CORSI BREVI ORGANIZZATI DAL DSCM - 2024|2025

Application of Deep Eutectic Solvents (DES) in chemistry, from organic synthesis to polymer science [10h]
Prof. Gianluca Ciancaleoni - Università di Pisa

This course will focus on the Deep Eutectic Solvents (DES), from the definition of what a DES is to their application in different fields of chemistry, as organic synthesis and polymer science. The initial part of the course will deal with the characterization of a DES, presenting the different techniques used and the information that can be derived. Their general properties will be analysed in detail, as well as their preparation and purification methodologies. The advantages of DESs over standard organic solvents will be discussed in detail: in general, it can be said that they are generally less toxic, flammable and volatile, and can be prepared from cheap and abundant materials. The course will also include a laboratory part, in which the most common DES will be prepared and compared.

Selected Issue from Separation Sciences: Theory and Praxis [10h]
Prof. Boguslaw Buszewski, prof. Jan Czochralski - Research & Development Centre, Toruń (Poland)

For over 100 years, physicochemical separation methods have been the dominant techniques in modern analytical chemistry. They are not only commonly applied in various configurations, but also widely used in the qualitative and quantitative determination of a wide range of numerous individuals. Combining these techniques with selective and specific methodologies and sample preparation technologies (extraction, distillation, adsorption-desorption, filtration, etc.) is a challenge for analysts. A particularly interesting case concerns the combination of these techniques with mass spectrometry and other detectors. This course will focus on these issues, but attention will also be paid to miniaturization and automation as well as statistical data processing - validation. Theoretical considerations will be supported and confirmed by examples from trace medical, pharmaceutical or environmental analyses.

Energy Materials: A physical chemistry perspective [8h]
Dr. Samuele Giannini, CNR

This course aims to provide students with a comprehensive understanding of the structural, electronic, and optical properties of a diverse range of energy materials crucial for emerging energy-efficient technologies. It specifically focuses on materials used in solar energy conversion and energy harvesting, such as organic and inorganic semiconductors for solar cells, semiconducting polymers, and thermoelectric materials. Additionally, it discusses materials involved in energy transformation, including light-emitting diodes, photodetectors, and photocatalysts and it briefly touches on materials relevant to energy storage, such as batteries, fuel cells, covalent and metal-organic frameworks. From a practical perspective, this course covers the most common theoretical and experimental methodologies employed to study the electronic structure and electronic dynamics of these systems. For instance, methodologies based on density functional theory and molecular dynamics as well as common spectroscopy and microscopy experimental techniques are discussed. The course also delves into the relationship between material properties and their morphological and chemical structures to ultimately provide an understanding of their interplay and materials design strategies. New perspectives and possible further development in the coming years are examined.

Surfaces & Interfaces: From Catalysis to Devices [8h]
Dr. Giacomo Melani, Novara Laboratories (NOLAB)

God made the bulk; surfaces were invented by the devil." - Wolfgang Pauli. Course Description: This advanced doctoral course provides an in-depth exploration of theoretical and phenomenological concepts concerning solid surfaces, emphasizing how their electronic structure properties intricately determine various applications. Through the lectures, students will gain comprehensive knowledge of the principles governing surface behaviour at an atomistic level.

Adsorption at surfaces: an essential toolkit to characterize porous materials [8h]
Prof. Valentina Crocellà, Università di Torino

Nanoporous materials are widely used in adsorption-related application such as catalysis, gas separation and storage, pollution control, as well as in the fields of pharmacy, medicine and agriculture. The use of adsorption phenomena is an old history. Indeed, the adsorption properties of porous materials have been known since Egyptian times, where carbon and clays have been applied in the purification of oils and water. The current extensive use of adsorption and adsorbent in industrial processes needs to gain a deeper understanding of the adsorption phenomena under conditions close to those of applications. However, before the "process evaluation" of these nanoporous materials, it is important to characterize such solids simply in terms of their textural properties (specific surface area, pore volume and pore size). This advanced characterization step can be used to disclose the intimate properties of porous solids, to possibly establish trends when a set of materials is under investigation or to shed light on the peculiar feature of a specific adsorbent. These experiments are carried out with specific molecular probes, exploiting readily available commercially instruments, that usually provide data of high quality. However, the theoretical exploitation of these raw data is generally employed by users in an automatic and aseptic way, using the software directly provided with the commercial instruments. Such a "black box" often leads to poor exploitation and misinterpreted results. This course, therefore, aims to give a "practical guide" for the interpretation of the adsorption phenomena at surfaces for the characterization of textural properties of porous materials, starting from the definition of "adsorption" up to the application of advanced physisorption methodologies for micro- and mesopores assessment.

