CORSO DI DOTTORATO IN SCIENZE E TECNOLOGIE DELLA CHIMICA E DEI MATERIALI

CONTENTS OF THE COURSES

OPENING LECTURE and TYPE "A" COURSES – 2024

The most up-to-date details can be found in file "Educational Offer 2024-2025_complete and updated on xx-yy-zz" available on: https://chimica.unige.it/dottorato/organizzazione and https://chimica.unige.it/en/dottorato/organizzazione.

PROGRAMS TYPE "B" COURSES – 2024

Aspects of soft matter (2 CFU)

Teacher: Prof. Annalisa Relini (UniGe, Dipartimento di Fisica).

Contents:

Soft matter and its features – intermolecular forces – hydrophobic effect and hydrophobic interactions – viscoelasticity. Colloidal dispersions – lyophobic and lyophilic colloids – DLVO interaction – critical coagulation concentration – Brownian motion and Langevin equation – zeta potential – stabilization of colloidal suspensions. Fluid–like structures and self–assembled systems: monolayers, micelles, bilayers and biological membranes – thermodynamic principles of self–assembly – conditions necessary for the formation of aggregates – critical micelle concentration – effects of interactions between aggregates – geometric packing considerations: micelles and bilayers – structure of biological membranes. Protein structure and protein aggregates – amyloid fibrils as protein nanostructures.

Course material:

[1] Israelachvili J. Intermolecular and surface forces, Academic Press – Elsevier, 2011.
[2] Jones, R. A. Soft condensed matter, Oxford University Press, 2002.
[3] Berg, J. C. An introduction to interfaces and colloids – The bridge to nanoscience. World Scientific, 2010.

Atomic force microscopy, theory and practice (2 CFU)

Teacher: Prof. Marco Salerno (UniGe, Dipartimento di Fisica).

Contents:

Atomic force microscopy (AFM) is the major technique of the scanning probe microscopy family born in the last 20 years of the past century. In AFM in particular the interaction force between probe tip and sample is used as a mechanism for detection and local mapping of the sample material properties. The course will unveil the principles and mechanisms of AFM operation as a force sensor, in the different configurations of static (contact mode) and dynamic interaction (tapping mode). In particular for the latter, the interpretation of the behavior of the observables, namely amplitude and phase of the cantilever oscillation, will be carried out in detail. The analysis of AFM operation will be done with both analytical means based on the theory of the damped, forced simple harmonic oscillator, as well as with computer simulation based on the freeware online program VEDA. Examples of real imaging and related issues on diverse materials (semiconductors, organics, composites etc) will be presented and discussed. The course will include practice on the different AFM systems available at IIT, as well as homework and exam tests for verification of learning of the main concepts involved.

Catalysts and adsorbents (2.5 CFU)

Teachers: Prof. Elisabetta Finocchio, Prof. Gabriella Garbarino (UniGe, Dipartimento di Ingegneria Civile, Chimica e Ambientale).

Contents:

The course, held in English, describes the main families of catalysts and adsorbents applied in industrial and environmental chemistry and the nature of their behavior. Insight will be provided on materials properties, technologies and molecular interactions, with focus on organo-inorganic composite materials. The course consists of classroom lessons.

Activation mode and teaching period:

The course will be held during the period January-February 2024. Please contact the teachers: Gabriella Garbarino, Gabriella.Garbarino@unige.it, Elisabetta Finocchio: email: Elisabetta.Finocchio@unige.it

Final exam:

Course participants will take an oral exam, by appointment with the teachers. The exam will be focused on a discussion on the topics covered during the course.

Design of magnetic nano–architecture (2 CFU)

Teacher: Prof. Davide Peddis (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

A physical property depends on the size of an object, if its size is comparable to a dimension relevant to that property. In magnetism typical size – as for example the dimension of magnetic domains or lengths of exchange coupling interaction – are in the nanometer range. For this reason, starting few decades ago, great attention has been directed towards nanostructured magnetic materials where constituent phase or grain structures are modulated on a length scale from 1 to 100 nm. In particular magnetic nanoparticles have generated much interest because of their application in high density data storage, ferrofluid technology, catalysts and biomedical application (drug delivery, contrast enhanced MRI). The course will treat magnetic properties and chemical synthesis methods of magnetic nanomaterials. Then, correlation between synthesis, structure and magnetic properties will be discussed trough several examples[1]–[4].

