

Dottorato di Ricerca in Scienze Chimiche - Università degli Studi di Firenze

PROPOSTA DIDATTICA 2021

“It could work!” – Unconventional reaction activation techniques in organic synthesis	2
Advanced design and synthesis of catalytic antioxidants	3
Anion Coordination Chemistry Fundamentals	4
Applications of ultrafast spectroscopy	5
Focal Plane Array (FPA) Imaging FTIR: principles and applications	6
Fractals in chemistry: from theory to practical applications	7
From micro- to femto-moles, from small to giant molecules: the route of Modern Mass Spectrometry	8
Introduction to Python for scientist	10
Metabolomics and Nutrition – analytical approaches to investigate human responses to dietary intervention in health and disease	11
Metal Complexes as Drugs and Chemotherapeutic Agents	12
Orbital Interactions in Chemistry	13
Orbital Interactions in Chemistry: Hands on	14
Organocatalysis and photocatalysis: principles and recent synthetic applications	15
Polypyridyl compounds: from their use as chemosensors to their employment in the design of transition metal complexes featuring biological applications in combination with light	16
Small molecule libraries: synthetic methods and cheminformatics approaches	17
Smart Polymers for photonics and medicine	18
STRUCTURAL PROPERTIES OF GLASSES: AN INTRODUCTION	19
THz spectroscopy: from water to aqueous solutions of biomolecules	20

TITOLO DEL CORSO /COURSE TITLE:	"It could work!" – Unconventional reaction activation techniques in organic synthesis
SSD:	CHIM06
DOCENTE:	Dr. Daniele Franchi / Dr. Daniele Dessì - CNR-ICCOM
ABSTRACT:	<p>Heating and stirring are the most common reaction conditions, but not always the optimal ones: overcoming the activation energy barrier is just one of the requirements to start a chemical transformation. For some reactions, favouring energetic collision between reagents, supporting entropy variations, or initiating single electron pathways could be a smart trick to access fast kinetics and high selectivity. In these cases, unconventional physical activation agents such as high pressure, microwaves, ultrasounds, light irradiation, and applied voltages can provide unexpected improvements in the reaction outcomes, even under mild conditions. In this course, we will explore the physical principles behind unconventional activation methods that gave rise to new branches of chemistry, such as mechanochemistry, sonochemistry, photochemistry, and electrosynthesis. Suggestions on how to take advantage of these innovative procedures, especially in organic synthesis, will be offered by analysing successful examples reported in the literature. Finally, since these activation techniques often offer important improvements when focusing on environmentally friendly synthetic methods, conventional and unconventional procedures will be compared according to green chemistry metrics (E-factor, Eco-points, Solvents usage).</p>
Periodo di Svolgimento /Time Schedule:	Maggio-Luglio 2021
Prova di accertamento /Final test:	Ricerca e presentazione di un recente articolo scientifico che confronti due o più metodiche trattate del corso.

TITOLO DEL CORSO /COURSE TITLE:	Advanced design and synthesis of catalytic antioxidants
SSD:	CHIM06
DOCENTE:	Dr. Damiano Tanini - Dip. Chimica "Ugo Schiff"
ABSTRACT:	Antioxidants include a variety of molecules with broad structural diversity, widely employed in industrial processes, biology, medicinal chemistry, and food chemistry. The design and the development of new antioxidants have been attracting considerable interest over the last decades. This course will be focusing on recent advances in the chemistry of organic catalytic antioxidants. The synthesis and the study of the thiol-peroxidase-like activity of chalcogen-containing antioxidant small molecules will be described. Key structural features of relevant catalytic antioxidants, as well as the possibility to modulate and enhance the antioxidant properties by exploiting intramolecular chalcogen bonding interactions, will also be discussed. The aim of the course is to provide advanced tools for the successful design and synthesis of potent chalcogen-containing catalytic antioxidants.
Periodo di Svolgimento /Time Schedule:	Giugno-Luglio 2021
Prova di accertamento /Final test:	Lettura critica e discussione di un articolo scientifico sugli argomenti del corso (prova in lingua Inglese)

