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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 of the research themes summarized in the call June, 2023.

Summary

Curriculum Drug Discovery and Nanobiotechnologies

1. Nanoparticle-based colorimetric biosensors

Tutor: 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.

2. Biological application of nanozymes

Tutor: 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.

3. Exploring new nanozyme functionalities and applications

Tutor: 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 ctivities, 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 Nanochemistry

4. Development of colloidal nanocrystals for energy related applications (3 scholarships)

Tutors: Liberato Manna, Luca De Trizio

The need to reduce the pollution connected with the combustion of petrol and carbon is increasingly pushing research toward the development of new materials that can be used in energy conversion devices and/or that can decrease the energy demand of devices (e.g. for telecommunications or light emitters). Solar cells or solar concentrators, for instance, enable the direct conversion of the solar energy into electrical power, thus generating “green” energy. Colloidal semiconductor nanocrystals (NCs) have been shown to be promising materials for low-cost and high efficiency solar cells, solar concentrators and light emitting optoelectronic devices thanks to their unique properties and to the low costs associated with their synthesis. For example, NCs having a stokes-shifted photoluminescence (PL) emission can be optimal candidates to be employed in plastic-based solar concentrators or even for scintillators. The latter are devices capable of detecting ionizing radiation which could be potentially employed for (clean) energy production (in particular in future fusion reactors) as well as for strategic technologies including homeland security, medical diagnostics and environmental monitoring. On the other hand, NCs emitting in the near infrared could be exploited in solar cells and/or low-cost near infrared based optoelectonic devices (e.g. night vision, optical telecommunications, food quality assessment ecc).

In general, the optical properties of colloidal NCs can be finely tuned to match the required standards, and the NCs, in the form of inks (i.e. dispersion of NCs in a desired solvent) can be readily employed in low cost ink-jet processes for the fabrication of devices. This research activity will be first focused on the synthesis of nanocrystals (targeting for example emerging metal halides, metal oxides, metal chalcogenides and pnictides) and heterostructures (i.e. nanocrystals composed of two (or more) domains of different materials). Doping/alloying strategies will be also pursued in order finely tune the optical properties of the above-mentioned nanostructures. The nanocrystalline products will be subjected then to a complete (structural, chemical, surface and optical) characterization. Both the nanocrystals and the heterostructures will be engineered in order to optimize their optical and/or electrical properties.

Requirements: The ideal candidate must have a Master Degree in one of the following areas: Material Science, Chemistry, Chemical Engineering or Physics.

For further details concerning the research theme, please contact: liberato.manna@iit.it, luca.detrizio@iit.it.

5. Synthesis and characterization of organic materials based on Sulfur (II)-containing polymers, and their biological anti-oxidant performance

Tutor: Nicola Tirelli

Sulfur (II) organic polymers (polysulfides, polythioacetals) can effectively scavenge biologically relevant oxidants (Reactive Oxygen Species, ROS) such as hydrogen peroxide or superoxide. Since ROS typically act as inflammatory mediators (both intra- and inter-cellularly), their removal has important anti-inflammatory consequences [1,2]. Further, ROS-scavenging polymers may also fulfil a protective (sacrificial) role for sensitive molecules such as therapeutic proteins, being oxidized in their stead [3].

This project aims to develop hydrophilic ROS-scavenging polymers, such as poly(thioglycidyl glycerol). The objective is to employ them as functional components of systems (nanoparticles), which are designed to intracellularly deliver nucleic acids.

The skills developed in the project will include monomer/polymer synthesis (including microfluidic-assisted scaled-up processes), nanomaterial/colloidal characterization, culture and molecular biology characterization of mammalian cell lines. Previous experiences in polymer synthesis are strongly preferred.

