A.D. 1308
unipg
DIPARTIMENTO DI CHIMICA,
BIOLOGIA E BIOTECNOLOGIE

PhD Program in Chemical Sciences

A PhD Program of the Dipartimento di Chimica, Biologia e Biotecnologie (DCBB) of the Università degli Studi di Perugia

Ad-Hoc Courses Offered for the Academic Years

2020/2021 (XXXVI cycle ongoing and previous ones)
2021/2022 (XXXVII cycle and previous ones)
2022/2023 (XXXVIII cycle and previous ones)
2023/2024
2024/2025

Coordinator: Prof. Luigi Vaccaro

Lectures will be held in room A of the DCBB at via Elce di Sotto 8, and/or at the PhD dedicated MicrosoftTeams room.
The exact time will be updated on the webpage and communicated via email to all PhD students.
Final schedule will be also advertised on the screens in the main entrance of the DCBB.

** Course organized in collaboration with the Dipartimento di Scienze Farmaceutiche (DSF) with the PhD Programme in Pharmaceutical Sciences.*

November 23 - December 7, 2020
Electron transfer in molecules and in condensed phases: Fundamentals and applications *(18, 3CFU)*
Dr. Francesco Ambrosio, IIT Genova, Italia

Electron transfer (i.e. the movement of an electron from one atom/molecule/material to another) is ubiquitous in a plethora of relevant chemical reactions, ranging from biological processes such as photosynthesis to electrochemistry in aqueous solution and charge transfer in materials and at homogenous or heterogeneous interfaces of relevance for photovoltaics and photocatalytic applications. In this course, the theory of electron transfer will be reviewed along with applications in different fields of chemistry. Furthermore, the interplay between experiment and theory in the study of charge-transfer processes will be discussed by analysing in detail some significant case studies.

January 11-15, 2021
Catalytic approaches in the synthesis of biologically relevant molecules *(12h, 2 CFU)**
Dr. Luca Sancineto, Università degli Studi di Perugia

In the era of a green new deal and given the importance of catalysis for the development of sustainable synthetic processes, the aim of the course is to provide an overview of the most recent advancements regarding biomimetic and metal-based approaches. Particular emphasis will be devoted to biomimetic approaches in oxidative transformations, and metal catalysts employed in C-C bond formation and activation of otherwise unreactive C-H groups.

January 18-29, 2021
Theoretical modelling of reactivity and energy transfer in astrochemistry and planetary atmospheres *(18 h, 3 CFU)*
Prof. Andrea Lombardi, Università degli Studi di Perugia

The amount of data sent by the probes exploring the solar system and planetary atmospheres, and the astronomical discovery of numerous molecules of increasing complexity in interstellar space, implicates a remarkable relevance of the modern chemistry for the science of the Universe. The interpretation of the resulting ample phenomenology needs to be assisted by theoretical and computational modelling of energy exchanges and reactions involving chemical species to set up data bases and improve kinetic models.

February 15– March 19, 2021
Continuous flow technologies for the preparation of pharmaceutically relevant molecules *(18 h, 3 CFU)*
Dr. Francesco Ferlin, Università degli Studi di Perugia

Modern chemical production relies on the development of innovative technologies that could allow the preparation of the desired chemicals at the highest chemical and economic efficiency.
Flow technologies have proved to be powerful synthetic tools for accessing complex molecular entities in a faster and user friendly manner. The use of flow reactors has also proven to be very effective for the definition of protocols featuring easier purification of the pure products leading to a minimal waste production and

consequently a lower cost of the synthetic process. In this course, the student will be introduced to the fundamental aspects of flow chemistry and some examples of application of this technology to relevant target will be also presented.

February, 2021
***Process Analytical Technology and Chemometrics in the Pharmaceutical Industry** (2h, 2CFU)**
Prof. Emidio Camaioni, Università degli Studi di Perugia
Dr. Remo Simonetti, Janssen

The course will show some recent PAT (Process Analytical Technology) implementations in the drug oral solid pharmaceutical industry. Examples of spectroscopic and non-spectroscopic applications will be discussed such as:
• PAT for the real-time evaluation of the particle size distribution during fluidized bed granulation;
• PAT for real-time evaluation of blending uniformity;
• PAT for real-time evaluation of the API content uniformity in the tablets.

February-March, 2021
***Concepts in Metabolomic Analysis. Applications to the analysis of medicinal plants and complex natural products** (12h, 2CFU)*
Dr. Luisa Mattoli, Aboca

Course description: Natural substances and plant metabolites. Mass spectrometry in the Metabolomic Analysis. Identification of metabolites. Targeted and untargeted metabolomics. Identification of metabolites and their quantitative determination. Regulatory implications and study of biological activity. Analysis of metabolites by phytochemical class: the case of alkaloids and phenols. Research applications and examples for quality control.