TITOLO DEL CORSO /COURSE TITLE:	Anion Coordination Chemistry Fundamentals
SSD:	CHIM03
DOCENTE:	Dr. Matteo Savastano - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<p>Anion Coordination Chemistry has a delay in its development of about $\frac{3}{4}$ of a century in comparison to its twin, Cation Coordination Chemistry. Such a setback arises both from practical limitations and chemists' general mindset. This course aims at telling the story from the beginning, guiding students in understanding that there is more than a vertical bar distinguishing a positive from a negative species. Once such differences are understood, it is possible to re-examine supramolecular forces holding together anion complexes. Among them, some are rarely known and fully understood by students, as their discussion can be hardly accommodated in today's already dense curricula. Examples include anion-π interactions, halogen bonding and solvent effect on complexation phenomena. Being unfamiliar at best, recognition, assessment, and quantification of such interactions is even less frequently discussed in academic courses, preventing full appreciation of the usefulness of these forces and perpetuating the false idea of Anion Coordination Chemistry as subordinate research field. This course intends to offer the basic tools required to join contemporary (and quite active) scientific discussion in this area.</p>
Periodo di Svolgimento /Time Schedule:	February 2020
Prova di accertamento /Final test:	Critical review and discussion of a scientific paper focusing on topics covered in the course

TITOLO DEL CORSO /COURSE TITLE:	Applications of ultrafast spectroscopy
SSD:	CHIM02 - ICCOM CNR
DOCENTE:	Dr. Mariangela Di Donato
ABSTRACT:	<p>The course aims at introducing the principal methodologies of ultrafast time resolved spectroscopies, giving an overview of the technical and experimental aspects connected with the use of ultrafast lasers. Examples of applications will be given concerning the study of photo-induced energy and electron transfer processes in complex molecular systems. Data analysis methods will be also presented. The specific content of the lectures will deal with:</p> <ul style="list-style-type: none"> -Introduction about ultrafast lasers and time resolved spectroscopic techniques -Pump-probe spectroscopy to study energy and charge transfer in multi-chromophore systems and proteins -Infrared and Raman time resolved spectroscopies -Two dimensional infrared and visible spectroscopies.
Periodo di Svolgimento /Time Schedule:	Marzo 2021
Prova di accertamento /Final test:	Lettura critica e discussione di un articolo scientifico sugli argomenti del corso

TITOLO DEL CORSO /COURSE TITLE:	Focal Plane Array (FPA) Imaging FTIR: principles and applications
SSD:	CHIM12
DOCENTE:	Dr. David Chelazzi - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<p>Coupling microscopy with Fourier Transform Infrared Spectroscopy (micro-FTIR) enables the non-invasive and non-destructive detection of molecular functional groups. The use of Focal Plane Array (FPA) detectors allows the simultaneous acquisition of spatially resolved IR spectra on an array of $n \times n$ pixels, each pixel corresponding to an independent spectrum. This technique can thus be used for the identification of low amounts of analytes that are heterogeneously distributed on relatively large areas (e.g. from millimeters to centimeters), with high spatial resolution (few microns), using arrays of 64×64 and 128×128 pixels. The possibility of working in transmittance, reflectance and ATR (Attenuated Total Reflectance) mode, makes the technique highly versatile: possible applications cover a wide range of fields, from biomedicine (analysis of tissues) and pharmaceutical research, to environmental chemistry (detection/identification of microplastics), and conservation of cultural heritage (assessment of the degradation and cleaning of artifacts).</p> <p>The course will focus both on fundamental principles and practical aspects, including some demonstration of the technique on a selection of samples.</p>
Periodo di Svolgimento /Time Schedule:	MARZO-APRILE 2021
Prova di accertamento /Final test:	Lettura critica e discussione di un articolo scientifico sugli argomenti del corso