Section 1:

After definition and classification of magnetic Nanomaterials, the new physical properties of the nanoscaled materials compared with the corresponding bulk materials will be discussed. Applications of the nanostructured spinel oxide will be described.

Section 2:

Brief introduction on the fundamental concept of magnetism– The correlation between crystalline structure, morphology and magnetic properties relevant to several applications (e.g. Biomedicine, energy, catalysis) will be discussed starting from the concept of magnetic anisotropy. Attention will also given to the most common experimental approaches used to investigate structure, morphology and the magnetic behavior of nanostructured materials

Section 3:

After a wide overview of to the different approaches to the synthesis of nanostructure materials, a detailed description of the most common chemistry method (e.g. sol–gel, self–combustion, polyol method, high thermal decomposition of mettallorganic precursor) will be given.

Section 4:

This section will describe some examples, highlighting the strong correlation between preparation method, composition, structure, and magnetic properties. Seminar of external experts will be scheduled in this section.

Form of examination:

At the end of the course each student should discuss a scientific paper about synthesis and characterization of nanostructured magnetic material. The contents of the article will be chosen on the basis of the background and on the scientific interest of each student. A short ppt presentation could be required.

Note:

A short CV describing the scientific background of each participant is required.

Course material:

[1] Binns, C. Ed., Nanomagnetism: Fundamentals and applications. Oxford: Elsevier, 2014.
[2] Peddis, D.; Jönsson, P. E.; Laureti, S.; Varvaro, G. Magnetic interactions: a tool to modify the magnetic properties of materials based on nanoparticles, vol. 6., 2014.
[3] Cannas C.; Peddis, D. Design of magnetic spinel oxide nanoarchitetures, La Chimica e l'industria, 2012.
[4] Suber L.; Peddis, D. Approaches to synthesis and characterization of spherical and anisometric metal oxide magnetic nanomaterials, in Nanomaterials for life science, Wiley., vol. 4, Kumar, C. S. S. R. Ed. Weinheim: Wiley, 2010, p. 431475.

Experimental design (2 CFU)

Teachers: Prof. Francisco Ardini, Prof. Barbara Benedetti (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

The course gives the basic knowledge on the experimental design approach. The most commonly used designs will be described, namely Full Factorial Designs, Screening Designs, Fractional Factorial Designs, Central Composite Designs, Doehlert Design. More advanced designs will be briefly presented, namely D–Optimal Design, Experimental Designs withqualitative variables at more than two levels, Mixture Designs, Mixture-Process Designs. During the course, several examples of applications in various fields will be illustrated and critically discussed.

Fundamentals of scanning electron microscopy (2 CFU)

Teacher: Prof. Paola Riani (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

- Structural characteristics: electro-optical column, electron guns, electromagnetic lenses, their aberrations.
- Electron beam – sample interaction: elastic and inelastic scattering, Rutherford and Bethe equations, interaction volume, Influence of beam and specimen parameters on the interaction volume.
- Types of signals: back scattered electrons and their properties; secondary electrons and their properties, characteristics X-rays and their properties, absorption and fluorescence.
- Image formation and detectors: Characteristics of detectors; for SE and BSE signals; image formation. Magnification, resolution, picture element size; depth of field; the roles of the specimen and detector in contrast formation, compositional and topographical contrast.
- EDX spectroscopy: qualitative and quantitative analysis.
- Quick reference to electron backscattering diffraction (EBSD).

Course material:

[1] Goldstein, J. I.; Newbury, D. E.; Joy, D. C.; Lyman, C. E.; Echlin, P.; Lifshin, E.; Sawyer, L.; Michael, J. Scanning electron microscopy and X-ray microanalysis. Third edition. Springer, 2003.

