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PhD Course in Chemical, Geological and Environmental Sciences
Call for Interest 39th cycle – session I - Curriculum Chemical Sciences

Nr. 1		**Supervisor**	**Davide Ballabio**
Title	**Chemometrics strategies for the prediction of the molecular structure by LC-MS/MS spectra**		

Liquid chromatography with tandem mass spectrometry (LC-MS/MS) is one of the most effective analytical techniques to characterize environmental, food, forensic and biological samples. The identification of substances in the sample is usually based on a similarity match between the experimental MS/MS spectrum and the spectra included in specific libraries. This process may be dependent on the experimental settings used for the spectrum measurement; moreover, it is likely that a detected molecule is not present in the reference spectral library, in particular when omics untargeted experiments are carried out.

Recent studies have shown that chemometrics can support the identification of substances from LC-MS/MS spectra by developing novel deep learning tools to directly correlate the chemical information encoded in MS spectra with the molecular structures of compounds. In this way, it may be possible to directly predict molecular structures (encoded in molecular descriptors) from large databases of spectra measured under different experimental conditions. Then, the descriptors can be used to search for the target compound in huge chemical database, containing millions of substances.

Being a novel development, there are many improvements in the approach to be evaluated, such as different representations of both spectra (input) and molecular structure (output), as well as the deep learning algorithms and their optimisation. The PhD student is expected to acquire knowledge on both the interpretation of the MS analytical information and on the development of proper chemometric approaches. The period abroad can be planned at the Eindhoven University of Technology (NL) to acquire knowledge on deep learning strategies.

Supervisor web page: https://www.unimib.it/davide-ballabio

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Nr. 2		**Supervisor**	**Fabio Gosetti**
Title	**Fate of emerging micropollutants in the environment**		
Every year the number of substances that the scientific community considers potentially dangerous to humans and the environment increases. It is therefore essential to deepen the knowledge, distribution, and territorial spread of these newly emerging pollutants (pharmaceuticals, pesticides, plasticizers, PFAS, etc…). Although there are often sufficiently sensitive analytical methods for their determination in water, the routine methods of analysis do not take into account the possible transformation products (TPs) that may originate in the environment by hydrolysis reactions, solar radiation or microbial degradation. In addition, TPs can have comparable toxicity or sometimes be even more toxic than the precursor compound, and for this reason, it is also necessary and important to monitor them in the environment. After simulating the conditions of pollutant degradation in the laboratory, the PhD student is expected to develop and validate innovative chromatographic methods for the identification of the generated species. Structural elucidation will be done by techniques based on the use of low- and high-resolution mass spectrometry using targeted and untargeted approaches.			
Supervisor web page: https://www.unimib.it/fabio-gosetti			

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Nr. 3		**Supervisor**	**Fabio Gosetti, Simona Binetti**
Title			

The constantly increasing number of new drugs on the market implies the presence of both the active principles and their metabolites or transformation products (TPs) in surface waters at concentrations of ng/mL or pg/mL. These compounds can be only partially removed during the treatment processes in wastewater treatment plants, and they are considered emerging micropollutants (EMPs). Therefore, the development and validation of sensitive analytical methods for their monitoring are mandatory.
On the other hand, it is necessary to develop innovative methods for their abatement. Preliminary laboratory tests have successfully demonstrated the use of a new material based on kesterite nanoparticles (CZTS NPs) both as a photocatalyst for the photodegradation of EMPs and as an adsorbent material. In the latter case, the NPs are able to totally release the adsorbed EMPs through a suitable desorption solvent and they can therefore be recovered and reused for a new process. Moreover, the CZTS NPs can be grafted on silica allowing their use in the flow process. They can be inserted into a support thus generating a sort of "filter" that can be used in an industrially scalable set-up.
This study aims to evaluate the use of CZTS NPs both dispersed in solution and grafted on a support for the degradation/abatement of several EMPs with different chemical-structural properties, optimizing the experimental conditions and testing the efficiency of the NPs after recycling..