March 30, 2021

STiBNite 1st Network Symposium: Global Challenges in Materials Science
This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 956923
https://zoom.us/j/95885450604?pwd=dW52M2dZUjhiMzhDdHBhMVhKbEY3Zz09
Meeting ID: 958 8545 0604

***09.50 – 10.00**: Opening address*
Prof. Tatiana Da Ros, Prof. Paolo Tecilla and Prof. Davide Bonifazi
***10.00 – 10.50**: Prof. Danila Moscone*
(Università degli Studi di Roma Tor Vergata, Italy)
Chair: Prof. Paolo Tecilla
***11.00 – 11.50**: Prof. Stephen Wuttke*
(Ikerbasque, Spain)
Chair: Prof. Jean-Christophe Charlier
***12.00 – 12.50**: Mr. Wolfgang Mildner*
(MSWTech, Germany)
Chair: Ms. Susana Otero

***15.00 – 15.50**: Prof. Mauricio Terrones*
(Penn State University, USA)
Chair: Prof. Tatiana Da Ros
***16.00 – 16.50**: Prof. Klaus Müllen*
(Max Planck Institute, Germany)
Chair: Prof. Davide Bonifazi
***17.00 – 17.50**: Prof. Brent S. Sumerlin*
(University of Florida, USA)
Chair: Prof. Ruben Costa

April 12-16, 2021
X-Ray powder diffraction for pharmaceutical applications in drug discovery
*(12h, 2 CFU)**
Prof. Riccardo Vivani, Università degli Studi di Perugia

Course description. Introduction to the solid state: crystals and amorphous state, crystal lattice, unit cell and asymmetric unit, elements of symmetry in crystals, forms of crystals, energetics of crystals and relationships with the main chemical-physical properties, polymorphism. Introduction to diffraction techniques. Basic theory of powder diffraction. Sample preparation. Description of the instrumentation. Phase recognition. Determination of the unit cell. Profile fitting, structure refinement (Rietveld). Hints on structural resolution. Crystallographic databases and description of the CIF file. Quantification of mixtures: tutorial session at the computer room

Giornate della Green Chemistry.
workshop verranno trasmessi sul ***Canale YouTube*** *del GC-CS in* ***diretta streaming****, raggiungibile al link:*
https://www.youtube.com/channel/UCcvxptABZ0j2jEiD31I0JHg
Il collegamento sarà anche disponibile dalla ***Pagina Facebook del GC-CS:***
https://www.facebook.com/SCIgreenchem

April 27, 2021
CO2 as a strategic green carbon source for the synthesis of target materials
14.45 Prof. Arjan Kleij, *Institute of Chemical Research of Catalonia (ICIQ)*
"Carbon Dioxide as a Feedstock for Reactive Monomer and Functional Polymer

15.30 Prof. Shoubhik Das, *University of Antwerp*
"Do we really need transition metals for CO2-Promoted reactions and others?"

May 4, 2021,
Ultrasound as a key modern tool for green synthesis and processing

14.45 Prof. Pedro Cintas Moreno, *Universidad de Extremadura*
"Introduction to Sonochemistry and Role of Ultrasound in Green Chemistry and Synthesis"
15.15 Dr. Judy Lee, *University of Surrey*
"Sonocrystallization Introduction, State of the Art and Applications"
15.45 Prof. Giancarlo Cravotto, *University of Turin*

"Cavitational Technologies, Current Applications and Perspectives"

11 Maggio, 2021
Microalgae, a source for future biobased green processes

14.45, Prof. Michel H. M. Eppink, *University of Wageningen*
"Multiproduct Microalgae Biorefineries Mediated by Ionic Liquids"

March 20-May 15 2021
Data Scientist with R *(18 h, 3 CFU)*
Dr. Gianandrea La Porta, Università degli Studi di Perugia

Data science is the practice of transforming data into knowledge, and R is one of the most popular programming language used by scientists. The course aims to provide students with: i) the skills necessary to use the R programming language, ii) the principles of statistics to analyze and transform data, and iii) the functions to create and interpret descriptive and multivariate statistics, graphic representations, and statistical models.
Note: Lectures will be held on Monday at 3pm.

June 7-20, 2021
Introduction to Theoretical Inorganic Chemistry *(18 h, 3 CFU)*
Dr. Giovanni Bistoni, Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr, Germany

Introduction to Theoretical Inorganic Chemistry

This course aims to present the theoretical framework that underlies modern theoretical inorganic chemistry. The theory behind the most popular computational methods will be briefly introduced. The students will gain a general understanding of what methods can be used to tackle specific chemical problems. About half of the available hours will be used to present and discuss research papers that rely

on computational methods to solve chemical problems, such as the calculation of reaction energies, barriers, as well as other properties of chemical reactions in gas phase and in solution. The methods used, their strengths and limitations, and how they were used to interpret the chemistry concerned, will be discussed.

January 17-26, 2022
***Introduction to retrosynthetic analysis and its application to the synthesis of antiviral drugs** (12h, 2 CFU)**
Prof. Andrea Temperini, Università degli Studi di Perugia

The aim of the course is to provide a rational approach to organic synthesis through disconnections and interconversions of functional groups. Synthons and synthetic equivalents as well as evaluation of the flexibility and convenience of a linear or convergent synthesis and together with the comparative study of industrial and laboratory synthetic strategies for the preparation of Oseltamivir phosphate will be discussed.

