

DOTTORATO IN INGEGNERIA DEI PRODOTTI E DEI PROCESSI INDUSTRIALI
Ciclo XL

	Proponent	Title of proposed activity (ENG)	Curriculum (ENG)
1	Paolo Aprea	Functionalization of microporous supports with bioactive vegetal molecules	Materials and Structural Engineering
2	Enrico Armentani - Michele Perrella	Modelling of the damage, fatigue and fracture behaviour of materials for applications in unconventional environments	Materials and Structural Engineering Technologies and Production Systems
3	Antonio Aronne - Aurelio Bifulco - Claudio Imparato	Design and development of new flame-retardant nanocomposite polymeric materials by sol-gel chemistry	Chemical engineering Materials and Structural Engineering
4	Antonello Astarita	Digital Twin development to reduce the environmental impacts of manufacturing processes in Industry 5.0 context	Technologies and Production Systems
5	Antonello Astarita (fater)	Sustainability and digitalization of production lines	Technologies and Production Systems
6	Sergio Caserta (Biofilm)	Role of biofilm contamination in microplastic formation	Chemical engineering Design of Sustainable and Safe Products and Processes
7	Sergio Caserta (Fater)	Skin-Product Interaction in Incontinence Pads	Chemical engineering
8	Sergio Caserta (Biofilm)	Biomechanics of Tumor Spheroids	Chemical engineering
9	Prof. Aniello Costantini, Dr. Tonia Mariarosaria Di Palma (CNR-STEMS)	Innovative materials for eco-sustainable metal-air batteries	Materials and Structural Engineering Chemical engineering Technologies and Production Systems

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			Design of Sustainable and Safe Products and Processes
10	Salvatore Costanzo	Role of chain branching on the processability and performance of poliolefins within circular economy	Chemical engineering
11	Gaetano D'Avino	Electrohydrodynamics of complex biological fluids for the detection of biomarkers	Chemical engineering
12	Bruno de Gennaro , Giuseppina Luciani	Natural zeolite-based biocomposites for catalytic removal of emerging contaminants.	Materials and Structural Engineering
13	Almerinda Di Benedetto	Insights into safety issues of Li-Batteries	Chemical engineering Design of Sustainable and Safe Products and Processes
14	Ernesto di Maio	Schiume polimeriche avanzate per applicazioni strutturali: proprietà controllate da instabilità meccaniche	Materials and Structural Engineering
15	Ernesto di Maio	Studio di schiume per la produzione di manufatti con mappe di densità ottimizzate nel 3D	Materials and Structural Engineering Chemical engineering
16	Alessandro Erto, Amedeo Lancia	CO2 capture from marine engines by adsorption onto honeycomb structured solids	Chemical engineering
17	Alessandro Erto, Amedeo Lancia	Production of synthetic natural gas (SNG) in advanced reactors for conversion of CO2 with renewable hydrogen	Chemical engineering

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18	Luca Esposito	Design and Development of Advanced Devices for Major Physics and Astrophysics Experiments	Technologies and Production Systems
19	Giovanni Filippone	Development of low environmental impact nanostructured polymer coatings for aerospace applications	Materials and Structural Engineering
20	Mose' Gallo, Giuseppe Converso	Development of decision support models to implement the concepts of sustainability and circularity within textile supply chains. These models, which fully take into consideration the recent technologies in the field of material recovery, are intended to support decision making from system configuration to short-term production planning, also by integrating the latest information and communication technologies made available by "Industry 4.0" paradigm.	Technologies and Production Systems
21	Andrea Grassi	Optimization of Coordination in the Supply Chain through the Reduction of Informational Asymmetry, using Advanced Models and Software Simulations	Technologies and Production Systems
22	Antonio Langella (SCpA)	Metal Additive Manufacturing for the aerospace industry	Technologies and Production Systems
23	Valentina Lopresto (ATM)	Innovative Composite Materials made by thermoplastic resins for industrial applications	Technologies and Production Systems

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24	Giuseppina Luciani, Antonella Macagnano	Biowaste valorization as smart nanostructured bio-stimulants for sustainable agriculture	Chemical Engineering Materials and Structural Engineering
25	Pier Luca Maffettone (Fater)	Set up of Digital version of manufacturing industrial plants to be used as a Modelling & Simulation tool	Chemical Engineering Design of Sustainable and Safe Products and Processes
26	Pier Luca Maffettone (3DnA)	Characterization of the 3D printing process of polymeric foams for the development of functional, environmentally friendly and high technological value materials for the various industrial sectors	Chemical Engineering Design of Sustainable and Safe Products and Processes
27	Giuseppe Mensitieri Giuseppe Milano	Multiscale Modeling of "Grafting-to" Processes for the Production of Functional Polymer Brushes	Materials and Structural Engineering Design of Sustainable and Safe Products and Processes
28	Tullio Monetta	Plasma Electrolytic Oxidation (PEO) coating of light metal alloys	Materials and Structural Engineering
29	Tullio Monetta	Low environmental impact processes for recovering precious metals from waste electrical and electronic equipment (WEEE)	Design of safe and sustainable products and processes Ingegneria dei materiali e delle Strutture
30	Teresa Murino	Sviluppo di modelli e soluzioni innovative per l'applicazione e l'ottimizzazione di problemi di packaging in ottica di Lean Manufacturing combinata a processi di "Industria 4.0"	Technologies and production systems Materials and Structural Engineering
31	Paolo Netti	IIT - Cell mechanoprogramming	Materials and Structural Engineering Chemical Engineering Technologies and production systems

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			Design of safe and sustainable products and processes
32	Paolo Netti	IIT - Cancer mechanobiology	Materials and Structural Engineering Chemical Engineering Technologies and production systems Design of safe and sustainable products and processes
33	Paolo Netti, Francesco Urciuolo	Muscle on Chip	Materials and Structural Engineering
34	Paolo Netti, Francesco Urciuolo	Tissue fibrosis on Chip	Materials and Structural Engineering
35	Roberto Nigro	Development of innovative techniques for the extraction and concentration of plant exosomes	Chemical engineering
36	Roberto Nigro	Biotechnological upcycling of wasted Spent Coffee Ground	Chemical engineering
37	Rossana Pasquino	Hydrogel fibers as optical waveguides in human tissues	Chemical engineering
38	Domenico Pirozzi	Development of advanced adsorbent materials for the removal of recalcitrant pollutants from wastewaters	Chemical engineering
39	Danilo Russo	Safe hydrogen storage in aqueous formate/bicarbonate	Chemical engineering

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40	Fabrizio Scala – Mariarosaria de Joannon Ceglia (STEMS- CNR)	Integrated carbon dioxide and nitrogen cycles for the GHG emission mitigation and the energy and material recovery.	Chemical Engineering
41	Fabrizio Scala	Reduction of ilmenite in a fluidized bed for the production of gaseous oxygen in a lunar environment	Chemical Engineering
42	Maurizio Ventre	Development of functionalized platforms and computational models for mechanobiology studies	Materials and Structural Engineering
43	Massimiliano Villone	Label-free opto-microfluidic technologies for early diagnosis	Chemical engineering

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Prof. Paolo Aprea

Proposed research topic: *Functionalization of microporous supports with bioactive vegetal molecules*

Reference curriculum:

Materials and Structural Engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) The pharmaceutical and cosmetics industry needs to develop efficient and modifiable active ingredient release systems over time. In particular, pharmaceutical and cosmetic formulations for topical use can present problems related to the release kinetics of the active ingredient, which quickly reaches a peak concentration, followed by a rapid decay. Microporous materials, including zeolites, have shown excellent retention/release capabilities of some active ingredients, whose concentration can thus be modulated in a more stable manner over time, allowing for a more efficient action. A further property of some zeolites is the ability to regulate skin hydration through water adsorption/desorption, improving dermatological tone and patient comfort after application of the drug. Based on these assumptions, the present doctoral project aims to investigate the retention and release properties of active ingredients for cosmetic use on supports made up of natural and synthetic zeolites.

Accordingly, some novel, plant-derived extracts, normally conveyed in glycerol-based cosmetic creams, will be selected. Suitable zeolitic supports, chosen based on their hydrophilicity and adsorption behavior, will be also selected. Then, the kinetics and thermodynamics of the retention of the active ingredients contained in the extracts on the selected zeolitic supports will be studied.

Based on the results of this experimental campaign, release tests will then be carried out in different systems (such as, for example, water and glycerol) and finally ex-vivo and subsequently/possibly in-vivo tests will be carried out on biological samples to evaluate the performance of the obtained formulations.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

the doctoral student will carry out his research activity for a minimum period of 6 months at the company Arterra Bioscience SpA (<https://arterrabio.it/>)

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The doctoral student will spend a minimum period of 6 months at a research centre/company among those with which the company co-financing the doctoral scholarship has active collaborations (<https://arterrabio.it/collaborazioni/>).

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Enrico Armentani, Michele Perrella

Proposed research topic:

Modelling of the damage, fatigue and fracture behaviour of materials for applications in unconventional environments

Reference curriculum:

Materials and Structural Engineering
Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The construction of complex structures, such as nuclear fusion reactors or liquid rocket engines, requires continuous improvement of components, materials and geometric configurations. Within this context, there is a strong interest in developing predictive models for evaluating the useful life of the various structural components. The study of the behaviour of machine elements, operating at high temperatures and subject to high stress states, through FEM elastic-plastic analysis, needs the modelling as realistic as possible of the elastic-plastic material constitutive law. Many efforts have been made over last years on numerical simulation of the elastic-plastic behaviour of materials and a great deal of numerical models have been proposed (Ramberg-Osgood, Hill, Chaboche, etc.). In the literature there are numerous models that describe the elastic-plastic behaviour of specimens subjected to well-defined types of load, but very few numerical-experimental validations on complex geometries and stress states are available. The choice of the most appropriate hardening model for the specific application is therefore crucial. Furthermore, the analysis of the multiaxial fatigue life of elements related to the safety and operation of machines involves the use of a reliable predictive model. Many authors have proposed criteria for calculating low-cycle multiaxial fatigue life (Brown-Miller, Fatemi-Socie, etc.). These criteria are based on the evaluation of stresses and / or strains in the cyclically loaded specimens, consequently correlating these quantities with the number of loading / unloading cycles required to the cracks onset in the specimens.

The research deals with the study of the fracture and damage of machine elements subject to load conditions varying over time by means of finite element (FEM) analysis. The elements to be investigated are parts subject to very high temperatures, in which considerable thermo-mechanical loads are generated (for example in components of magnetic plasma confinement systems or in liquid rocket thrust chambers). Hence the need to correctly evaluate the fatigue life of these elements, due to complex thermo-structural load spectra. A series of elastic-plastic FEM analysis will be performed, in order to numerically simulate temperature, stress and strain fields over time and crack propagation. The interaction between the creep phenomenon and fatigue will be also investigated and the effect of residual stresses on the durability of the structure will be evaluated. Subsequently, the fatigue life of the components under investigation will be estimated by means of FEM results.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity,

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collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The proposing research group have been involved for a long time in the study of the behaviour of materials and the response of structures. They have dealt in depth with various aspects, with particular regard to mechanical characterization, structural and material instability, damage and fracture. The commitment and qualifications achieved are proven by participation in European research and agreements and collaborations with industry. The Ph.D. student will have at his disposal both a laboratory for virtual experimentation equipped with workstations and finite element method codes and a laboratory for the experimental investigations of materials and structures.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

During the Ph.D. period, the student will have the opportunity to spend a period abroad at universities or research centres with which the research group collaborates on these topics. During this period, the student will have the opportunity to improve his knowledge of both finite element methodologies and those relating to experimental tests.

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PhD Project Proposal

Proponent: Prof. Antonio Aronne, Dott. Aurelio Bifulco, Dott. Claudio Imparato

Proposed research topic: Design and development of new flame-retardant nanocomposite polymeric materials by sol-gel chemistry

Reference curriculum:

Chemical engineering

Materials and Structural Engineering

Summary of the Research Project:

Unquestionably, polymeric materials are used in our daily lives. High-performance applications need for an increasing number of low-flammable, mechanically superior products based on polymers. However, one of the biggest issues that the modern society must face is the massive release of polymeric wastes, whose inappropriate handling is posing a threat to human health and the environment, particularly when additives are involved. Governments and the scientific community are fostering the adoption of a circular economy model in order to address these problems, as well as the advancement of more efficient and sustainable technologies. Epoxy resins and other high performance polymers are mostly used in the transportation industry due to their good mechanical behavior, chemical resistance, and thermal stability, although flame retardance is frequently required to meet certain criteria. While halogen-based flame retardants (HFRs) are very good at enhancing the fire behavior of epoxy composites, the European Union has recently passed legislation outlawing several of them because of their negative effects during the recycling of polymeric wastes containing these chemicals. In comparison to HFRs, phosphorus (P)-based flame retardants (FRs) such as ammonium polyphosphate, phytic acid, and bio-based P-compounds are considered greener, since they can be used to create more environmentally friendly polymer-based materials and vitrimers (recyclable thermosets and thermoplastics), as they do not produce toxic gases along their tertiary recycling. Nevertheless, with respect to HFRs, high concentrations of P-based FRs (2, 3 wt.%) are required in the polymer matrix to produce excellent results; additionally, synergistic effects are frequently needed to maintain the lowest feasible flame retardant loading. During the combustion of the epoxy matrix, silica and metal oxides with basic and acidic sites on their surface can act as barriers to the transport of heat and oxygen and as char promoters. In addition to their physical barrier properties, natural metal silicates (e.g., clays) and synthetic nanostructures containing metal ions, like titanium or magnesium, have been demonstrated to enhance charring or suppress smoke. The combined use of P-based FRs and functional biowastes can lower the concentration of P-containing additives needed and thereby prevent phosphorus depletion while also adding value to waste materials. The PhD student selected for the project will be involved in the following activities:

1) design and synthesis of new greener flame retardants (e.g., P-based compounds and mixed metal oxides) for the manufacturing of polymeric materials, vitrimers, and recyclable thermosets with

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improved mechanical, thermal and fire behavior;

2) functionalization and treatment of biowastes and/or textile for the synthesis and development of new composites with enhanced mechanical, thermal and fire behavior;

3) synthesis of new ex/in-situ nanostructures for the preparation of flame retardant multifunctional composites showing better hydrophobicity, optical properties, reshaping capability, and overall performances.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

This research project will be performed jointly with the Chemistry of Materials Laboratory of the Department of Chemical, Materials and Production Engineering of the University of Naples Federico II and the Fire Test Laboratory "PIROS" of the Italian Technological District for the Engineering of Polymeric and Composites Materials and Structures (IMAST).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....) A research period abroad is planned with some of our national and international partners (Politecnico di Torino, Swiss Federal Laboratories for Materials Science and Technology (EMPA)) and the details will be later defined.

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PhD Project Proposal

Proponent: Antonello Astarita

Proposed research topic:

Digital Twin development to reduce the environmental impacts of manufacturing processes in Industry 5.0 context

Reference curriculum:

Technologies and Production Systems

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Additive manufacturing (AM) has surfaced as a pivotal component in intelligent manufacturing, offering many benefits compared to conventional production techniques. Nevertheless, the industry grapples with manufacturing instability and inconsistent repeatability issues, making it challenging to meet desired microstructure and performance standards. The optimization of processing variables within specific equipment and parameter sets often necessitates expensive trial-and-error experiments, given the diversity and complexity of AM process parameters.

To mitigate these challenges, the digital twin (DT) technical concept represents an opportunity for real-time projection and mirroring of physical attributes for both the fabricated products and the AM machinery, thereby facilitating real-time feedback control to alleviate AM-induced defects and achieve optimal performance of the manufactured parts.

Thus, the creation of digital twins that allow continuous improvement of processes represents a fundamental step for achieving sustainable development objectives. The research project will start from the study of Additive Manufacturing and conventional technologies and then define: the quantities to be monitored and consequently the sensors to be implemented; the most used simulation methodologies and related software; the most suitable types of DT; the most useful artificial intelligence algorithms. After this phase, a methodology for the development of digital twins of 3D printing processes of components made of metallic materials will be developed. Also include the post process machining phases which are often required for the production of high-performance components. The developed DT will then be validated both in a virtual environment and experimentally, thanks to the collaboration with companies where the measurements will be carried out, and the developed methodologies will be tested. Achieving the objectives of the research project passes through a detailed knowledge of both the manufacturing processes and the methodologies to be applied for the sensing of processes and the development of digital twins.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

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The doctoral student will work in the DICMAPI laboratories and will be able to use both sets of dedicated sensors and specific software for the simulation of manufacturing processes and the calculation of the environmental impacts linked to the production of mechanical components (LCA analysis software, Tecnomatix Plant Simulation, and so on). The activities will be carried out in collaboration with research institutions and companies, in particular with CIRA (Italian Center for Aerospace Research) and with local companies.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The doctoral student will choose to carry out his period abroad at OSU (Ohio State University) within the Additive Manufacturing center, at DCU (Dublin City University) within the Advanced Manufacturing center or at other groups of research of international importance that should carry out activities useful for its training.

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PhD Project Proposal

Proponent: Antonello Astarita

Proposed research topic:

Sustainability and digitalization of production lines

Reference curriculum:

Technologies and Production Systems

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The research project on the sustainability of Fater production plants aims to find innovative technical solutions to make production lines more sustainable, both from the point of view of materials and from an energy point of view. The project aims to identify alternatives to bonding technologies currently found in absorbent products, in order to reduce environmental impact and improve product sustainability. At the same time, the research lies in reducing the energy consumption of production lines. Reducing energy consumption is not just an economic necessity, but a crucial environmental priority. In an era where energy resources are limited and energy demand is constantly increasing, optimizing energy efficiency becomes essential for the long-term sustainability of industrial activities. This could involve implementing more efficient technologies or reviewing some processes to monitor and minimize energy waste. Adopting measures to reduce energy consumption also means reducing CO₂ emissions, thus contributing to the fight against climate change. Furthermore, a more responsible and conscious use of energy resources can lead to a significant reduction in operating costs, freeing up resources that can be reinvested in further sustainable innovations. The transition towards an energy efficient production system therefore represents not only an environmental advantage, but also an economic and social one, promoting a model of sustainable and responsible growth

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The doctoral project will be carried out in collaboration with the company Fater SpA (<https://fatergroup.com/it>), the doctoral student will therefore have full access to both the DICMAPI and Fater Group laboratories. If necessary, collaborations will be activated with research institutes of national and international importance.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The doctoral student will have to spend a period abroad in research groups of the TU Delft University in order to learn the most modern methodologies for analyzing the sustainability of processes.