TITOLO DEL CORSO /COURSE TITLE:	Fractals in chemistry: from theory to practical applications
SSD:	CHIM02
DOCENTE:	Dr. Giovanni Ferraro - Dip. Chimica "Ugo Schiff"
ABSTRACT:	Introduction to the fractal concept and examples: nanostructures, polymers, supramolecular systems. Fractals in chemistry: description of different surface patterns, processes affecting the cluster fractal dimension, link between colloidal dispersion, fractal dimension and macroscale properties. Experimental techniques available to estimate the fractal dimension at different length scale: small-angle X-ray scattering, microscopy, rheology and gas adsorption. Description of a surface pattern: differences between fractality and lacunarity. Practical activity: introduction to the use of the FracLac software and measurement of fractal dimension and lacunarity of a 2D image using the box counting approach.
Periodo di Svolgimento /Time Schedule:	Giugno - Settembre 2021
Prova di accertamento /Final test:	Da concordare con studenti

TITOLO DEL CORSO /COURSE TITLE:	From micro- to femto-moles, from small to giant molecules: the route of Modern Mass Spectrometry
SSD:	CHIM06/CHIM08
DOCENTE:	Dr. Domenico Garozzo - CNR-IPCB
DOCENTE PROPONENTE:	Prof. Cristina Nativi - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<p>The mass spectrometer: a chemical lab</p> <p>The definition of a mass spectrometer from the American Society for Mass Spectrometry (ASMS) is: "A mass spectrometer is an instrument that measures the masses of individual molecules that have been converted to ions; i.e., molecules that have been electrically charged"; using simply words: a machine used to weigh molecules. This definition is obviously correct, but the mass spectrometer is much more than an instrument. It is a complete laboratory for the investigation of molecules, clusters, and other species under the environment-free conditions of the gas phase. For this reason, Mass Spectrometry (MS) is widely used today by almost all chemists and many researchers from neighboring disciplines such as physics, medicine, or biology as a powerful analytical tool. Today the mass spectrometer is more and more present in the pharmaceutical industry, in the biological labs, in the hospitals and in many other bio-labs, while until few years ago it was present only in specialized chemical lab. This revolution starts at the end of 1980s with the introduction of two different methods able to desorb and ionize molecules with molecular weights in a range from few hundreds daltons to millions. Until then, a few techniques, fast atom bombardment (FAB), plasma desorption (PD) and desorption chemical ionization (DCI) were able to carry out in the gas phase and to ionize molecules with a molecular weight greater than one thousand, but they all required high concentrations of sample and they did not work at all for larger molecules such as proteins or polymers. Then, in 1988, Electrospray ionization (ESI) invented by John B. Fenn and Matrix assisted laser desorption (MALDI) introduced by Franz Hillenkamp and Michael Karas appeared almost simultaneously. These desorption-ionization methods revolutionized MS and are the main forms of ionization to this day. In the beginning the two techniques were not believed robust enough, but at the end of 1990s almost all MS instruments on the market were MALDI or ESI.</p> <p>Few application examples</p> <p>Pharmacokinetics</p> <p>Pharmacokinetics is often studied using mass spectrometry because of the complex nature of the matrix (often blood or urine) and the need for high sensitivity to observe low dose and long time point data. The most common instrumentation used in this application is LC-MS with a triple quadrupole mass spectrometer. Tandem mass spectrometry is usually employed for added specificity. Standard curves and internal standards are used for quantitation of usually a single pharmaceutical in the samples. The samples represent different time points as a pharmaceutical is administered and then metabolized or cleared from the body. Blank or t=0 samples taken before administration are important in determining background and ensuring data integrity with such complex sample matrices. Much attention is paid to the linearity of the standard curve; however, it is not uncommon to use curve fitting with more complex functions such as quadratics since the response of most mass spectrometers is less than linear across large concentration ranges. There is currently considerable interest in the use of very high sensitivity mass spectrometry for microdosing studies, which are seen as a promising alternative to animal experimentation.</p> <p>Protein characterization</p> <p>Mass spectrometry is an important emerging method for the characterization and sequencing of proteins. The two primary methods for ionization of whole proteins are electrospray ionization (ESI) and matrix-assisted laser desorption/ionization (MALDI). In keeping with the performance and mass range of available mass spectrometers, two approaches are used for characterizing proteins. In the first, intact proteins are ionized by either of the two techniques described above, and then introduced to a mass analyzer. This approach is referred to as "top-down" strategy of protein analysis. In the second, proteins are enzymatically digested into smaller peptides using proteases such as trypsin or pepsin, either in solution or in gel after electrophoretic separation. Other proteolytic agents are also used. The collection of peptide products are then introduced to the mass analyzer. When the characteristic pattern of peptides is used for the identification of the protein the method is called peptide mass fingerprinting (PMF), if the identification is performed using the sequence data determined in tandem MS analysis it is called de novo sequencing. These procedures of protein analysis are also referred to as the "bottom-up" approach.</p> <p>Bottom-Up Proteomics</p> <p>In bottom-up proteomics, the analytes introduced into the mass spectrometer are peptides generated by enzymatic cleavage of one or many proteins. The proteins can first be separated by 2Dgel, SDSGel or chromatography, in which case the sample will contain only one or a few proteins. Alternatively, a complex protein mixture initially can be digested to the peptide level, then separated by on-line chromatography coupled to electrospray mass spectrometry (ESI-MS). In the latter case, the digest can contain thousands to hundreds of thousands of peptides, and require separation in two or more chromatographic dimensions before MS analysis. The identity of the original protein is determined by</p>