February 1-15, 2022
***Raman micro-spectroscopy: theory and applications** (18 h, 3 CFU)*
Prof. Paola Sassi, Università degli Studi di Perugia

The course aims to provide students with the tools necessary to use Raman spectroscopy in the microscopic characterization of different types of materials, from clays to cells. Starting from the description of the Resonant Raman and Raman effect (6 h), passing through the concepts that underlie microspectroscopy (2 h), the theoretical and experimental aspects of the most recent techniques of light scattering spectroscopy will be illustrated. In particular, the following techniques will be presented: SERS (Surface Enhanced Raman Scattering; 2 h); TERS (Tip Enhanced Raman scattering; 2 h); ROA (Raman Optical Activity; 2 h) and EDLS (Extended Depolarized Rayleigh Scattering; 2 h). A two-hour practice exercise will also give the students the possibility to analyze different samples with

the micro-Raman instrumentation available in the "Molecular Spectroscopy" Lab of this Department.

10-20 February, 2022
Multiple applications of enantioselective liquid chromatography: from the control of asymmetric synthesis to the study of biological matrices *(12h, 2 CFU)**
Prof. Roccaldo Sardella, Università degli Studi di Perugia

Course description. The Course intends to provide information on the different fields of application of enantioselective liquid chromatography. Focus will be mostly given on the way to identify the best chiral stationary phase-mobile phase combination, according to the matrix of interest, and the detection system. in this framework, the basic principles of the method development process will be given. The basic notions of the preparative-scale chiral chromatography will be given as well.

February 15-28, 2022
Homogeneous catalysis by theoretical chemistry *(18 h, 3 CFU)*
Prof. Paola Belanzoni, Università degli Studi di Perugia
Dr. Leonardo Belpassi, CNR-SCITEC

The enormous challenge of moving our societies to a more sustainable future offers several exciting opportunities for computational chemists. The first principles approach to "catalysis by design" will enable new and much greener chemical routes to produce vital fuels and fine chemicals. This prospective outlines a wide variety of case studies to underscore how the use of theoretical techniques can be applied to biocatalysis and homogeneous catalysts to provide invaluable insights into the reaction mechanisms. In particular, homogeneous catalysis by transition metal complexes and biomimetic catalysts will be addressed through a density functional theory (DFT) approach, based on the state-of-the-art computational protocols.

March 01-15, 2022
An introduction to synchrotron radiation based X-ray methods: fundamentals and applications *(18 h, 3 CFU)*
Dr. Letizia Monico, CNR-SCITEC

The course will provide an introduction to the general properties of synchrotron radiation and details about the design of current beam-lines in synchrotron radiation facilities. Lectures will include explanations of the basic principles of X-ray interactions with matter and description of different x-ray techniques, including X-ray absorption and emission spectroscopy methods (both in 2D and 3D mode) and X-ray scattering techniques.
For each method, some applications will be presented and examples will cover chemical/structural studies in the fields of materials and life sciences, environmental chemistry, catalysis, earth and planetary sciences, heritage science.

March 28-31, 2022
Nuclear magnetic resonance for structure elucidation of organic compounds, *(12h, 2 CFU)**
Prof. Claudio Santi, Università degli Studi di Perugia

Focusing on novel aspects of method and instrumentation development, applications in emerging fields and new techniques and technologies, the course will illustrate the main relevant advances in the field of NMR. The aim is to facilitate greater understanding and encourage wider use of NMR techniques in structural elucidation of small and macromolecules as well as in metabolomics and host-guest interactions. Particular enphasis will be given on the relevance of this techniques in the early phase drug discovery.

April 25 – April 29, 2022 (in presence)
Introduction to Industrial Catalysis *(6h, 1CFU)*
Dr. Roger Kuhlman, Texas, USA

Chemistry students naturally experience an academic environment while training, but many obtain their final degrees with very limited exposure to the nature of industrial research. This course will provide: (1) A comparison of academic and industrial research, including funding decisions, project team structures and collaborations; (2) A high-level overview of chemical manufacturing considerations, such as safety, supply-demand, margin velocity, competitive advantages; (3) Important factors for implementation of catalysis in industrial processes, featuring things like cost, purity, safety and compliance.

May 2 – May 20, 2022, (in presence)
***Catalysis in Industrial Processes** (12h, 2CFU)*
Dr. Roger Kuhlman, Texas, USA

This course will feature various homogenous and heterogenous catalyzed processes across the value chain of commodity chemicals, starting with raw materials such as oil, natural gas and naphtha and ending with high-value products like emulsion polymers and chiral drug precursors. About one catalyzed reaction will be presented per lecture, whenever possible including aspects of process considerations, history of catalyst development, current best mode, mechanism, and persisting challenges. Some of the processes to be covered are hydrocracking, epoxidation, amination, arene alkylation, hydroformylation, and multiple types of polymerizations.