[1]. F. El Mohtadi et al., A 'tandem' nanomedicine approach against osteoclastogenesis. Polysulfide micelles synergically scavenge ROS and release rapamycin, *Biomacromolecules*, **21** (2020) 305-318. DOI: 10.1021/acs.biomac.9b01348

[2]. Z.Y. Turhan et al., Dual thermal- and oxidation-responsive polymers synthesized by a sequential ROP-to-RAFT procedure inherently temper neuroinflammation, *Biomacromolecules*, **24** (2023), in press. DOI: 10.1021/acs.biomac.2c01365

[3]. R. d'Arcy et al., A Reactive Oxygen Species-scavenging 'stealth' polymer, poly(thioglycidyl glycerol), outperforms poly(ethylene glycol) in protein conjugates and nanocarriers and enhances protein stability to environmental and biological stressors, *Journal of the American Chemical Society*, **144** (2022), 21304–21317. DOI: 10.1021/jacs.2c09232.

For further details concerning the research theme, please contact: Nicola.tirelli@iit.it.

6. Development and preparation of colloidal nanocrystals with chiroptical activity

Tutors: Francesco Di Stasio, Paola Lova

The quest for new medical drugs demands reliable, ultrasensitive and fast techniques to identify, refine and test small volumes of molecules for clinical trials. The efficacy of pharmaceuticals depends to

a large extent on their chiral composition, and thus enantiomeric purity and selectivity is an important issue for the development of new drugs and to test their biotoxicity. Project TwistedNano (EIC-Pathfinder OPEN 2021) addresses this need with a new generation of integrated nanophotonic devices enabling ultrasensitive chiroptical spectroscopy of sub-nanolitre volumes, revolutionizing at-source the sensing technological toolbox for drug discovery and nanomedicine.

The project aims at developing a photonics-enabled chiral sensing technology that integrates vectorial structured light fields with almost arbitrary control onto a microfluidic chip, providing ground-breaking advantages compared to current instrumentation: (i) remote/distributed analysis, (ii) reduced sample consumption, (iii) cost reduction, (iv) parallelization, (v) increased diagnostic speed and sensitivity.

At IIT, the PhD candidate will focus on the development of photonic nanostructures via colloidal chemistry. In view of this, the activities will focus on chemical synthesis, together with extensive optical characterization (steady-state and time-resolved). Importantly, the PhD candidate will develop synthesis protocols leading to chiroptical active colloidal nanostructures based on noble metals, transparent conductors, and/or colloidal semiconductors. Such nanostructures will then be exploited by other consortium members (in the framework of project TWISTEDNANO) in combination with miniaturized twisted photonic platforms for efficient radiation confinement and programmable super-chiral field design.

Within the research team, your main responsibilities will be:

- Colloidal synthesis of nanoparticles.
- Manipulation and characterization of nanomaterials. Comprehensive investigation of their structural and morphological properties.
- Fabrication and characterization of nanophotonic architectures, with the specific aim of realizing strongly coupled hybridization between chiral light and semiconductor nanocrystals.

Requirements: the candidate should have a master's degree in material science, chemistry or related disciplines, with possibly some experience in colloidal chemistry. Importantly, candidates should be driven by strong work dedication and experience in working in an international environment will be positively considered.

Funding for this position is provided by European Innovation Council through the project Pathfinder OPEN 2021 "TWISTEDNANO", for more information please visit: https://www.twistednano-horizon.eu/.

For questions concerning the research theme, please contact Francesco.DiStasio@iit.it.

7. Physical chemical interactions of magnetic based nanomaterials with immune cells

Tutor(s): Teresa Pellegrino, Davide Peddis

Magnetic hyperthermia (MHT) is a new therapeutic approach that enables to 'burn' tumor cells by means of the heat generated by magnetic nanoparticles under time varying fields. Different clinical trials are now ongoing to treat different types of solid tumors. In GIULIa project, we will apply MHT for the treatment of metastasized tumors. MHT treatment of cancer metastases is now not doable because of scarce MNP dose accumulation at the spreading tumor sites. In GIULIa, MNPs designed for MHT, will be loaded in/on immune cells, which will work as Trojan horses to deliver the right dose of magnetic materials needed for mild or hot MHT to the metastases.

