CORSI ORGANIZZATI DAL DSCM - 2023|2024

Application of infrared spectroscopy to the study of reaction mechanisms (10 h)
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Time-resolved IR spectroscopy is widely used in the study of reaction mechanisms in many fields of chemistry. This is related to recent developments of new instrumental approaches, as well as to the huge diffusion - in the last 2 - 3 decades - of commercial instruments capable of time-resolved measurements. Furthermore, in several cases static IR spectroscopy can also provide key pieces of information on reaction mechanism.This cycle of seminars is organized as follows:

1) I will first show the experimental methods, highlighting the most recent developments
2) I will then focus on band assignment and on the issue of reaction triggering
Finally, I will show selected examples from:
3) photochemical reactions
4) photobiological reactions
5) non-photoinduced reactions - catalysis, biochemistry, and reactions in solutions.

Examples will show that some key results can be obtained with relatively cheap instrumentation.

Chemistry and Materials Science Challenges in the Batteries Field (10 h)
Prof. Federico Bella, Politecnico di Torino
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Lithium (and post-lithium) batteries represent the main energy storage technology in the ongoing ecological transition. Although they have been marketed for over 30 years, their production is currently mainly located outside Europe and is based on critical raw materials and – often – on unsustainable processes. This course focuses on the current challenges of chemistry and materials science aimed at the development of anodes, cathodes and electrolytes for new battery generations. Particular attention is paid to the preparation of cobalt-free electrodes, to processes carried out in an aqueous environment and to the formulation of electrolytes capable of self-repair and guaranteeing long life to the batteries in which they are used. Finally, these aspects are contextualized in the European scenario where gigafactories for the production of lithium and post-lithium batteries are growing.

Advanced NMR methods: from molecular characterization to hyperpolarization (8 h)
Dr. Andrea Cesari, University of Pisa
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Nuclear Magnetic Resonance (NMR) spectroscopy is generally considered one of the most powerful and versatile analytical techniques. Stereochemical, dynamic, and thermodynamic features of a wide range of molecular entities (from small organic/organometallic species to macromolecules and polymeric materials) can be obtained. After briefly providing the basic NMR spectroscopy concepts and tools, the main objective of this course is to introduce the

students to the deepening of more advanced methodologies based on both 1- and 2-dimensional experiments. No prerequisite specific knowledge is required. Several case-studies on NMR methodologies accompanied by practical examples on pharmaceutical, optoelectronics, and chemosensing research fields will be discussed. The final part of the course will be dedicated to cutting-edge NMR techniques (e.g., hyperpolarization, SABRE, DNP). At the beginning of the course the students will be warmly invited to propose one or more problems of interest concerning their project. At the end of the course some solutions using the techniques proposed throughout the course will be discussed.

Atomic-level characterization methods in modern materials chemistry (10 h)

Prof. Dominik Kubicki, University of Warwick, Coventry (UK)
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The course will explore local structure characterization techniques, such as solid-state NMR, pair distribution function (PDF), muon spin relaxation (μSR), X-ray absorption (XAS), and Mössbauer spectroscopy. We will discuss them in the context of different classes of materials, such as metal-organic frameworks (MOFs), inorganic semiconductors (GaN, CdS etc.), halide perovskites, and glasses. You will learn about the physical principles underlying these techniques, and their applications in materials science. Through hands-on activities and case studies, you will develop a deeper understanding of the complementarity of local and long-range structure characterization techniques and the importance of using both. The course will be particularly useful for students interested in pursuing careers in materials science, chemistry, or related fields. Upon completion, you will have a strong foundation in local structure characterization techniques and their role in modern materials chemistry.

Gene therapy: a chemical perspective (8 h)

Prof. Lorenzo Di Bari, University of Pisa
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Gene therapy is at the frontline of current research for the treatment of acute, chronic and genetic diseases and conditions. It is based on synthetic oligonucleotides sequences, that interfere with gene expression. Nucleic acids therapeutics are conceptually very different from standard drugs, because they separate two actions: their target is controlled by the sequence and for this reason it is highly modular, while delivery and potency depend strongly on the chemical modification that one can introduce on the oligonucleotide itself. The course will briefly recall basic concepts of gene expression and of splicing, presenting siRNA, miRNA, shRNA, antisense oligonucleotides. The main classes of modified nucleotides will be presented, covering their chemical design, synthesis and stereochemistry features. The use of carriers to enhance delivery profile in vivo will be discussed. Among the methods to reveal and monitor hybridization with the target sequence and to determine the pairing thermodynamics and kinetics, we shall discuss calorimetry, fluorescence, circular dichroism, surface plasmon resonance. Finally, one can quantify efficacy e.g. by measuring protein expression downregulation (western blotting and other methods) and follow the fate of the nucleic acid therapeutic with imaging techniques, after coupling the synthetic oligonucleotide with suitable reporters.

Carbenes, Metal Carbenes & Carbenoids, Diazo Decomposition and Subsequent Reactivity (3 h)

Prof. Jerome Lacour, Universite de Geneve (CH)
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Carbenes, neutral compounds featuring a divalent carbon atom with only six electrons in its valence shell, have evolved from transient laboratory curiosities to diverse, and surprisingly impactful, synthetic intermediates. In this context, diazo compounds are a particularly useful class of carbene precursors – by reacting them in different manners like photochemically, thermally or with metal catalysts. Further, the use of metals as a catalyst generates metallocarbenes in the reaction medium which has similar reactivity to free carbenes. Several transition metal catalysts like Cu, Rh, Pd, Ru, etc. are employed to generate metal bound carbenes in the reaction medium. Many catalysts are used extensively in industry as well as in academia to catalyze series of subsequent transformations such as Wolff rearrangements, cyclopropanation and related reactions (including skeletal rearrangements), C-H / X-H insertions, cross-coupling organometallic reactions and, last but not least, ylide synthesis and subsequent reactivity. After discussing the intrinsic nature of carbenes and their metal analogues (Fischer vs. Schrock for instance), the course will concentrate on modern synthetic applications of the transient reactive species.

Design and analysis of experiments (12 h)

Prof. Fabio Di Francesco, University of Pisa
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The course is intended to provide the students with a toolbox of methods allowing them to develop empirical models describing the behaviour of complex systems for which a theoretical framework is not available. After a quick reminder of basic concepts (determination of model coefficients and their significance, significance and validation of a model) and a brief overview of the basic screening designs and response surface methodology, the student will delve into more advanced techniques including blocking in response surface design, mixture experiments and calibration designs to be used for multivariate calibration procedures. During the course, the student will be encouraged to use these techniques to design experiments concerning his/her research activity, whose results will be discussed in the classroom to turn theory into an everyday practice.

Communicating and disseminating research results: organization of a scientific event

Prof. Fabio Marchetti and Prof. Elisa Martinelli, University of Pisa
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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 2024. 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 2024.

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.