15-31 May , 2022
***Single Crystal X-Ray diffraction. Fundamentals, techniques and applications** (18 h, 3 CFU)*
Prof. Ferdinando Costantino, Università degli Studi di Perugia

The course will focus on the XRD single crystal diffraction techniques and it will be organized in three parts:
-Fundamentals of crystallography and diffraction theory
-X-ray single crystal diffractometry: instruments and methodologies
-Applications: from small molecules to functional materials to macromolecules

16-27 May, 2022 (first week online, second in presence)
Mass spectrometry: principles and applications to Omics *(18 h, 3 CFU)*
Dr. Maria Fedorova, University of Leipzig, D

The course will cover an introduction to mass spectrometry, from principles to applications to Omics. Instrumentations and acquisition modes will be described, together with methods design, development and optimization. Finally, applications to OMICs will be described and discussed. In particular, the course will cover: introduction to mass spectrometry; static and direct infusion MS; principles of LC-MS coupling; Hybrid MS instruments and principles of method designs; data-dependent and data-independent acquisitions – principles of method development and optimization; Targeted MS – multiple reaction monitoring and parallel reaction monitoring; Quantitative MS; proteomics, lipidomics and metabolomics.

June 1-15, 2022
Computational Chemistry and Classical Molecular Dynamics: carbon-nano structures applications *(18 h, 3 CFU)*
Dr. Noelia Faginas Lago, Università degli Studi di Perugia

This course treats advanced molecular dynamics (MD) methodology for classical simulations in order to evaluate uptake and adsorption properties of small gases on carbon based materials like graphene, γ-graphynes, COFs. MD simulations provide atomistically detailed information on structural and dynamic quantities, but often at a high computational cost. This course introduces to programming and numerical methods that are useful to solve problems in chemistry. Classical molecular dynamics simulations are performed using the public domain software Dl_POLY.

June 27-Luly 10, 2022
The micro-mechanism of chemical reactions *(18 h, 3 CFU)*

Dr. Gianmarco Vannuzzo, Università degli Studi di Perugia
The mechanism of chemical reactions is of central importance in organic-, inorganic-, physical-, and bio-chemistry. All macroscopic chemical processes are the results of many elementary (uni-, bi- and termolecular) reactions. Bimolecular reactions, usually involving at least one transient species, are at the heart of chemical transformation and, therefore, it is of great interest to explore and characterize them at the atomic and molecular level to derive the "micro-mechanism" of reaction. The aim of this course is to gain an understanding of reaction micro-mechanisms. In the first part, I will introduce key concepts and the experimental techniques used to probe them. In the second part, I will use these concepts to discuss the observed reaction micro-mechanisms in a wide range of chemical reactions of both fundamental and practical interest, such as those of relevance in atmospheric chemistry, combustion chemistry, and astrochemistry.

September 26 -October 28, 2022
***Processes and Technologies for accessing valued chemicals from biomass valorization** (18 h, 3 CFU)*
Dr. Federica Valentini, INSTM , UdR Perugia, Università degli Studi di Perugia

This course intends to give introduce the student to the fundamental technologies and approaches utilized for the manipulation of biobased chemicals to access value added products including, energy carriers, fuels, pharmaceutical ingredients, and catalytic systems for a more sustainable and greener chemical production.
An overview of the recent literature as well as the applications available at the moment will be presented.

October 15-28, 2022
***Ab Initio Molecular Dynamics Simulations: Theory and Applications to Energy Materials** (18 h, 3 CFU)*
Dr. Waldemar Kaiser, CNR-SCITEC

This course introduces the fundamentals of ab initio molecular dynamics (AIMD) methods for computer-based simulations of dynamical material properties. A peculiarity of AIMD methods is the on-the-fly calculation of forces from accurate electronic structure calculations without the need for prior parameterization. The fundamental concepts of AIMD methods, particularly Born-Oppenheimer and Car-Parrinello molecular dynamics, will be introduced and applied using illustrative examples. The potential of AIMD to describe research problems in solution chemistry, material growth and degradation, and condensed matter phases will be outlined with a focus on energy materials. Furthermore, most recent advancements in the acceleration of AIMD simulations by Machine Learning strategies will be discussed.

November 22 - December 10, 2022
***Electron transfer in molecules and in condensed phases: Fundamentals and applications** (18, 3CFU)*
Dr. Francesco Ambrosio, IIT Genova, Italia

Electron transfer (i.e. the movement of an electron from one atom/molecule/material to another) is ubiquitous in a plethora of relevant chemical reactions, ranging from biological processes such as photosynthesis to electrochemistry in aqueous solution and charge transfer in materials and at homogenous or heterogeneous interfaces of relevance for photovoltaics and photocatalytic applications. In this course, the theory of electron transfer will be reviewed along with applications in different fields of chemistry. Furthermore, the interplay between experiment and theory in the study of charge-transfer processes will be discussed by analysing in detail some significant case studies.

February 15-28, 2023

Introduction to proteolysis targeted chimeras (PROTACs): design principles, synthetic approaches, and applications. (18 h, 3 CFU)

Dr. Jenny Desantis, Università degli Studi di Perugia

Proteolysis targeting chimeras (PROTACs) represent an innovative class of compounds that are emerging in drug discovery and are opening the way to a next generation idea of therapeutic agents aimed at the removal of disease-related target proteins. Structurally, PROTACs are hetero-bifunctional molecules composed of two ligands, one binding the protein of interest (POI) and the other one recruiting an E3 ubiquitin ligase, concatenated through a linker. The chemically-induced formation of ternary complexes (POI-PROTAC-E3) leads to ubiquitination and proteasomal degradation of the target protein.
In this course, after an introduction to the principles used for PROTACs design and optimization, an overview of the different synthetic approaches exploited so far for the preparation of such tricky molecules will be presented. Furthermore, different examples of applications of PROTAC technology will be discussed.