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PhD Project Proposal

Proponent: Sergio Caserta

Proposed research topic: Role of biofilm contamination in microplastic formation

Reference curriculum:

Chemical engineering

Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

State of the Art

Biofilms are complex communities of microorganisms that adhere to surfaces, embedded within a self-produced matrix of extracellular polymeric substances (EPS). Biofilm formation on surfaces poses significant challenges in various sectors, including medical, industrial, and environmental fields. Despite the relevance of the topic, most studies, mainly focused on lab surfaces (e.g. agar plates), and not on industrial and sanitary relevant surfaces (e.g. metal, water, plastics).

This project has as aim the investigation of the stresses mechanisms that led bacterial adhesion and the subsequent biofilm formation on plastics surfaces. In particular, the focus of the research will be on the role of biofilm and bacteria contamination in the fragmentation of plastics in the oceans, leading to the formation of microplastics. Once biofilms establish on plastic surfaces, they can lead to severe consequences such as biodeterioration, biofouling, and the dissemination of pathogens. For instance, in the medical field, biofilms on plastic medical devices can result in persistent infections and increased antibiotic resistance, as in the case of catheters contamination. However, in marine environments, biofilm formation plays a key role on the degradation of microplastics.

Research on biofilm-plastic interactions has advanced, yet several aspects remain inadequately understood. Key areas of interest include the initial stages of biofilm attachment, the specific roles of various microbial species in biofilm development, and the interaction between biofilms and different types of plastic polymers. Understanding these factors is crucial for developing effective strategies to prevent or mitigate biofilm formation on plastic surfaces.

Short Program of Planned Activities

The candidate activities are here planned to be distributed during the duration of the 3 years project.

Activates of the first year are here proposed:

- Literature Review and Preliminary Research (Month 1-6)
- Selection of plastics and microbial strain of interest (Month 6-12)
- Experimental Design and Methodology Development (Month 6-12)

Activities of the second year are here proposed:

- Develop of experimental protocols to study biofilm formation on different plastic surfaces, for example Calgary device, and inflow systems (Month 1-6)
- Laboratory Experiments (Month 1-12)
- Use of microscopy (e.g., Time lapse and CLSM) to analyze biofilm structure (Month 6-12)
- Data Analysis and Interpretation (Month 9-12)

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Activities of the third year are here proposed:

- Compare findings with existing studies and to contextualize results and original scientific publication writing (1-8)
- Test the efficacy of selected strategies in preventing biofilm formation on real plastic surfaces (e.g. catheters) (Month 1-8)
- Dissemination of Findings (Month 1-12)
- Thesis writing (6-12)

Objectives

The objective of this project is to understand how shear stress, chemical exposure, and temperature affect the adhesion of diverse bacterial strains to different types of plastic surfaces. The methodologies developed will be employed to create a screening protocol to identify the specific shear stress values that trigger bacterial adhesion for the studied strains on solid surfaces.

The knowledge acquired during the project will be employed for two practical cases of studies:

1: Enhance bacterial attachment to microplastics for environmental studies.

2: Re-engineer catheter surfaces to prevent bacterial attachment, contributing to improved medical device safety.

By achieving these objectives, the project aims to provide valuable insights into the factors influencing bacterial adhesion to plastics and develop practical solutions for both promoting and preventing biofilm formation in specific applications.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The main part of the project will be hosted in the DICMaPI facilities of the University of Naples Federico II, particularly in the Reottica and Bioengineering laboratories. Potential collaborations may include the Industrial Biotechnology laboratory within the same department. In these facilities, the candidate will use a laminar flow hood and all the necessary equipment for microbial handling (Type 1 security). Additionally, the candidate will have access to advanced microscopy facilities such as high-speed time-lapse microscopy and a confocal laser scanning microscope.

Other important equipment for the project includes oxygen plasma technology for materials modification and a wetting platform for interfacial analysis.

Possible collaboration with foreign research bodies such as INRAE (France National Institute of environmental and agriculture research) and University such as Aristotle University of Thessaloniki will be considered.

1. Available at DICMaPI Laboratories:
 - a) 2 Automated Time-Lapse Video Microscopy Workstations, equipped with XYZ motors, high-sensitivity or high-speed cooled cameras, and a micro-incubator for observations in bright field, phase contrast, fluorescence, and confocality.
 - b) Cell Culture Laboratory, equipped with a sterile hood, benchtop incubator, and centrifuges.
 - c) Flow and Chemotaxis Cells.
 - d) Image Analysis Software.
 - e) Data Analysis Software.
 - f) Finite Element Numerical Simulation Software.
2. Available at Other Departments of Federico II or Affiliated Institutes:

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- a) Mass Spectrometer in collaboration with the Department of Chemical Sciences.
- b) Advanced Microscopy Facility equipped with FRAP, FRET, Super-resolution at CEINGE Advanced Biotechnologies.
- c) Immunochemistry Facility at CEINGE Advanced Biotechnologies.
- d) Cell Culture Bank at CEINGE Advanced Biotechnologies.
- e) Computational Software and Resources for in silico analysis of tumor growth and invasiveness through multiscale models, in collaboration with Houston Methodist Research Institute (USA).
- f) SCOPE GRID Computing Platform (Unina).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

During the second year of activities the candidate will spend a 6-month period at the INRAE to develop a microbial strain able to report through fluorescence the level of c-di-GMP, a molecular reporter for the cellular stress. This strain will be used to correlate shear stress level and cell adhesion on surfaces

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Sergio Caserta

Proposed research topic:
Skin-Product Interaction in Incontinence Pads

Reference curriculum:
Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

In the field of healthcare products, it is essential to deepen our understanding of the interactions between human skin and the materials used in incontinence pads. This research project aims to systematically explore the physico-chemical dynamics between the skin and absorbent products.

The main objectives include analyzing moisture transfer mechanisms, skin irritation, and the permeability of various materials, with the goal of optimizing the composition and structure of the products to maximize comfort and minimize the risks of dermatitis and other skin complications. Through advanced experimental methodologies and mathematical modeling, the project intends to identify innovative solutions that positively influence the daily lives of users, incorporating principles of environmental sustainability and potentially impacting current laboratory tests to measure product performance.

This research will not only deepen the material science applied to skin health but also stimulate the development of new absorbent technologies that can be implemented in the company's future production. Collaboration with the academic world promises to open new horizons in the design and functionality of incontinence products, with a constant focus on individual well-being and eco-sustainability.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

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PhD Project Proposal

Proponent: Sergio Caserta

Proposed research topic: Biomechanics of Tumor Spheroids

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Metastases represent the primary cause of cancer-related death, as cancer cells spread from the primary site to distant organs through the circulatory system. This dissemination process is complex and involves several stages, including the invasion of surrounding tissue, entry into the bloodstream or lymphatic system, survival in circulation, exit from the vessels, and colonization of new tissues. Studying the mechanical properties of cells during these stages can provide fundamental insights into the mechanisms of cancer cell dissemination and improve therapeutic strategies. In fact, the mechanical properties of biological samples, from single cells to entire tissues, are effective biomarkers that allow for the distinction between healthy and pathological tissues and the identification of metastatic potential.

This research project aims to examine the mechanical properties of cells during metastasis to understand the mechanisms of cancer cell dissemination and improve therapeutic strategies. The three-dimensional model used to simulate a tumor mass is known in literature as a cellular spheroid. Spheroids are aggregates of cancer cells capable of reproducing *in vivo* conditions due to the formation of internal chemical gradients resulting from the accumulation of nutrients and catabolites. These three-dimensional models are considered more representative of physiological reality compared to traditional two-dimensional models, as they better replicate the natural tumor environment.

A primary objective will be to evaluate the difference in mechanical properties, in terms of Young's modulus, of spheroids obtained from immortalized breast cells. Specifically, the biomechanics of spheroids obtained from three cell lines will be compared: non-tumorigenic (MCF-10a), which will be used as controls, tumorigenic (MCF-7), and tumorigenic with a higher metastatic potential (MDA-MB-231). To evaluate the mechanical properties, the compression assay developed by us, known as the Rheo-optical Compression Assay (patent pending), will be used. This assay involves applying a load to the spheroids to correlate the observed morphological deformation with stress, thereby determining Young's modulus.

Subsequently, to better simulate physiological conditions, our objective will be to evaluate the effect of the extracellular matrix and fibroblasts on biomechanical characteristics, creating spheroids with a certain ratio of Collagen I and co-cultures of the aforementioned cell lines with NIH/3T3 fibroblasts. The extracellular matrix plays a crucial role in regulating cellular behavior, influencing adhesion, migration, and survival of cancer cells. Fibroblasts, on the other hand, are known for their ability to remodel the extracellular matrix and influence the mechanical properties of the tumor microenvironment. The correct penetration of collagen and fibroblasts will be verified using microscopy and/or Western blot techniques, thus ensuring the accurate integration of these components into the spheroid model.

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Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Scientific operational facilities include the use of microscopes, laminar flow hoods, and cell culture incubators. During the proposed activities, the doctoral candidate will have the opportunity to collaborate with Italian research entities such as CEINGE Advanced Biotechnologies Franco Salvatore scarl, as well as international research institutes like the Houston Methodist Research Institute. The research activities are part of a recently approved project funded by Compagnia di San Paolo to support the development of industrial invention patents. The project budget can be used to support doctoral activities.

The candidate will have access to the following facilities:

3. Available at DICMaPI Laboratories:
 - g) 2 Automated Time-Lapse Video Microscopy Workstations, equipped with XYZ motors, high-sensitivity or high-speed cooled cameras, and a micro-incubator for observations in bright field, phase contrast, fluorescence, and confocality.
 - h) Cell Culture Laboratory, equipped with a sterile hood, benchtop incubator, and centrifuges.
 - i) Flow and Chemotaxis Cells.
 - j) Image Analysis Software.
 - k) Data Analysis Software.
 - l) Finite Element Numerical Simulation Software.

4. Available at Other Departments of Federico II or Affiliated Institutes:
 - g) Mass Spectrometer in collaboration with the Department of Chemical Sciences.
 - h) Advanced Microscopy Facility equipped with FRAP, FRET, Super-resolution at CEINGE Advanced Biotechnologies.
 - i) Immunochemistry Facility at CEINGE Advanced Biotechnologies.
 - j) Cell Culture Bank at CEINGE Advanced Biotechnologies.
 - k) Computational Software and Resources for in silico analysis of tumor growth and invasiveness through multiscale models, in collaboration with Houston Methodist Research Institute (USA).
 - l) SCOPE GRID Computing Platform (Unina).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The potential period abroad could be carried out at the Houston Methodist Research Institute, with which a bilateral research agreement is already in place with DICMaPI. Collaboration would be with the research groups of Prof. Cristini and Prof. Taraballi, with whom Prof. Caserta's group has established previous collaborations. Alternatively, it could be at the University of Glasgow, collaborating with the research group of Prof. Tassieri.

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PhD Project Proposal

Proponent:

Prof. Aniello Costantini, Dr. Tonia Mariarosaria Di Palma (CNR-STEMS)

Proposed research topic:

Innovative materials for eco-sustainable metal-air batteries

Reference curriculum:

Materials and Structural Engineering

Chemical engineering

Technologies and Production Systems

Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The current batteries show several problems about safety and environmental impact, so, it is necessary to identify new types of more sustainable batteries with similar or better performances. Metal-air batteries, based on the metal oxidation and oxygen reduction, could be a viable alternative. However, at the moment there many limitations especially related to the cathode and the electrolyte which hinder the large-scale production. The purpose of the research project is the identification of eco-sustainable materials to use in the preparation of cathodes and electrolytes with superior performances than those currently discussed in literature, in order to develop new battery prototypes.

Considering the described objectives and the three-year length of the PhD course, it is foreseen to organize the activities in the following way:

1. During the first year the research will be focused on the study and preparation of the cathodic electrodes.
2. The second year will be principally dedicated to the electrolyte design.
3. During the third year the activity of optimization and prototyping of the battery will be carried out.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The research activity will be carried out in cooperation with the CNR-STEMS institute at which the Dr. Tonia M. Di Palma is related. In particular, the preparation of the materials (cathodes and electrolytes) and the electrochemical tests on the materials and on the entire galvanic cell will be carried out in the chemistry laboratories of the CNR-STEMS institute. The main instruments used will be tubular ovens and muffles, electrochemical stations, scanning electron microscope (SEM) equipped with elemental analysis (EDX) and a porosimeter.

Moreover, the PhD student will also have access to the new equipment of the “Centro di Eccellenza Sustainable Energy Sources” situated in the CNR-STEMS institute.

The physico-chemical characterizations of the materials will be conducted at the “Laboratorio di Chimica dei Materiali del DICMAPI”. In particular, the following techniques will be used: thermogravimetric analysis, UV-vis and FTIR spectroscopy and X-ray diffraction analysis.

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Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A possible period abroad could be carried out in the research groups specialized in the synthesis of polymeric materials at the Institute for Chemical Technology and Polymer Chemistry (ITCP) of the Karlsruhe Institute of Technology (KIT) in Germany.

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Ciclo XL

PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Salvatore Costanzo

Proposed research topic: Role of chain branching on the processability and performance of polyolefins within circular economy

Reference curriculum:
Chemical engineering

Summary of the Research Project

Polyolefins with a branched molecular structure show better mechanical properties than the linear counterpart. In particular, branched polyethylene and polypropylene are characterized by a marked viscoelasticity and better processability, for example in foaming processes. These properties make the presence of long-chain branching (LCB) a desired feature in polyolefin products. However, in most cases of practical interest, the difficulties in precisely controlling the degree of branching during industrial-scale synthesis lead to the production of linear and branched polymer mixtures. Furthermore, linear and branched polyolefin mixtures are the usual outcome of recycling processes. Currently, despite the amount of scientific literature on the subject, the relationship between the degree of LCB within a mixture of linear and branched chains and the final properties of polyolefin materials is not well defined, and most industrial processes exploit empirical knowledge to produce materials with certain mechanical properties.

This research project aims to assess the influence of LCB on linear and branched polyolefin mixtures in fast flows, under conditions similar to those encountered during industrial processes. In this context, particular attention will be paid to the link between microstructure and rheological response, in relation to both flow-induced crystallization and to the final mechanical properties.

Using several experimental techniques, including differential scanning calorimetry, rheology, rheo-spectroscopy, scattering, and foaming tests, the aim is to create a chain of knowledge at both microscopic and macroscopic levels, to control the mechanical properties of polyolefin products from the molecular structure of the synthesized mixtures.

The expected results will allow design and optimization of the recycling process of polyolefins to obtain materials with improved performance.

The proposed activity will be carried out in the Rheolab I laboratory, located in Piazzale Tecchio, currently equipped with both stress- and strain-controlled rotational rheometers, with temperature control and nitrogen generator to provide inert atmosphere. With these rotational rheometers, it is possible to carry out experiments both in shear and extensional flows. In addition to the Rheolab I laboratory of P.le Tecchio, the Re-Ops laboratory of the San Giovanni a Teduccio is also available. The Re-Ops laboratory is equipped with additional rheometric setups. The new structure of the “Polymer Hub” will also be available soon, in the same location, where a capillary rheometer will also be installed.

Regarding the analysis of foaming of materials, it will be carried out in collaboration with Prof. Ernesto di Maio, head of the laboratory FoamLab of DICMaPi, equipped with different experimental setups to carry out foaming tests of materials under controlled conditions.

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This PhD project is in collaboration with the Dutch branch of the multinational SABIC, which is project co-founder, therefore, part of the experimental activity, related to the processability of materials, will be carried out at the company laboratories that are equipped with different process setups (extruders).

Regarding rheo-spectroscopy, a collaboration will be established with the University of Groningen, in particular with Prof. Daniele Parisi, an expert in rheo-RAMAN experiments. Any extensional rheology tests that require the use of " filament stretching " rheometers can be performed in collaboration with the FORTH-IESL research institute in Heraklion (Greece).

The project comprises 6 months of activity in the Netherlands at SABIC's laboratories. A further period of 3 months, between the second and the third year, will be spent in the group of prof. Daniele Parisi at the University of Groningen (Netherlands) for rheo-RAMAN spectroscopy.

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Ciclo XL

PhD Project Proposal

Proponent: Gaetano D'Avino

Proposed research topic: Electrohydrodynamics of complex biological fluids for the detection of biomarkers

Reference curriculum: Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The objective of this PhD proposal is to characterize the electrohydrodynamics of biological liquids having peculiar rheological properties to deposit small quantities of sample to be analyzed for the detection of biomarkers. As part of a previous project between UNINA and the Agenzia Spaziale Italiana, a super-sensor was developed capable of depositing small quantities of a biological sample on a slide by exploiting the pyroelectrohydrodynamic effect, i.e., by generating an electric field through heating/ cooling of a lithium-niobate crystal. The electric field deforms the meniscus of a drop hanging from a perforated plate forming the so-called "Taylor cone" (p-jet) with consequent release of a small amount of material onto a glass slide [1].

The main innovation of this doctoral proposal with respect to this project is to consider biological liquids that show peculiar rheological properties, defined as "non-Newtonian". As an example, blood shows a variety of non-Newtonian characteristics such as pseudoplasticity, viscoelasticity, thixotropy [2]. Another example concerns tears that show a viscosity that is not constant with the rate of deformation [3], especially in conditions of dry eyes, a pathology that affects astronauts on long-duration space missions [4]. The non-Newtonian properties of such fluids have a significant effect on the fluid dynamics which, consequently, translates into a different response to the electric field compared to classical Newtonian fluids. Therefore, the rheological properties of the liquid can influence the optimal parameters of the device both with regard to the formation of the meniscus of biological liquid, and for the generation of the Taylor cone and the consequent deposition of material to be analyzed. In this project we aim to comprehensively characterize the effect of non-Newtonian properties such as shear-thinning, viscoelasticity and plasticity on the dynamics of the liquid subjected to an electric field. The final objective will therefore be to identify the optimal conditions to implement in the super-sensor depending on the type of biological fluid used for the detection of biomarkers, making the lab-on-chip device more widely applicable.

The research activity will be carried out through experiments and numerical simulations. The first part of the experimental activity will focus on the analysis of the deformation of the liquid between two electrodes to understand the effect of the rheological properties. In the next phase, the device with lithium-niobate crystal will be used, which represents the setup of interest for space missions. The experimental activity will be supported by a computational study to model: i) the meniscus of liquid exiting the micro-hole of the load support, ii) the dynamics of the liquid due to the effect of the electric field. To this end, the electro-hydrodynamic equations in the liquid and gas domains will be solved numerically. The air-liquid interface will be tracked through the Volume-Of-Fluid method which allows to account for high deformations, liquid breakage and droplet coalescence. Particular

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importance will be given to the effect of gravity on the deformation of the drop to simulate microgravity conditions.