Fundamentals of spectral imaging (2 CFU)

Teachers: Prof. Cristina Malegori, Prof. Paolo Oliveri (UniGe, Dipartimento di Farmacia).

Contents:

The course presents the fundamentals of spectral imaging, from standard RGB, to multichannel, to hyperspectral devices. Instrumentation operating under different principles (point-scan, line-scan, plane-scan) will be described, embracing the main spectroscopic techniques used for chemical imaging (UV-Vis, fluorescence, NIR, MIR, Raman, XRF, MS), at both the microscopic and the macroscopic scale. The main strategies for data mining and processing (pixel-based, object-based and image-based) will be described, with a focus on the extraction of relevant chemical information. Applications in several fields (biomedical, environmental, cultural heritage, forensic sciences, food sciences) will be presented.

Innovative pharmaceutical dosage forms: preparation and control methods (2 CFU)

Teachers: Prof. Sara Baldassari, Prof. Gabriele Caviglioli, Prof. Eleonora Russo, Prof. Guendalina Zuccari (UniGe, Dipartimento di Farmacia).

Contents:

Some theoretical and practical aspects of the development of drug release systems will be described. Preformulation: theoretical aspects relative to characterization of the solid state of drugs, devoted to rational development of dosage forms. Mucoadhesive dosage forms: preparation methods, determination of adhesiveness, excipients used, with particular attention to adhesive polymers, also in relation to systems based on nano and microparticles. Nanoparticle and micellar systems based on polymeric carriers for sustained drug release. Cyclodextrins and poloxamers as solubilizing agents for poorly soluble drugs.

Instrumental techniques for trace elements determination in pharmaceuticals, inorganic nanomaterials, food products, environmental samples, and *in vivo* biokinetics evaluation (2 CFU)

Teacher: Prof. Giuliana Drava (UniGe, Dipartimento di Farmacia), Prof. Valerio Voliani (UniGe, Dipartimento di Farmacia).

Contents:

The most important instrumental analytical techniques for trace element determination in complex matrices (*i.e.*, organic and mineral) are presented, with a focus on atomic spectrometry and on the elements of interest for living organisms. Each step of the analytical procedure is discussed, from sampling and sample preparation to data analysis. Single chemical species analyses are presented in detail and matrix effects are discussed together with the calibration methods to overcome interferences. The assessment of analytical result accuracy is illustrated. The application of statistical techniques of experimental design and multivariate analysis at the various analytical steps is shown using a set of case studies. In addition, a focus on the application of atomic spectrometry for *in vivo* biokinetics evaluation of inorganic nanomaterials is presented.

Introduction to functional ceramic materials. Structure, properties, preparation and applications (2 CFU)

Teacher: Dr. Vincenzo Buscaglia (ICMATE–CNR, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia).

Contents:

The specific and sometimes unique magnetic, electrical and optical properties of ceramic materials has promoted their broad application in many electronic and optoelectronic devices. Typical examples include barium titanate ($BaTiO_3$) as a dielectric material with high dielectric constant for multilayer ceramic capacitors, lead zirconate titanate ($Pb(Zr,Ti)O_3$) as fundamental component of piezoelectric actuators and transducers, lithium niobate ($LiNbO_3$) for its use in optoelectronic devices and yttrium–doped zirconia ($Y{:}ZrO_2$) as solid electrolyte in solid–oxide fuel cells (SOFCs). The scope of this course is to provide an overview of the main types of functional ceramic materials and their commercial applications. The lessons will be mainly focused on dielectric, piezoelectric and ferroelectric oxides, multiferroic materials, ionic and mixed conductors. The initial lessons will be dedicated to some topics of general interest, such as the technologies for ceramic processing and the role of grain boundaries on functional properties. This to ensure a better comprehension of following more specialized topics. For each specific class of materials a representative compound will be selected and the corresponding composition–microstructure–property relationships will be illustrated and discussed. Typical examples of most common applications and case histories about the optimization of materials and devices in terms of performances, performance to cost ratio and processing will be provided.

