POLITECNICO DI MILANO

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

Number of scholarship offered	6
Department	DIPARTIMENTO DI CHIMICA, MATERIALI E INGEGNERIA CHIMICA "GIULIO NATTA"

Description of the PhD Programme

The specific research activity sharing this broad research area might be focused on one of the following topics: **Micro and nanostructured materials:** Production of innovative nanostructured thin films and surfaces, and their physical characterization (e.g. morphology, structure and electronic properties). Focus will be on the study of materials for energy-related applications, with a condensed matter physics approach (e.g. materials for thermoelectric, photovoltaic and catalytic applications). **Functional organic materials for applications in photonic and electronic**. The research will deal with the synthesis and characterization of organic functional materials with tailored optical and electrical properties.**Surface engineering and advanced coatings:** Surface treatments play an important role in several fields: energy, environment, design, architecture, electronics, biomaterials, etc.. The activity will be focused on the production of innovative coatings and thin films by electrolytic or PDV/CVD techniques. The approach combines electrochemistry, surface engineering, physical chemistry and metallurgical competences.**Mechanical and physical properties of micro and nano-structured materials for biomedical applications:** The objective is to improve the knowledge on the relationship between properties and structure of micro and nano-structured biomaterials, such as ceramic based nano-structured coating.**Polymeric Materials for Advanced Applications:** The activity is aimed at developing and/or improving materials and products for new applications through macromolecular structure design, new polymer production routes and appropriate bulk and surface physico-mechanical characterization in the following areas: Polymer Nanocomposites; Advanced rubbers; Composites for aeronautic and marine applications; Innovative textiles; Materials for energy; Polymeric Lab on Chip Devices; Materials and technologies for environment**Scattering, Spectroscopy, Modelling and theoretical approaches to the structure of materials**: Development of structural models, from sub-nanometric to micrometric scales, allowing to rationalize the behaviour of new functional and nanostructured materials. Fields of application : Polymer Nanocomposites; Advanced rubbers; Innovative textiles; Materials for electronic, photonic and energy; Biomaterials**Production and characterisation of titanium oxides:** The alterations caused by anodising treatments of titanium oxide will be exploited to functionalize titanium surfaces. Applications range from photocatalytic systems for wastewater treatment and air purification, to the implementation of a new generation of photovoltaic cells, to the biomedical field.**Innovative**

materials for civil and industrial engineering works: The main objectives are: - development and characterization of novel low-friction materials with high wear resistance and strength; - prediction of mechanical properties of composite materials depending on aging and fatigue loading conditions; - reinforcement of steel and concrete structures by composite materials (FRP).**Materials and techniques in the Cultural Heritage**

POLITECNICO DI MILANO

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 Reasearch,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.
Educational objectives	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.
Job opportunities	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.).
Composition of the research group	2 Full Professors 1 Associated Professors 1 Assistant Professors 3 PhD Students
Name of the research directors	Prof. G. Raos / Prof. C. Alippi

Contacts
guido.raos@polimi.it +39 022399 3051 cesare.alippi@polimi.it +39 022399 3512

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	662.5 €
By number of months	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.

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

OPEN SUBJECT Research Field: MATERIALS ENGINEERING

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 Reasearch,during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	1. Polymeric Materials for Advanced Applications; 2. Surface engineering and advanced coatings; 3. Functional organic materials for applications in photonic and electronic; 4. Production and characterization of micro and nano-structured materials for catalysis, photovoltaic, electronic, biomedical applications; 5. Innovative materials for civil and industrial engineering works; 6. Scattering, Spectroscopy and modeling of materials; 7. Materials and techniques in the Cultural Heritage
Methods and techniques that will be developed and used to carry out the research	Advanced methods for materials preparation and characterization, ranging from mechanical tests, physical properties determination, chemical and structural analysis, will be learned and used. Quantum Chemical modelling of molecular materials and polymers
Educational objectives	The objective is to combine the theoretical knowledge with technological skills in order to train a qualified researcher who can guide the design, manufacturing and use of traditional and/or new materials.
Job opportunities	PhD course offer specialized curricula aimed to the formation of specialized people with skills in: i) development and innovation in the production, processing, application and conservation of traditional materials; ii) development of innovative materials for the production of new manufactured goods or devices to cope with the growing demands of modern technologies.