- [1] Ferrato et al., Nat. Nanotechnol., 5, 2010, 429
- [2] Beris et al., Soft Matter, 17, 2021, 10591
- [3] Recchioni et al., Exp. Eye Res., 219, 2022, 109083
- [4] Ax et al., Front. Physiol., 14, 2023, 1281327

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The experiments will be carried out in the laboratories of the Bottega della Materia Soffice (in P.le Tecchio) and at the ISASI-CNR Institute (Pozzuoli) using the p-jet device already developed in the previous collaboration between UNINA and ASI. The computational tool to be used for numerical simulations will be Basilisk (www.basilisk.fr), an open-source software specialized for the simulation of multiphase systems.

The PhD project is in collaboration with the Agenzia Spaziale Italiana (which funds the doctoral scholarship) and the ISASI-CNR Institute.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A period abroad of at least 6 months is envisaged in the group of Prof. J. M. Lopez-Herrera of the Department of Ingeniería Aeroespacial y Mecánica de Fluidos dell'Universidad De Sevilla (Seville, Spain).

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PhD Project Proposal

Proponent: Prof. Bruno de Gennaro e Prof. Giuseppina Luciani

Proposed research topic: Natural zeolite-based biocomposites for catalytic removal of emerging contaminants.

Reference curriculum:

Materials and Structural Engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

In a constantly changing society with exponentially increasing industrialization, ensuring access to uncontaminated drinking water resources is a priority goal. Major threats to the water body include emerging contaminants released by the textile, food, pharmaceutical and cosmetic industries. The class of emerging contaminants includes all those substances that are hardly removed by conventional treatment plants as well as all compounds for which limits to their concentration have been proposed but not yet translated into regulatory obligations. Among the methods commonly used for their removal from wastewater, adsorption with porous materials is considered the most reliable, simple and economical. There is increasing interest in applications of zeolite-based materials due to their ion exchange capacity and biocompatibility. Recent studies have also demonstrated the effectiveness of biopolymers, such as polydopamine, chitosan, cellulose, and alginate, to functionalize the surface of zeolites, improving their adsorption properties. In particular, the reducing and chelating characteristics of such biopolymers toward metal ions can be effectively exploited to produce environmentally friendly catalysts for the adsorption and degradation of contaminants.

In this scenario, a biocomposite obtained from the combination of polydopamine/zeolite with metallic silver has been employed in recent studies by the proponent group to adsorb dyes by studying their adsorption and reduction cycles using Sodium Borohydride as a reducing agent. The composites have shown high efficacy in the removal of selected dyes over multiple treatment cycles, promoting interest in an in-depth study of such materials to enable their technological application and use in wastewater treatment.

The present Ph.D. project proposal, focuses on the development of adsorbent materials, based on suitably modified natural zeolites for the removal and degradation of emerging contaminants. The initial phase of the project will focus on literature research aimed at both selecting appropriate materials for the realization of the biocomposite and identifying the best techniques for its synthesis and regeneration, as well as identifying current techniques in use in different industries.

Materials based on bioavailable polymers and natural zeolites will be synthesized, the produced systems will be subjected to thermodynamic and kinetic adsorption tests considering contaminant concentrations close to the real ones. In addition, the behavior of these materials in mixed pollutant systems will be evaluated with the aim of assessing possible affinities and interferences. Thereafter, the PhD project will focus on optimizing the biocomposite regeneration process through the use of

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environmentally friendly reducing agents by implementing a circular and more sustainable approach involving its reuse in multiple adsorption cycles.

The proper functionalization aims at making zeolite a reusable material in successive adsorption/desorption cycles due to the presence of metallic silver particles that act as a catalyst for contaminant degradation. Finally, in a logic of industrial scale-up, the research goal is to implement an appropriate column system to investigate the efficiency of the composite system under dynamic settings.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The Ph.D. project involves the development of systems based on zeolites, natural or synthetic, functionalized with bioavailable polymers and a metal catalyst to promote their reuse in the removal, through adsorption and reduction, of emerging contaminants. At the same time, in-depth physicochemical characterizations will be carried out on the synthesized systems using common investigation techniques, including:

- XRPD, for characterization of the obtained composites by X-ray analysis;
- SEM-EDS, for checking the obtained structure and evaluating elemental content;
- Microporosimetry, for evaluation of BET surface area;
- FT-IR, to obtain information on the composition of the formulated biocomposite and the functional groups present;
- TGA/DTA, for monitoring the mass loss of the material and enabling the study of thermo-degradation and thermo-oxidation;
- UV-Vis, to measure the goodness of adsorption in terms of residual concentrations of contaminants in solution;
- ICP-OES, for elemental composition analysis, of cationic species in solution.
- Microwave mineralizer, for digestion of solid phases to be prepared for their characterization, as well as for synthesis of new phases
- Molds for high-temperature treatments (1500°C)
- LC liquid chromatography for elemental analysis of cationic and anionic species constituting biocomposites

The project will be carried out in collaboration with Prof. Brigida Silvestri of the Department of Civil, Building and Environmental Engineering (DICEA) of the University of Naples Federico II.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

Due to the decades-long collaboration with Dr. Aleksandra Dakovic's group at the INSTITUTE FOR TECHNOLOGY OF NUCLEAR AND OTHER MINERAL RAW MATERIALS (ITNMS), Belgrade, Serbia, and the experience this group has in modifying and subsequent characterization of zeolitized materials, a period of at least 6 months at ITNMS is planned to further explore the proposed topic.

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PhD Project Proposal

Proponent: Prof.ssa Almerinda Di Benedetto

Proposed research topic: Insights into safety issues of Li-Batteries

Reference curriculum:

Chemical engineering

Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The rapid advancement in battery technology, especially in lithium-ion batteries, has revolutionized energy storage solutions across various sectors, including electric vehicles, consumer electronics, and renewable energy systems. Despite their widespread use and high energy density, these batteries present significant safety challenges.

Battery safety is strongly related to thermal management. The battery thermal management system must dissipate the heat generated during operation to avoid temperature rise. Temperatures may exceed the threshold value for two main reasons:

- 1) External heating
- 2) Abuse conditions and/or insufficient cooling

If one or both these conditions are met, battery temperature may go out of control with the consequence of activation of undesired (exothermic) reactions between battery materials which eventually lead to thermal runaway (TR).

As shown in figure 1, the optimal (safe) operating temperature window for Lithium-ion cell operating window is $T < 60^{\circ}\text{C}$. (*Languang Lu, Xuebing Han, Jianqiu Li, Jianfeng Hua, Minggao Ouyang, A review on the key issues for lithium-ion battery management in electric Vehicles, Journal of Power Sources 226 2013 272-288*).

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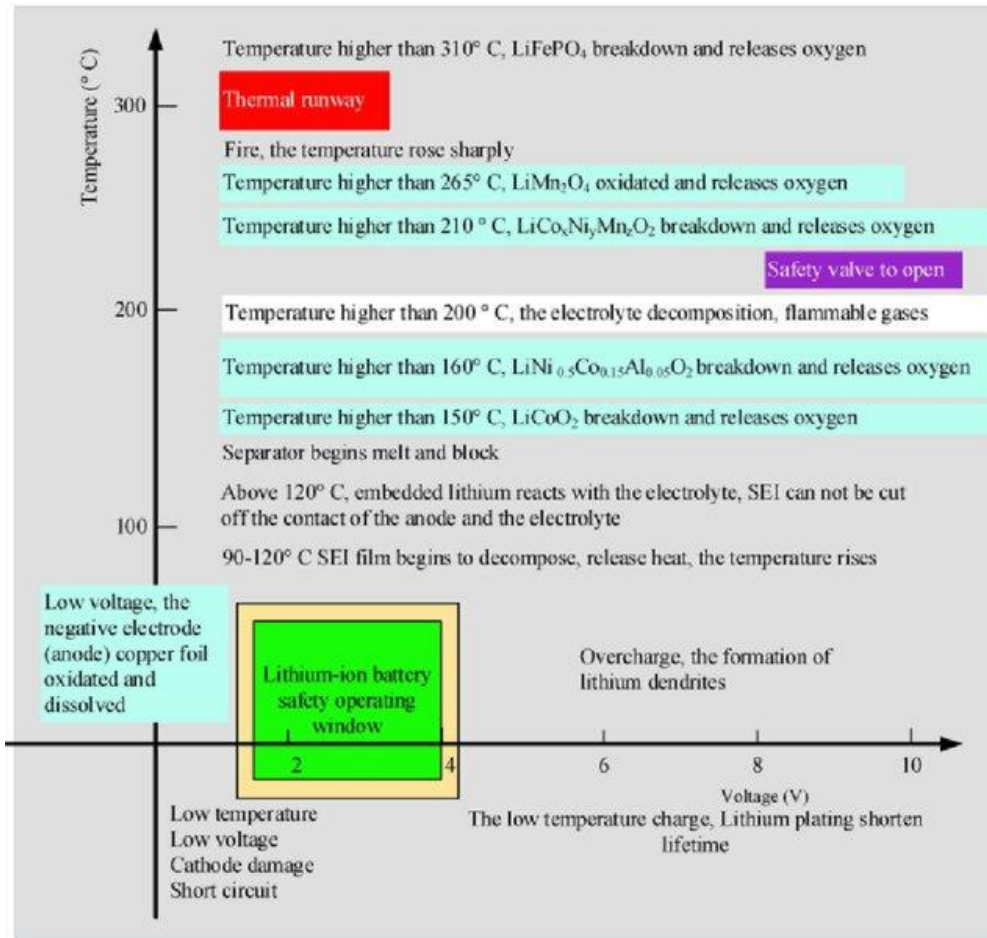


Figure 1 – Operating window of Li-batteries

If this temperature limit is exceeded undesired events may arise like fires and explosions (Figure 2). Incidents of thermal runaway, fires, and explosions have highlighted the urgent need for comprehensive safety measures.

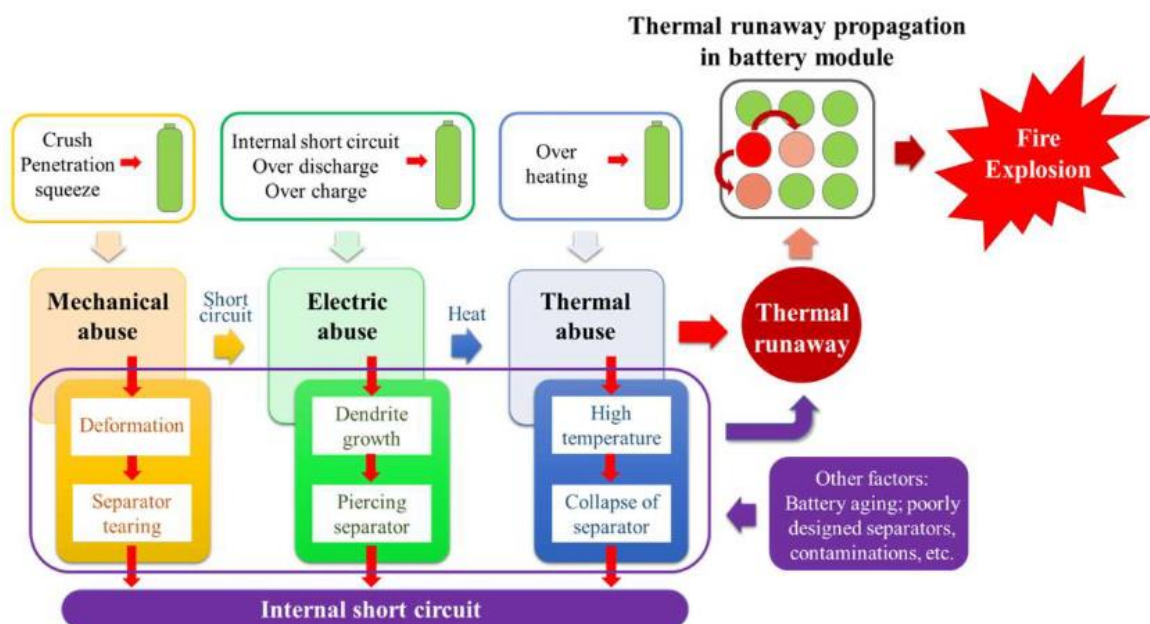


Figure 2 – Sequence to fires and explosions from A review of early warning methods of thermal runaway of lithium-ion batteries (Depeng Kong , Hongpeng Lv, Ping Ping, Gongquan Wang, Journal of Energy Storage 64 (2023) 107073)

Current research has focused on understanding the mechanisms of battery failures, improving materials and design, and thermal management systems (Depeng Kong , Hongpeng Lv, Ping Ping, Gongquan Wang, Journal of Energy Storage 64 (2023) 107073).

Many questions in terms of electrolyte nature, interaction with the other materials, optimal thermal management and geometrical configuration remain a critical need for further research to address unresolved issues and to develop solutions that ensure the safe operation of batteries under all the operating conditions.

2. Objectives

In this context, the primary objective of this research is to significantly enhance the safety of batteries through innovative approaches in materials science, thermal management, and system/process integration, utilizing advanced experimental techniques and modeling tools

1. Characterize all the battery materials that exhibit superior thermal and chemical stability to mitigate risks of thermal runaway and fires;
2. Thermal Management Optimization: design effective thermal management solutions that ensure stable temperature profiles and prevent overheating.

3. Program of Planned Activities

The proposed research project will undertake a multidisciplinary approach to study battery safety, encompassing materials science, thermal management, and system integration. The project will be structured into the following key activities:

First Year

Conduct a comprehensive review of existing literature on battery safety, also identifying current knowledge gaps and limitations in existing safety measures.

Develop and use a kinetic model to evaluate the flammability/explosion parameters of the gas produced by battery overheating

Plan the experimental activities for thermal studies.

Second Year

Investigate the flammability properties (flash point) of advanced materials such as solid-state electrolytes and liquid electrolytes and their mixing

Perform extensive testing to evaluate thermal stability through DSC analysis, also with high quantities by using RADEX calorimetry.

Develop and use an advanced model (CFD and bifurcation model) for thermal management evaluation

Third Year

Simulation of the thermal management of batteries.

Development of safety maps as function of operating conditions and materials.

Design and optimize thermal management systems to prevent overheating and thermal runaway.

Thesys

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Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Experimental Tests

The experimental tests for evaluation of the flammability/explosion properties of the Li-battery materials will be performed by means of:

1. Flash Point Test Apparatus available at the SaRAH lab
2. Thermal/chemical stability analysis will be performed by means of Differential Scanning Calorimetry (DSC) available at STEMS/CNR
3. Radex experimental tests to simulate and evaluate the thermal behavior of batteries under various operational conditions, including abusive scenarios.

Modeling

1. Chemkin software (available at the calculus Lab of SaRAH);
2.) to model the chemical kinetics and combustion properties of the gases produced by batteries under thermal runaway and other failure conditions;
3. Employ bifurcation analysis modeling to study the stability and runaway conditions of battery systems, identifying critical thresholds and failure points (AUTO software, available at the calculus Lab of SaRAH);
4. Simulate the integrated system for thermal management optimization (ANSYS software available at calculus Lab of SaRAH).

Collaborations will be established with ing. Roberto Sanchirico from STEMS/CNR

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A period of at least 6 months will be spent abroad.

Different possibilities are:

1. Prof. Olivier DUFAUD, University of Lorraine, Nancy
2. Prof. Alfredo Ursúa, Institute of Smart Cities (ISC), Department of Electrical, Electronic and Communications Engineering, Public University of Navarre (UPNA), Campus de Arrosadia, Pamplona, 31006, Navarra, Spain

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Proponente: Ernesto Di Maio

Tematica di ricerca proposta:

Schiume polimeriche avanzate per applicazioni strutturali: proprietà controllate da instabilità meccaniche

Curriculum di riferimento:

Ingegneria dei Materiali e delle Strutture

Sintesi del Progetto di Ricerca (stato dell'arte, breve programma previsto per le attività e obiettivi)

Negli ultimi anni, il controllo delle instabilità meccaniche sta giocando un ruolo chiave nella progettazione di metamateriali. I materiali convenzionali possono infatti essere strutturati sia alla microscala che alla macroscala per essere resi suscettibili di instabilità meccaniche, le quali portano spesso a importanti variazioni di proprietà. Materiali che sono di per sé strutturati alla microscala sono le schiume polimeriche, in cui le instabilità meccaniche sulla scala microscopica determinano le proprietà meccaniche sulla scala macroscopica.

Recentemente sono state sviluppate schiume polimeriche avanzate a gradiente di densità, ovvero schiume polimeriche in cui la densità è distribuita in maniera non-uniforme nel materiale al fine di soddisfare requisiti meccanici e/o funzionali.

Il progetto di dottorato ha come obiettivo quello di progettare le instabilità meccaniche su due scale: la scala microscopica (scala delle celle) e la scala macroscopica (scala della densità), al fine di ottenere materiali estremamente leggeri ma con proprietà meccaniche non convenzionali, in grado di garantire performance meccaniche nettamente superiori rispetto alle attuali schiume polimeriche presenti sul mercato.

Si prevede perciò che il candidato sviluppi nel primo periodo di dottorato conoscenze inerenti sia al processo di schiumatura che alla meccanica del continuo, sviluppando uno stato dell'arte sulla meccanica non lineare di schiume polimeriche.

Dopodiché, si passerà alla modellizzazione analitica e prototipazione virtuale (tramite CAD e FEM). Il materiale verrà poi prodotto in laboratorio e testato presso centri di ricerca specializzati, con l'aiuto di tecniche di imaging per verificare sperimentalmente che i meccanismi di instabilità meccanica diano effettivamente le proprietà desiderate.

Informazioni sintetiche relative a: strutture operative e scientifiche (attrezzature, software, laboratori,...) a disposizione del dottorando per lo svolgimento dell'attività proposta, collaborazioni con altri enti di ricerca italiani ed esteri (eventualmente anche con aziende) potenzialmente rilevanti alla tematica proposta.

Il lavoro verrà svolto presso il foamlab del DICMaPI, nonché presso laboratori e centri di ricerca pubblici e privati con i quali sussistono collaborazioni scientifiche e progetti di sviluppo, come l'*École Polytechnique* (Parigi, Francia) e l'Università di Pavia.

Informazioni sintetiche relative ad eventuale periodo all'estero previsto per il dottorando (periodo, gruppo di ricerca, Università, ente di Ricerca....)

