University of Milano-Bicocca
PhD Course in Chemical, Geological and Environmental Sciences
Call for Interest 41st cycle – session I – Curriculum Chemical Sciences

1		**Supervisor**	**Dario Narducci**
Title	**Efficiency at maximum power in dynamically operated thermoelectric generators**		
Heat harvesting, namely the conversion of low-enthalpy heat into electric power, provides ways both to boost energy circular economy, partially reusing waste heat, and to power low-consumption electronic devices such as sensing nodes in distributed sensing networks. In principle, thermoelectric generators (TEGs) offer a convenient way to achieve such goals. However, their efficiency, especially at low temperatures, is low. We demonstrated that the efficiency at maximum power of TEGs may be largely increased by modulating the supplied heat fluxes due to their increased enthalpy. The PhD student will participate in the theoretical and experimental investigation of such a new class of devices. S/he will further advance the thermodynamic analysis of the system and will participate in the experimental development of a proof-of-concept device, corroborating the model. A 6-month stage is planned at the Korea Electrotechnology Research Institute, Changwon (RoK). Research costs will be partially covered in the frame of the Program Agreement between ENEA and the Italian Ministry of Environment & Energy Security (MASE), Three–Year Realization Plan of the Electrical System Research 2022–2024, Project 1.4, 'Frontier materials for energy uses' (contract number I53C22003040001).			
Supervisor webpage: https://sites.google.com/unimib.it/thermoelectrics/home			
Notes:			

2		**Supervisor**	**Davide Ballabio**
Title	**Machine learning and deep learning approaches for the modelling of complex analytical data**		

Chemometrics is a powerful modelling approach that has found extensive application in the field of analytical chemistry, specifically in the prediction of chromatographic retention times (tR). Retention time is a critical parameter, influencing the separation and identification of compounds in a mixture, and chemometrics leverages the relationship between the physicochemical properties and molecular structural characteristics of chemicals to predict their behaviour in a chromatographic system. By employing chemometric multivariate techniques based on machine learning and deep learning approaches, we can establish quantitative correlations between molecular descriptors, which encode structural characteristics, and the chromatographic retention times. This enables the prediction of the elution order and separation efficiency of compounds, which is fundamental in the design and optimization of chromatographic methods. In this context, chemometric models serve as important tools for accelerating method development, reducing experimental efforts, and providing insights into the underlying physicochemical interactions governing the chromatographic process.
In this project, the PhD student is expected to initially acquire the data to be used to train the models and then develop proper modelling methods, to be eventually validated with experimental tests. Therefore, the student will acquire knowledge on both the chromatographic framework and on all the modelling steps, from data acquisition and curing to the development of advanced modelling pipelines. The period abroad can be planned at the Eindhoven University of Technology (NL) to acquire knowledge on deep learning strategies (6-12 months).

Supervisor webpage: https://en.unimib.it/davide-ballabio

Notes:

3		**Supervisor**	**Luca Beverina**
Title	**Heterogeneous and heterogenized catalysis for cross coupling reactions in water**		
Our group was amongst the first to develop efficient arylation protocols in aqueous solution of surfactants, dedicated to the synthesis of a wide variety of organic conjugated derivatives of interest for printed (opto)electronics. Over the last 10 years, we have developed protocols based on both industrial and designer surfactants for the preparation of monodisperse and polymeric materials. Alongside efficiency, we also focus on selectivity, exploiting both selective surfactant/reactants interactions and compartmentalization effects. Mostly, our methods are based on metal catalyzed cross coupling reactions. Recently, we also introduced a specific surfactant capable of promoting metal free photo-redox arylations while in aqueous environment. So far, we have developed methods based on soluble catalysts, metallic and not. Within this project we plan to move to heterogenized catalysts, still suitable for reactions in aqueous environment. Catalysts will be based on partially crosslinked conjugated polymers having a structure designed to provide specific interactions with reagents and/or products of polyconjugate materials. We will develop both photoredox, metal free catalysts and supported palladium catalysts. In both cases, we will study the interaction between the light absorbing and photoredox active support and the reaction mixture. The heterogenized catalysts will be prepared in the presence of polymeric surfactant to produce interpenetrated polymeric networks between the polyconjugated, active component and the surfactant. The final catalyst will be water dispersible thanks to the intertwined surfactant. Staying abroad period: 6 months, in leading European and American institutions involved in research fields thematically correlated. Funding supporting the position: PRIN PNRR INPOWER. EU Pathfinder GRETA. The supervisor also applied for 1 ITN project, under evaluation.			
Supervisor webpage: https://www.unimib.it/luca-beverina			
Notes:			