Composition of the research group	15 Full Professors 10 Associated Professors 20 Assistant Professors 30 PhD Students
Name of the research directors	Chiara Bertarelli

Contacts
chiara.bertarelli@polimi.it +39 022399.3224 http://www.dottorato.polimi.it/corsi-di-dottorato/corsi-di-dottorato-attivi/ingegneria-dei-materiali/

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	662.5 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Educational activities (purchase of study books and material, funding for participation in courses, summer schools, workshops and conferences) financial aid per PhD student about 5.500 euros *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 regulations. *Computer and desk availability*

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

INTERDISCIPLINARY Research Field: SELF-ASSEMBLING COMPOSITE MATERIALS FOR INDUSTRIAL AND CIVIL WASTEWATER TREATMENT VIA PHOTOCATALYTIC PROCESSES

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 Reasearch,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 "**INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING**". See https://www.dottorato.polimi.it/?id=422&L=1 for further information. The management of water resources, in terms of rational use, purification treatments and recycling, is a long-standing and crucial issue that is increasingly considered to be the basis of sustainable global development. In particular, reduction of the level of inorganic and organic contaminants in water streams for industrial, domestic or agricultural use, has a paramount importance for reasons primarily related to human health, but also to environmental, technical and regulatory issues. It is therefore necessary to implement technological solutions aimed at reducing the content of undesirable species in wastewater coming from various processes in order to reusing such streams within the original process or disposing of them in a safe and sustainable way. There are two main methods used today: liquid-liquid processes (e.g., extraction with organic solvents) and solid-liquid processes (filtration and adsorption). The selection of the most appropriate technique depends on the correct evaluation of different parameters, such as, for example, reliability, flexibility, cost, environmental sustainability, process scalability and efficiency in contaminant removal.

	In this scenario, the research proposes to address two urgent problems such as metal accumulation and pollution caused by pesticides and herbicides, by employing adsorbent materials in the form of self-assembling reduced graphene oxide (rGO) membranes and TiO_2-based photocatalysts. The final goal is to develop a composite filter to be used in photocatalytic reactors able to adsorb hybrid contaminants degrading the organic fraction. At the same time, it has to reduce the content of heavy metals, synergistically exploiting the well-known properties of TiO_2 and the innovative capabilities, demonstrated by the proponents, of rGO.
Methods and techniques that will be developed and used to carry out the research	The activity will be carried out by integrating chemical and materials science knowledge with catalysis and photocatalysis knowledge. In particular, a method for GO reduction will be refined using reagents that are neither dangerous to humans nor harmful to the environment, such as, for example, ascorbic acid instead of hydrazine, still widely used as a reducing agent in the scientific literature. Self-assembling composite membranes will be produced by adopting TiO_2-containing formulations, and morphological and photocatalytic properties of the membranes will be investigated. All of them will be tested in photocatalytic reactors in order to evaluate the correlations between their morphological properties and performance in removing target pollutant species.
Educational objectives	The research activity will strengthen the following skills:- materials selection in several operating conditions;- design of experiments to fulfil pre-defined targets;- team-working and human interactions in research and industrial environments
Job opportunities	The research activity will strengthen the following skills:- materials selection in several operating conditions;- design of experiments to fulfil pre-defined targets;- team-working and human interactions in research and industrial environments
Composition of the research group	2 Full Professors 3 Associated Professors 3 Assistant Professors

	5 PhD Students
Name of the research directors	Prof. Dotelli - Prof.ssa Nova

Contacts
Telephone: +39 0223993232 (prof. Dotelli); +39 0223993228 (prof. Nova) Email: giovanni.dotelli@polimi.it; isabella.nova@polimi.it Web-pages of the research group: Mat4En^2 group:https://mat4en2.cmic.polimi.it/ - LCCP group: https://www.lccp.polimi.it/

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	662.5 €
By number of months	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 5.500 euros. **Teaching assistantship**: availability of funding in recognition of supporting teaching activities by the PhD student:There are various forms of financial of 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.