Raman spectroscopy applied to heritage science [10h]
Prof. Peter Vandenabeele, University of Ghent, Ghent (Belgium)

This course provides a comprehensive exploration of Raman spectroscopy and its integration with cultural heritage research. We discuss the theoretical foundations of Raman spectroscopy in detail, and address pertinent side effects and interferences. Following this, we examine the essential components of Raman instrumentation, including lasers (and laser safety protocols), detectors, and sample interfaces (e.g. Raman microscopes and fibre optics). A dedicated section explores spectral interpretation, digital filtering techniques, and advanced data processing algorithms. Moreover, we explore various strategies for enhancing the Raman signal, such as the use of resonance enhancement and surface enhanced Raman spectroscopy. Throughout the course, numerous real-world examples demonstrate the practical application of Raman spectroscopy in cultural heritage research, enriching the learning experience.

Programming and Data Visualization for PhD students [8h]
Dr. Federico Maria Vivaldi, Università di Pisa

This advanced course is tailored for PhD students seeking to enhance their data analysis and visualization skills using R, a versatile and widely used programming language in the field of research. The student will learn the fundamentals of R programming, covering syntax, data types, and operations. Additionally, data manipulation and cleansing techniques for effective analysis will be discussed. Finally, ggplot2 package will be introduced for creating a wide range of static visualizations. By the end of this course, participants will be equipped with advanced R programming skills, a deep understanding of data visualization principles, and the ability to apply these techniques to enhance their research output. Students are invited to bring their own laptop to the lesson in order to apply the concepts learned.

Lignin: the challenges of its structural characterization and of its application as advanced material [8h]
Dr. Rosarita D'Orsi, Università di Pisa

Lignin is one of the main components of the cell wall of a plant. It is a non-carbohydrate polymer rich in aromatic rings with a highly complex structure, variable across different types of plant species due to the biosynthetic process. Due to the prominence of aromatic derivatives in strategic chemical sectors, several areas have explored the use of pure lignin. Nevertheless, the use of lignin in material sciences have been limited by the scarce knowledge on its structure. Several spectroscopic techniques could be used to achieve different information. This course will give an overview of the extraction methods to obtain a valuable form of lignin, the characterization methods to obtain useful information on its structure and its utility on chemicals production. Finally, the application of this material in different fields of advanced

materials will be discussed. This course could be attractive to all Ph.D. students working on biomass in various fields of application, from industry, valorisation, to cultural heritage and to students working on bio-based materials.

Isotopic Chemistry for the Radiolabeling of Pharmaceuticals [8h]
Dr. Antonio Del Vecchio, Università di Pisa

Isotope labeling represents a major chemical challenge in the fields of organic and inorganic research, in both academic and industrial settings. Among the many different uses, the practical application of (radio)isotopes spans from fossil datation to diagnostics, where the choice of the radioelement becames crucial for the patient. The present course aims to deliver the basic notions related to synthetic and applicative (radio)isotopic chemistry. A focus will be provided on the characteristic of the most important and frequently encountered isotopes, with a particular focus on applicative methodological syntheses for the incorporation [13C], [14C], [11C] and [18F] into drug precursors and biologically active compounds. Real examples regarding the radiolabeling of pharmaceuticals and PET tracers will be also critically discussed.

Communicating and disseminating research results: organization of a scientific event
Prof. Fabio Marchetti and Prof. Elisa Martinelli, University of Pisa

The course dedicated to PhD students in the second year is a laboratory-practical course aiming at providing PhD students with the knowledge and experience necessary for the organization of an international scientific dissemination event. The course will be followed by the allocation of practical tasks, and in particular the involved PhD students will live the experience of taking part in the scientific committee of an international scientific conference, i.e. the Chemistry for the Future (CFF) Conference which will be held in June-July 2025. Students will be guided by the teachers in all stages of the organization process, furthermore they will have the opportunity to test their acquired skills by contributing to the organization of Bright "European Researcher Night", which will be held in September 2025.

Students will be divided into groups and will be engaged in the following steps:

- determining the theme, scope, and goals of the conference;
- establishing a timeline outlining the key milestones in the conference planning process, such as the deadline for submitting abstracts, the date for finalizing the program, and the date of the conference itself;
- developing a budget plan, ensuring that the budget is realistic and feasible, and raising funds;
- choosing a suitable venue for the conference, taking into account different aspects such as capacity, accessibility and cost, and ensuring that the venue is equipped with the necessary facilities, such as audiovisual equipment, seating arrangements, and catering services;
- individuating and inviting plenary and keynote speakers to be involved in the conference, and ensuing that and that their travel and lodging expenses are covered;
- defining a detailed program of events, session titles, and speaker names, ensuring that the program is in alinement with the conference themes and objectives and with gender balance, and provides opportunities for networking and discussion;
- spreading the event through various channels, such as social media, email, and online advertising, ensuring that the conference website is constantly up-to-date and provides all the necessary information (registration details, speaker bios, and program updates);
- managing the logistics aspects, and in particular catering, display stands and audiovisual services;
- leading the conference according to the established program and timeline, facilitating networking opportunities and a positive experience for the participants;
- follow up with participants after the conference to obtain feedback and evaluate the strengths of the event and understand those aspect which could be improved with a view to other future events.