Supervisor web page: https://www.unimib.it/fabio-gosetti

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Nr. 4		**Supervisor**	**Simona Binetti**
Title	**Wet chemistry process for new generation solar cells based on sustainable chalcogenide thin film**		
This research project is focused on the optimization of the wet low-cost deposition methods for the synthesis of inorganic chalcogenide thin films (employable as absorbers in new generation solar cells). The quaternary alloys involved in this research are structured as Cu2XY(S,Se)4 (with X = Zn, Mn and Y = Sn, Ge), already known and well-documented in the literature thanks to their good performances, high stability, high sustainability and possibility to modulate the energy gap, aiming to make them suitable for tandem applications with silicon or perovskites. The thin films deposition will be performed on rigid and flexible substrates, transparent or otherwise. The corresponding Cd-free n-type buffer layer that will be examined in this project are Zn(O,S), ZnS, ZnSnO e TiO2, and the most performing deposition techniques among chemical-bath deposition, film applicator deposition, spray pyrolysis, ink-jet printing and Atomic Layer Deposition (ALD) will be investigated. The optimization of the back contact with a proper transparent conductive oxide will make the devices suitable for bifacial or tandem application, allowing to overcome theoretical efficiency limitations. The collaborations with other European research centers such as Tallinn University of Technology, Technische Universiteit Delft and Institut Photovoltaique d'Ile-de-France will allow the candidate to spend a period abroad, expanding its knowledge by learning complementary characterisation skills and techniques for the above-mentioned materials.			
Supervisor web page: https://www.unimib.it/simona-binetti			

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Nr. 5		**Supervisor**	**Laura Bonati**
Title	**Molecular dynamics methods for the study of properties and interactions of biomolecules**		

Biology largely runs on the operation of complex biomolecular systems involving protein folding and dimerization, binding of small molecules, and allosteric communication. The study of these processes at atomistic level is of great relevance for the comprehension of mechanisms behind physiological processes, human diseases, pharmacological and toxicological activity of chemical compounds, as well as for the development of new drugs. The PhD project will be focused on the use of Molecular Dynamics (MD) simulations to study diverse biological processes. Such processes, however, involve large systems up to thousands or even millions of atoms and may happen on timescales of seconds, thus their study requires the use of methods based on the Molecular Mechanics approximation. When the timescale of the mechanism under study is beyond current computational limits, enhanced sampling methods (such as steered MD, Metadynamics, or accelerated MD) will be used to speed-up the calculation and obtain a deeper understanding of the underling free-energy landscape. Furthermore, to achieve a good level of accuracy and keep the computational cost affordable, hybrid QM/MM simulation approaches will be evaluated. During the PhD period the candidate will be part of a research group and collaborations with international groups will be carried out.

Supervisor web page: https://www.unimib.it/laura-bonati

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Nr. 6		**Supervisor**	**Dario Narducci**
Title	**Novel materials for thermoelectric heat harvesting and cooling**		
Thermoelectricity has been a cornerstone in irreversible thermodynamics. At the same time, it has been largely used as a tool either to convert heat into electric energy or to pump heat in refrigerating machines – in both cases with no need for moving parts. Still, efficiency of both classes of devices needs to be improved to fully exploit thermoelectricity as a viable strategy for heat harvesting and management. To this aim, this research activity explores different routes to enhance the efficiency of thermoelectric materials (and devices, thereof), all making use of nanotechnology. This includes bottom-up and top-down strategies to energy filter charge carriers, and fabrication of dimensionally constrained inorganic nanostructures as well. The project is carried out in collaboration with several European universities and research centres, including the University of Warwick (UK), Aix-Marseille University (France), and the Institute of Micro and Nanotechnology of the Spanish National Research Council of Madrid (Spain), where the Ph.D. candidate might spend research stages.			
Supervisor web page: https://www.unimib.it/dario-narducci			