March-April, 2023

Cosmochemistry (18 h, 3 CFU)

Prof. Nadia Balucani and Dr. Gianmarco Vannuzzo, Università degli Studi di Perugia

The chemistry of the interstellar medium

Molecules in the interstellar and circumstellar medium; Physical conditions in the interstellar medium; Chemical reactions in the interstellar medium; The role of dust grains; Chemical models of molecular clouds

Meteorite and comet chemistry

Formation of the solar system; Comet chemistry; Structure of a comet; Physicochemical conditions in a cometary coma; Chemical composition of comets; Classification of meteorites

Planetary atmospheres

The case of Mars, Venus, Jupiter and Titan

10 marzo-5 giugno, 2023

The theory of Complex Systems to address the XXI Century Challenges **(**18 h, 3 CFU)

Prof. Pier Luigi Gentili, Università degli Studi di Perugia

Despite significant achievements in science and technology, humankind still needs to win global challenges. Whenever we face the XXI century global challenges, we deal with Complex Systems. Complex Systems are natural systems that science is unable to describe exhaustively. This course presents the features of Complex Systems by using the theories of Out-of-Equilibrium Thermodynamics, Non-linear Dynamics, and Natural Computing. The contents are interdisciplinary. Subjects regarding chemistry, biology, physics, economy, and philosophy are presented. This course intends to give the PhD students new ideas and methodologies to face their specific research.

Note: Lectures will be held on Friday at 3pm.

March-May 2023

Data Scientist with R **(**18 h, 3 CFU)

Dr. Gianandrea La Porta, Università degli Studi di Perugia

Data science is the practice of transforming data into knowledge, and R is one of the most popular programming language used by scientists. The course aims to provide students with: i) the skills necessary to use the R programming language, ii) the principles of statistics to analyze and transform data, and iii) the functions to create and interpret descriptive and multivariate statistics, graphic representations, and statistical models.

Note: Lectures will be held on Monday at 3pm.

March- May, 2023

Advanced NMR techniques for investigating molecular and supramolecular structures in solution *(*18 h, 3 CFU)
Prof. Cristiano Zuccaccia. Università degli Studi di Perugia

The course is separated into two modules. In the first part (14 hours) the main theoretical aspects of NMR spectroscopy will be summarized. After a brief recall of the basic principles, such as chemical shift and scalar coupling, 1D (spin echo and multi-pulse experiments) and 2D techniques (COSY, HMQC, HMBC, NOESY, ROESY) will be illustrated in some detail. In addition, the main principles and applications of diffusion NMR experiments (PGSE and DOSY) will be presented. In the second part (4 hours), a series of practical exercises will be carried out, including, if possible, direct acquisition and data processing at the NMR spectrometer. Organic molecules, organometallic complexes or samples provided by the students themselves, will be used as examples to illustrate how different NMR experiments can be combined together to investigate their molecular and supramolecular structures in solution.

June 1-30 2023
Theoretical modelling of reactivity and energy transfer in astrochemistry and planetary atmospheres *(*18 h, 3 CFU)
Prof. Andrea Lombardi, Università degli Studi di Perugia

The amount of data sent by the probes exploring the solar system and planetary atmospheres, and the astronomical discovery of numerous molecules of increasing complexity in interstellar space, implicates a remarkable relevance of the modern chemistry for the science of the Universe. The interpretation of the resulting ample phenomenology needs to be assisted by theoretical and computational modelling of energy exchanges and reactions involving chemical species to set up data bases and improve kinetic models.
In this course the theoretical grounds of quantum and classical molecular dynamics and a number of computational applications to astrochemistry will be reviewed.

June 19-30, 2023
Isotope effect in chemistry: from theory to environmental applications (18 h, 3 CFU)
Prof. David Cappelletti, Università degli Studi di Perugia

Isotopes are atoms that have the same atomic number (and, hence, generally the same chemistry) but different mass. The difference in mass becomes chemically relevant when specific conditions are satisfied. Theoretical (thermodynamic and kinetic) basis of isotope effect will be illustrated. Applications of synthetic, radiogenic and stable isotopes in chemistry including organic chemistry, spectroscopy and environmental chemistry will be reviewed.

July 2023
An introduction to Python programming language for chemists (18h, 3 CFU)
Dr. Leonardo Belpassi, Instituto di Scienze e Tecnologie Chimiche del CNR (SCITEC-CNR), Perugia, Italia.

Programming in Python empowers chemists to apply their domain knowledge to scales unreachable by manual effort. Learning Python is easy, but contextualizing chemical problems in Python is not always obvious. In this course the students will develop the skill to identify problems, also from their PhD students' research activity, for which code may automate operations and scale a large volume of data or calculation.

September 11-23, 2023
Introducton to Nanophotonics (18 h, 3 CFU)
Prof, Loredana Latterini, Università degli Studi di Perugia

This course presents the fundamental aspects of the interactions between radiation and nanomaterials and the criteria to prepare and engineer materials to achieve tailored optical responses. Examples of ordered nanostructures to harvest, guide,

shift and concentrate the radiation in the nanometer-scale are going to be presented.