Course organization:

- Functional ceramic materials: generalities.
- Processing of ceramic materials. Powder synthesis, forming and sintering.
- Effect of grain boundaries on electrical properties. Nanoceramics.
- Ceramics for electronics: ferroelectric and piezoelectric ceramics. Multilayer ceramic capacitors, piezoelectric actuators and transducers, ferroelectric memories. Miniaturization of devices and related issues. Lead–free materials.
- Multiferroic materials (BiFeO3, magnetoelectric composites): a challenge for materials science.
- Ceramics for energy: ionic and mixed high–temperature conductors, solid–oxide fuel cells, ceramic membranes for gas separation.
- Ceramici per l'energia: conduttori ionici e misti ad alta temperatura($Y{:}ZrO_2$). Celle a combustile SOFC, membrane per la separazione di gas.

Introduction to polymer physical chemistry and characterisation techniques (2 CFU)

Teacher: Prof. Nicola Tirelli (IIT, Polymers and biomaterials).

Contents:

- The concept of molecular weight distribution. What this entails in terms of polymer properties, and the key features of a statistical approach to molecules as opposed to the deterministic one typical of well-defined, single-valued and low molecular weight values.
- Seeing macromolecules in 3D: random walk and freely jointed chains, more realistic (rigid chains) in unperturbed conditions and in solution. Why in polymers longer does not necessarily mean bigger.
- Characterization techniques, with a specific emphasis on viscosimetry and size exclusion chromatography (SEC, also known as Gel Permeation Chromatography, GPC). Differences between the entropy-based SEC/GPC and all the other (enthalpy-based) chromatographic techniques.
- Wrap-up and assessment.

Mathematical methods for chemistry (2 CFU)

Teachers: Prof. Massimo Ottonelli (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

Matrix algebra: mathematical features and spectroscopic uses:
Types of usually employed matrices: two–dimension matrices, square matrices, row matrices, column matrices. Matrix product. Elementary methods for obtaining transposed and inverse matrices. Diagonalization of symmetrical square matrices. Properties of diagonal eigenvalue matrices and orthogonal eigenvector matrices. Spectroscopic matrix approaches for obtaining normal coordinates to be used in the treatment of molecular motions.

Numerical techniques for treating large matrices: theory and applicative examples:
From a square matrix to the corresponding inverse matrix. Gauss decomposition, pivot strategy, an example of matrix conditioning supported by a finite arithmetical procedure. LU (Lower–Upper) factorization. Iterative Jacobi and Gauss–Seidel methods. A numerical matrix inversion obtained by applying the Jordan method. Evaluation of the eigenvalues concerning a square matrix put in its related diagonal form. Power method. Jacobi method for hermitean matrices. Givens–Householder method. Introductive approach to the QR factorization method (Q and R being, respectively, an orthogonal matrix and an upper triangular matrix.).

Fourier transform: mathematical features and spectroscopic uses:
Evaluation of the terms enclosed in the Fourier series corresponding to a given function. Inadequacy of the representation provided by the Fourier series for the related function when it is needed to cover the entire existence range. The Fourier transform as the result of an attempt to improve the Fourier series. Fast identification of the single frequencies superimposed in a radiative spectroscopic beam through an analysis suitably involving a Fourier transform.

Optical properties of materials (2 CFU)

Teachers: Dr. Francesco Bisio (SPIN-CNR, Superconducting and other innovative materials and devices institute), Prof. Maurizio Canepa (UniGe, Dipartimento di Fisica), Dr. Michele Magnozzi (UniGe, Dipartimento di Fisica).

Contents:

Classical description of light-matter interaction. Lorentz oscillators and optical properties of dielectrics. Free carriers and Drude formula. Local field corrections and effective models for the treatment of non-homogeneous media.

Porous media. Interfaces. Fresnel formulae. Thin films and dielectric multilayers. Semi-classical description of light-matter interaction. Interband transitions. Optical properties of semiconductors, direct and indirect gap, and metals. Luminescence. Photoconductive devices. LEDs. Experimental methods and laboratory activities.