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Nr. 7		**Supervisor**	**Luca Bertini**
Title	**Enzymatic degradation of recalcitrant compounds**		
The demand for technological and industrial processes with a low environmental impact that degrade recalcitrant pollutants is growing. In this field, bioremediation processes are very promising. These exploit bacterial and fungal enzymes whose function in these organisms is precisely to degrade recalcitrant substrates. Most of these systems are metalloenzymes with catalytic sites typically containing Fe or Cu ions featuring the highest standard reduction potentials among biological systems. More in detail, the interest of this project is focused on some metalloenzymes capable of oxidizing non-phenolic substrates, including some polymers and aromatic hydrocarbons, such as Laccase, Lignin peroxidase and some monooxygenases involved in the aerobic degradation of aromatic hydrocarbons. Interestingly, although many studies have been conducted over the years in this regard, the oxidation mechanisms of different classes of aromatic hydrocarbon compounds and polymers are not known in detail at the molecular level. The main goal of this project is to characterize these mechanisms at the multiple level using all the toolbox of techniques available in molecular modeling, from the classical level (molecular docking and dynamics) to the quantum chemistry level (Density Function Theory) and the combination of the two (quantum mechanics/molecular mechanism level). The substrates of choice are aromatic hydrocarbons and, in particular, polycyclic ones, in order to shield light on the nature of electron transfer processes following their oxidation.			
Supervisor web page: https://www.unimib.it/luca-bertini			

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Nr. 8		**Supervisor**	**Roberto Nisticò**
Title	**Development of anisotropic magnetic nanomaterials through soft-chemistry approaches for the environmental remediation of contaminated wastewater**		

The shortage of available clean water is a serious global emergency affecting both the domestic and agricultural use of water. Anthropic pollution is among the major causes of the negative impact on fresh water quality. From this, it clearly emerges the importance of exploring integrated water reuse and water treatment processes seeking for a transition toward a more circular water management. Currently, many studies are focusing on the exploitation of innovative methods for wastewater treatments, particularly focused on the removal of emerging micro-contaminants by exploiting either heterogeneous photo-catalysis or advanced sorption approaches.
In this context, the project aims at the preparation of anisotropic magnetic nanomaterials (i.e., mostly iron oxides) through soft chemistry approaches. These magnetic nanomaterials are extremely advantageous as easily recoverable due to their magnetic nature, and usable in heterogeneous photo-catalytic processes. Besides intense efforts in the morphologically controlled synthesis of these nanomaterials, a comprehensive structural and morphological characterization will be pursued. The photo-catalytic activity of these anisotropic magnetic nanomaterials will be evaluated in the abatement of a model emerging micro-contaminant from wastewater. The project will be developed in collaboration with other national and foreign University groups, offering important educational and professional tools that will encourage career perspectives.

Supervisor web page: https://www.unimib.it/roberto-nistico

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Nr. 9		**Supervisor**	**Giovanni Di Liberto, Livia Giordano, Gianfranco Pacchioni, Sergio Tosoni**
Title	**Modelling of Inorganic Materials for Energy and Environment**		
The research line is devoted to the modelling of inorganic materials for applications in energy and environment, by means of state-of-the-art theoretical approaches. Inorganic materials are primary actors in several processes of technological interest for the energy transition. Computational models allow to interpret experiments, provide insight, and design new systems useful to solve problems in clean energy production, energy storage and ambient remediation. The project will be dedicated to the investigation of the properties of new materials for catalysis and for batteries. This allows to obtain the i) nature of the materials in real conditions, ii) their chemical behaviour, and iii) to predict strategies for the rational design of new candidates based on observed structure-relations properties and universal descriptors. The project will face several key chemical processes such as water splitting, CO2 valorisation and nitrogen fixation. The materials of interest range from classical semiconductor oxides, low-dimensional carbon-based materials, MXenes to perovskites.			
Supervisor web page: https://www.unimib.it/giovanni-liberto			

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Nr. 10		**Supervisor**	**Giuseppe Zampella, Federica Arrigoni**
Title	**DFT investigation on molecular determinants influencing the selectivity toward H_2, N_2, CO_2 of enzymes and related biomimicry involved in bio-energy production and storage.**		