The project aims at developing strategies to maximize the association or uptake of magnetic based nanomaterials to immune cells while maintaining intact the functionality of immune cells at no cell

toxicity, providing ground-breaking advantages including i) infusion of the minimal dose of immune cells at the highest dose of magnetic nanoparticles: (iii) reduced magnetic material consumption, (iii) fast loading process at the minimal cost reduction, (iv) safe conditions, (v) providing enough dose of magnetic materials for magnetic hyperthermia (vi) track and quantify magnetic nanoparticles by magnetic particle imaging (MPI) and magnetic resonance imaging (MRI) in phantoms.

At IIT, the PhD candidate will focus on the development of different functionalization coating of magnetic based nanomaterials via different wet colloidal approaches. Among them, the candidate will learn and apply polymer preparation and polymer functionalization with different moieties, polymer coating and lipid coating, ligand exchange procedures and inorganic silica growth methods of magnetic based nanomaterials. An important part of the study will be dedicated to correlate the physical and chemical parameters of the nanomaterials, including magnetic properties, shape, size, assembly structure, surface charge to the uptake or association to/on immune cells in terms of materials uptake, preservation of cell functions and survival, magnetic properties of interest in particular magnetic hyperthermia heating performance, MPI and MRI signaling, magnetic manipulation under different magnetic stimulation.

The PhD candidate will also develop loading protocols which will lead to scalable and reproducible processes and they will be possibly implemented to different types of immune cells.

Within the research team, the candidate main responsibilities will be:

- Preparation of water soluble magnetic nanomaterials.
- Magnetic, physical and chemical characterization of nanomaterials.
- Magnetic, physical and chemical characterization of immune cells loaded with magnetic based nanomaterials.
- Full investigation of structural and morphological features of immune cells loaded with magnetic materials.
- Full investigation of MPI, MRI, magnetic accumulation studies and magnetic hyperthermia study of immune cells loaded with magnetic materials.
- Deep investigation of the functional and molecular profiling of immune cells treated with magnetic based materials.

Requirements: The ideal candidate should have a master's degree in biology, biotechnology, medical chemistry or related disciplines, with possibly some experience in cell culturing, drug delivery with different materials. High motivation and strong dedication to research are considered basic requirements. The candidate will join an interdisciplinary and international group therefore the ability to cooperate and integrate in such an international environment will be positively considered.

Funding for this position is provided by project ERC consolidator GIULIa (PI Teresa Pellegrino).

For questions concerning the research theme, please contact teresa.pellegrino@iit.it. For administrative issues, please contact iulia.manolache@iit.it.

Curriculum Science and Technology of Materials (Regione Liguria)

8. **Synthesis and electrochemical production process of sodium hypochlorite: investigation and optimization of key process parameters** (grant within PROGRAMMA REGIONALE FONDO SOCIALE EUROPEO+ 2021-2027 PRIORITÀ 2 - ISTRUZIONE E FORMAZIONE - ESO 4.6 (OS-f), with the contribution of Angelini S.p.a.)

Tutor: Paola Riani, Maria Paola Carpanese

The research activity will focus on the optimisation of the electrochemical process of industrial production of sodium hypochlorite, by identifying solutions to reduce environmental impact, decreasing waste production and resources consumption.

The chemical process optimization will be aimed at reducing the risks of non-conformity of the product, to avoid the consequent generation of wastes; moreover, optimization will be studied and applied in the industrial context to move towards an automated and digital process.

It is expected that at the end of the PhD improvements related to the process have been explored and analysed; improvements are identified and compared with other similar industrial processes available in the literature; solutions able to reduce waste disposal are identified and the efficiency of the production lines improved.

For further details concerning the research theme, please contact paola.riani@unige.it, maria.paola.carpanese@unige.it.