E' previsto un periodo compreso tra i tre e i nove mesi presso l'*University of Maryland* (Washington, D.C.) presso il *Tubaldi Lab* della Prof. E. Tubaldi, esperta in meccanica non lineare e controllo delle instabilità.

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Proposta di progetto di dottorato
borsa di studio, ai sensi del D.M. n. 630 del 24.04.2024

Proponente: Ernesto Di Maio

Tematica di ricerca proposta: Studio di schiume per la produzione di manufatti con mappe di densità ottimizzate nel 3D

Curriculum di riferimento:

Ingegneria dei Materiali e delle Strutture
Ingegneria chimica

Sintesi del Progetto di Ricerca (stato dell'arte, breve programma previsto per le attività e obiettivi)

Il lavoro di dottorato si propone come primo obiettivo quello di studiare ed analizzare i principi chimico-fisici che regolano i processi di espansione e di reticolazione di compounds a base di miscele poliolefine-elastomeri all'interno di uno stampo per la produzione di schiume flessibili. Dal punto di vista applicativo questo studio si propone di migliorare le tecnologie ed i prodotti.

I benefici attesi riguardano la possibilità di migliorare l'efficienza del processo di stampaggio, in particolare in termini di tempo di ciclo e sostenibilità energetica, nonché di migliorare le proprietà del manufatto grazie all'ingegnerizzazione della schiuma.

In quest'ottica, un ulteriore obiettivo riguarda l'esplorazione della tecnologia di espansione a gradiente per produrre manufatti, con le stesse matrici elastomeriche, caratterizzati di una mappa 3D di densità e morfologia progettate sulla base della specifica applicazione. Questo studio sarà eventualmente affrontato attraverso la progettazione di apparecchiature di processo dedicate.

Il lavoro verrà svolto presso il foamlab del DICMaPI e presso Versalis SpA, nonché presso laboratori e centri di ricerca pubblici e privati con i quali sussistono collaborazioni scientifiche e progetti di sviluppo.

È previsto un periodo all'estero per un periodo non inferiore a sei mesi presso l'École Polytechnique (Laboratoire de Mécanique des solides), Palaiseau (Paris, France).

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent:

Prof. Amedeo Lancia/Prof. Alessandro Erto

Proposed research topic:

CO₂ capture from marine engines by adsorption onto honeycomb structured solids

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The rapid increase in world population has caused huge growth in energy consumption during the 20th century, and more than 85 percent of that demand is now met by fossil fuels. Against this backdrop, environmental issues related to pollutant emissions from the transportation sector have attracted worldwide attention, particularly to the rising levels of greenhouse gases in the atmosphere, which can disrupt the energy balance.

The introduction of environmental regulations and energy efficiency improvements in the shipping industry are generating major changes in the design of new ships, which must include innovative solutions in terms of naval architecture, propulsion systems, and depollution systems to comply with the constraints imposed in a cost-effective manner.

The need for a reduction in greenhouse gas emissions, and in particular CO₂, has resulted in the development of numerous technologies aimed at abating pollutants and reducing emissions of these compounds. The use of exhaust gas treatment plants is a useful option, and sometimes the only one available, to be able to comply with these regulatory requirements.

Adsorption represents a well-established removal technology because of its high potential for efficiency and operational flexibility, low cost and, when combined with a high-efficiency regeneration process, for the absence of by-products. In addition, it represents among the best technologies for retro-fitting pre-existing plants and combustion engines, as it can be made into treatment units that are easily implemented in existing units. The main disadvantages associated with the use of this technology lie in the cost of the sorbent and the possibility of it being saturated or "poisoned" by the co-presence of other pollutants, first and foremost NO_x and SO_x. In any case, the prospects for research in this field portend developments such that these drawbacks can be overcome. Numerous porous solids can be usefully employed for CO₂ capture from exhaust gases (activated carbons, zeolites, MOF's, etc.); most of these solids, although possessing good adsorption capacity, can be subjected to functionalization processes with amines, alkaline compounds, ionic liquids, etc., which modify their surface structure in a way that results in increased capture performance, making the process more cost-effective.

In an industry such as marine where additional factors such as minimizing space requirements, reducing pressure drops and maximizing specific yields are of particular importance and interest, the use of honeycomb-structured adsorbents functionalized with appropriate active phases (amines) appears to be a particularly attractive solution.

Specifically, the main objectives of the project are as follows:

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- Study of adsorption processes for the removal of CO₂ from combustion gas from marine engines, assuming the use of different fuels (natural gas, diesel);
- Definition of a structured adsorbent solid, of different chemical nature, and functionalized with different amines at varying concentration;
- Designing and operating a prototype CO₂ capture plant, possibly coupled with a CO₂ regeneration/recovery stage;
- Modeling of experimental results geared toward preliminary scale-up study and economic feasibility.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The project is based on an existing scale-lab CO₂ capture plant located in the Adsorption Laboratory of the Department of Chemical, Materials and Industrial Production Engineering, University Di Napoli Federico II.

The project is being developed with the co-funding partner company (Corning GmbH).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The project involves a 6-month period abroad at the University of Edinburgh (Scotland) - Department of Materials and Processes. Responsible: Prof. Stefano Brandani.

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PhD Project Proposal

Proponent:

Prof. Amedeo Lancia/Prof. Alessandro Erto

Proposed research topic:

Production of synthetic natural gas (SNG) in advanced reactors for conversion of CO₂ with renewable hydrogen

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

One of the greatest challenges that scientific research and technological development must face is to be able to profitably and efficiently combine the need to reduce CO₂ emissions to curb global warming with meeting ever-increasing global energy needs. However, the replacement of carbon-based energy sources with renewable ones is not easily feasible and in the short term. The current energy scenario is based on the use of fossil-fueled power plants that can continuously provide electricity or heat, while renewables suffer from several limitations, such as the intermittency of sources (e.g., photovoltaics and wind) and the low energy density of corresponding carriers (e.g., hydrogen).

In this panorama, CCU (Carbon Capture and Utilization) technologies could represent an interesting element of energy transition, between the current fossil economy and the future renewable economy: in particular, Power to Gas (PtG) processes represent a valid synergistic approach to the problems mentioned above, as they involve the reaction between CO₂, captured from anthropogenic emissions, and H₂ produced from renewable sources. Among the different products that can be obtained, methane (CH₄) assumes a very prominent role, even in light of recent events that have so affected world energy policies. It is a compound with medium energy density and easily deployable by injection into the natural gas grid: for this reason, methane produced by PtG processes is also called synthetic natural gas (SNG).

The strategic importance of this process is further underscored by both the centrality of natural gas as a means of meeting national energy needs and the need to diversify its sources of supply due to the current international political situation, in accordance with the REPowerEU plan recently announced by the European Commission.

For these reasons, the main purpose of this project is to provide a substantial boost to the technological development of PtG processes, through the realization of a state-of-the-art reactor that, coupled with the identification of a state-of-the-art catalyst, would enable the optimization of the CH₄ productivity of the CO₂ hydrogenation process, while ensuring effective temperature and reaction heat management to maximize the economic and energy yield of the system. The research results would enable the establishment of design criteria for the construction of a demonstration unit, an important step toward the large-scale application of this technology.

Specifically, the main objectives of the project are as follows:

- Design, construction and validation of an advanced reactor (e.g., micro-reactor or three-phase reactor) in laboratory scale for the catalytic hydrogenation of CO₂;
- Screening and synthesis of advanced bimetallic catalysts (e.g., Ni and Ru on mesoporous supports) and optimization of system operating parameters;

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- Modeling of experimental results oriented to preliminary scale-up study and economic feasibility.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The project is based on an existing scale-lab methanation plant located in the Sala Impianti of the Department of Chemical, Materials and Production Engineering, University of Naples, Federico II. The project is being developed with the co-financing partner company (Oiltech S.r.l.).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The project involves a 6-month period abroad at the University of Alicante (Spain) - Inorganic Chemistry Department (Laboratorio de Materiales Avanzados). Responsible: Prof. Joaquin Silvestre-Albero.

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PhD Project Proposal

Proponent:

Prof. Luca Esposito

Proposed research topic:

Design and Development of Advanced Devices for Major Physics and Astrophysics Experiments

Reference curricula:

Technologies and Production Systems

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Successful scientific experiments in physics and astrophysics often require the design and fabrication of prototypal devices with extraordinary performance. To achieve these ambitious objectives, it is essential to combine cross-functional skills ranging from mechatronics to physics. This entails not only mastering advanced mechanical design techniques but also gaining a deep understanding of the physical principles governing the operation of these devices. In particular, the ability to perform detailed structural analyses using FEM (Finite Element Method) calculations is crucial to ensure the reliability and effectiveness of the developed prototypes.

An example of such complex equipment is the Einstein Telescope, a third-generation gravitational wave observatory designed to significantly enhance our ability to detect and study these cosmic phenomena. Another example is the nuclear fusion reactor, an advanced technology aimed at replicating the processes occurring in the core of stars to generate clean and sustainable energy. The complexity of such systems requires professionals adequately trained to find innovative technological solutions to specific problems.

A possible doctoral research topic in this field requires an integrated approach of Mechatronics and Structural Analysis." This research project focuses on: This research project focuses on:

1. **Advanced Mechanical Design:** Development of innovative methodologies for the design of experimental devices, with a focus on optimization and the integration of multiple functionalities.
2. **Structural Analysis:** Application of FEM calculation techniques to evaluate the strength, deformation, and overall performance of prototypes under various operating conditions.
3. **Interdisciplinarity:** Integration of knowledge from mechatronics, physics, and materials engineering to optimize the design and functionality of devices.
4. **Experimentation and Validation:** Fabrication of prototypes and their experimental validation in the laboratory, with particular attention to applications in physics and astrophysics.
5. **Technological Innovation:** Exploration of new technologies and advanced materials to improve the performance of devices, for instance, using next-generation sensors, high-precision actuators, and smart materials.

The ultimate goal of this doctoral project is to train experts capable of combining theory and practice, developing advanced technological solutions for scientific research. These experts would be able to

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tackle the complex challenges posed by modern physics and astrophysics experiments, significantly contributing to the advancement of knowledge in these fields.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The proposed topic falls within a broader collaboration between Professor Esposito's research group, the National Institute of Nuclear Physics (INFN) section of Naples, and the University of Trento. The collaboration with the University of Trento is active under the PRIN project titled "ADaptive OPTics for Asymmetric light shaping in gravitational wave detectors (ADOPTA)". At the INFN section of Naples, the collaboration focuses on the study and prototyping of a New Generation of Super Attenuators (NGSA) for third-generation interferometers. Depending on the needs, the PhD candidate will have access to equipment, software, and personnel from the three entities involved in the topic.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

International collaborations and INFN's participation in international consortia are beneficial in creating opportunities for the PhD candidate to spend a training period abroad to deepen specific topics.

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Giovanni Filippone

Project proposed in collaboration with Centro Italiano Ricerche Aerospaziali (CIRA) in the framework of DM630 - Dottorati Innovativi cofinanziati da Aziende/Enti di Ricerca

Proposed research topic: Development of low environmental impact nanostructured polymer coatings for aerospace applications

Reference curriculum:

Materials and Structural Engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

Ice formation that occurs in cold and humid atmospheres can pose a danger to flight safety. The formation of ice on the surface of an aircraft alters the aerodynamic flow, causing a reduction in lift and an increase in drag, making the aircraft unmanageable. To reduce ice formation and its associated dangers, two protection systems are commonly used: anti-icing, which prevents ice formation, and de-icing, which removes ice once it has formed. The objective of this research project is to develop, optimize, and validate nanostructured coatings for aerospace applications, with reference to anti-icing and de-icing functional properties. The project is divided into five main phases:

- a) investigation of current models and technological solutions used for de-icing and anti-icing
- b) Coating design, selection of raw materials based on information derived from benchmark analysis, and preparation of nanostructured coatings
- c) Structural characterization and functional validation of nanostructured coatings
- d) Scale-up of the optimized process
- e) Comparison of the newly developed technology with benchmarks

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The research activities will be conducted within the research laboratories of DICMaPI and CIRA, which are well-equipped for carrying out the planned activities, both for the preparation/synthesis of new materials and for their characterization.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution)

The research activity will be conducted through a synergistic collaboration between the University and Industry. In particular, the Ph.D. student will carry out continuous periods of activity at the company (first and second year, at least 12 months). A period of research at foreign universities (third year, 6 months) is also planned, to be selected based on the results obtained in the first two years of research, particularly with research groups specializing in the development of self-healing coating formulations and/or research groups specializing in the functionalization of nanoparticles.

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PhD Project Proposal

Proponent:

Prof. GALLO MOSE'

Dott. CONVERSO GIUSEPPE

Proposed research topic:

Development of decision support models to implement the concepts of sustainability and circularity within textile supply chains. These models, which fully take into consideration the recent technologies in the field of material recovery, are intended to support decision making from system configuration to short-term production planning, also by integrating the latest information and communication technologies made available by "Industry 4.0" paradigm.

Reference curriculum:

Technologies and Production Systems

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The textile industry sector is undergoing a significant transformation towards the circularity and sustainability of its production processes. Such an objective could be pursued both by developing "reverse logistics" strategies, also exploiting innovative production paradigms such that of "Industry 4.0", and by developing and implementing new "short supply chain" circularity models, of an intra- and inter-district nature. The main areas, in which transformation processes (although still in an embryonic state) determined by this new production orientation are found, include: 1) Design for Durability; 2) Recycled and Biodegradable Materials; 3) Product Life Cycle Analysis; 4) Production planning models. This latter area involve the development of integrated models between the various supply chain actors and which include the systemic feedback generated by the new production paradigms.

In a sort of self-induced phenomenon, this industrial vision shift is causing a strong drive for innovation in technological terms, regulatory policies, supply chain and district interactions, but also, and above all, new production management logics which, in turn, would make it possible a brand-new production paradigm permitting the textile sector to achieve significant results towards reducing environmental impact and improving working conditions along the whole supply chain.

In this context, the objective of the research will consist in analyzing the existing relationship between industrial production planning, on the one hand, and the new vision on circularity, end of life product recovery, lowering of environmental impacts and operational risks, which characterize the textile industry sector, in order to harmonize and, above all, optimize its production processes by significantly contributing to raising its effectiveness and efficiency.

Consistently with this general objective, the research will focus on the development, verification and validation of proper mathematical models leading decision-making. These models, also developed by leveraging the most advanced Artificial Intelligence tools, will at least be validated by means of the simulative methodology, where ground-testing is not possible.

The research program, will involve a preliminary stage, in which emerging scientific issues for the specific field will be punctually and integrally analyzed by means of an in-depth literature review that, although never interrupted throughout the three-year research project, will be mainly conducted in the first ten/twelve months of the project itself.

Next, the most suitable modeling methods to address the "research questions" emerged from the previous research stage will be scrutinized. At the same time, a field data collection phase will be

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launched among those industrial actors operating in the closest production districts and interested in the aims of the research activity.

The model development phase will characterize the fourth and fifth semesters of the project, while the last semester will be devoted to the implementation of the model, its validation and, above all, the analysis of the results obtained.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The research activities will be possibly conducted in collaboration with University of Parma (Prof. Giovanni Romagnoli principal investigator of the PRIN project “Sustainable Textile - SusTex: exploring and adapting good practices for valorizing wastes in the textile and apparel supply chain” – CUP D53D23011410006” which has objectives that are complementary to the present research) and companies located in the Campania region and operating in the textile industry. Similarly, although with different objectives specifically aimed at investigating the potential of models to be implemented in relation to circularity issues between related industry sectors (e.g., leather industry), part of the scientific activities could be carried out in collaboration with academic and industrial research facilities, coordinated at MICS within the framework of the PNRR project 'Made in Italy Circular and Sustainable - MICS _ PNRR MUR _ M4C2 _ I 1.3' – CUP E63C22002130007– Project Code: PE00000004 - Spoke 7.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

At the moment, any period abroad for the PhD student has been planned but, considering the interest that the research question holds, especially at the European level, this possibility is not excluded, conditioned on the availability of research institutions interested in the development of the project.

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PhD Project Proposal

Proponent:

Andrea Grassi

Proposed Research Topic:

Optimization of Coordination in the Supply Chain through the Reduction of Informational Asymmetry, using Advanced Models and Software Simulations

Reference Curriculum:

Production Technologies and Systems

Project Summary:

The proposed research project aims to improve coordination in the Supply Chain to reduce informational asymmetry, focusing on the interaction between actors at the operational rather than strategic level. The main objective is to develop new models and algorithms that address this issue over an extended and dynamic time horizon.

State of the Art:

Currently, the Supply Chain operates in a dynamic and complex context, where demand variability and the need for customization require rapid responses and integrated strategies across various levels of the chain. However, informational asymmetry among different actors can lead to suboptimal decisions due to a lack of transparency and the willingness of some actors to withhold relevant information. Previous studies have proposed various coordination mechanisms to mitigate these effects, but they often rely on simplified assumptions that do not adequately reflect the complexity and dynamics of operational reality.

Research Program:

The project will be structured into four main phases:

1. Literature Review: Existing research on informational asymmetry and coordination mechanisms will be examined, focusing on those applicable to dynamic operational contexts.
2. Development of New Models: Models incorporating variability and temporal dynamics will be proposed to analyze interactions between subjects and their decisions in cooperative and non-cooperative scenarios.

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3. Model Validation: The new models will be tested through simulations and practical experiments to evaluate their effectiveness in improving Supply Chain performance.

4. Dissemination of Results: Results will be published in academic journals and presented at conferences to stimulate further research and practical applications.

Objectives:

The project aims to:

- Reduce informational asymmetry through the development of new coordination mechanisms that incentivize honest information sharing.
- Improve the Supply Chain's adaptability to market changes and disruptions through a more flexible and responsive coordination approach.
- Generate knowledge that can be generalized for applications in different Supply Chain contexts, thereby contributing to more efficient and transparent global supply chain management.

This innovative approach not only addresses the limitations of current models but also offers a new perspective for continuous improvement of long-term performance and competitiveness.

Laboratories and Equipment:

Virtual Simulation Laboratories: These will be used to conduct experiments in a controlled and replicable environment. These laboratories are essential for testing Supply Chain models in variable scenarios and evaluating the effectiveness of the proposed new coordination mechanisms.

Software and Platforms:

AnyLogic and AnyLogistix: These advanced simulation software tools enable the modeling of complex systems and the simulation of logistics and supply chain processes. AnyLogic supports Java programming, which facilitates the customization of simulation scenarios according to the specific needs of the project.

Visual Studio Development Environment: Used for programming in Python, this integrated development environment (IDE) supports code writing, debugging, and testing. Visual Studio will be employed to develop algorithms that analyze collected data and to program dynamic interaction models between Supply Chain actors.