Nitrogenases and hydrogenases are metalloenzymes able to catalyze the crucial step of the nitrogen cycle (N_2 fixation to bio-available form, NH_3) and the of H_2 oxidation/H+ reduction interconversion, respectively. Nitrogenase reduces N_2, (NH_3 synthesis, Haber-Bosch-like reactivity) and a series of other substrates, including CO and CO_2 that are converted to a mixture of unsaturated hydrocarbons with potential relevance for biofuel production (Fischer Tropsch-like reactivity).
Both systems share the common feature to have cofactors containing Fe, S, C, O clusters (Mo/V ions only in nitrogenases). A Fe_2S_2 core is considered the minimal functional subunit for catalyzing both proton reduction and nitrogen fixation. Presently, bioinspired models of both enzymes exist that are active, although not as much as related biosystems. Remarkably, nitrogenases can process different substrates. Our aim is detecting determinants that underlie to substrate promiscuity in nitrogenase and to understand if biomimicry possessing a Fe_2S_2 core, can activate CO_2 to HCOO- production. That could clarify whether the enzyme substrate promiscuity and selectivity can be applied to new biomimetics.
Density Functional Theory (DFT) will be used to characterize CO_2 binding affinities, redox potentials and the mechanism of CO_2 hydrogenation by Fe2S2 containing systems. Molecular Docking and DFT will be used to study CO_2 binding to V-nitrogenase and its activation by the active site of the enzyme and its mimics.

Supervisor web page: https://www.unimib.it/giuseppe-zampella

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Nr. 11		**Supervisor**	**Silvia Bracco**
Title	**Photoactive porous materials**		
The project will focus on the synthesis and characterization of high surface area porous coordination polymers containing suitably engineered photoactive ligands capable of interacting with light. The versatility of these porous metal-organic structures makes them suitable both for the inclusion of catalytic sites for the conversion of absorbed CO2 and for the fabrication of luminescent sensors.			
Supervisor web page: https://www.unimib.it/silvia-bracco			

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Nr. 12		**Supervisor**	**Angiolina Comotti**
Title	**Three-dimensional nanoporous dynamic polymers for gas storage**		
The project will focus on the synthesis and characterization of high-surface area porous materials. These materials, consisting both of crystalline structures generated from metal ions connected by organic ligands through coordination bonds and 3D-polymers, exhibit permanent porosity and have applications in the selective capture, separation and storage of gases and vapours, and in the insertion of ultrafast molecular rotors within porous architectures.			
Supervisor web page: https://www.unimib.it/angiolina-comotti			

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Nr. 13		**Supervisor**	**Alessandro Abbotto**
Title	**Solar generation of green hydrogen and other artificial photosynthetic processes**		
The activity consists in the development of organic and hybrid molecules, active in processes promoted by sunlight to obtain fuels and other sustainable and renewable chemical compounds, to meet the zero emission targets of the European Union for 2030 and 2050. In particular, three processes are investigated: 1) generation of green hydrogen from water and sunlight; 2) use and transformation of carbon dioxide into fuels and chemical intermediates with net zero emission; 3) green synthesis of ammonia starting from nitrogen and sunlight (artificial nitrogen fixation) for the green synthesis of fertilizers (synthesis of ammonia is currently one of the most important chemical processes for the planet). The study will involve the synthesis and characterization of the molecules and their use and investigation in photocatalytic, electrocatalytic, and photoelectrochemical devices. A second line of research also involves the study of new generation photovoltaic devices with high sustainability and low impact for use under ambient light (indoor, offices, homes, etc.).			
Supervisor web page: https://www.unimib.it/alessandro-abbotto			