Spectroscopic reflectivity and ellipsometry measurements from thin and ultrathin dielectric films, nanoporous materials, films organic ultrathin. Magneto-optical Kerr Effect measurements on ultrathin magnetic films.

Course material:

[1] Appunti del corso disponibili su AulaWeb.
[2] Mark Fox Optical Properties of Solids. Oxford Un. Press.
[3] Stenzel, O. The physics of Thin films Optical Spectra Springer.
[4] Born, M.; Wolf E. Principles of Optics.

Organic materials for photonics (2 CFU)

Teacher: Prof. Davide Comoretto (UnIGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

Introduction. Optional: (Basic Mathematics with vectors operations, complex numbers and Euler's Formula).

Refractive index:

- Propagation in dielectrics and metals: Lorentz oscillator and Free electron models
- Complex refractive index and optical properties: interface and bulk effects
- Optical anisotropy and birefringence.
- Optical response of organic materials (molecular, polymeric, hybrid, photochromic,…).
- How to change the refractive index in organic materials

Photonic crystals:

- Dielectric lattices
- The role of the dielectric contrast (refractive index in polymer and inorganic dielectrics)
- Growth of photonic crystals: top–down vs. bottom up.
- Natural (biological and mineral) photonic crystals
- Structural color
- Bulk photonic crystals: properties and applications (sensing, design)
- Structural defects: waveguides and microcavities. Properties and applications (laser, optical switch).

Organic photochemistry (2 CFU)

Teacher: Prof. Andrea Basso (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

Organic photochemistry is not a modern research field, in fact pioneering works date back to the beginning of 20th century. Nevertheless, organic photochemistry is a cutting–edge research area, since it fulfills most of the requirements of green (sustainable) chemistry.

This short course will illustrate the basic principles of photochemistry and the differences between photoinduced and photocatalyzed reactions. Examples from the recent literature will be taken and analyzed. A practical activity will be also part of the course.

Principal plants used in phytocosmetics and their constituents (2 CFU)

Teacher: Prof. Angela Bisio (UniGe, Dipartimento di Farmacia).

Contents:

The principal plant-compounds (lipids, carbohydrates, polyphenols, isoprenoids) characterizing the plant-derivatives used in phytocosmetics are described. Subsequently a list, of the most utilized botanical species used is given with a description of their properties.

New:

The main plants, tallophytes and cormophytes, used in phytocosmetics are described, with a focus on their bioactive secondary metabolites.

Introduction: Common myths and misconceptions; Decorative cosmetics and care cosmetics; Herbal cosmetics; Brief historical outline.

Herbal market and herbal products: From planting to product: the herbal value chain; Some hints about quality assurance of medicinal and aromatic plants; European harmonization efforts for the quality of medicinal and aromatic plants

The protective chemistry of plants: Secondary metabolites; Processes and Products from aromatic plants; Potential of plant cells in culture for cosmetic application; Molecular bio-liquefaction: safety and effectiveness of enzyme bio-catalysis.

Applications of herbs in cosmetic products: Plants for skin with notes on the plants used in diseases of the skin; Plants for hair; Use of essential oils; Cosmeceuticals; Nutricosmetics; Neurocosmetics

Formulation and evaluation: Herbal cosmetics; Novel approaches.

Surface science (3 CFU)

Teacher: Prof. Luca Vattuone (UniGe, Dipartimento di Fisica).

Contents:

Surface structure. Structure of bare surfaces. Adsorbate induced reconstruction of surfaces. Solid band structure and its modification in presence of interfaces. Phonon vibrations. Experimental techniques applied to surface analysis.

Scanning tunneling Microscopy and spectroscopy. Low Energy Elecron Diffraction. Electronic and vibrational spectroscopy. Microcalorimetry on single crystals. Gas surface interaction: physisorption and chemisorption dynamics. Physisorption. Non dissociative chemisorption. Dissociative chemisorption. Influence of translational and internal degrees of freedoms of gas phase molecules on their sticking probability at surfaces. Experimental study of sticking probability and of simple reactions by molecular beams. Langmuir Hinshelwood and Eley – Rideal reaction mechanisms.

