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RESEARCH THEMES
DOCTORATE SCIENCES AND TECHNOLOGIES OF CHEMISTRY AND MATERIALS

NOTE: In this file you can find additional information on some research themes summarized in the call June, 2024.

Summary

Curriculum Nanosciences – Code 10563

1. Development of functional graded layered nanomaterials (funded by 2023 ERC Consolidator Grant EVA, programme Horizon Europe, GA 101124411)

Supervisor(s): Milena Arcignegas

Short title	Development of functional graded layered nanomaterials
Expanded Title	Design and synthesis of intrinsically functional graded layered nanomaterials in solution
Background	Advanced functional devices require the integration of distinct materials (polymers, ceramics, metals) with different properties to achieve high performance in aerospace, biomedicine, electronics, and automotive. A major structural challenge is associated with localized (mechanical, thermal, electrical) stresses due to property mismatch at different scales, thus causing premature malfunction

	and failure. Research has focussed on compositional or structural material gradients (in at least one spatial direction) to enable the fabrication of "in-one" body parts (mostly inorganics) with exceptional properties. Examples at rather macroscale include AlGaAs with graded bandgap for solar cells, or Al2O3/Ti with graded mechanical stiffness for bioimplants. However, in light of miniaturization technology, there is a need to translate this concept to nanomaterials. The Automated Nanomaterials Engineering group at IIT aims to unveil the deep relationships between the composition of 2D layered nanomaterials and their properties towards functionally graded nanostructures
Description	In this PhD project, we will focus first on the synthesis of structures that intercalate different organic and inorganic components and investigate the role of, for example, organic cations, solvents, concentrations, and injection rates, to carefully build layered nanomaterials with graded properties. In parallel, the developed protocols will be translated into automated processes. These nanostructures will be subjected then to a complete (structural, chemical, surface, mechanical, and optical) characterization. The layered nanomaterials will be engineered to optimize their graded mechanical and optical properties
Main Supervisor	Dr. Milena Arciniegas, Milena.Arciniegas@iit.it
Essential expertise	
i)	Excellent Master Degree in Chemical Engineering, Chemistry, Material Science, Physics, or similar
ii)	Highly motivated
iii)	Creative
iv)	Excited to work in an interdisciplinary team
Desirable expertise	
i)	Experience in organic chemistry
ii)	Experience in structural and optical characterization
iii)	Experience in materials synthesis
iv)	Knowledge in robot-assisted synthesis

2. Rapid fabrication of graded layered nanomaterials (funded by 2023 ERC Consolidator Grant EVA, programme Horizon Europe, GA 101124411)

Supervisor(s): Milena Arcignegas

Short title	Rapid fabrication of graded layered nanomaterials
Expanded Title	Design and synthesis of intrinsically functional graded layered nanomaterials through rapid liquid deposition
Background	Advanced functional devices require the integration of distinct materials (polymers, ceramics, metals) with different properties to achieve high performance in aerospace, biomedicine, electronics, and automotive. A major structural challenge is associated with localized (mechanical, thermal, electrical) stresses due to property

	mismatch at different scales, thus causing premature malfunction and failure. Research has focussed on compositional or structural material gradients (in at least one spatial direction) to enable the fabrication of "in-one" body parts (mostly inorganics) with exceptional properties. Examples at rather macroscale include AlGaAs with graded bandgap for solar cells, or Al2O3/Ti with graded mechanical stiffness for bioimplants. However, in light of miniaturization technology, there is a need to translate this concept to nanomaterials. The Automated Nanomaterials Engineering group at IIT aims to explore rapid fabrication strategies for constructing 2D layered nanomaterials with graded properties, aiming to revolutionize the landscape of advanced materials engineering
Description	In this PhD project, we will exploit different rapid fabrication routes based on controlled liquid deposition to deliver functional graded layered nanomaterials. This will include direct laser writing and drop-on-demand injection to intercalate consecutive organic and inorganic layers, as a means to create mechanical and optical gradients in the final layered films. These nanostructures will be subjected then to a complete (structural, chemical, surface, mechanical, and optical) characterization, including the assessment of their stability against moisture and temperature. The layered nanomaterials will be engineered to optimize their graded mechanical and optical properties
Main Supervisor	Dr. Milena Arciniegas, Milena.Arciniegas@iit.it
Essential expertise	
i)	Excellent Master Degree in Materials Science, Chemical Engineering, Chemistry, Physics, or similar
ii)	Highly motivated
iii)	Creative
iv)	Excited to work in an interdisciplinary team
Desirable expertise	
i)	Experience in direct laser writing and controlled liquid deposition
ii)	Experience in structural and optical characterization
iii)	Knowledge in materials wet-chemical synthesis
iv)	Knowledge in automated synthesis methods