	<p>comparison of the peptide mass spectra with theoretical peptide masses calculated from a proteomic or genomic database. There are two approaches for protein identification using the bottom-up approach, peptide mass fingerprinting and tandem MS (MS–MS).</p> <p>Peptide mass fingerprinting: In peptide mass fingerprinting, peptide masses obtained from an MS scan are compared to calculated peptide masses generated by "in silico" cleavage of protein or gene sequences in the database using the same specificity as the enzyme that was employed in the experiment. One disadvantage of peptide mass fingerprinting is the requirement for pure proteins or simple mixtures of proteins. The purification steps therefore limit the throughput of the peptide mass fingerprinting approach. Another disadvantage is the requirement for several peptides to uniquely identify a protein. Peptide mass fingerprinting can be performed with ESI or MALDI instruments. Mass accuracy better than 100 ppm is mandatory.</p> <p>Tandem MS: In MS-MS, peptide ions are isolated in the mass analyzer and subjected to dissociation to produce product ion fragments. The product ion spectra are compared with databases by crosscorrelation analysis to identify the intact protein. (see below)</p> <p>Glycan analysis</p> <p>Mass spectrometry (MS), with its low sample requirement and high sensitivity, has been the predominantly used in glycobiology for characterization and elucidation of glycan structures. Mass spectrometry provides a complementary method to HPLC for the analysis of glycans. Intact or permethylated glycans may be detected directly as singly charged ions by matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) or, Electrospray ionization mass spectrometry (ESI-MS) also gives good signals for the smaller glycans. Various free and commercial software are now available which interpret MS data and aid in Glycan structure characterization</p> <p>Differences between MALDI mass spectra of permethylated Tf N-glycans from three patients with unsolved CDG type II: (a) healthy control, (b) CDG-IIx(1) patient showing a remarkable hyposialylation and a less intense galactosylation defect, (c) CDG-IIx(2) patient with a severe sialylation and galactosylation deficiency and (d) CDG-IIx(3) patient presenting a pure sialylation defect.</p>
<p>Periodo di Svolgimento /Time Schedule:</p>	<p>periodo febbraio-marzo 2021 / settembre 2021</p>
<p>Prova di accertamento /Final test:</p>	<p>Da concordare con gli studenti</p>