Curriculum Chemical Sciences and Technologies (D.M. 118 and Regione Liguria)

9. **Sustainable design of new permanent magnets** (research theme for grant funded within D.M. 118 del 2.3.2023 - Azione Dottorati di ricerca PNRR)

Tutor: Davide Peddis

Permanent magnets (PMs) are fundamental components in a wide variety of primary applications ranging from energy-conversion devices, household appliances, to rapidly developing green technologies (i.e., hybrid vehicles, wind turbines). Current high-performance PMs owe their extraordinary properties to the presence of rare-earth elements (REEs), whose mining and refining processes require large amounts of energy and water, while generating vast volumes of CO_2 emissions as well as pollutants and radioactive secondary materials. The present PhD project is mainly aimed at developing innovative and sustainable design of new permanent magnets to face the REE criticality issue. RE-free hard/soft exchange coupled nanocomposite powders containing $BaFe_{12}O_{19}$ hexaferrites as the hard phase and $CoFe_2O_4$ (CoFe) spinels as the softer phase will be synthesized by ball milling and/or chemical approaches, to manufacture mid-range PMs filling the gap between HFs and RE-PMs.

For further details concerning the research theme, please contact: davide.peddis@unige.it.

10. **Synthesis and characterization of magnetic nanocomposites** (research theme for grant funded within D.M. 118 del 2.3.2023 - Azione Dottorati di ricerca PNRR)

Tutor: Stefano Alberti

The PhD project includes the study of a polymer-based hybrid nanocomposite material, in which nanoparticles with magnetic properties of different compositions are dispersed. The hybrid material is processed using the electrospinning technique, which allows the production of fibrous fabrics. The fibers have dimensions ranging between micrometres and nanometres, endowing the material with high porosity, high surface area, and mechanical resistance features. Depending on the final composition of

the hybrid material, it is possible to foresee uses in the bio-technological and bio-medical sectors, in line with the "Health" theme of the PNRR.

For further details concerning the research theme, please contact: stefano.alberti@unige.it.

11. **Synthesis of high value organic molecules from renewable lignocellulosic resources through innovative synthetic methodologies** (research theme for grant funded within D.M. 118 del 2.3.2023 - Azione Dottorati di ricerca PNRR)

Tutor: Andrea Basso

The valorization of renewable feedstocks, which accounts to more than 130 mln*ton/year, is crucial to fulfill the Fitfor55 strategy of the EU and the more stringent scenario of a net-zero community by 2050. The contribution of synthetic chemistry to this issue can be considerable. The present project is focused at developing high-value synthetic applications of renewable synthons, which can be readily applied in the fine chemical, material and pharmaceutical area. Specifically, a series of lignin derived synthons will be at the core of innovative synthetic methods, ranging from the use of photoactive species to multicomponent reactions. The strategy is perfectly coherent with the present PNRR initiative. Indeed, within the strategic emerging topic "SUSTAINABILITY AND PROTECTION OF NATURAL RESOURCES", it is precisely found that the "sustainable and circular management and use of natural resources as well as prevention and removal of pollution" is a key element that should drive academic and industrial research.

For further details concerning the research theme, please contact: andrea.basso@unige.it.

12. **Metallurgical investigations on the production and reproduction of objects in copper alloys that replicate the findings from various eras belonging to the Samnite Museum of Campobasso** (research theme for grant funded within D.M. 118 del 2.3.2023 - Azione Dottorati per il patrimonio culturale)

Tutor: Paolo Piccardo

The Samnite Museum is rich in metal findings from the Bronze Age to the Medieval period and most of them were never submitted to deep metallurgical and chemical investigations. Such studies are considered of the utmost importance to reveal the material knowledge behind the object. The results gathered through the research activities performed during the PhD will be enriched with the archaeological information to offer a picture of the societies with their culture and habits that manufactured and used such objects. The investigations are performed using the protocols designed and consolidated at the M.E.T.A.L. research group which are inspired by the industrial failure analysis and adapted to the high specificity of the objects. To complete the research activities some of the objects will be replicated using the same alloy and by methods as close as possible to the ancient ones. The goal of this activity is to acquire information on the empirical practice of ancient metallurgists. The candidate will work at the Museum for at least 6 months, will participate to international meetings and publish the results of the research in international peer-reviewed journals.

For further details concerning the research theme, please contact: paolo.piccardo@unige.it.