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Nr. 14		**Supervisor**	**Cristina Airoldi**
Title	**Advanced bioorganic and bioanalytical techniques for drug discovery, drug delivery and diagnostics**		
The research project involves the use and the implementation of advanced techniques, mainly NMR spectroscopy, for the study of molecular recognition processes of biological relevance. These studies allow the identification of the structural determinants of ligand-receptor interactions involving biomolecules. The experimental work also requires the organic synthesis of bioconjugates as potential multifunctional ligands to be used as molecular tools in the in the fields of drug discovery, drug delivery and diagnostics. Collaboration with research groups form other European Universities and Research Centers, as well as participation in international congresses, seminars and workshops is expected.			
Supervisor web page: https://www.unimib.it/cristina-airoldi			

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Nr. 15		**Supervisor**	**Luca Beverina**
Title	**Sustainable approaches to the synthesis of organic semiconductors for plastic electronics**		
Plastic electronics uses semiconducting polymers and molecules instead of traditional inorganic semiconductors for the manufacturing of low cost, flexible electronic components. The research in the field developed very efficient materials and sound structure property relationships, thus making a case for a transition from laboratory to industrial environment. At this critical juncture, sustainability and ease of scaling up are at least as important as performances, to the point that efficient materials on a lab scale could become unpractical for the industry. The development of more efficient synthetic protocols and the complete removal of all organic solvents from both the synthesis and the processing of semiconducting polymers can help tremendously to improve sustainability and reduce costs. In the last 5 years we have demonstrated that the use of an aqueous dispersion of surfactants (including food grade lecithin), enables the synthesis and processing of representative semiconducting polymers. In this project we aim at producing more complex materials according to the same techniques. We also aim at developing techniques for the direct production of aqueous inks not requiring the purification of the polymer. Results will have a transformative impact on the growing printed electronics industry. The development of micellar chemistry will also impact in more traditional synthetic chemistry fields like pharmaceutical and specialty chemicals.			
Supervisor web page: https://www.unimib.it/luca-beverina			

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Nr. 16		**Supervisor**	**Laura Cipolla**
Titile	**Carbohydrate and proteins from waste: feedstock for added value chemicals and materials**		
Biomass and some industrial waste are rich in polysaccharides and proteins, that can be considered as renewable source alternative to fossil-based raw materials. In addition, the use of biomass and waste fits within bioeconomy and circular economy approaches, in compliance with the ONU agenda for the sustainable development goals. Natural polymers (i.e. starch, chitin, chitosan, cellulose, silk fibroin and sericin) by themselves possess poor mechanical properties when compared to fossil-based synthetic polymers. These drawbacks can be overcome by crosslinking, eventually in blends with suitable additives, and by chemical modification. The project will be focused on the design of innovative bio-based materials with suitable mechanical properties as an alternative to fossil-based polymers, through the development cross-linking chemistry and polymer modification. The use of biocatalysis will also be considered. Biodegradation, and biocompatibility will be assessed. The obtained materials will be considered for packaging applications, and as drug delivery platforms. The project may benefit of international mobility (potential destination Boku, Vienna).		
Supervisor web page: https://www.unimib.it/laura-cipolla			

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Nr. 17		**Supervisor**	**Laura Cipolla**
Titile	**Design, preparation, and characterization of bio-based hydrogels**		
Hydrogels have become popular as three-15 dimensional (3D) scaffolds for cell culture providing robust platforms for different applications, such as investigation of cell physiology, pathology, tissue regeneration, drug discovery, and delivery. Depending on the desired application, hydrogel chemico-physical features should be tuned by cross-linking strategies. In this framework, the search for new hydrogels and cross-linking strategies is still ongoing, in order to ameliorate their performances toward the desired application. The increasing need for advancements in hydrogels as robust platforms as 3D cell culture scaffolds (i.e., for cell therapies, tumor models, drug delivery systems, and tissue engineering) is prompting the research in the field, that is expected to boost the market growth in the next years (CAGR of 10.7% from 2021 to 2028, https://www.grandviewresearch.com/industry-analysis/3d-cell-culture-market). The project will focus on the study of innovative chemical cross-linking strategies for hydrogel preparation, starting from natural polymers including proteins (i.e. gelatin, silk sericin), and polysaccharides (i.e. chitosan, starch). The effectiveness of chemical cross-linking will be assessed by analytical spectroscopic techniques such as NMR and FT-IR, while morphology will be assessed by SEM. Biological behavior and drug release studies will also be performed in collaboration with research groups at UNIMIB. The project may benefit of international mobility (potential destination Houston Medical Center, US).			
Supervisor web page: https://www.unimib.it/laura-cipolla			