October 15-28, 2023

Ab Initio Molecular Dynamics Simulations: Theory and Applications to Energy Materials *(*18 h, 3 CFU)

Dr. Waldemar Kaiser, CNR-SCITEC

This course introduces the fundamentals of ab initio molecular dynamics (AIMD) methods for computer-based simulations of dynamical material properties. A peculiarity of AIMD methods is the on-the-fly calculation of forces from accurate electronic structure calculations without the need for prior parameterization. The fundamental concepts of AIMD methods, particularly Born-Oppenheimer and Car-Parrinello molecular dynamics, will be introduced and applied using illustrative examples. The potential of AIMD to describe research problems in solution chemistry, material growth and degradation, and condensed matter phases will be outlined with a focus on energy materials. Furthermore, most recent advancements in the acceleration of AIMD simulations by Machine Learning strategies will be discussed.

November15-December 15, 2023

Theoretical foundations of light-matter interaction *(*18 h, 3 CFU)

Prof. Enrico Ronca, Università degli Studi di Perugia

Light-matter interaction is our way of understanding nature and is at the foundation of several fundamental physical, chemical and biological (photosynthesis, etc.) processes as well as the basic principle of many technological applications (photovoltaics, optical manipulation of matter etc.).

The aim of the course is to provide a general theoretical framework to study light-matter interaction that could be applied to standard spectroscopic techniques, to intense lasers up to optical manipulation of matter by quantum fields. The students will gain a general understanding of the approximations that need to be applied to

describe the different situations. Several subtle aspects of the interaction with light will be clarified.

February 19– March 15, 2024
Continuous flow technologies for the preparation of pharmaceutically relevant molecules (18 h, 3 CFU)
Dr. Francesco Ferlin, Università degli Studi di Perugia

Modern chemical production relies on the development of innovative technologies that could allow the preparation of the desired chemicals at the highest chemical and economic efficiency.
Flow technologies have proved to be powerful synthetic tools for accessing complex molecular entities in a faster and user friendly manner. The use of flow reactors has also proven to be very effective for the definition of protocols featuring easier purification of the pure products leading to a minimal waste production and consequently a lower cost of the synthetic process. In this course, the student will be introduced to the fundamental aspects of flow chemistry and some examples of application of this technology to relevant target will be also presented.

February 2024
Advanced spectroscopic techniques for the study of solid and heterogenous solid matrices: the artistic heritage materials *(18 h, 3 CFU)*
Dr. Laura Cartechini, Dr. Francesca Rosi, (SCITEC-CNR), Perugia,
Prof. Aldo Romani, *University of Perugia*

During the course some of the most widely used spectroscopic techniques for the characterization of solid and heterogeneous matrices such as those present in many objects of our Cultural Heritage will be presented. The discussion of the techniques, based on the use of a wide spectral range (X-rays, ultraviolet, visible, near and medium infrared), will be addressed by evaluating and quantifying the advantages and disadvantages of the various analytical approaches, from the

study of microsamples to non-invasive measurements both point and imaging/mapping.

April 2024
High-throughput methods for rational drug design, hit-to-lead optimization and safety risk assessment *(18 h, 3 CFU)*
Prof. Laura Goracci, University of Perugia

15-31 May , 2024
Single Crystal X-Ray diffraction. Fundamentals, techniques and applications *(*18 h, 3 CFU)
Prof. Ferdinando Costantino, *Università degli Studi di Perugia*

The course will focus on the XRD single crystal diffraction techniques and it will be organized in three parts:
-Fundamentals of crystallography and diffraction theory
-X-ray single crystal diffractometry: instruments and methodologies
-Applications: from small molecules to functional materials to macromolecules

June 3-17, 2024
Synchrotron radiation spectroscopy (18 h, 3 CFU)
Dr. Barbara Rossi, Elettra Sincrotrone Trieste
Prof. Marco Paolantoni, Università degli Studi di Perugia

There are many advantages in the use of synchrotron radiation (SR) compared to conventional “laboratory” source for the characterization of liquid systems and materials. First of all, the high brightness, wavelength-controlled and tunable emission of SR allows to tune in a very efficient way cross sections and atomic edges of the systems under investigation. The SR emission is a coherent and multiply polarized radiation that can be used for probing dichroic effects and

bonding orientation. Finally, there are a great variety of SR-based spectroscopies that provide elemental, chemical and magnetic information and a large variety of imaging contrasts based on photon absorption, scattering or spectroscopic feature. The purpose of this course is to give an overview of the SR-based techniques useful for the characterization of liquid systems, soft matter and materials. Moreover, basic information helpful to successfully applying for obtaining beamtime at SR facilities will be provided.
The following topics will be presented and discussed:

- SR production and operation of SR sources;
- SR-based spectroscopic techniques: Infrared Absorption and UV Resonance Raman scattering;
- Selected case studies on different systems including, biological systems, ionic liquids, materials of interest for cultural heritage;
- Writing a proposal to perform experiments at SR facilities.