4		**Supervisor**	**Carlo Santoro**
Title	**Electrocatalysts development for electrochemical applications**		
Electrocatalysis and electrochemical systems will be paramount for the Green Revolution. Development of electrocatalyst that are affordable and can replace precious and noble metals are also important and crucial to a successful deployment. This PhD proposal intends to develop novel platinum-free (PGM-free) materials based on transition metals (TMs) for reactions of interests. These reactions can be for example oxygen reduction reaction (ORR), hydrogen evolution reaction (HER), oxygen evolution reaction (OER), small molecules oxidation, carbon dioxide reduction reaction (CO2RR), nitrate reduction reaction (NO3RR) and so on. Depending on the interest of the candidate, a specific reaction can be pursued and specific type of electrocatalyst can be synthesized including atomically dispersed (TM-Nx-C), oxides, mixed oxides, nanoparticles, alloys, etc. These materials will undergo microscopic, spectroscopic and electrochemical characterizations. Period Abroad: 6-12 months period abroad is expected that can be done in EU or Korea or USA, depending on nationality and VISA availability.			
Supervisor webpage: https://en.unimib.it/carlo-santoro			
Notes:			

5		**Supervisor**	**Giovanni Di Liberto**
Title	**Developing a Computational Approach for Accurate Predictions of Single Atom Electrocatalysts**		
Catalysis is at the core of the energy transition. Electrochemistry is demonstrating a viable way to use renewable energy to make possible at room temperature energy intensive processes such as water splitting, ammonia synthesis and CO 2 reduction. The optimization of catalyst is usually based on trial-and-error procedure, as the fundamental understanding of the chemistry behind a reaction requires an atomistic description. Computational chemistry is a valid tool in this respect. The power of theory nowadays is not only restricted to the understanding and characterization of the nature of a catalyst or a process, but it can be pushed up the limit of the so-called rational design. This research project aims at modeling different catalysts for advanced electrochemical applications, including synthesis of ammonia, CO 2 reduction, water splitting, and hydrogen peroxide synthesis. The computational framework will address challenges of the current methodologies, including the need to describe the stability in reaction conditions, reproducing electrochemical polarization curves, and describe charge transfer reaction in long timescales. The project will include a visiting period of six month in a leading institution in the field.			
Supervisor webpage: https://qclab.mater.unimib.it/home/people			
Notes:			

6		**Supervisor**	**Luca De Gioia**
Title	**From Computational Insights to Tailored Design: Investigating Stereo-Electronic Relationships in Molecular Ratchets for Enhanced Performance**		
Autonomous chemically fueled information ratchets play a crucial role in synthetic molecular motors and pumps, mimicking biological processes. This research aims to investigate the relationship between stereo-electronic properties and the reactivity of molecular ratchets, focusing on their speed, power, and efficiency. The study will employ computational approaches, including Molecular Dynamics, DFT calculations, and Knowledge-based methods, to guide the rational design of optimized molecular ratchets. The project includes a planned six-month research period abroad at the University of Manchester (UK). This international experience aims to strengthen collaborations and enhance the research outcomes. The laboratory has already secured the necessary funding to support the research activities required for this project.			
Supervisor webpage: https://www.unimib.it/luca-de-gioia			
Notes:			

7		**Supervisor**	**Giorgio Moro**
Title	**Study of collective motion of water molecules in liquid water under illumination of microwave**		

Liquid water is warmed up with an electromagnetic wave at a frequency of approximately 2.45 GHz. Since a single water molecule lacks any degrees of freedom which corresponds to this energy level, it has been suggested that the absorption of microwaves may induce "collective motion" of multiple water molecules. Several studies have been reported in terms of molecular dynamics simulation of liquid water under illumination of microwave. However, few studies provide clear molecular level insights into this collective motion.

On the other hand, liquid water is renowned for its hydrogen bond network, characterized by donor-acceptor interactions, which provide additional degrees of freedom compared to other substances. The topology of the hydrogen bond network in small water clusters (H2O)n has been extensively studied. In this study we aim to apply the concept of hydrogen bond topology to liquid water to give better picture of collective motions which may be stimulated by microwaves.