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Prof. Antonio Langella

Proposed research topic:

Metal Additive Manufacturing for the aerospace industry

The project is within the framework of Ministerial Decree No. 630 of 04/24/2024 in collaboration with CIRA SCpA (Center for Aerospace Research)

Reference curriculum:

Technologies and Production Systems

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

The project aims to study the manufacturing process by additive technologies of special materials such as shape memory materials for aerospace applications.

Shape memory alloys represent a class of innovative materials that offer unique properties such as shape recovery by simple heating (Shape Memory Effect) or the ability to exhibit large deformations without any yielding (Superelasticity). Within this class of materials, the possibility of printing Nitinol (a Nickel-Titanium alloy) with EBM technologies will be evaluated.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The activity will be carried out according to the following training plan:

- 12 months at the Department of Chemical, Materials and Industrial Production Engineering where activities of theoretical/scientific investigation and characterization of materials and elements made in the experimental phases will be carried out mainly;
- 18 months at the facilities of CIRA SCpA in Capua (Ce) where machines for additive technologies for EMB available for the experimental phases will be used.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The period that will be spent at foreign research facilities is 6 months. The facility will be identified later.

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Valentina Lopresto
Advanced Tools and Mouldes S.r.l. (ATM S.r.l.)

Proposed research topic: Innovative Composite Materials made by thermoplastic resins for industrial applications Theoretical and experimental study of thermoforming and joining processes for thermoplastic matrix composites and their reuse and recycling processes

Reference curriculum:
Technologies and Production Systems

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The research project will be about the fabrication of fiber reinforced panels made by thermoplastic resin for industrial applications and to the subsequent thermoforming and joining. The reuse and the recycling processes of the used materials represent an important aspect of the research. The student will cooperate to the chemical-physical characterization of material and will develop knowledge on composites. The experimental characterizations will be supported by the internal facilities. ATM cooperates with Universities and Research center in the Campania Region which will enrich the experience of the student. Thermoplastic composites answer nowadays the need to support the sustainability. The demand for thermoplastic composites is, in fact, continuously increasing because they offer many advantages over their thermoset counterparts, such as high toughness, long storage time, easy repairing and recycling, and ability to be thermoformed and heat-welded. However, the manufacturing of thermoplastic composite parts requires high processing temperatures and expensive equipment. These issues may be overcome by means of reactive processing where a fibrous preform is first impregnated by a low viscosity mono- or oligomeric precursor and the polymerization of the thermoplastic matrix then occurs in-situ. Acrylic reactive thermoplastics for manufacturing thermoplastic composites by liquid molding was already successfully employed. Aim of the activity is to investigate the suitability of such material in a relevant industrial applications. What done up to now is in fact at laboratory level and the scale factor as well as the industrial validation due to the particular needs of the industries represent an important aspect to be faced.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

ATM and DICMAPI are equipped with all the necessary operational and scientific structures necessary to develop the proposed topic. In particular in ATM all the most common fabrication technologies are available to obtain high quality composite laminates and the FEM programs for the simulation of the processes.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

At least 6 months will be spent abroad depending on the development of the project and its results at one of the industrial customer of ATM mainly interested in the results obtained

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PhD Project Proposal

Proponents: Giuseppina Luciani, Antonella Macagnano

Proposed research topic:

Biowaste valorization as smart nanostructured bio-stimulants for sustainable agriculture

Reference curriculum:

Chemical engineering

Materials and Structural Engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives):

Traditional agriculture poses risk to the environment and significantly contributes to climate change and ecosystem degradation. There is a close relationship between soil security, water security, climate security, and economic security, so there is an urgent need to replace these conventional practices with environmentally friendly processes. The use of bio-fertilizers, smart nanomaterials and nanotechnologies can decrease environmental pollution and improve soil health. Lignin, cellulose, and other bioactive compounds such as polyphenols and essential oils can be extracted from fruits and vegetables and embedded in polymer nanofibers with electrospinning. This technology has gained significant traction in agriculture for producing nanostructured materials that can be used for active substance delivery and environmental sensing. At the same time the formulation of nanomaterials based on bioavailable compounds as well as their combination with an inorganic nanostructured phase, through the ceramic templated approach, can enhance the intrinsic bioactive features and address reproducibility issues related to their heterogeneous composition.

This PhD proposal aims to advance sustainable and precision agriculture through the development of functional materials utilizing the synergistic combination of wet chemistry synthesis of nanomaterials with electrospinning technology using agricultural by-products and waste, containing high levels of valuable bioactive compounds like polyphenols, flavonoids, and lignocellulose. The project focuses on creating composite nanofibrous systems capable of both providing controlled release of biofertilizers and biopesticides to soil-plant ecosystems and serving as nanofibrous sensors for monitoring their health. The project will involve a comprehensive methodology, including the selection and preparation of suitable agricultural by-products, the design of nanomaterials from waste to optimize release control and effectiveness under different environmental conditions, the development and characterization of nanofibers, and the testing of their efficacy in real-world agricultural settings.

The project will use electrospinning and wet chemistry routes (solvothermal, antisolvent precipitation) to create organo-mineral nanocomposites by combining lignocellulose, lignin, cellulose, and organo-mineral nanoparticles. These will be encapsulated into nanofibrous scaffolds to form aggregates of varying sizes, to be applied to the soil as stable organic amendments,

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enhancing carbon stock compared to typical compost processes. Additionally, it will be focused on developing nano-biopesticides from biowastes (polyphenols, flavonoids). Electrospun nanofibers can encapsulate these active substances, allowing for their gradual release into the soil-plant ecosystem. This approach reduces the need for frequent applications, decreases resource waste, and mitigates the risk of over-fertilization and pest resistance. Also the combination of lignin with carbon nanomaterials can exploit the natural affinity of lignin for ammonia, leading to more pronounced and measurable changes in sensor output upon ammonia exposure. So lignin can be processed to form nanostructures that integrate well with carbon nanoparticles or carbon nanofibers resulting in a composite material with enhanced mechanical and thermal stability, crucial for sensor durability.

First year: Literature Review and Initial Training; Material Preparation and Characterization

Second year: Nanostructures Optimization and Functionalization

Third year: Sensor Development and Field Testing

Expected outcomes:

- Development of nanofibrous materials for controlled release of biofertilizers and biopesticides;
- Creation of high-sensitivity, field-deployable VOC sensors for monitoring soil and crop health;
- Valorization of agricultural by-products into high-value functional materials;
- Contributions to the circular economy model and sustainable agriculture practices.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Electrospinning equipment (CNR) for designing nanofibrous matrices for each proposal aim

Materials characterization

(CNR-IIA): Stereomicroscopy, Optical-Fluorescent Microscopy, Electronic Microscopy, atomic force microscope, Spectrophotometry UV-Vis (reflectance, absorbance and transmittance); WCA home-made tool, Open-Source software of image analysis.

("Federico II"-University): - Transmission Electron Microscopy (TEM) or Scanning Electron Microscopy (SEM) for identifying morphology and size; X-Ray Diffraction (XRD) for verifying structure; BET porosimetry to determine surface area and pore distribution; Infrared Spectroscopy (FTIR) for identifying major functional groups present; and Simultaneous Thermogravimetric Analysis (TGA-DSC) combined with FTIR gas analysis

Electrical Measurements (CNR-IIA):

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Mass-flow controllers for gas and VOCs generation for sensors calibrations; electrometers; interdigitated electrodes; electronic bench; interface electronics

Data Analysis (CNR-IIA)

Data analysis and collection software

Applications:

test in cooperation with laboratories of Federico II UNINA and CNR

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....) :

The period abroad is foreseen in the third year of the PhD at the university of Gent (Belgium) with Karen De Clerck's research group.

DOTTORATO IN INGEGNERIA DEI PRODOTTI E DEI PROCESSI INDUSTRIALI

Ciclo XL

PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proposer: Pier Luca Maffettone
3DnA

Proposed research topic: Characterization of the 3D printing process of polymeric foams for the development of functional, environmentally friendly and high technological value materials for the various industrial sectors

Reference curriculum:

Chemical engineering
Design of sustainable and safe products and processes

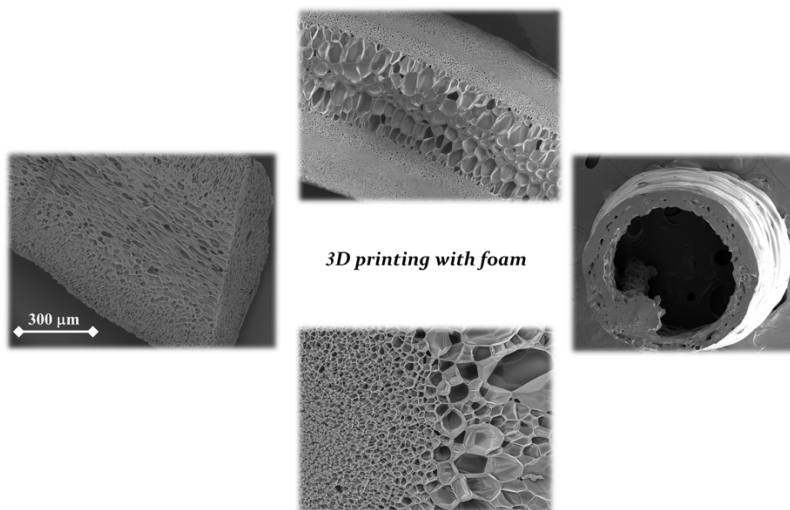
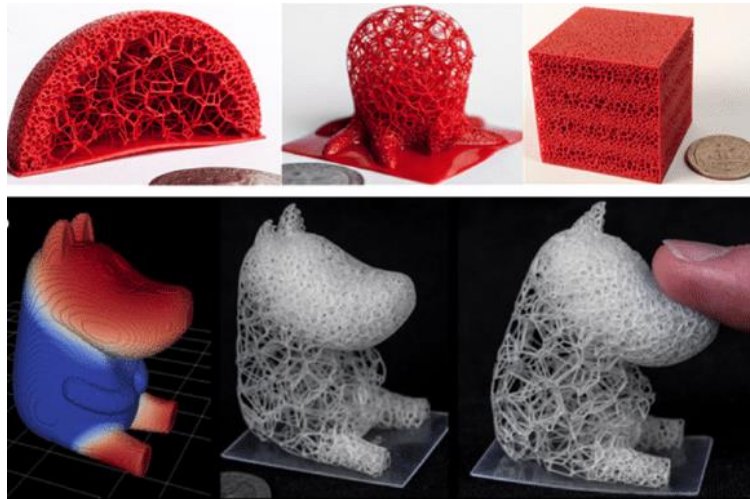
Summary of the Research Project (state of the art, short program planned for the activities and objectives) max 500 words

3D printing of polymer foams has attracted significant attention in multiple recent research studies, as it represents a technologically advanced process whose products guarantee good acoustic and thermal insulation, lightness and high specific resistance [1,2,3].

It is an emerging technique that combines the advantages of additive manufacturing (material savings, design flexibility and low costs) with those of foaming (low density, dimensional stability and greater functionality) [3,4,5]. This combination allows the production of cellular polymeric materials with a defined periodic matrix, optimized for specific applications of interest such as the creation of insulating structures, food packaging and components for chemical processes [2,3,4,6,7].

Recently, the focus has shifted towards environmentally friendly materials and sustainable production processes. Polymeric foams based on biodegradable materials or materials derived from renewable sources represent a promising solution [1,7,8].

Currently, foams are 3D printed but without a specific methodology and standards that can allow control of the dimensions and final thermomechanical characteristics (e.g., stiffness, resistance, thermal transport). The precise modeling and characterization of these materials in 3D printing contexts, in fact, require further developments to optimize the properties of the final product and guarantee its economic and environmental feasibility.



The research project will be divided into three main phases:

1. Selection and preparation of materials:
 - a. Identification of polymers derived from renewable and non-renewable sources, suitable for 3D printing.
 - b. Scientific in-depth analysis of the filament extrusion and pressure solubilization stages.
 - c. Production of polymeric foams obtained through the integration of environmentally friendly blowing agents.
2. Characterization and evaluation of properties:
 - a. Characterization of the mechanical, thermal and structural properties of printed foams.
 - b. Evaluation of the biodegradability and environmental impact of the developed materials.
 - c. Comparison of the performance of environmentally friendly foams with that of traditional foams in terms of strength, density and durability.
3. Development of a methodology for controlling, predicting and optimizing the properties of polymer foams
 - a. Analysis of key parameters and operating conditions of the 3D printing system.
 - b. Using numerical simulation tools to predict polymer behavior during phase transition.

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- c. Optimization of printing parameters (e.g., temperature, extrusion speed, deposition pattern) to guarantee the reproducibility of the process and the desired functionality of the products obtained.
- d. L'obiettivo principale del progetto sarà l'elaborazione di una metodologia che permetta di controllare la morfologia cellulare, la densità e, di conseguenza, le proprietà della schiuma polimerica prodotta, utilizzando la tecnologia di stampa 3D a filamento (FDM).

3D printing profiling and calibration studies, together with the definition of optimal printing parameters and components, will be fundamental elements for the development of cutting-edge functional materials.

Furthermore, we aim to ensure that polymer foams, particularly environmentally friendly and sustainable ones, obtained from this innovative process offer comparable or superior properties to those obtained using conventional techniques.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

3DnA equipment:

- Digital and scanning electron microscope
- 3D Printers (FDM, FFF)
- Software: Materialize, nTopology, CATIA

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The PhD student could carry out a complementary part of the experimental 3D printing activities of printed products at the Materia Nova Innovation Center of the University of Mons (<https://web.umons.ac.be/materiaux/en/materia-nova/>), in Belgium, under the guidance of professor Jean Marie Raquez. Furthermore, the PhD student could carry out part of the characterization activities on printed structures at the University of Bath (<https://researchportal.bath.ac.uk/en/>) in the United Kingdom, under the guidance of Professor Davide Mattia (<https://researchportal.bath.ac.uk/en/persons/davide-mattia>).

References

- [1] Tuan D Ngo et al. "Additive manufacturing (3D printing): A review of materials, methods, applications and challenges". In: *Composites Part B: Engineering* 143 (2018), pp. 172–196.
- [2] Mohammadreza Nofar et al. "Foam 3D printing of thermoplastics: a symbiosis of additive manufacturing and foaming technology". In: *Advanced Science* 9.11 (2022), p. 2105701.
- [3] Daniele Tamaro, Ernesto Di Maio, and Pier Luca Maffettone. "3D foam printing by physical blowing agent". In: *AIP Conference Proceedings*. Vol. 2607. 1. AIP Publishing, 2023.
- [4] Daniele Tamaro, Massimiliano Maria Villone, and Pier Luca Maffettone. "Microfoamed strands

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by 3D foam printing”. In: *Polymers* 14.15 (2022), p. 3214.

[5] Matteo Gregorio Modesto Marascio. “3D Printing and Supercritical Foaming of Hierarchical Cellular Materials”. Tech. rep. EPFL, 2018.

[6] D. Flagiello et al. “Performances of a Y-type structured packing produced by 3D foam-printing for the intensification of gas absorption processes”. In: *Chemical Engineering Research and Design* 195 (2023), pp. 637–650.

[7] Faba S. et al., “Foaming of 3D-Printed PLA/CaCO₃ Composites by Supercritical CO₂ Process for Sustainable Food Contact Materials” (2024), *Polymers*, 16, 798.

[8] Litauszki et al., “Environmentally friendly packaging foams: Investigation of the compostability of poly (lactic acid)-based syntactic foams” (2024), *Sustainable Materials and Technologies*, 35.

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent: Pier Luca Maffettone
FATER S.p.A.

Proposed research topic:

Set up of Digital version of manufacturing industrial plants to be used as a Modelling & Simulation tool

Reference curriculum:

Chemical engineering
Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Last stages of liquid products industrialization in Fater plants usually foresee physical tests to evaluate how variation of operative conditions affects its effectiveness. The PhD project aims to develop Digital Twins, intended as actual virtual copies of existing production plants with fluid dynamics, heat and mass transport models implemented in.

The processes for which the digital twins will be developed are:

- static mixers
- free surface problems in tanks for addition sequence
- Batch and continuous mixers with mechanical agitation
- Batch with air bubbling agitation
- Continuous systems with static mixers
- Continuous systems with dynamic mixers

This would allow the company to obtain numerous advantages:

- significant reduction of projects' costs: the execution of physical tests requires production downtime for the time necessary for the tests with consequent loss of productivity; the amount of savings can be as high as one million euros
- the speed up of tests which, taking place in a virtual environment, can be accelerated by focusing only on the interesting process phase, reducing execution times by up to months
- scenarios evaluation through virtual modifications of the plant that could not be realized in physical tests
- more effective scaling up, having more immediate feedback on the pilot scale

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

At Fater:

- Use of formulation/testing/analysis laboratories: about 2500 square meters equipped with state-of-the-art equipment
- pilot plant, 550 square meters set up as scale-down of the production plants
- visit to production facilities both as for knowledge and to test case studies

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....) N.A.

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PhD Project Proposal

Proponent:

Prof. Giuseppe Mensitieri
Prof. Giuseppe Milano

Proposed research topic:

Multiscale Modeling of “Grafting-to” Processes for the Production of Functional Polymer Brushes

Reference curriculum:

Materials and Structural Engineering
Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Polymer brushes are nanostructures formed by polymer chains tethered to a solid substrate via a stable covalent or noncovalent bond. The features of these structures make them captivating for surfaces and interfaces that respond to the surrounding environment, useful for sensor applications from electronics to medicine. Under this perspective, several polymeric materials such as homopolymers, gradient and block copolymers, polyelectrolytes and responsive polymers were successfully used in the preparation of coated surfaces with polymeric brushes.

Polymer brushes can be prepared by grafting from and grafting to processes. The first process consists in the functionalization of the substrate by including chemical groups which promote the polymerization from the solid surface. The latter process consists in the reaction of functional polymer chains (prepared prior to the grafting reaction) with the substrate, and it is better suited for applications in which it is fundamental to tune the brush thickness and control the reproducibility (e.g., materials for advanced energy, photonics and nanolithography [1]).

The main mechanisms that regulate the morphological features of the polymer brush formation by the grafting to process are: (a) the diffusion-controlled step of the reaction which rules the self-limiting nature of the process in which the polymer chains find increasing difficulty in diffusing through the previously grafted chains; (b) the MW partition of the macromolecules that constitute the brush which is responsible for surface enrichment or depletion of species with different MW due to the distinct diffusion rates of long and short chains combined with different entropic penalties paid during the transport process.