TITOLO DEL CORSO /COURSE TITLE:	Introduction to Python for scientist
SSD:	CHIM03
DOCENTE:	Dr. Giuseppe Cucinotta - Dip. Chimica "Ugo Schiff"
ABSTRACT:	For today scientists (and not only) the knowledge of a programming language is one of the most valuable skills. Python represents one of the most widespread program languages used in very different fields including, just to name a few, mobile apps realization, web development, machine learning. This course intends to give an overview of the possibilities offered by Python to scientists and to provide the students with the basic instruments to start using Python for data analysis. No particular programming knowledge is requested to attend the lessons, indeed this course will at first introduce Python fundamentals including main built-in types (numbers, strings, lists), flow control tools (if... then... else statement, for and while loops) and functions. Following, principal scientific libraries (NumPy, SciPy, Matplotlib) will be presented and how to use them to create arrays, make computations, plot and analyse data. Input/output methods to read and write data to files will also be explained.
Periodo di Svolgimento /Time Schedule:	Giugno 2021
Prova di accertamento /Final test:	The assignment will consist in writing a Python program to be discussed with the teacher.

TITOLO DEL CORSO /COURSE TITLE:	Metabolomics and Nutrition – analytical approaches to investigate human responses to dietary intervention in health and disease
SSD:	CHIM01
DOCENTE:	Dr. Maria Ulaszewska - San Raffaele Scientific Institute, Proteomics and Metabolomics Facility
DOCENTE PROPONENTE:	Prof. Massimo Del Bubba - Dip. Chimica “Ugo Schiff”
ABSTRACT:	<p>Nutrimetabolomics, which represents the intersection of metabolomics and nutrition research, offers an opportunity to investigate the effects of whole diets, specific foods, and food components on the human metabolome. Nutrimetabolomics plays an important role in the discovery of new food intake biomarkers, validation of food frequencies questionnaires and assessment of dietary compliance or dietary patterns. Furthermore, the application of nutrimetabolomics within dietary interventions might help to characterize the molecules responsible for modulating health and identifying their mechanism of action.</p> <p>This course will provide students with entire workflow for metabolomics science applied to nutrition from study design to interpretation of results. Particular emphasis will be put on analytical chemistry and instrumental aspects of the work.</p>
Periodo di Svolgimento /Time Schedule:	6-10 Settembre 2021
Prova di accertamento /Final test:	Lettura critica e discussione di un articolo scientifico sugli argomenti del corso.

TITOLO DEL CORSO /COURSE TITLE:	Metal Complexes as Drugs and Chemotherapeutic Agents
SSD:	CHIM03
DOCENTE:	Dr. Lara Massai - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<ul style="list-style-type: none"> - brief overview of the physical and chemical properties of metal complexes - metallo-drugs and their action; nature and structure of biological targets, - illustration of the steps from drug discovery to marketplace - focus on individual metallo-drugs, drug candidates and metal-containing agents used to treat and diagnose disease, their synthesis, structures and known mechanisms of action.
Periodo di Svolgimento /Time Schedule:	Giugno/Luglio 2021
Prova di accertamento /Final test:	Oral presentation (five/six slides) on a paper related to the topics covered

TITOLO DEL CORSO /COURSE TITLE:	Orbital Interactions in Chemistry
SSD:	CHIM03
DOCENTE:	Prof. Federico Totti - Dip. Chimica "Ugo Schiff"
ABSTRACT:	The course will cover the construction of molecular orbital interactions through a perturbative theoretical approach. In this framework, the operative applications will cover both organic and inorganic species. The aim of the course is to make the student able to sketch the electronic structure of the species under study in order to understand and predict their reactivity and electronic properties.
Periodo di Svolgimento /Time Schedule:	Febbraio 2020
Prova di accertamento /Final test:	Colloquio: verrà discussa l'applicazione degli argomenti presentati nel corso alla propria attività di ricerca

TITOLO DEL CORSO /COURSE TITLE:	Orbital Interactions in Chemistry: Hands on
SSD:	CHIM03
DOCENTE:	Prof. Tulika Gupta - Banaras Hindu University
DOCENTE PROPONENTE:	Prof. Federico Totti - Dip. Chimica "Ugo Schiff"
ABSTRACT:	The course will give the basics to perform simple calculations on ab initio packages of programs on inorganic complexes. The course includes the building and running of inputs. Theoretical aspects learned at the course Orbital Interactions in Chemistry will be exploited to rationalize the computed electronic structure. At request, organic systems will be also considered.
Periodo di Svolgimento /Time Schedule:	Da definire in base ad emergenza Covid
Prova di accertamento /Final test:	Building, running of one input and interpretation of the results.