We will conduct ab initio molecular dynamics (MD) simulations of liquid water under microwave illumination. Information regarding the hydrogen bond network will be preserved in the form of a hydrogen bond matrix. The collective motion of water molecules will then be extracted based on the hydrogen bond network topology. The PhD student involved in this study is expected to gain expertise in both ab initio MD simulation and hydrogen bond network topology analysis, also by means of research stays for a period at least six months in a selected foreign institution.

Supervisor webpage: https://www.unimib.it/giorgio-moro

Notes:

8		**Supervisor**	**Claudio Greco, Stefano Motta**
Title	**Molecular modelling of ligand-dependent activation mechanisms: the role of the Ah receptor in inflammatory and autoimmune disease**		

The aryl hydrocarbon receptor (AhR) is a ligand-activated transcription factor involved in immune regulation and inflammation, making it a promising target for drug discovery in autoimmune diseases such as psoriasis. Computational chemistry approaches may greatly contribute to identify new compounds with the potential to bind and activate AhR and to exert therapeutic effects, as well as to characterize the ligand-induced conformational changes and allosteric communication for the comprehension of the AhR activation mechanisms.
The aim of the PhD project will be to identify the molecular determinants of drugs able to modulate AhR leading to therapeutic effects against psoriasis-related inflammation. To achieve this, the PhD student is expected to acquire knowledge in: virtual screening techniques to process large libraries of chemical compounds; molecular docking to describe ligand-protein interactions; and Molecular Dynamics (MD) simulations, also employing enhanced sampling methods (such as steered MD, Metadynamics, or accelerated MD) to speed-up the calculation and obtain deeper understanding of the underling free-energy landscape.
The project will be developed in collaboration with the molecular biology laboratory of the Università Politecnica delle Marche under a project supported by the US National Psoriasis Foundation.
During the PhD period the candidate will participate in collaborations with international groups and will dedicate a minimum of 6 months to the period abroad

Supervisor webpage: https://www.unimib.it/claudio-greco
https://www.unimib.it/stefano-motta

Notes:

9		**Supervisor**	**Simona Binetti, Fabio Gosetti**
Title	**Use of kesterite nanoparticles for the abatement of emerging micropollutants**		

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) as an efficient photocatalyst for the photodegradation of EMPs. Interesting results have been achieved in the catalytic photodegradation of Diclofenac (one of the most dangerous emerging micropollutants) with efficiencies close to 90%, compared to the current 20-40% efficiency of the industrial water treatments plants, also avoiding the formation of even higher-toxicity byproducts. CZTS NPs recorded comparable performances also when irradiating with a visible-light-only source, making this system suitable also for indoor applications with visible light sources, looking forward to possible industrial implementation.
To do so, the CZTS NPs can be furtherly grafted on a properly functionalized silica, allowing their use in the flow process through the aid of a photoreactor. The resulting photocatalytic setup can be employed for a deep screening on the degradation of micropollutants belonging to different compound families, thus demonstrating the broad scope of the photocatalytic study. This investigation 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. The abroad period (6 months) can be planned at the Université Clermont Auvergne or other Universities in Spain or Greece to investigate the photochemical reactions of EMPs in the environment.

Supervisor webpage: https://www.unimib.it/fabio-gosetti
https://www.unimib.it/simona-olga-binetti

Notes:

10		**Supervisor**	**Fabio Gosetti**
Title	**Determination of contaminants in waste materials for their reuse or recycling**		
More and more attention is being paid to the reuse and recycling of raw or waste materials in the context of a circular economy that minimizes waste and maximizes the production of more sustainable goods. We need only think of the reuse of materials for the production of food packaging, whose controls must guarantee the health of the consumer, and the safety of the food contained, or the extraction of bioactive molecules from waste materials. These compounds, in fact beneficial to human health, could be introduced into cosmetic products or food supplements in order to improve their properties or functional characteristics (functional food). To do this, it is necessary to check for the presence of any organic and inorganic contaminants within the waste materials and ensure that the purified extract containing the bioactive molecules is free of them. First of all, it will be necessary to develop and validate proper analytical methods. The search for organic pollutants will be carried out in both target and non-target modes mainly through chromatographic techniques coupled to low- and high-resolution mass spectrometry, while for the inorganic contaminants inductively coupled plasma - optical emission spectroscopy will be used. The abroad period (6 months) may be spent at the Universities in Spain, France or Greece with which collaborations are in place.			
Supervisor webpage: https://www.unimib.it/fabio-gosetti			
Notes:			