Combination of molecular simulations with statistical thermodynamics approaches provide an insight of the molecular level mechanisms of the grafting process which is fundamental to tailor the properties of the system.

This project consists of the set-up of a modelling framework which comprises (i) combination of reactive Grand-Canonical Monte Carlo [2] and coarse-grain Molecular Dynamics simulations to study the equilibrium properties of bidisperse brushes. Once the equilibrium grafting density has been predicted by molecular simulations, (ii) a self-consistent statistical thermodynamic approach based upon compressible lattice-fluid models (such as, Sanchez-Lacombe model) [3] will be implemented to properly describe the macroscopic topology of the brush chains displaying different flexibilities. Finally, macroscopic model outcomes (e.g., average grafting density and brush height) will be validated against experimental data both available in literature as well as collected on new systems specifically synthesized.

[1] Goldmann, A. S.; Boase, N. R.; Michalek, L.; Blinco, J. P.; Welle, A.; Barner-Kowollik, C. (2019). Adaptable and reprogrammable surfaces. *Advanced Materials*, 31, 1902665.

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- [2] Brondi, C.; Baldanza, A.; Chiarcos, R.; Laus, M.; Scherillo, G.; Mensitieri, G.; Milano, G. (2024). Partition by Molecular Weight of Polymer Brushes: a Combined Re active Grand Canonical Monte Carlo and Self-Consistent Field Investigation of Grafting to Processes. *Polymer*, [294](#), 126737.
- [3] Lakkas, A. T.; Sgouros, A. P.; Theodorou, D. N. (2019). Self-Consistent Field Theory Coupled with Square Gradient Theory of Free Surfaces of Molten Polymers and Compared to Atomistic Simulations and Experiment. *Macromolecules*, *52*, 5337–5356.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The activity will be performed by using the parallel cluster available in the Department of Chemical, Materials and Industrial Production. In particular, regarding the Molecular Dynamics simulation, models will be developed by using Gromacs and OCCAM codes. For the Statistical Thermodynamics modelling, codes will be developed by adopting Matlab environment. The experimental results required to validate the models will be collected in cooperation with the research group of prof. Michele Laus (Università del Piemonte Orientale - Italy).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

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PhD Project Proposal

Proponent: Prof. Tullio Monetta

Proposed research topic:

Plasma Electrolytic Oxidation (PEO) coating of light metal alloys

Reference curriculum:

Materials and Structural Engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Light metals such as Al, Ti, Mg, find increasingly diversified applications in the electronics, aerospace and mechanical engineering sectors, thanks to the favorable ratio between mechanical characteristics and mass of the substance, also in relation to the energy savings allowed by their use in cars, planes, trains, etc. They require an accurate surface finish to ensure their durability and performance in service.

Plasma electrolytic oxidation (PEO), also known as micro-arc oxidation (MAO), is a surface coating technology that produces ceramic layers on the surface of light metals, valve metals and their alloys. The porous outer layer of the coating allows the impregnation of different substances, thus customising the performance characteristics of the coating. Surface coatings formed through PEO offer hardness levels two to four times higher than those obtained through hard anodising. The PEO process uses an electrolytic bath consisting of a dilute aqueous solution, with the addition of other chemical compounds depending on the desired surface coating properties. In the PEO technique, a high potential difference, usually between 200 and 600 V, is applied, causing plasma discharges on the surface to be modified. The plasma, in turn, creates the high temperature and pressure conditions that result in the formation of a predominantly crystalline oxide on the metal substrate. Plasma Electrolytic Oxidation, used under conditions of high potential difference, pulsed, bidirectional, varying duty cycle, is a recently developed surface modification technique. By varying the process parameters, it is possible to design coatings that exhibit specific microstructural characteristics, chemical composition, thickness, rate of accretion, porosity, etc., which determine the chemical/physical characteristics of the surface in terms of morphology, composition, reactivity, biocompatibility, mechanical properties, etc., with the possibility of controlling the degree of porosity of the formed layer. An innovative approach consists of introducing microparticles into the electrolyte, with the aim of incorporating them in situ into PEO coatings during growth. These substances can lead to a change in the hardness of the layer, its corrosion resistance, etc., depending on the intended application.

As part of the project's activities, the aim is to study the effect of process parameters on the structural, morphological and degradation resistance behaviour of ceramic oxide coatings developed by means of (PEO) generated in DC and AC on light alloys, in particular magnesium and titanium, in relation to the applied potential, duty cycle and chemical composition of the electrolyte used containing micro-particles with the aim of incorporating them in situ into PEO coatings during growth.

Work to date has focused on the use of magnesium alloys in the biological environment. Magnesium and its alloys are characterised by low corrosion resistance in such environment; this characteristic can be exploited to make resorbable medical devices. The aim of the work focused on the design of devices capable of controlling the degradation kinetics of the alloy at a rate comparable to the growth

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rate of the host tissue (bone). To achieve this goal, coatings consisting of one or more layers made up of oxide obtained by PEO with appropriate chemical compounds added were used. The results obtained showed that it is possible to design coatings that can control the degradation kinetics of the substrate.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

DICMAPI's Materials Surface Treatment Laboratory is equipped with modern apparatus for the modification and characterisation of materials' surfaces, such as: temperature-controlled electrochemical cells, DC 600V/5.5A voltage/current generator, AC 600V/5.5A with programmable duty cycle voltage/current generator, digital microscope, SEM scanning electron microscope with EDX and EBDS probe, Pt target metalliser for specimens (SEM), metallographic cut-off machine, automatic lapping machine, DC and AC potentiostats/galvanostats, Electrochemical Interface for EIS, electrometers, magnetic induction (Fe) & eddy current (NFe) thickness gauges, pull-off adhesion tester, automatic contact angle meter, differential scanning calorimeter (DSC), micro-Ohmmeter for surface electrical resistance measurements.

Collaborations with IPCB- CNR Pozzuoli, University of Manchester and Biocera Medical Limited (UK).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

As part of the PhD student's activities, a research period at Biocera Medical Limited (UK) is planned.

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PhD Project Proposal

Proponent: Prof. Tullio Monetta

Proposed research topic:

Low environmental impact processes for recovering precious metals from waste electrical and electronic equipment (WEEE)

Reference curriculum:

Materials and Structural Engineering
Design of Sustainable and Safe Products and Processes

Summary of the Research Project

Conventional methods to recovery waste electrical and electronic equipment are pyrometallurgical, hydrometallurgical or a combination thereof, which can only be applied downstream of treatment with physical-mechanical methods. Hydrometallurgical treatments involve the use of organic solvents or strong acids in which the metals are dissolved and can subsequently be recovered chemically or electrochemically. Pyrometallurgy uses very high temperature treatments. These processes have a very high environmental impact.

Recently, the use of solvometallurgical processes based on 'Deep Eutectic Solvents' (DES) is being experimented. DES are systems formed from an eutectic mixture of Lewis or Brønsted acids and bases, they can be 'designed' to obtain selective solvents. DES exhibit low vapour pressure and non-flammability. From a toxicological point of view, DES constituents are well characterised and not harmful to humans and animals. Solvometallurgical processes based on DES therefore have a low environmental impact.

This research project involves the leaching of gold and silver from WEEE using DES solutions. In the preparatory phase, gold and silver samples will be used to determine the kinetics of the dissolution process, into the test solution, as the operating parameters governing the process change, such as: bath temperature, solution agitation speed, process duration, etc.. In relation to these, the need to add oxidising substances to the test solution to increase the kinetics of the process will be assessed. Plasma mass spectrometry (ICP-MS) will be used to assess the concentration of metals in solution. This will make it possible to close the mass balance of the materials used and define the theoretical yield of the leaching process.

The recovery of dissolved metals in DES will be carried out using electrochemical deposition processes using the same solvent. The deposition window to be used for the reduction, at the cathode surface, of the cations dissolved in solution will be determined using Cyclic Voltammetry (CV). The study of the oxidation and reduction potentials of the individual species in the test solution will be conducted using a test solution made of AuCl and/or AgCl at a concentration of 0.05M or the maximum obtainable as determined by the leaching tests. The scanning speed will be varied between 10 and 100 mV/s. Once the deposition windows of the various elements have been defined, it will be possible to proceed with the recovery of the dissolved metals in solution using the solutions obtained from the leaching of the WEEE in DES. After this step, the purity of the metals deposited at the cathode can be assessed, the kinetics of the process can be evaluated, and the amount of energy used can be estimated as a function of the bath temperature, the stirring speed of the solution in the electrolysis cell, and the interelectrode distance.

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Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

DICMAPI's Materials Surface Treatment Laboratory is equipped with modern apparatus for the modification and characterisation of materials' surfaces, such as: temperature-controlled electrochemical cells, DC 600V/5.5A voltage/current generator, AC 600V/5.5A with programmable duty cycle voltage/current generator, digital microscope, SEM scanning electron microscope with EDX and EBDS probe, Pt target metalliser for specimens (SEM), metallographic cut-off machine, automatic lapping machine, DC and AC potentiostats/galvanostats, Electrochemical Interface for EIS, electrometers, magnetic induction (Fe) & eddy current (NFe) thickness gauges, pull-off adhesion tester, automatic contact angle meter, differential scanning calorimeter (DSC), micro-Ohmmeter for surface electrical resistance measurements.

Collaborations with Politecnico di Milano and the University of Leuven (Nederland).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

As part of the PhD student's activities, a research period at University of Leuven (Nederland).

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PhD Project Proposal

Proponent:

Prof. Teresa Murino

Proposed research topic: Sviluppo di modelli e soluzioni innovative per l'applicazione e l'ottimizzazione di problemi di packaging in ottica di Lean Manufacturing combinata a processi di "Industria 4.0"

Reference curriculum:

Tecnologie e sistemi di produzione

Progettazione di prodotti e processi sostenibili e sicuri

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

Lean Manufacturing, or Lean Production, is a business management methodology focused on eliminating waste and optimising processes to generate value for the customer. Based on Japanese manufacturing techniques, the Lean philosophy has become a global practice that has proven its effectiveness in improving business efficiency. Lean techniques are not limited to production, but affect every aspect of the company, from the supply chain to human resource management, improving working conditions, reducing stress and promoting teamwork and continuous improvement. At the same time, bin-packing problems represent a complex optimisation challenge, which require in-depth studies in order to aim for an increasingly lean and optimised management of industrial production. A subcategory of these problems is the 3D Bin Packing problem, which consist of placing three-dimensional objects in bins as efficiently as possible. The project in question involves the study of innovative solution methods to the proposed problem, which can aim to optimise industrial production in terms of both processes and sustainability. The study of these problems also extends to areas such as logistics, which problems involve optimising the load on means of transport in order to better manage all stages of product delivery. By minimising the number of containers and thus the number of vehicles required to transport goods, companies can reduce shipping costs and the number of vehicles required to transport goods, and reduce emissions.

Activities Program

- Literature study of Lean Manufacturing principles and currently used technologies.
- Study of technologies for solving one-dimensional, two-dimensional and three[1]dimensional bin packing problems.
- Study of the application of these technologies in the literature and their impact in terms of industrial and sustainable optimisation.
- Development of Hybrid Models: Integrating Lean techniques with heuristic and meta[1]heuristic approaches for 3D-BPP. This will include the creation of mathematical models that combine Lean waste reduction with optimal packing strategies.

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- **Experimentation and Validation:** Conduct experiments on real and simulated datasets to test the effectiveness of the developed hybrid models. Performance will be evaluated in terms of waste reduction, packing efficiency and calculation time.
 - **Dynamic Optimisation:** Apply the principles of Lean continuous improvement to 3D-BPP models, constantly refining the algorithms based on feedback and experimental results.
 - **Waste Reduction:** Combining Lean principles with 3D-BPP optimisation techniques to minimise waste of space and resources in logistics and production processes.
 - **Sustainability:** Promoting sustainable practices by reducing waste and optimising the use of resources, with a positive impact both economically and environmentally.
 - **Continuous Improvement:** Implement a continuous improvement cycle that allows 3D[1]BPP solutions to be constantly adapted and refined in response to new needs and data.
 - **Research in an International Framework:** Collaborate with institutions and companies globally to share knowledge, methodologies and results. This international approach will foster the development of innovative and scalable solutions applicable in different cultural and industrial contexts. International collaboration will be important for the success of the project, allowing global best practices to be exploited and adapted to specific research and business contexts.
- Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic. The PhD student could have access to operational and scientific facilities to carry out the proposed activity. Equipment and software, specialised in optimisation and lean manufacturing, may be available. In particular, the software used will include Python, Matlab and C++, which are fundamental for developing and testing optimisation algorithms. The project could also benefit from collaborations with Italian and foreign research institutions, as well as with companies in the logistics and manufacturing sector.
- Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....) The research project includes a six-month period abroad for the PhD student at a prestigious international university. During this period, the PhD student will collaborate with a research group specialising in optimisation and lean production. This experience will allow the student to deepen his or her knowledge of Lean Manufacturing techniques and three-dimensional packaging problem solving, benefiting from the advanced scientific and operational resources of the host institution

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PhD Project Proposal

Proponent:

Paolo A. Netti -IIT

Proposed research topic:

Cell mechanoprogramming

Reference curriculum:

Materials and Structural Engineering

Chemical engineering

Technologies and Production Systems

Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The project aims at developing cell-mechanomodulator chips capable to coherently control and tune the mechanical identity of tens of thousands cells seeded on their surface. Cell mechanomodulator chips are indented to provide a valuable tool to study and disclose the underpinning mechanism of cell mechanobiology and to provide a viable platform to administer in a highly controlled manner mechanomedicine doses. Mechanomodulator chips operate the control of the cell transcription activity by regulating the direction and the intensity of cytoskeleton forces acting on the nuclear envelop. As consequence, a control of nuclear shape is possible that, in turn, induces selective chromatin deformation thus regulating cell genetic expression.

The ultimate goal is engineering materials surfaces and devices to modulate and coherently control the cell nuclear shape and therefore the 3D chromatin structural organization. The mechanomodulator chips will be realized to generate a distinctive nuclear shape library spanning from prolate to oblate. Starting from these quasi-static nuclear shape, a dynamic stretcher will be used to scan through a full library of tens of thousands generated nuclear shapes while acquiring the intensity and distribution of cytoskeleton forces, nuclear deformation, chromatin condensation and gene expression. These data will be used to define the role of mechanical stretching on the distribution and compaction of heterochromatin regions and their degree of transcription. It is indented to generate specific domain Knowledge Graph whose (causal chain) connection will be scouted then used to generate a general mechano-modulation Knowledge Graph acting as a learning framework for the development of an Intelligent Data Analysis System. The deriving AI model will enable to identify the optimal mechanical trail dosage to manipulate/control the degree of expression of selected gene sequences.

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The main expected results will be (a) to disclose the functional relationship between nuclear stretch and genetic expression; (b) provide technology for assessing for the first time mechano-medicine dose response – drawing the limit between mechanotoxicity and mechanotherapy; provide the fundamental to develop a novel mechanoprogramming technology.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The PhD work will be carried out at the Centre for Advanced Biomaterials for Health Care of the Italian Institute of Technology in Naples. The center is equipped with cutting-edge instrumentation enabling synthesis, micro and nano-fabrication and characterization of material platforms and microfluidic devices, along with state-of-art cell culture facilities for in vitro testing and organotypic tissue fabrication. Furthermore, the laboratory include microscopy and spectral microscopy facilities for cell and material imaging and cell-material interface characterization.

Collaboration with national and international laboratories are foreseen including prof. Giancarlo Ruocco, University of Rome, Prof. Francesco Nicassio, IIT Milan, Prof. Stefano Piccolo, University of Padua.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A period abroad of at least 6 months will be programmed.

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Ciclo XL

PhD Project Proposal

Proponent:

Paolo A. Netti -IIT

Proposed research topic:

Cancer mechanobiology

Reference curriculum:

Materials and Structural Engineering

Chemical engineering

Technologies and Production Systems

Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

In the context of cancer mechanobiology, a large body of knowledge is continuously growing providing a better comprehension of the role of the local mechanical microenvironment as a co-conspirator of the onset of cancer cells transformation and tumor progression. It is now appreciated that, during tumor growth, morpho-physical features of cells Extracellular Matrix (ECM) are altered, and these alterations result into a departure from the homeostatic cell-ECM mechanical equilibrium towards a new status characterized by an increased stiffness of the cell microenvironment. The tissues affected by malignant tumors are characterized by ECM accumulation, that leads to a severe fibrotic response, known as desmoplasia, and consequent tumor stiffening. Furthermore, the degree of stiffened tumor mechanical microenvironment (TMME) appears to be correlated with very important pathways associated with the cell malignant transformation. The stiffening process occurring at the level of the TMME appear to promote the invasive nature of tumor cells through the activation of specific molecular pathways. In this regard, three recent experimental evidences are worth to be taken into account: (a) only a coordinated interplay between oncogene-mediated transformation and changes in the rigidity of the microenvironment can power up the process of tumorigenesis; (b) a growing body of evidence indicates that the TMME can instruct tumor cells to undergo an even more profound reprogramming, termed epithelial-mesenchymal transition (EMT), that makes the cell more motile and able to invade and metastasize; and (c) tumor cells are characterized by a less structured cytoskeleton, lower mechanical and cyto-adhesive properties compared to their physiological counterpart (ie, healthy cells). These evidences enlighten the pivotal role of TMME in mediating tumor cell transformation state and call for systematic approach to disclose the collaborative and synergistic interaction between cells and ECM, and its role in cancer development and progression.

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The unveiling of the intricate reciprocal relationship between TMME and tumor cell status and stage, is the main objective of this doctoral proposal.

To unveil the dynamic and reciprocal relationship between mechanical microenvironment and tumor cell status and stage, the proposal aims to construct a **cell-TMME mechanoscore diagram** for lung adenocarcinoma. It is intended to represent, in an instructive graphical tool, the cell departure from a normal/physiological state of the lung under different TMME conditions. In particular, a three-dimensional (3D) graph will be designed to describe the correlations between TMME and the activation of a tumor cell condition: the graph will show the TMME condition (mechanical and structural composition), as independent variable, on the first axis (TMME axis), the cell cytoskeleton mechano-phenotype on the second one and known mechanobiology transcriptional factors activation, as parameter to designate the oncogenic activation of a tumor cell condition, on the third one. This graph will delineate the existing relationship between cell and tissue mechanical properties and its effects on cell oncogenetic mechano-reprogramming process. The construction of cell-TMME mechanoscore diagrams will provide a new quantitative approach for tumor diagnosis and prognosis, along with useful clinical therapeutic tools. Specifically, by assessing the mechanical status of cells and their microenvironment in response to classical therapeutic approaches, such as chemotherapy and radiotherapy, it could provide new and complementary information for the optimization of the treatments and their therapeutic outcome. The definition of the cell-TMME mechanoscore diagram, will help to elucidate the behavior of lung adenocarcinoma cells in relationship to their TMME, and unveil its potentiality as a diagnostic and/or prognostic and /or therapeutic tool.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The PhD work will be carried out at the Centre for Advanced Biomaterials for Health Care of the Italian Institute of Technology in Naples. The center is equipped with cutting-edge instrumentation enabling synthesis, micro and nano-fabrication and characterization of material platforms and microfluidic devices, along with state-of-art cell culture facilities for in vitro testing and organotypic tissue fabrication. Furthermore, the laboratory include microscopy and spectral microscopy facilities for cell and material imaging and cell-material interface characterization.