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Nr. 18		**Supervisor**	**Barbara La Ferla**
Titile	**Functionalization of cellulose nanocrystals for biomedical application**		

Cellulose nanocrystals and nanofibres (CNC, CNF) have gained increasing interest thanks to their wide availability, sustainability, and low cost (compared to other nanoparticles), especially from the view of a circular economy. They feature high strength, possibly acting as a reinforcing filler to improve a composite material's mechanical, thermal, chemical, and optical properties, leading to enhanced performance. Interestingly, in recent studies, CNC exhibited activity against microbial adherence due to their unique surface chemistry [1]. In addition, thanks to their rod-like shape, they have demonstrated unique biodistribution characteristics with promising applications as drug carriers.

Considering all these factors, this nanomaterial shows excellent potential in the biomedical field. Among them are their use as drug carriers through the linkage and/or adsorption of drugs, their improvement of antibacterial properties through the introduction of synergistic compounds, and their incorporation in nanocomposites to prepare prostheses with antibacterial properties. However, CNC and CNF are too hydrophilic to be used as is in hydrophobic resin matrixes. Therefore, the grafting of different functional groups onto their surface to change and improve their performance can be done. Such materials are highly promising as innovative biomedical nanocomposites with enhanced mechanical, aesthetic, and microbiological/biological performance. One example of composite to be developed in this project consists into methacrylate-based resin incorporating functionalized CNC and CNF. The mechanical properties and microbiological behaviour (activity against microbial adherence and biofilm formation) of light-curable functionalized CNC/CNF nanocomposites will be evaluated. Fields of application may include materials for dental restorations, implantable stents, and tissue grafts. [1] D'Orazio G. et al J. Mater. Chem. B. (2017) 5, 7018-7020; 2] Colombo L et al. Biomacromolecules (2015) 16, 2862-2871; 3] Zoia L. et al Nanomedicine (2020) 15(23) 2271-2285.

Supervisor web page: https://www.unimib.it/barbara-ferla

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Nr. 19		**Supervisor**	**Alessandro Palmioli**
Titile	**Discovery of bioactive compounds from natural sources**		

Recently, the research of bioactive natural compounds is gaining renewed interest. Natural extracts obtained from medicinal plants, foods, and algae, but also fungi and bacteria, are considered fundamental sources for exploring a large chemical diversity of healthy ingredients with pharmacological and nutraceutical applications. Our group combines expertise in bioorganic and medicinal chemistry as well as in advanced analytical techniques (including NMR and LC-HR-MS) for the preparation and characterization of bioactive-enriched extracts and for the identification and isolation of bioactive compounds from natural complex mixtures.
In this context, the PhD student involved in this research project will have the chance to develop different and complementary skills concerning:
• extraction and purification of bioactive compounds from natural sources;
• NMR spectroscopy for extract component identification and molecular recognition studies (with the target(s) of interest);
• mass spectrometry coupled with chromatographic techniques for extract component identification and isolation;
• biophysical, biochemical, and biological assays to assess extract biological activities (as amyloid inhibitors, antioxidants and modulators of autophagy, antitumoral, antibacterial agents).