11		**Supervisor**	**Federica Arrigoni, Luca Bertini**
Title	**Machine Learning for the Prediction of Standard Reduction Potentials in Metalloenzymes for Energy Conversion**		
Metalloenzymes play a crucial role in bioinorganic chemistry, particularly in energy conversion processes, where their catalytic sites drive key redox reactions. This PhD project aims to develop machine-learning models to accurately predict the standard reduction potentials of catalytic sites in metalloenzymes, with a particular focus on Iron-Sulfur FeS motifs and their possible modification. The study will focus on the integration of quantum mechanical calculations, molecular dynamics simulations, and experimental electrochemical data to train and validate predictive algorithms. The project foresees a research stay abroad for 6 months. The preferred partner institution will be identified based on expertise in computational chemistry and machine learning applications in bioinorganic. The laboratory has already secured the necessary funding to support the research activities required for this project (SMARFeS: Small Molecule Activation by Redesigned iron-sulfur (FeS) proteins;2022-NAZ-0498).			
Supervisor webpage: https://www.unimib.it/federica-arrigoni			
Notes:			

12		**Supervisor**	**Cristina Airoldi**
Title	**Discovery of bioactive compounds from natural sources**		

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 chemistry and 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.

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);
- organic synthesis for compound derivatization and functionalization.

The research and training activity will include a period abroad with a duration varying between six months and one year. Possible joint supervision: Prof. Jimenez-Barbero (Center for Cooperative Research in Biosciences (CICbioGUNE) and University of the Basque Country (UPV/EHU)). Any additional funds to carry out the research activities will be provided by the research group.

Supervisor webpage: https://www.unimib.it/cristina-airoldi

Notes:

13		**Supervisor**	**Laura Russo**
Title	**AI based predictive and automated synthesis of hydrogels for biomedical applications**		

The proposed project will develop AI based predictive and automated synthesis hydrogels for 3D-printing, with two main objectives: a) development of human tissue mimetics for regenerative medicine and personalized drug screening applications; b) hydrogels and microneedles for drug delivery. The human tissue mimetics (healthy and pathological) will be generated by exploiting natural and synthetic biopolymers (collagen, gelatine, hyaluronic acids, chitosan, PEG, PCL) and glycans as signaling molecules. The polymers will be functionalized with different glycans, and crosslinked by click chemistry approaches, to generate "bioinks" suitable for 3D printing in presence of cells (3D-bioprinting). AI based approaches will be employed in the selection of synthetic protocols to generate the in vitro tissue with the expected properties. The predictive tools will provide instructions to an automated robotic platform to fasten the process. The project includes accurate chemical and morphological characterization of the obtained constructs. Clinical partners will collaborate on biomedical applications. Furthermore, microfluidic apparatus containing the synthesized artificial organs (organ on chip) will be generated to study the "ex vivo" performance. A potential stage abroad at the University of Maastricht (NL) can be considered to optimize the organ on chip providing angiogenetic properties.

Supervisor webpage: https://www.unimib.it/laura-russo

Notes:

14		**Supervisor**	**Luca Beverina**
Title	**Development of Green Chemistry compliant methods for the synthesis of X-ray and MRI contrast agents and their intermediates**		

Iodinated contrast agents (ICAs) are non-ionic, water soluble molecules containing iodine atoms which are currently employed worldwide in X-rays diagnostic imaging. Their excellent safety profile, effectiveness, and versatility have made ICAs a crucial tool in modern medicine for accurate diagnosis and treatment planning. Iodinated contrast agents have been on the market for more than 40 years since the launch of Iopamidol, the pioneer compound of this category, and they are manufactured on a commodity scale of thousands of tons annually. MRI contrast agents are also well developed and represent an invaluable tool for diagnosis of a plethora of conditions. The European Union's Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) legislation is imposing increasingly strict limitations on the use of crucial reagents and solvents for the industrial preparation of iopamidol and other related compounds. Also, the continuous efforts of the chemical industry to reduce wastes and implement protocols having minimized energy consumption and resources depletions demand for the development of alternative protocols starting from sustainable raw materials.
The project leverages recent advancements in chemistry in water and other benign solvents as well as various solventless approaches as valuable tools for process intensification and reduction of overall environmental impact. The PhD student will be involved in the Bracco Open Science Platform (Avalanche) benefiting from constant feedbacks and discussion with leading national teams and international experts active in various fields of green chemistry.

Supervisor webpage: https://www.unimib.it/luca-beverina

Notes: scholarship funded by Bracco Imaging S.p.a. (Green Chemistry applied to industrial processes for the preparation of APIs for diagnostics and intermediates thereof)