TITOLO DEL CORSO /COURSE TITLE:	Organocatalysis and photocatalysis: principles and recent synthetic applications
SSD:	CHIM06
DOCENTE:	Prof. Daniele Leonori - University of Manchester
DOCENTE PROPONENTE:	Prof. Franca Cordero - Dip. Chimica "Ugo Schiff"
ABSTRACT:	Organocatalysis and photocatalysis have made remarkable progress in modern chemical synthesis. Organocatalysts are small organic molecules that catalyse organic transformations by regulating the chemical reactivity of the substrates. Photocatalysts absorb visible light to induce their photoexcited states which can activate unreactive substrates via electron or energy transfer mechanisms. Moreover, in the last few years, several achievements have been obtained using the combination of photocatalysis and organocatalysis. In this course fundamentals and recent developments of these techniques will be discussed.
Periodo di Svolgimento /Time Schedule:	Settembre 2021
Prova di accertamento /Final test:	written test

TITOLO DEL CORSO /COURSE TITLE:	Polypyridyl compounds: from their use as chemosensors to their employment in the design of transition metal complexes featuring biological applications in combination with light
SSD:	CHIM03
DOCENTE:	Dr. Luca Conti - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<p>Polypyridyl compounds are attractive molecules that have been largely used, especially in combination with polyamine macrocyclic frameworks, to develop efficient receptor systems for selected substrates in aqueous solution, including ions of environmental and biological relevance. However, the use of these compounds is not limited to such purpose. In fact, they can be successfully combined with transition metal ions affording challenging metal complexes with application in the bio-medical field, as anticancer as well as antibacterial agents. Their high biological relevance arises from their rich chemical-physical repertoire, which permits to achieve, upon irradiation with low-energy light, different mechanisms of action. A fine choice of the characteristics of the metal ion along with those of the polypyridyl ligands, makes it possible to easily switch from a pure Photodynamic Therapy (PDT) approach to a more intriguing Photo-Activated Chemotherapy (PACT) strategy, being the latter less dependent on molecular oxygen and thus offering a valuable alternative for the treatment of pathologies with a marked hypoxic nature. The aim of this course is to introduce the fundamentals of the rationale design of polypyridyl-based systems for application as chemosensors and as therapeutic agents. A comprehensive and multidisciplinary understanding of the different mechanisms that underlie their biological potential will be also provided.</p>
Periodo di Svolgimento /Time Schedule:	May/June 2021
Prova di accertamento /Final test:	Critical review and discussion of a scientific paper focusing on topics covered in the course.

TITOLO DEL CORSO /COURSE TITLE:	Small molecule libraries: synthetic methods and cheminformatics approaches
SSD:	CHIM06
DOCENTE:	Dr. Elena Lenci - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<p>Drug discovery is a long and arduous process, as only 1 molecule out of 5000 hit candidates can reach the market. Thus, the generation of large compound collections to be applied in high-throughput screening (HTS) and phenotypic assays is necessary to maximize the chance of finding new bioactive chemical entities. New frontiers in the synthesis of small molecule libraries have been recently explored in order to improve the quality and quantity of small molecules representing a library. Also, cheminformatics approaches are very much used for the design and the evaluation of chemical libraries. This class aims to give an overview on the main synthetic and cheminformatics approaches used in this context. The topics of the class can be summarized as follows:</p> <ul style="list-style-type: none"> - Chemical libraries: concepts, historical perspective and applications in drug discovery. - Synthetic methods: combinatorial chemistry, diversity-oriented synthesis, multicomponent reactions, late-stage functionalization. - Cheminformatics approaches: computer representation of chemical structures, database management systems, descriptors of similarity and diversity. - Selected case studies of the application of both synthetic and cheminformatics methods to generate and evaluate new chemical libraries.
Periodo di Svolgimento /Time Schedule:	Febbraio 2021
Prova di accertamento /Final test:	Critical review and discussion of a scientific paper focusing on topics covered in the course