Supervisor web page: https://www.unimib.it/alessandro-palmioli

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Nr. 20		**Supervisor**	**Francesco Peri**
Titile	**Sustainable synthesis of bioactive compounds; drug discovery and development**		

In our lab several different projects are running in the fields of drug discovery and green synthesis of bioactive molecules. In particular, the candidate will participate to basic research and industrial projects on the development of new immunostimulant compounds that are drug leads as vaccine adjuvants and tumor immunotherapeutics. We also develop new antagonists of the human receptor TLR4 as drug candidates targeting autoimmune and rare diseases.
The chemical processes and syntheses of bioactive compounds and drug leads are designed to be sustainable and green.
The PhD candidate will be exposed to an international environment (several collaborations in Europe and USA) and secondment in foreign groups for a period from 6 to 12 months are favoured.
During the PhD period the candidate will be trained to read scientific literature, to project experimental work, to carry out lab work, to use of several instrumental (analytical) techniques, to grant and scientific paper writing. The PhD student will have the possibility to present the results of his/her own research to international congresses and to develop industrial projects in collaboration with the spinoff CP2 Biotech founded by F. Peri in 2020.
We are also committed to science dissemination in public initiatives as the European Research Night also aimed to communicate Responsible Research and Innovation.

Supervisor web page: https://www.unimib.it/francesco-peri

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Nr. 21		**Supervisor**	**Luca Zoia, Veronica Termopoli**
Titile	**Valorisation VFAs within an integrated set-up for the anaerobic digestion of waste biomasses: continuous isolation, reduction, and monomer separation using membrane technologies and in-line analysis**		

The PhD project aims at optimising the valorisation of the volatile fatty acids (VFAs) generated within the anaerobic digestion of waste biomasses. So far, valorisation of VFAs is achieved in the form as feedstocks for PHA production, or in the form of the acids themselves after separation.

Within the wider context of the Green Transition and the thus needed integrated biorefineries furnishing starting materials for the chemical industries in the form of platform chemicals, the project will develop a technology based on membranes that will allow the (segmented) continuous isolation of VFAs from a bioreactor, their continuous reductive functionalisation to C2, C3, and C4 monomeric building blocks, and the separation of the mixture of monomers for the polymer industries.

The extraction and separation technologies, based on membranes, are supposed to be compatible, i.e., readily capable to be integrated, with common bioreactors, and realisable in (segmented) continuous fashion. Reductive functionalisation and separation of monomers is supposed to be run alongside the continuous extraction, such as to arrive at an overall parallel processing.

In detail, the project will i) screen existing membranes for filtering VFAs out from the bioreactor slurry, and eventually change their properties by chemical and/or biotechnological surface modification; ii) identify a working catalytic transformation of VFAs into unsaturated C2, C3 and C4 building blocks; iii) screen existing membrane systems for separating alkenes, and eventually develop new ones compatible with the reductive derivatisation. The solutions are expected to be compatible such as they can be integrated with proven reactor technologies, scalable, and run in parallel in (segmented) continuous mode.

The strongly inter- and transdisciplinary project will combine analytical, synthetic, and polymer chemistry, catalyst design, and material sciences, and will in part be performed at the Luleå University of Technology in Sweden (one or two stays, 6-12 months).

Supervisor web page: https://www.unimib.it/luca-zoia

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Nr. 22		**Supervisor**	**Luca Ferrero**
Titile	**Study of the thermodynamic properties of atmospheric aerosol deposited on high voltage insulators in function of its chemical composition: applications to prevention of flashover phenomena**		
The atmospheric aerosol, due to its hygroscopic nature which makes it conductive, is a critical element for the continuity of the national electricity service. Failure events occur when the soluble salts present in the deposit, in conditions of high ambient humidity, dissociate into ions, creating a conductive liquid film on the surface of the insulator and triggering electric discharge phenomena (flashover). The project aims to study the phase transitions (deliquescence and crystallization) and the conductive effect of the aerosol deposition (on specimens simulating the surface of the insulators exposed in the environment) in an Aerosol Exposure Chamber, as a function of the variation of its chemical composition and relative humidity. With a view to prevention, the thermodynamic model of the atmospheric aerosol Isorropia will be used to predict the deliquescence point (DRH) as a function of the chemical composition of the deposit collected on the insulators.			
Supervisor web page: https://www.unimib.it/luca-ferrero			