3. Light-matter interaction in solution-processed nanomaterials

Supervisor(s): Roman Krahne

Short title	Light-matter interaction in solution-processed nanomaterials
Expanded Title	Light-matter interaction and photonics in emerging solution-processed nanomaterials with complex and anisotropic architectures
Description	We are investigating emerging nanomaterials for light emission and their integration into optical resonators to obtain nonlinear

	optical properties and emitting devices with novel functionalities. Towards the emitters we focus on low-dimensional metal-halide perovskites and colloidal nanocrystals that can be tailored for the compatibility with photonic cavities in size, emission wavelength and surface functionalisation. For the optical resonators we are interested in photonic cavities that can consists of the emitting material itself, or in which the emitters can be readily integrated. We will also consider plasmonic nanosystems that can be realized either by self-assembly or top-down fabrication. This PhD project will target the fabrication of the photonic cavities and explore different strategies for the integration of emitting nanomaterials, with the aim to discover novel approaches that can boost the performance of optoelectronic devices in light emission and photodetection.
Main Supervisor	Dr. Roman Krahne, roman.krahne@iit.it
Essential expertise	
i)	Master Degree in Physics, Chemistry, Mechanical Engineering, Nanotechnology, Material Science, or similar
ii)	Profound knowledge in solid-state physics and semiconductor devices
iii)	Knowledge in optoelectronic and/or structural characterization tools
iv)	Enthusiastic to work in a creative and international environment
Desirable expertise	
i)	Experience in optical spectroscopy
ii)	Experience in nanofabrication (clean room)
iii)	Experience in nanomaterial fabrication
iv)	Experience in electrical characterization

4. Development of light-sources based on colloidal quantum dots

Supervisor(s): Francesco di Stasio, Paola Lova

Short title	Quantum dots light-emitting devices
Expanded Title	Development of light-sources based on colloidal quantum dots
Background	The Photonic Nanomaterials group aims at developing both classical and quantum light-sources exploiting the unique properties of colloidal quantum dots (QDs). The motivation for such aim lies in the versatility of QD chemistry, which enables on-demand tailoring of the light-emission properties of the final nanomaterial. In addition, solution processing of QDs allows the fabrication of small-footprint, CMOS compatible light-emitting devices that can be integrated into complex photonic architectures, retaining tuneable emission wavelength from the blue to the near-infrared. Importantly, one must consider that the lack of miniaturized light-sources is the current bottleneck of photonic technologies, holding back their full integration. One can

	draw a comparison with the development of integrated electronics, which was driven by the constant decrease in size of field-effect-transistors in the last decades of the 20th century
Description	Currently, the group is focusing on the development of three main types of light-sources exploiting QDs (either small or large-footprint ones): Near-infrared light-emitting diodes (940 – 1300 nm) based on InAs QDs, optically and electrically driven single-photon sources operating in the visible and near-infrared spectral ranges, and integrated photonic nanostructures/QDs light-emitting devices presenting circularly polarized emission. The PhD candidate will focus on the implementation of colloidal quantum dots in such light-sources currently under development in the Photonic Nanomaterials group. In this context, the activities will either focus on chemical synthesis, optical characterization (steady-state and time-resolved photoluminescence, photon statistics, etc…) or device fabrication depending on the expertise and the interest of the selected candidate. Importantly, the PhD candidate will engage in collaborations with other group members, given the interdisciplinary nature of the proposed research theme, which requires a variety of skills for implementation
References	Advanced Science, 2312482 (2024), Advanced Optical Materials, 2400554 (2024), ACS Photonics, 10, 1662–1670 (2023), ACS Energy Letters, 7, 3788-3790 (2022)
Main Supervisor	Dr. Francesco Di Stasio, Francesco.DiStasio@iit.it
Additional Supervisor	Dr. Paola Lova
Essential expertise	
i)	Master degree in Materials Science, Chemistry, Physics or related disciplines
ii)	Highly motivated
iii)	Willing to undertake a challenging research project
iv)	Interest in working in an interdisciplinary team
Desirable expertise	
i)	Colloidal synthesis of quantum dots (II-VI, III-V, perovskites)
ii)	Functionalization of quantum dots (ligand exchange procedures both in solution and solids)
iii)	Fabrication and electro-optical characterization of light-emitting devices
iv)	Characterization of quantum dots (comprehensive investigation of their structural, optical and morphological properties)