Collaboration with national and international laboratories are foreseen including prof. Paolo Decuzzi University of Stanford, Prof. Stefano Piccolo, University of Padua..

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A period abroad of at least 6 months will be programmed.

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PhD Project Proposal

Proponente: Paolo Netti/Francesco Urciulo

Tematica di ricerca proposta: Tissue fibrosis on Chip

Curriculum di riferimento:

Ingegneria dei Materiali e delle Strutture

Ingegneria chimica

Tecnologie e sistemi di produzione

Progettazione di prodotti e processi sostenibili e sicuri

Sintesi del Progetto di Ricerca (stato dell'arte, breve programma previsto per le attività e obiettivi)

Impaired tissue repair processes in humans are associated with either the formation of fibrotic tissue or non-healing processes. Fibrosis are often associated with an inflammatory state that generally influences the nature, the composition the amount and the superstructure of the de-novo synthesized extracellular matrix (ECM). Inflammatory state associated with both pathologic status (e.g. hepatic cirrhosis, chronic obstructive pulmonary diseases, intestinal bowel diseases, tumors) and deep skin wounds generally induces a the formation of fibrotic tissue characterized by a denser packing of fibrillar component of the ECM with an enhanced stiffness and reduced hydration degree. This anomalous assembly induces formation of fibrotic ECM in the connective compartment, which strongly compromises functionality of the affected. Fibrotic tissue in lung can compromise its elasticity and impair the functions of cells involved in gas exchange. Fibrosis in liver compromises metabolism, immunity regulation, digestion, detoxification and vitamin storage. Sever scarring of the human skin induces impaired thermoregulation, sensitization, limbs mobility and critical aesthetical issues. metabolism, immunity, digestion, detoxification, and vitamin storage. In diabetic patients, on the contrary, the inflammation status induce the formation of chronic wound as cells loss the capability to synthesize and assemble the components of the ECM. It is widely accepted that dysfunctional tissue repair process are a consequence of an aberrant/compromised immune and response which governs both he fibrotic response and non-healing phenomena. This still represent a clinical and social issue and makes the mechanistic and molecular understanding of repairing mechanisms a very actual need. Recently, three-dimensional (3D) models have revolutionized our ability to study these processes in a controlled context, allowing the cultivation of fibroblasts and other cells in a 3D matrix that better simulates the native environment. However, most currently available 3D models lack both extracellular matrix, vascularity, and immune response limiting their ability to faithfully replicate dynamic of wound healing. This deficiency is particularly significant in

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the context of pathological conditions, which drastically compromise the immune reaction. Starting from the expertise of the proponent group in the field of tissue engineering, biomaterials and tissue-on-chip systems, this project proposal aims at realizing an immunocompetent 3D model of skin-on-chip able to recreate the interactions between tissue repairing mechanisms and immune system under both normal and pathological conditions. In particular the main tasks can be summarized as follows: i) fabricating a wounded immune competent tissue on chip model using advanced bio fabrication techniques (e.g. modular tissue engineering / 3D bioprinting approaches; ii) modelling the pathological conditions on chip by integrating immune cells from normal and non-healthy patients; iii) use of advanced characterization such as omics-based techniques. This will pave the way for to better elucidate key pathways involved in impaired healing under different conditions and will speed up the development of new treatments in a personalized manner.

Informazioni sintetiche relative a: strutture operative e scientifiche (attrezzature, software, laboratori,...) a disposizione del dottorando per lo svolgimento dell'attività proposta, collaborazioni con altri enti di ricerca italiani ed esteri (eventualmente anche con aziende) potenzialmente rilevanti alla tematica proposta.

The research activity will take place at Interdepartmental Research Center on Biomaterials (CRIB) and Department of Chemical, Materials and Production Engineering (DICMAPI) at University of Naples Federico II. The project will be carried out in collaboration with other research centers such as Istituto Italiano di Tecnologia, and Scuola di Meicina e Chirurgia – Federico II.

Available instrumentation and facilities comprise: advanced bioreactors for 3D tissue culture, 3D cell culture lab, 3D printing and 3D bioprinting systems, microfabrication machines, histological, mechanical and rheological characterization of biomaterials and biological tissues, confocal and multiphoton microscopy, fluid dynamic and mechanical computation.

Informazioni sintetiche relative ad eventuale periodo all'estero previsto per il dottorando (periodo, gruppo di ricerca, Università, ente di Ricerca....)

A period abroad of at least 6 months will be programmed.

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PhD Project Proposal

Proponente: Francesco Urciuolo and Paolo Netti

Tematica di ricerca proposta: Muscle on Chip

Curriculum di riferimento:

Ingegneria dei Materiali e delle Strutture

Sintesi del Progetto di Ricerca (stato dell'arte, breve programma previsto per le attività e obiettivi) max 500 parole

Engineered skeletal muscles have the potential to revolutionize medical robotics (i.e. advanced prosthetic systems) by acting as living actuators. In the field of medical and soft robotics the actuation is a critical step and, nowadays, different working principles can be exploited to mimic the actuation capability of skeletal muscles such as hydraulic-, pneumatic-, piezoelectric-, electromagnetic-, shape memory alloys-, twisted and coiled polymer- muscles. Such systems allow miniaturization, integration and actuation, but still possess different drawbacks. Electromagnetic-based systems, for instance, are heavy and do not guarantee large contractile strokes; pneumatic and hydraulic actuators, require cumbersome actuation systems, whereas electroactive polymers need large voltages.

Based on the consolidated expertise of the proponent groups in the tissue engineering field, microfabrication, organ on chip and 3D bioprinting, this project aims at realizing a muscle-on-chip system able to elucidate the mechanisms of muscle regeneration, contraction and actuation. The final goal of the project would be the development of living actuator based on the skeletal muscle logic. To achieve this, a tissue-on-chip system, that integrates engineered muscle with stimulation system and either kinematic and/or deformable elements, would be built. This system would allow to study and monitor muscle tissue development and functions (i.e. twitch / tetanic force) under several stimulation conditions. As the engineered muscle still feature different limitations such as (i) small value of the output force (in the order of 10 mN) (ii) high metabolic request hampering long lasting in vitro cultures and (iii) difficulties in modulating and controlling the contraction, the project aims at developing new strategies and devices to increase and to control the force contraction and to overcome metabolic constraints.

This project aims at integrating different approaches such as engineering optimal biomaterials formulation, bio fabrication techniques (e.g. 3D bioprinting) and cell culture conditions as well. Force modulation can be obtained by exploiting different techniques, to evoke muscle contraction on chip such as the use electroactive systems capable to generate local action potential under different "wireless" stimulation. The full "-on chip" system composed by engineered muscle, stimulation/modulation systems and force collection will represent a powerful tool to better

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understand the mechanism of muscle contraction/modulation for the development of a new class of actuation systems for soft robotics.

Finally, such project has the potential to contribute to the improvement of quality of life of people suffering of musculoskeletal disorder. By using pathological muscle cells the developed system can be used as a flexible and potent platform to replicate and study severe pathologies impacting on force generation and control such as sarcopenia and dystrophy. This will contribute to advancements in personalized and precision medicine to significantly improve both diagnostic and therapeutic strategies.

Informazioni sintetiche relative a: strutture operative e scientifiche (attrezzature, software, laboratori,...) a disposizione del dottorando per lo svolgimento dell'attività proposta, collaborazioni con altri enti di ricerca italiani ed esteri (eventualmente anche con aziende) potenzialmente rilevanti alla tematica proposta.

The research activity will take place at Interdepartmental Research Center on Biomaterials (CRIB) and Department of Chemical, Materials and Production Engineering (DICMAPI) at University of Naples Federico II. The project will be carried out in collaboration with other research centers such as Istituto Italiano di Tecnologia, CNR-Nanotech and Università Campus Biomedico di Roma (UCBM).

Available instrumentation and facilities comprise: advanced bioreactors for 3D tissue culture, 3D cell culture lab, 3D printing and 3D bioprinting systems, microfabrication machines, histological, mechanical and rheological characterization of biomaterials and biological tissues, confocal and multiphoton microscopy, fluid dynamic and mechanical computation.

Informazioni sintetiche relative ad eventuale periodo all'estero previsto per il dottorando (periodo, gruppo di ricerca, Università, ente di Ricerca....)

A period abroad of at least 6 months will be programmed.

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PhD Project Proposal
D.M. n. 630 del 24.04.2024

Proponent:

Roberto Nigro
I.T.P. Innovation & Technology Provider Srl

Proposed research topic:

Development of innovative techniques for the extraction and concentration of plant exosomes

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

Exosomes are one of the classes of so-called extracellular vesicles, measuring between 20 and 150 nm, released by cells into the surrounding environment. They contain a variety of biological molecules, including proteins, lipids, metabolites, miRNAs, RNA, and DNA. Initially considered cellular waste, exosomes have attracted the attention of biomedical research in recent years due to their multiple functions and potential applications. Thanks to their complement of surface proteins, loading capacity, and stability, exosomes are very efficient extracellular messengers capable of transferring genetic and molecular information between cells, thus influencing various biological and pathological processes. They regulate inflammation, modulate the immune response, and promote tissue repair. Current knowledge also suggests their use in diagnostics as biomarkers of specific pathological processes, including tumors, and in therapy as vehicles for the targeted delivery of drugs, miRNAs, or other molecules.

Plant exosomes, with their similar morphology and structure to animal exosomes, offer a unique potential for therapeutic and nutraceutical purposes. In addition to the components found in animal exosomes, they also contain secondary metabolites exclusive to plants. These metabolites possess peculiar biochemical properties, such as antioxidants, which can be harnessed for therapeutic and nutraceutical applications, opening up a new frontier in biomedical research.

The availability of exosomes from plant sources, produced in a controlled and reproducible way, paves the way for new nanotherapeutic platforms. These platforms can be used in a wide range of applications, from aesthetic and regenerative medicine to the treatment of inflammatory states linked to various pathologies. They also hold promise for the development of new drugs. This innovative tool has the potential to significantly impact human health and improve the quality of life, inspiring a new wave of research and development in the field of biomedical science.

However, the purification of plant exosomes is a complex process due to their low concentration in cellular fluids and the presence of contaminants. It, therefore, requires developing sophisticated techniques and methodologies, generally based on very high-speed ultracentrifugation processes and repeated ultracentrifugations, which make the separation and concentration of such nanovesicles very expensive and challenging. The project aims to develop an innovative technology

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based on refrigerant fluids in the liquid phase, allowing the extraction and classification of plant exosomes contained in plant species with high biological functionality.

The general program of the research project is as follows:

1st year: Study of the impact of refrigerant fluids on the chemical, physical, and biological characteristics of exosomes. Preliminary definition of extraction and concentration conditions;

2nd year: Design and development of a lab-scale system. extraction, concentration, and classification of exosomes;

3rd Year: Scale-up of the process developed in the second year.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The company makes available to the research:

N° 2 lab-scale extraction units;

N° 1 Agilent 1200 HPLC with UV and ELS detector;

N°1 Agilent 7850 GC

N° 1 Freeze Dryer

N° 1 laboratory for chemical and physical analyses;

N° 1 centrifuge (18,000g) at controlled temperature

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A research period abroad is planned at the WUR in Wageningen (NL), where it will be possible to delve deeper into the physical and biochemical interaction between exosomes and refrigerant fluids.

They are expected to stay abroad for between 3 and 6 months, locating between the second and third years of PhD activity.

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PhD Project Proposal

Proponent:

I.T.P. Innovation & Technology Provider Srl

Proposed research topic:

Biotechnological upcycling of wasted Spent Coffee Ground

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

The primary goal of this innovative project is to develop a novel postbiotic ingredient, rich in LA (linoleic acid) and CLA (linoleic acid conjugates), both of which are known for their anti-obesity and anti-cancer properties. Postbiotics, a cutting-edge category of functional ingredients, are derived from probiotics through specific inactivation processes. By fermenting spent coffee (SCG) with specific lactic microorganisms, we can convert the LA load of the SCG into CLA, significantly enhancing the functionality of the recovered material and making it particularly effective against the aforementioned diseases.

The dry postbiotic product, derived from exhausted SCG (from various processes) and enriched with high concentrations of CLA, holds significant potential as an ingredient in formulations across the food, nutraceutical, cosmetic, and pharmaceutical sectors.

The general program of the research project is as follows:

1st year: definition of the waste materials to be used and the microorganisms suitable for the conversion of LA into CLA;

2nd year: development of the fermentation protocol and the inactivation and drying processes of the fermented matrix. Lab scale tests and characterization of the fermented and functional elements in the wet and dry postbiotic. Determination of the biological effect of the postbiotic using 2D cellular models

3rd Year: Scale-up of the postbiotic production process developed in the 2nd year. Determination of the biological effect of the postbiotic produced on a pilot scale.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The company makes available to the business:

N° 2 laboratory-scale fermentation stations with 1 and 2-liter stirred reactors,

N° 2 systems for treatment and thermal inactivation of the fermented product

N° 1 Spray Dryer of 2lt/h equipped with a 1lt stirred fermentation reactor;

N° 1 Agilent 1200 HPLC with UV and ELS detector;

N°1 Agilent 7850 GC

N° 1 Freeze Dryer

N° 1 microbiology laboratory for the characterization of the fermented products produced.

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N°1 Pilot plant for the in-line production of postbiotics starting from fermented matrices consisting of a 200 lt fermenter, 1 sterilizer, and 1 15 lt/h Spray Dryer

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

A research period abroad is planned at the KraftHeinz R&D Center in Nijmegen (NL). This is a significant opportunity as it will allow us to utilize the 200 liter pilot scale fermentation plant and a 15 liter/h spray dryer, which are crucial for obtaining postbiotic powders. These powders, when scaled up, have the potential to make a substantial impact on our research, developed at the company's laboratories and at the DICMAPI-University of Naples Federico II.

A stay abroad of between 3 and 6 months is expected.

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PhD Project Proposal

Proponent:

Rossana Pasquino

Proposed research topic:

Hydrogel fibers as optical waveguides in human tissues

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

Solid-state optics has been one of the pillars of modern digital age. Conventional optical fibers are generally fabricated by drawing silica glass, crystals, and plastics. They are all much stiffer than biological tissues and have low bio-compatibility and bio-degradability, which can cause damage to the surrounding biological environment, thus limiting their applications in tissue engineering. Integrating soft hydrogel materials with micro/nano-optics will expand the horizons of photonics for bioengineering. The idea is to implement light-based therapies in the clinic, patient-friendly devices that can deliver light inside the body while offering tunable properties and by mimicking the mechanical properties of the interested tissue.

The project deals with the formulation of biocompatible hydrogels and with the production of hydrogel-based optical waveguides (mono or multilayers) used as multifunctional platform (actuators, detectors, skeleton for cells growth, biophotonics active biomaterials) for investigating and manipulating photochemical, biological and optogenetic processes in close-to-physiological environments. The high-water content environments guarantee a low refractive index and a good optical match for releasing light into tissues. Physical and chemical hydrogels will be designed, based on data already available in the literature. Natural polysaccharides will be involved, as well as proteins and synthetic biocompatible polymers (e.g. Pluronics, Polyethyleneglycol etc). Chemical or physical processes will be used to create the desired gel properties, with mechanical properties tunable within a tissue-compatible range. Rheology, scattering and calorimetry will be used to characterize both the transitions from a sol to a gel state, as well as the final properties of the gel structure.

For the production of the hydrogel/based fibers, two approaches will be pursued: 3D printing and microfluidic fabrication. The 3D printing is an accomplished - widely studied - process to create long hydrogel fibers, in which their shape and dimension are controlled by the design of the nozzle and can be easily tunable. To create more complex designs, such as a multi-core system for multi-wavelength delivery or duplex communication, microfluidic fabrication is another option. The shape and arrangement of the microcapillaries will guide the final fiber structure, providing various geometries, including single-fibril, hollow-tube, and double-walled fibers.

Finally, the optical delivery performances will be also evaluated by using green and red laser lights, and in vitro performances analyzed through drug release studies and light interaction with living cells.

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In conclusion, the Phd final aim is to formulate and produce innovative fibers for advances in biomaterial-based photonics and biosensing platforms.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The PhD student will use the laboratories and the instruments already available at DICMaPI. The necessary equipment for the formulation and characterization of the hydrogel-based optical fibers is already available, as well as a bioprinter for the 3D production of a one-core fiber. The microfluidic device, and/or suitable add-ons to the 3D printer, will be developed by the PhD student for the creation of multiwall optical soft fibers. The PhD will be run in collaboration with Prof. Andrea Cusano, Università degli Studi del Sannio. He is well known as an expert in the development of innovative optical sensing systems. A research agreement between our department and the Engineering Department of Università degli Studi del Sannio is already in place. The laboratories in Benevento will be available to study the optoelectronics performances of the produced fibers, to host cellular and molecular experiments, to set up biophotonics investigations devoted to assess drug uptake, cells proliferation, light assisted dose-response. The PhD student will take advantage from the advanced labs of the Regional Research Infrastructure "Optoelectronics and Nanophotonics Center for Human Health", recently established in Benevento and in tight connection with the University of Sannio and the group coordinated by Prof. Andrea Cusano (<https://www.cerict-cnos.it/>).

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The PhD student will probably spend part of his/her project at the Okinawa Institute of Science and Technology (OIST), Micro/Bio/Nanofluidics Unit, during the last 18 months of the Phd period (at least 6 months abroad). There, Prof. Amy Shen and Dr. Vincenzo Calabrese, experts in microfluidics, are available to host her/him for the planned time period.

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PhD Project Proposal

Proponent: Domenico Pirozzi

Proposed research topic: Development of advanced adsorbent materials for the removal of recalcitrant pollutants from wastewaters

Reference curriculum: Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

Recalcitrant pollutants are chemical substances that can persist in the environment for long periods and eventually accumulate in the tissues of living organisms, causing potential risks to human health and the ecosystem.