TITOLO DEL CORSO /COURSE TITLE:	Smart Polymers for photonics and medicine
SSD:	CHIM04
DOCENTE:	Dr. Camilla Parmeggiani - Dip. Chimica "Ugo Schiff" Dr. Daniele Martella - INRIM
ABSTRACT:	We will briefly describe selected class of smart polymers (stimuli responsive networks, hydrogel, etc.) together with their application in different research field, such as photonics and medicine. The examples will spine from tunable micro lasers and innovative approach to cryptography, to cell scaffold, biosensors and cardiac devices.
Periodo di Svolgimento /Time Schedule:	2-4-9-11 febbraio 2021
Prova di accertamento /Final test:	lettura critica e discussione di un articolo scientifico sugli argomenti del corso

TITOLO DEL CORSO /COURSE TITLE:	STRUCTURAL PROPERTIES OF GLASSES: AN INTRODUCTION
SSD:	CHIM02
DOCENTE:	Dr. Giorgio Signorini - Dip. Chimica "Ugo Schiff"
ABSTRACT:	Glass structure description: pair distribution function $g(r)$ and other structural parameters. Overview of experimental methods of glass structure investigation: methods based on scattering/diffraction; principles of NMR and vibrational spectroscopy. Computational methods: Monte Carlo and Molecular Dynamics simulations. Structural models of glasses: continuous random network, bonding models; random close packing. Structure of various groups of glasses and structure/properties relationship. Simple, one component, oxide glasses: silica glass and boron oxide glass. Oxide glasses with modifiers. Borate glasses with more than one glass former. Non-oxide glasses: mainly covalent glasses, metallic glasses, mixed-salt glasses
Periodo di Svolgimento /Time Schedule:	Marzo 2021
Prova di accertamento /Final test:	analisi di letteratura recente su un argomento trattato nel corso

TITOLO DEL CORSO /COURSE TITLE:	THz spectroscopy: from water to aqueous solutions of biomolecules
SSD:	CHIM02
DOCENTE:	Dr. Federico Sebastiani - Dip. Chimica "Ugo Schiff"
ABSTRACT:	<p>Terahertz (THz) frequencies span the range of low-energy excitations in electronic materials, low-frequency vibrational modes of condensed phase media, and vibrational and rotational transitions in molecules, making this a key spectral range for probing fundamental physico-chemical properties as well as for practical applications. This frequency region, broadly defined as 0.1–30 THz ($\nu=3\text{-}1000\text{ cm}^{-1}$, $\lambda=3000\text{-}10\text{ }\mu\text{m}$), occupies a large portion of the electromagnetic spectrum between (and partially overlapping to) the infrared and microwave ranges.</p> <p>THz radiation is an ideal tool to probe the collective intermolecular dynamics of water molecules. Such dynamics i) play an active role in the structural plasticity of proteins, ii) are involved in bio-reactions like drug intercalation into DNA, iii) are thought to be the drive of the structural rearrangements of the molecular network. The collective dynamics of the hydrogen-bonded network dictate the unique solvation properties of water, and are at the origin of the puzzling physical and chemical properties of this special liquid.</p> <p>The intention of this course is to provide an overview of THz and far infrared spectroscopy, introducing the fundamentals of the technique, and briefly illustrating the ability of THz spectroscopy to study water and its interaction to biomolecules.</p>
Periodo di Svolgimento /Time Schedule:	01 LUGLIO 2021-30 LUGLIO 2021; 01 SETTEMBRE 2021-10 SETTEMBRE 2021
Prova di accertamento /Final test:	Lettura critica e discussione di un articolo scientifico sugli argomenti del corso