5. Nanoparticle-based colorimetric biosensors

Supervisor(s): Pierpaolo Pompa

The project will focus on the development of new sensing platforms able to identify and quantify low concentration biomarkers in non-invasive fluids such as saliva and urine. Combining nanotechnology with biotechnology (exploiting the unique physical-chemical properties of nanoparticles, e.g., plasmonics

and catalysis) will lead to innovative and smart colorimetric diagnostic tests with naked-eye or smartphone-based readout (powered by machine learning algorithms).

Requirements: a background in chemistry, biotechnology, physics, engineering, and related disciplines would be appreciated.

For further details concerning the research theme, please contact: pierpaolo.pompa@iit.it.

6. Biological application of nanozymes

Supervisor(s): Pierpaolo Pompa

Nanozymes are catalytic nanoparticles able to mimic natural enzymatic activities even in conditions where natural enzymes are ineffective. This project will focus on the investigation of the therapeutic potential of nanozymes exploiting their unique antioxidant and anti-inflammatory properties. Biofunctionalization of nanoparticles for specific biological targeting will be also part of the project.

Requirements: a background in chemistry, biotechnology, and related disciplines would be appreciated.

For further details concerning the research theme, please contact: pierpaolo.pompa@iit.it.

7. Exploring new nanozyme functionalities and applications

Supervisor(s): Pierpaolo Pompa

Nanozyme are nanoparticles that can mimic natural enzymes, however one single nanozyme can present multi-catalytic activity, mimicking even three or more natural enzyme altogether, with no need for specially prepared functionalization. The catalytic activity can be switched by using co-factors or specific environmental conditions. As a matter of fact, for several nanozymes new properties are yet to be found and so are their potential applications. This project aims to explore new nanozyme activities, investigate some properties recently found in our group and their potential applications in sensing, nanomedicine, and environmental remediation.

Requirements: a background in chemistry, biotechnology, physics, engineering, and related disciplines would be appreciated.

For further details concerning the research theme, please contact: pierpaolo.pompa@iit.it.

Curriculum Science and Technology of Materials – Code 10564

Research themes Decreto Ministeriale n. 630 – 24/04/2024

8. Archaeological wood objects with the presence of metal elements: physico-chemical characterization and evaluation of new consolidants. Co-funded by: Conservazione e Restauro di Ilaria Bianca Perticucci, Milano

Supervisor(s): Davide Peddis, Federico Locardi

The restoration of waterlogged archaeological wood poses a complex challenge involving not only the preservation of the wood structure but also the conservation of any metallic fastening elements that may be present (e.g., nails, bolts, hinges) The presence of these metal elements can trigger degradation processes in the wood, making a detailed characterization of the artifacts essential, with particular reference to the chemical and physical interactions between wood and metal. Furthermore, during restoration, the use of consolidants (such as polyethylene glycol (PEG), for example) may promote the corrosion of metal elements. The aim of this thesis is the study of the degradation processes resulting from the interaction between wood and metal, employing advanced characterization techniques that allow the identification of the chemical composition, crystalline structure, and degradation products, thus providing an in-depth understanding of the ongoing deterioration mechanisms. Another objective is to study and select consolidating materials compatible with both components of the artifact. These consolidants will need to be optimized in terms of penetration capacity, conferred mechanical resistance, and aesthetic outcome.

For further details concerning the research theme, please contact: Davide.Peddis@unige.it, Federico.Locardi@unige.it.

9. Study and optimization of the parameters for the electrochemical synthesis of sodium hypochlorite. Co-funded by: Angelini S.p.A.

Supervisor(s): Diego Colombara

The research activity of this PhD project is related to the study and optimization of the parameters for the electrochemical synthesis of sodium hypochlorite.

The electrochemical synthesis of sodium hypochlorite from sodium chloride is a well established process; nevertheless, it is amenable to improvements and optimizations with an eye to the final product. For example, the process layout may be innovated to maximise its efficiency. In this context, the research activity is devoted to the identification of means to reduce wastes, resources utilization and environmental footprint, taking into account the industrial viability, i.e. process automation and digitization, to increase resilience. The project targets the production lines of disinfectants, according to the principles of green chemistry, and may make use of micro/nano-structuration and identification of alternative materials for electrodes intended for the chlorine evolution reaction.

