounts of data and machine learning algorithms. In addition to the above technical skill, the candidate will also be expected to acquire a range of soft skills, such as writing and presenting one's work at conferences.
<b>Job opportunities</b>	The successful PhD candidate will have access to jobs in the academic track (typically, a post-doc position in a university or research institute), as well as in industry and the service sectors (materials development, high performance computing, data science, machine learning, etc.).
<b>Composition of the research group</b>	2 Full Professors 1 Associated Professors 1 Assistant Professors 3 PhD Students
<b>Name of the research directors</b>	Prof. G. Raos / Prof. C. Alippi

#### Contacts

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#### Additional support - Financial aid per PhD student per year (gross amount)

<b>Housing - Foreign Students</b>	--
<b>Housing - Out-of-town residents (more than 80Km out of Milano)</b>	--

#### Scholarship Increase for a period abroad

<b>Amount monthly</b>	662.5 €
<b>By number of months</b>	6



**Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information**

Educational activities (funding for participation in courses, summer schools, workshops and conferences) - financial aid per PhD student about 5.500 euros per student.

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student: there are various forms of financial aid for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.