This project is aimed at the development of adsorbents based on the use of nanosponges of cyclodextrins, nanostructured polymers which have particular "cage" structures that can easily trap a wide spectrum of organic and inorganic substances.

These complexing properties of nanosponges can be exploited in the capture and removal of pollutants present in wastewater, but also for the immobilization of biomolecules. Consequently, in order to make the removal of pollutants more effective, enzymes capable of degrading pollutants will be immobilized on the nanosponges (for example laccases which are able to degrade different classes of antibiotics). In this way the pollutants are captured by the nanosponges and then degraded by the enzymes immobilized within the nanosponges themselves, making the wastewater purification process more efficient.

In the second part of the research, based on the results obtained, a continuous laboratory-scale purification plant will be designed and built.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

This research activity is carried out in collaboration with the University of Coimbra (Portugal), with the Department of Agriculture of the Federico II University and with the Agri-food Cluster of the Emilia-Romagna region.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The PhD student will spend a period of 6 months at the University of Coimbra or other European universities.

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PhD Project Proposal

Proponent: Russo Danilo

Proposed research topic: Safe hydrogen storage in aqueous formate/bicarbonate

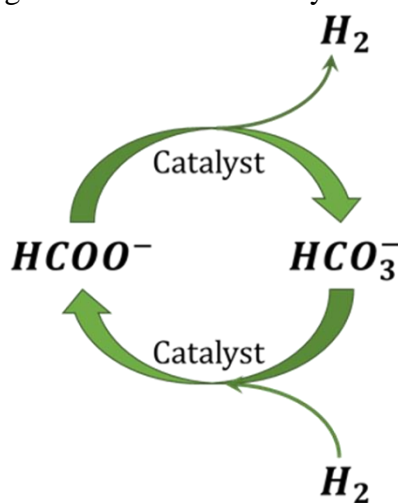
Reference curriculum:

Chemical engineering

Design of Sustainable and Safe Products and Processes

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The project aims at developing catalytic systems for the interconversion of aqueous formate/bicarbonate for hydrogen release and uptake. The system was recently proposed in the literature [1], showing potentialities of the state of the art. The catalytic reaction is shown in the figure. Thermodynamic assessment showed that the equilibrium reaction can be easily shifted by working at near-ambient conditions, i.e. 20 – 90 °C, 1 – 20 atm [2]. This, alongside the presence of water and non-toxic salts, makes the system intrinsically safer both under normal operating conditions and accidental process deviations [3]. Therefore, the system is of great interest with respect to traditional storage at high pressure or cryogenic conditions, as well as to innovative material-based storage, often requiring a complex thermal management and/or limited cyclability.



State-of-the-art catalytic systems [1] are palladium-based on carbonaceous or semiconductor materials. Catalysts preparation proposed are highly energy-consuming (pyrolysis, high temperature treatment) or require toxic materials (wet impregnation followed by chemical reduction). Volumetric energy density depends critically on salt concentration, and it can be comparable with high-pressure or cryogenic storage if supersaturated solutions are employed. Up to date, supersaturated solutions are not investigated in the literature.

On this basis, this project has the following objectives:

- Investigate different preparation techniques and active phase compositions, including transition metals in the palladium matrix, to improve activity and reduce costs.
- Test catalysts and their cyclability for aqueous formate dehydrogenation and bicarbonate hydrogenation, investigating the effect of operating conditions and the relation between morphology, preparation and activity
- Investigate the adoption of supersaturated solutions to increase volumetric energy density.

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To achieve these objectives, activities will be organized as follows:

- Year 1: literature review integration. Synthesis of catalysts changing composition of the active phase and hydrogenation/dehydrogenation tests.
- Year 2: for the most promising identified catalysts investigate the effect of process conditions: catalyst load, salt concentration, temperature, pressure, pH. Recovery and cyclability tests will be carried out. Pre- and post- reaction characterization will show the relation between preparation, morphology and activity.
- Year 3: completion of the activities, process condition optimization, kinetic modeling, thesis writing.

[1] Calabrese et al., Renewable and Sustainable Energy Reviews 173 (2023) 113102

[2] Russo et al., International Journal of Hydrogen Energy 47 (2022), 31370 - 31380

[3] Russo et al., International Journal of Hydrogen Energy 65, 2024, 421 - 427

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

DICMaPI research groups were already involved in preliminary investigations of this system and can provide the necessary pieces of equipment. Specifically:

- Thermo-regulated glass reactors for ambient pressure tests
- Fumehoods and reactants for catalysts synthesis
- Reactors for the safe pressurization of hydrogen. With regard to this, an agreement being defined between the proposing members of the DICMaPI and Saipem SPA, scheduled the purchase of another batch reactor for hydrogen pressurization (reduce volume 160 mL), that will be completely dedicated to the project. (Purchase scheduled by the end of 2024).
- Analytics: HPLC, GC
- Collaborations with other research groups within the department and with foreign universities (Khalifa University - United Arab Emirates) will ensure access to characterization techniques such as SEM, TEM, XRD, TPR, TPD, FTIR.

Modeling will be carried out by available softwares Matlab and Aspen Plus.

Moreover, the agreement being defined with Saipem SPA, will allow further development in the study of the proposed system also for different industrial purposes, with a focus on economic and life cycle assessment of the proposed technology. This agreement will also allow the Ph.D. student to spend a period of time in the company, acquiring new skills.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

Preferably, a 6 months period abroad will be spent in other European research groups working on similar topics and having available the necessary infrastructure. Specifically, a potential collaborating Institution may be:

- Fau: Friedrich-Alexander-Universität-Erlangen-Nürnberg, Germany, for their specific know-how and infrastructure in the field of liquid hydrogen carriers.

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PhD Project Proposal

Proponent:

FABRIZIO SCALA

Proposed research topic:

REDUCTION OF ILMENITE IN FLUIDIZED BED FOR THE PRODUCTION OF GASEOUS OXYGEN IN A LUNAR ENVIRONMENT

Reference curriculum:

CHEMICAL ENGINEERING

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

As part of a collaboration between the Department of Chemical, Materials and Industrial Production Engineering (DICMaPI) and the Italian Center for Aerospace Research (CIRA), an experimental research activity on Technologies for Space Exploration is being launched which concerns ISRU (In-situ Resource Utilization) chemical/physical processes, i.e. the exploitation of material and energy resources present on site in extra-terrestrial environments such as on the Moon.

In particular, the research activity focuses on the production of oxygen gas (for the life support of a possible stable inhabited base on the Moon) through a high-temperature hydrogen reduction process of ilmenite (derived from lunar rocks) using the technology of fluidized bed reactors, followed by the electrolysis of the water generated by the reduction reaction.

The thesis will consist of the experimental study on a laboratory scale of the ilmenite reduction process in a fluidized bed, aimed at the "proof of concept" and the optimization of the operating conditions. The experimental study will be accompanied by modeling of the entire process using the AspenPlus software.

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Numerous fluidized bed reactors ranging from laboratory scale to pilot scale are available in the laboratory, as well as appropriate auxiliary equipment for the characterization of gaseous and solid flows. In particular, in the proposed activity a laboratory-scale fluidized bed apparatus will be used. The activity will be carried out in collaboration with the Italian Center for Aerospace Research (CIRA) which has guaranteed possible co-financing, as part of the Innovative Doctorates co-financed by Companies/Research Institutions.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution.)

During the PhD, a stay of 3-6 months will be required at a foreign research laboratory to be defined, most likely at the end of the 2nd year or at the beginning of the 3rd year.

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PhD Project Proposal

Proponent:

Fabrizio Scala (DICMaPI-UNINA) - Mariarosaria de Joannon Ceglia (CNR-STEMS)

Proposed research topic:

Integrated carbon dioxide and nitrogen cycles for the GHG emission mitigation and the energy and material recovery.

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

In the swiftly change scenario of the energy transition, the main objective is to maximize the energy sources while keeping the goal of the net zero emission target. The proposed research topic is part of a comprehensive approach that aim to address this issue by studying a versatile and integrated process for management and valorization of CO₂. More specifically, the focus of the proposed research is the utilization of the biogas and bio-oil coming from pyrolysis process of different typologies of biomasses, finalized to produce energy and fuels. As first step, the dependence of biogas and bioliquid composition on the process variables, such as temperature, of the pyrolysis stage will be studied. The effect of gas carrier will be also extensively considered. In particular, the usage of CO₂ as a carrier gas will be studied in detail and the potentials of its usage will be evaluate as a preferential way to recycle CO₂ rich gaseous streams in the whole process chain. Biogas and bio-oil, formulated on the ground of the pyrolysis stage process products in order to mimic their physical and chemical characteristics, will be then utilized for successive studies aimed at recover significant amount of thermal energy and to activate a dry reforming process to produce a syngas from the pyrolysis products stream eventually added with suitable amounts of CO₂. Looking at the energy transformation process, both biogas and bio-oil can be used as energy carrier in an advanced combustion process, such as MILD combustion. Therefore, the characterization of the carrier conversion as function of process parameters (temperature, pressure, inlet composition, carrier characteristics) will be carried out in different fluid-dynamic configurations, looking at the efficiency of the process in term of stability and composition of the flue gases. On the other hand, CO₂ dry reforming of bio-oil for producing syngas will be the second relevant process that will be considered. Differently from the common approach that consider the catalytic reforming, the homogeneous dry reforming will be the focus of the research. The syngas production will be analyzed as a function of inlet parameters, the heating temperature and the bio-oil composition.

Both biogas and bio-oil MILD combustion and reforming will be studied with a twofold approach. Indeed, lab scale facilities, instrumented with remote monitoring and control tools, are available to carry on the experimental studies for the characterization of carrier conversion for either processes. Sampling and advanced chemical diagnostics will be done to characterize the outlet streams. Possibly, optical diagnostic techniques will be implemented for in situ, non intrusive detection of un-stable intermediate species. Moreover, numerical tools for kinetic and kinetic/fluid-dynamic studied will be also used with the aim to make available a numerical model of the processes.

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Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Fully instrumented pyrolysis reactors from the very small scale (few grams of feedstock in batch mode) to large lab-scale continuous reactor capable of transforming some kg per hour of feedstock will be used in order to characterize different aspects of the process. Feedstocks and pyrolysis products, solid (biochar), gaseous and condensable fractions, will be characterized by using a wide range of diagnostics for their chemical composition and morphological nature. Test on ammonia adsorption on the biochar will be systematically made in order to clarify the role of physical properties and surface chemical activity on the adsorption process. At STEMS-CNR a very rich instrumentation capable of producing a detailed characterization of all these materials is available and it will be used according to the research needs.

Elementary (i.e. CSTR and PFR) and cyclonic turbulent reactors, to be used for MILD combustion and dry reforming studies, are available in STEMS-CNR laboratories. Main processes parameters (temperatures, pressures, chemiluminescence emission and heat transfer) are monitored by means of advanced multipoint diagnostics. Products of the processes will be characterized by using advanced monitoring and control distributed sensors network. Online chemical sampling and analysis and in-situ optical diagnostics are available and will be used according to the research needs.

The doctoral work is framed in some European and Italian research frameworks and networking initiatives. The research group has many national and international collaborations that will be exploited to enrich the experience and widen the competences of the enrolled PhD students.

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

In an EU collaborative framework, the candidate will be in contact with Lund University for the diagnostics implementation and with the Technical University of Denmark for the kinetic models studies. In the framework of the European Innovation Council (EIC) "CO₂ & Nitrogen" challenge projects portfolio the candidate will be involved in a wide collaborative network of more than 50 research institutions and industrial operators aimed at gathered together research efforts and available know-how toward the promotion of innovative intrapreneurial initiatives. In the framework of the doctoral activities at least a period in an European laboratory is planned.

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PhD Project Proposal

Proponent: Maurizio Ventre

Proposed research topic: Development of functionalised platforms and computational models for mechanobiology studies

Reference curriculum:

Materials and Structural Engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives) max 500 words

The biophysical characteristics of the cellular microenvironment (with particular reference to the microstructure and mechanical properties) are known regulators of different aspects of the cellular functions and differentiation of various cell types, including embryonic, stem and immune cells. In recent years, research has mainly focused on identifying molecular signals that underlie the process of mechanotransduction (i.e. the transduction of mechanical signals into biochemical signals). Comparatively fewer are the studies dedicated to the analysis of the intracellular mechanical determinants, such as cytoskeletal assembly, cytoplasmic and nuclear mechanics, in the dynamics of mechanotransduction. Yet, recent literature has demonstrated how different cellular architectures regulate the activation of specific cellular programs and, furthermore, intracellular stresses are sufficient to alter nuclear morphology and consequent gene expression. The aim of this proposal is to develop experimental and computational models to understand how the cell alters its mechanics in response to biophysical signals and how this response influences specific biochemical processes.

The project activities aim to fabricate culture systems, of synthetic (hydrogels or elastomers) or natural (collagen networks) origin, that present specific biophysical signals, such as topography, porosity, stiffness, ligand patterns, in order to analyze the response of cells in terms of morphology, mechanical properties, molecular and functional profile. The central point of the project is to develop and implement manufacturing, manipulation or functionalization techniques capable of controlling the characteristics of the biophysical signals to be integrated into the culture systems (e.g. size of topographic patterns, degree of porosity, stiffness, ...). This goal enables performing a systematic study that relates the cellular response to specific arrays of biophysical signals. The starting point will be to fabricate culture systems that replicate biophysical characteristics of "physiological" systems and then develop "pathological" models that - for example - replicate microenvironments similar to fibrotic or cancerous environments (for example more rigid, aligned and dense). The data obtained from this activity will subsequently be used as input to a micro-mechanical model in FEM (in a preliminary version already developed by the project promoter) with the dual purpose of refining the interpretation of how mechanical signals are transmitted internally to the cell, and to predict the cellular response to certain sets of mechanical stimuli.

The objectives of the project can be summarized as:

1. Creation of functionalized synthetic/natural substrates;
2. Characterization of the cellular response in terms of adhesion, cytoskeletal structuring and evolution of cellular mechanics;
3. Development of a computational model of cellular mechanical-mechanical microenvironment interaction.

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Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

The student will carry out research activities at the DICMAPI laboratories and those affiliated with the Department. These are equipped with apparatuses for the manufacturing of culture systems (chemical hoods, 3D printers, micromilling machines, photopatterning); for cell cultures (incubators, biological hoods), for their morphological, mechanical (optical, confocal and AFM microscopes) and molecular characterization (implementation of immunofluorescence, histological and rt-PCR techniques).

The project proposal is partly linked to collaborations with the following teachers:

Prof. Alessandra Cambi, Cell Biology Department of the Radboud University Medical Center in Nijmegen in The Netherlands

Prof. José Manues García Aznar, Department of Mechanical Engineering, University of Zaragoza

Prof. Costantino Menna, DIST, University of Naples Federico II

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

The student will be able to complete a training/research period at European institutes involved in research activities related to mechanotransduction such as Radboud University Medical Center (for the cellular part), the 2mbe institute of the University of Zaragoza (for the of computational modeling).

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PhD Project Proposal

Proponent:

Massimiliano M. Villone

Proposed research topic:

Label-free opto-microfluidic technologies for early diagnosis

Reference curriculum:

Chemical engineering

Summary of the Research Project (state of the art, short program of the planned activities and objectives)

The objective of this doctoral proposal is the design and implementation of a microfluidic platform to identify, count and isolate cells in concentrated biological fluids (for example, blood) and provide morphological information on them, even in conditions of microgravity.

The project continues the activities defined in WP 1400 of the ASI-UNINA framework agreement "Development Activities for Innovative Technologies Related to Health in Space" and falls within the theme "Lab-on-Chip for rapid, portable, low-cost diagnostics, weight and bulk" foreseen in the ASI PTA 2022-2024. Where, for simplicity of processing, the WP 1400 focused on the analysis of isolated cells and diluted samples, this PhD proposal focuses on untreated biological fluids, similar to concentrated suspensions. Such multiphase systems exhibit, as a whole, non-Newtonian rheological properties. Blood, for example, exhibits pseudoplasticity (i.e., the existence of a stress threshold below which the material does not flow), viscoelasticity (i.e., a mechanical behavior in between that of a viscous liquid and that of an elastic solid) and thixotropy (corresponding to a viscosity varying over time when the system flows) [1]. Furthermore, given the large volume fraction of the particles contained in these suspensions (for example, red blood cells, white blood cells and platelets in blood), it is relevant to consider the effects of the interactions among them, which can induce phenomena such as the formation of aggregates [2]. The above-mentioned fluid mechanical and rheological aspects have significant effects on the dynamics of untreated biological fluids in microfluidic channels, which can significantly influence the design and operational parameters of a cell flow imaging device. In this project, we aim to comprehensively characterize the effects of non-Newtonian rheological properties and inter-cellular interactions on the dynamics of untreated biological fluids in microfluidic devices designed with the aim of performing holographic flow tomography of the cells themselves, thus to extend the scope of applicability of the device developed under WP 1400 of the ASI-UNINA framework agreement.

The research activity will be carried out both through experiments and numerical simulations. The experiments will be conducted using (and, if necessary, updating) the setups developed under the aforementioned framework agreement. The first part of the experimental activity will focus on the separation of cells of different types within untreated biological fluids, while, in the next phase, holographic flow tomography of the different types of cells will be implemented. The experimental activity will be accompanied by a modeling-simulation activity aimed at supporting and directing the experiments themselves, studying, in particular, the effects of non-Newtonian rheological properties and inter-cellular interactions on the dynamics of untreated biological fluids in microfluidic channels. For this purpose, advanced computational techniques based on the finite element method and the CFD-DEM method will be used, which allow the description of fluids with complex rheological properties and very concentrated suspensions. Particular importance will be given to the study of the

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effects of microgravity conditions. Part of the simulation activities will be carried out during the period abroad.

[1] Beris et al., *Soft Matter*, 17, 2021, 10591

[2] Harris et al., *NPJ Micrograv.*, 16, 2023, 17

Brief information relating to: operational and scientific structures (equipment, software, laboratories,...) available to the PhD student for carrying out the proposed activity, collaborations with other Italian and foreign research bodies (possibly also with companies), potentially relevant to the proposed topic.

Availability of advanced computing resources for numerical simulations and laboratories for experimental activities in the field of microfluidics, also in collaboration with the group led by Pietro Ferraro at CNR-ISASI

Brief information relating to any period abroad planned for the PhD student (period, research group, University, research institution....)

6-12 month stay in Mahdi Saeedipour's group at the Department of Particulate Flow Modeling of the Johannes Kepler University of Linz (Austria)