18-30 June 2024

Classical Molecular dynamics: BIO molecules applications (18 h, 3 CFU)

Dr. Noelia Faginas Lago, *Università degli Studi di Perugia*

This course treats advanced molecular dynamics (MD) methodology for classical simulations in order to design, development and molecular dynamics of RNA aptamers for Sars-Cov-2 M-Pro. MD simulations provide atomistically detailed information on structural and dynamic quantities, but often at a high computational cost. This course introduces to programming and numerical methods that are useful to solve problems in chemistry. Classical molecular dynamics simulations are performed using the public domain software Dl_POLY.

June 1-30 2024

Classification of complex molecular systems by invariant coordinates: structure, dynamics and kinetics

Prof. Andrea Lombardi, *Università degli Studi di Perugia*

The complex spatial arrangements and interaction networks of large molecular systems, such as biomolecules and composite materials, require a classificatory approach to ease the unveiling of hidden patterns and deep relationships between structure, dynamics and properties. In this cycle of lectures, invariant parameters and coordinates to be associated with a given molecular structure will be illustrated and applied to model systems. Theory for the application to molecular dynamics and kinetics will be also reviewed and applications to simple exemplary cases will be illustrated.

July 1-15, 2024
Advances in biogeochemistry (18 h, 3 CFU)
Prof. David Cappelletti, Università degli Studi di Perugia

Interdisciplinary course, applying concepts from chemistry, physics, biology and geology to Earth systems including terrestrial, ocean and freshwater environments; water and energy cycles; carbon, nitrogen, phosphorus and sulfur cycles; biogeochemical cycles through Earth history. Advanced examples from state-of-the-art research work will be illustrated and discussed.

July, 2024
Advanced topics in organometallic chemistry (18 h, 3 CFU)
Dr Luca Rocchigiani, Università degli Studi di Perugia

This series of lectures will provide graduate students with a general background on the fundamentals and recent trends in contemporary organometallic chemistry, with a particular focus on the applicative aspects. The first part of the course will review on the general thermodynamic considerations dictating stability and reactivity of metal-carbon bonds, ligand/complexes classification, preparation methods and fundamental properties. In the second part, the most relevant applications of organometallics in organic synthesis and industrial catalysis will be discussed, focusing on mechanistic considerations. In the last part, selected literature examples on the most recent hot topics in organometallic chemistry (e.g.

turbo-Grignard reagents, gold chemistry, Frustrated Lewis pairs, organometallic luminescent compounds) will be highlighted and contextualized.

June 2024
Relativistic quantum chemistry per il 2023-2024 (18h, 3 CFU)
Dr. Leonardo Belpassi, Instituto di Scienze e Tecnologie Chimiche del CNR (SCITEC-CNR), Perugia, Italia.

Students learn principles of chemistry on examples of light elements, the ones from the first three periods, and the rest of elements are mentioned only sporadically. Thus, most students thus have little opportunity to be acquainted with heavy elements in purely chemical sense, that is, to learn something about structure of their compounds and their properties. In this course I will introduce, in a gentle manner, some basics of relativistic effects in the electronic structure of atoms and molecules, relativistic theory of many-electron systems including the Dirac equation and some transformations of the Dirac equation to two-component form. A particular attention will be devoted to the understanding of the spin-orbit coupling effects in atoms and molecules. Applications of relativistic methods of quantum chemistry will be introduced and examples of their application in heavy-element chemistry will be presented.

September 20-October 28, 2024
Processes and Technologies for accessing valued chemicals from biomass valorization *(*18 h, 3 CFU)
Dr. Federica Valentini, INSTM , UdR Perugia, Università degli Studi di Perugia

This course intends to give introduce the student to the fundamental technologies and approaches utilized for the manipulation of biobased chemicals to access value added products including, energy carriers, fuels, pharmaceutical ingredients, and catalytic systems for a more sustainable and greener chemical production.
An overview of the recent literature as well as the applications available at the moment will be presented.

February 1-15, 2025
Raman micro-spectroscopy: theory and applications *(18 h, 3 CFU)*
Prof. Paola Sassi, Università degli Studi di Perugia

The course aims to provide students with the tools necessary to use Raman spectroscopy in the microscopic characterization of different types of materials, from clays to cells. Starting from the description of the Resonant Raman and Raman effect (6 h), passing through the concepts that underlie microspectroscopy (2 h), the theoretical and experimental aspects of the most recent techniques of light scattering spectroscopy will be illustrated. In particular, the following techniques will be presented: SERS (Surface Enhanced Raman Scattering; 2 h); TERS (Tip Enhanced Raman scattering; 2 h); ROA (Raman Optical Activity; 2 h) and EDLS (Extended Depolarized Rayleigh Scattering; 2 h). A two-hour practice exercise will also give the students the possibility to analyze different samples with the micro-Raman instrumentation available in the "Molecular Spectroscopy" Lab of this Department.