13. **The etruscan and roman bronzes of San Casciano dei Bagni, study of the alloys, the patinas of alteration and the impact of the post-excavation deposition and conservation environment** (research theme for grant funded within D.M. 118 del 2.3.2023 - Azione Dottorati per il patrimonio culturale)

Tutor: Paolo Piccardo

Recent excavations performed in San Casciano dei Bagni revealed an incredibly rich archaeological site in correspondence to a thermal source used since the 4th cen. B.C. for its recognized healing properties. Beside the nowadays sporadic usage the ancient official frequentation corresponds to 800 years half of which during the Etruscan period followed by 4 centuries ca. during the Roman period. The pools system where the thermal water was collected was organized as a temple and numerous bronzes decorated the surrounding area. Other bronzes were used as "ex-voto" to thank or to obtain the grace of the local divinities. The practice was to deep the bronzes with the shape of the sick person or of the part of the body needing to be treated. At the same time statues of various gods were also used. At the passage from the Etruscan to the Roman period the ancient bronzes were substituted and introduced into the pool bottom before to be covered with marble stones and part of the columns. In this way it is possible to distinguish the bronzes as Roman or Etruscan, which is important for archaeological studies. The findings remained for a period ranging from 15 to 25 centuries submerged into the mud arising from the thermal source which is rich of sulfide ions among others. The underwater corrosion was in part occurring in anaerobic conditions and with $S^{=}$ as main aggressive anion. The study of the bronzes and of their related corrosion process is a unique opportunity that will reveal important information from technical and conservational point of view. Beside the fact that some of the findings look poorly corroded it is important to notice that after the extraction and the preliminary cleaning process the findings enter in contact with a differing environment and some alteration processes might start. The PhD research will operate in this direction by defining the nature of the alloys, their behavior, and their stability. The corrosion process will be replicated in laboratory on alloys corresponding to the original ones and used as reference to establish the further reactivity/stability of the objects after restoration. The candidate will work in strict contact with the restoration and conservation team and with the specialists of the Central Institute of the Restoration of Rome where a part of the research work will be performed. The candidate will participate to international meetings and publish the results of the research in international peer-reviewed journals.

For further details concerning the research theme, please contact: paolo.piccardo@unige.it.

14. **Treatment of end-of-life wind turbine blades for the recycling of glass fibers** (grant within PROGRAMMA REGIONALE FONDO SOCIALE EUROPEO+ 2021-2027 PRIORITÀ 2 - ISTRUZIONE E FORMAZIONE - ESO 4.6 (OS-f), with the contribution of Exacto S.p.a.)

Tutor: Maila Castellano, Silvia Vicini

The PhD project aims to analyze the problem of the end-of-life treatment of wind turbine blades, with regard to the recycling of fiberglass in the composite materials. Different existing recycling methods (mechanical, thermal, and chemical) will be evaluated, analyzing the strengths and weaknesses of each treatment, and taking into consideration the following aspects: environmental impact, energy requirements, industrial scalability of the process, technical characteristics and stability of the product obtained following the recycling process. Finally, a technical-economic feasibility study of a pilot plant will be conducted.

For further details concerning the research theme, please contact maila.castellano@unige.it, silvia.vicini@unige.it.

15. **Circular economy for the sustainable closure of the waste cycle: use of secondary solids fuels for syngas production** (grant within PROGRAMMA REGIONALE FONDO SOCIALE EUROPEO+ 2021-2027 PRIORITÀ 2 - ISTRUZIONE E FORMAZIONE - ESO 4.6 (OS-f), with the contribution of Italiana Coke S.r.l.)

Tutor: Antonio Comite

The research project aims to study and develop a new pyrolytic process of waste and solid secondary fuels to produce syngas and an industrially reusable solid residue char. The pyrolytic process is proposed as an effective way to close the waste cycle following the circular economy approach to meet the sustainability goals. Representative solid waste materials (e.g. plastics that are not recyclable otherwise) will be identified and studied at both laboratory and pilot scale in an industrial environment in order to generate high syngas yields even with a variable inlet composition. The experimental data will support a theoretical and preliminary techno-economic evaluation of the pyrolytic gasification process of the waste material.

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