For further details concerning the research theme, please contact: diego.colombara@unige.it.

Research theme for grant funded by ENI S.p.A., Rome

10. Technical, economic, and sustainability analysis of remediation technologies

Supervisor(s): Marco Vocciante

The doctoral candidate's work will focus on the technical, economic and sustainability analysis of remediation technologies of interest to Eni, aimed at assessing the applicability and effectiveness of different approaches to targeted sites under actual site-specific conditions.

In addition to experimental activities for the chemical-physical characterization of a given site, from matrix texture to contaminant speciation, the candidate will be responsible for setting up and conducting specific experimental campaigns on a laboratory and/or higher scale to evaluate the effectiveness of the solutions identified for the remediation of the site in question under its specific conditions. In order to deepen the analysis and identify potential improvements in the materials and methods employed, various modeling approaches may be considered, including computational numerical simulation of the systems and processes involved, where useful to expand what can be obtained experimentally. Aspects of sustainability assessment of remediation processes using LCA-based techniques will be an integral part of the feasibility analysis of the investigated approaches, and will be a key optimization criterion along with the economic feasibility aspects of the intervention.

For further details concerning the research theme, please contact: marco.vocciante@unige.it.

Curriculum Chemical Sciences and Technologies – Code 10565

Research theme Decreto Ministeriale n. 629 – 24/04/2024

11. Membrane processes and reactors for water treatment e valorization

Supervisor(s): Antonio Comite

Membrane processes are now fundamental for an efficient and correct management of the water resource and will be increasingly so in a circular economy as well as environmental sustainability. The doctorate project aims at the recovery of waste water and its possible exploitation from waste to resource through both conventional (pressure-driven) and emerging membrane processes (e.g. membrane distillation, biofilm membrane reactors, electrodialysis). For some processes it will be necessary to study the most suitable membranes and possibly to prepare special membranes in the laboratory. The waters to be treated will be both model solutions that real waters with environmental problems also coming from the production agro-industrial beyond that municipal (e.g. waters of vegetation). A particular attention will be dedicated to the treatment of wastewater by biological membrane reactors studied in different configurations (e.g. filtration mode and supporting a biofilm). The processes will involve the study of the different operating parameters. Valuable products will be identified and eventually concentrated for their eventual valorization. The water recovery from the processes will be studied in order to meet the application requirements (e.g. irrigation use).

For further details concerning the research theme, please contact: antonio.comite@unige.it.

Curriculum Chemical Sciences and Technologies – Code 10566

Research themes funded by 2023 ERC Starting Grant CIRCULARIZE, programme Horizon-ERC, GA 101114664

12. Processing of biomass for the extraction of platform molecules for the synthesis of novel solvents and polymeric materials

Supervisor(s): Alessandro Pellis

As part of the CIRCULARIZE project financed by the European Research Council (ERC) of the European Union as Starting Grant project (ERC-2023-STG) this PhD position is advertised on the topic: processing of biomass for the extraction of platform molecules for the synthesis of novel solvents and polymeric materials.

The project aims to process various biomasses (bamboo, spent coffee grounds, etc.) to extract the bio-oil which composition will be evaluated by LC-MS, GC-MS ed NMR techniques. After the characterization, the main components of the bio-oil will be isolated and utilized for the preparation of novel solvents and polymeric materials by using chemo-enzymatic processes and using solely green and sustainable chemistry techniques.

For further details concerning the research theme, please contact: alessandro.pellis@unige.it.

13. Chemo-enzymatic synthesis of novel macromolecular architectures by using biobased functional monomers

Supervisor(s): Alessandro Pellis

As part of the CIRCULARIZE project financed by the European Research Council (ERC) of the European Union as Starting Grant project (ERC-2023-STG) this PhD position is advertised on the topic: chemo-enzymatic synthesis of novel macromolecular architectures by using biobased functional monomers.

The project aims to conduct the selection and the chemical modification by means of carba-, aza- and thia-Michael reactions of platform molecules deriving from biomass. The new building blocks will be processed by means of enzymatic techniques to polymeric materials that will be characterized via NMR, GPC, TGA, DSC and FT-IR techniques. All the steps will be carried out utilizing solely green and sustainable chemistry techniques.

For further details concerning the research theme, please contact: alessandro.pellis@unige.it.