February 15-28, 2025
Introduction to proteolysis targeted chimeras (PROTACs): design principles, synthetic approaches, and applications. (18 h, 3 CFU)
Dr. Jenny Desantis, Università degli Studi di Perugia

Proteolysis targeting chimeras (PROTACs) represent an innovative class of compounds that are emerging in drug discovery and are opening the way to a next generation idea of therapeutic agents aimed at the removal of disease-related target proteins. Structurally, PROTACs are hetero-bifunctional molecules composed of two ligands, one binding the protein of interest (POI) and the other one recruiting an E3 ubiquitin ligase, concatenated through a linker. The chemically-induced formation of ternary complexes (POI-PROTAC-E3) leads to ubiquitination and proteasomal degradation of the target protein.

In this course, after an introduction to the principles used for PROTACs design and optimization, an overview of the different synthetic approaches exploited so far for the preparation of such tricky molecules will be presented. Furthermore, different examples of applications of PROTAC technology will be discussed.

February 15– March 19, 2025
Continuous flow technologies for the preparation of pharmaceutically relevant molecules *(18 h, 3 CFU)*
Dr. Francesco Ferlin, Università degli Studi di Perugia

Modern chemical production relies on the development of innovative technologies that could allow the preparation of the desired chemicals at the highest chemical and economic efficiency.
Flow technologies have proved to be powerful synthetic tools for accessing complex molecular entities in a faster and user friendly manner. The use of flow reactors has also proven to be very effective for the definition of protocols featuring easier purification of the pure products leading to a minimal waste production and consequently a lower cost of the synthetic process. In this course, the student will be introduced to the fundamental aspects of flow chemistry and some examples of application of this technology to relevant target will be also presented.

16-27 May, 2025 (first week online, second in presence)
Mass spectrometry: principles and applications to Omics *(18 h, 3 CFU)*
Dr. Maria Fedorova, University of Leipzig, D

The course will cover an introduction to mass spectrometry, from principles to applications to Omics. Instrumentations and acquisition modes will be described, together with methods design, development and optimization. Finally, applications to OMICs will be described and discussed. In particular, the course will cover: introduction to mass spectrometry; static and direct infusion MS; principles of LC-MS coupling; Hybrid MS instruments and principles of method designs; data-dependent and data-independent acquisitions – principles of method development

and optimization; Targeted MS – multiple reaction monitoring and parallel reaction monitoring; Quantitative MS; proteomics, lipidomics and metabolomics.

March-May 2025
Data Scientist with R (18 h, 3 CFU)
Dr. Gianandrea La Porta, Università degli Studi di Perugia

Data science is the practice of transforming data into knowledge, and R is one of the most popular programming language used by scientists. The course aims to provide students with: i) the skills necessary to use the R programming language, ii) the principles of statistics to analyze and transform data, and iii) the functions to create and interpret descriptive and multivariate statistics, graphic representations, and statistical models.
Note: Lectures will be held on Monday at 3pm.

March-May, 2025
Advanced NMR techniques for investigating molecular and supramolecular structures in solution *(*18 h, 3 CFU)
Prof. Cristiano Zuccaccia. Università degli Studi di Perugia

The course is separated into two modules. In the first part (14 hours) the main theoretical aspects of NMR spectroscopy will be summarized. After a brief recall of the basic principles, such as chemical shift and scalar coupling, 1D (spin echo and multi-pulse experiments) and 2D techniques (COSY, HMQC, HMBC, NOESY, ROESY) will be illustrated in some detail. In addition, the main principles and applications of diffusion NMR experiments (PGSE and DOSY) will be presented. In the second part (4 hours), a series of practical exercises will be carried out, including, if possible, direct acquisition and data processing at the NMR spectrometer. Organic molecules, organometallic complexes or samples provided by the students themselves, will be used as examples to illustrate how different NMR experiments can be combined together to investigate their molecular and supramolecular structures in solution.

March 20-June 15, 2025

The theory of Complex Systems to address the XXI Century Challenges **(**18 h, 3 CFU)

Prof. Pier Luigi Gentili, Università degli Studi di Perugia

Despite significant achievements in science and technology, humankind still needs to win global challenges. Whenever we face the XXI century global challenges, we deal with Complex Systems. Complex Systems are natural systems that science is unable to describe exhaustively. This course presents the features of Complex Systems by using the theories of Out-of-Equilibrium Thermodynamics, Non-linear Dynamics, and Natural Computing. The contents are interdisciplinary. Subjects regarding chemistry, biology, physics, economy, and philosophy are presented. This course intends to give the PhD students new ideas and methodologies to face their specific research.

Note: Lectures will be held on Friday at 3pm.

June 1-30 2025

Chirality in dynamics and kinetics in elementary molecular processes

Prof. Andrea Lombardi, *Università degli Studi di Perugia*

Chirality is a phenomenon that permeates the natural world, with implications for atomic and molecular physics, for fundamental forces and for the mechanisms at the origin of the early evolution of life and biomolecular homochirality. The manifestations of chirality in chemistry and biochemistry are numerous, the striking ones being chiral recognition and asymmetric synthesis with important applications in molecular sciences and in industrial and pharmaceutical chemistry. Chiral discrimination phenomena, due to the existence of two enantiomeric forms, very well known in the case of interaction with light, but still nearly disregarded in molecular collision studies. We will review some ideas and recent advances about the role of chirality in elementary molecular processes, designing and illustrating

molecular beam experiments for the demonstration of chiral effects and suggesting a scenario for a stereo-directional origin of chiral selection.