The ideal synthesis nowadays: lessons from the synthetic chemist Nature (2 CFU)

Teachers: Prof. Chiara Lambruschini, Prof. Lisa Moni (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

The aim of this course is to give an overview of the modern strategies for the ideal multistep synthesis, taking examples from natural biosynthesis and the state of the art in organic synthesis. Those methodologies, including for instance multicatalysis, domino reactions, iteration and compartmentation, are able to change "traditional" synthetic chemistry and open up rapid access to a world of biologically active compounds or functional materials. In particular, multicomponent reactions (MCRs), multicatalytic reactions (MCRs) and their combination will be presented as original opportunity to obtain molecular complexity in a short and simple way. The course includes both traditional lessons and active learning methods, such as flipped lesson and Jigsaws activity.

Theory of crystalline solids (3 CFU)

Teachers: Dr. Sergey Artyukhin (IIT, Quantum Materials Theory).

Contents:

In this course we will discuss how elastic, optical, magnetic and transport properties emerge in crystalline solids. We will start with an overview of basic math and single-particle quantum mechanics, discuss band theory of solids and its violations, thermodynamics and optical properties of metals and dielectrics. Particular attention will be given to crystal field theory, bonding, symmetries, phonons, Jahn-Teller effect. Finally, collective phenomena, such as ferroelectricity and magnetism, will be discussed within the mean field theory. Numerical techniques, such as density-functional theory and its extensions, Monte-Carlo methods will be covered. Material from recent research papers will complement the discussion. Homework problems will help the attendees to get comfortable with the material.

PROGRAMS TYPE "F" COURSES – 2024 and 2025

Materials characterization 1 (1 CFU)

Teachers: Dr. Matteo Lorenzoni, Dr. Luca Ceseracciu, Dr. Lea Pasquale, Dr. Silvia Dante (IIT, Materials Characterization).

Contents:

An overview of different characterization techniques will be given, through a combination of theory classes and examples in the laboratory.

In particular, the course will deal with (a) X-ray based techniques The theoretical basis as well as the practical application of X-ray Diffraction (XRD) will be presented. The course will also include lectures on X-ray techniques for the characterization of non-crystalline or partially ordered materials (small-angle scattering, SAXS); (b) Mechanical Characterizations The course will cover the basic theory of deformation of different classes of materials and their relationship with microstructure. The most common mechanical characterization techniques will be presented, with a special focus on uniaxial tension tests; (c) Atomic Force Microscopy (AFM) The lecture will present the basic principles underlying AFM operation, and will shortly comment on the meaning of roughness for 3D surface images obtained by whatever imaging technique. Examples of the different physical quantities that can be probed (e.g. stiffness, friction, electrical potential, surface current) will be shown.

Materials characterization 2 (1 CFU)

Teachers: Dr. Mirko Prato, Dr. Lea Pasquale, Dr. Silvia Dante, Dr. Luca Goldoni (IIT, Materials Characterization).

Contents:

An overview of different characterization techniques will be given, through a combination of theory classes and examples in the laboratory.

In particular, the course will deal with (a) X-ray based techniques The theoretical basis as well as the practical application of X-ray Photoelectron Spectroscopy (XPS) for the study of the surface chemistry of materials will be presented, along with micro-X-ray fluorescence (μ-XRF) for the examination of the elemental composition of a wide variety of sample types. (b) Nuclear Magnetic Resonance The course will cover the basic theory of NMR for structure elucidation, as well as some notions for studying the dynamic of molecules in solution; (c) Raman The lecture will present the basic principles underlying Raman data acquisition and interpretation, to provide a structural fingerprint by which molecules can be identified.

Nanomaterials and nano heterostructures: colloidal synthesis and chemical transformation (1 CFU)

Teachers: Dr. Luca De Trizio (IIT, Chemistry Facility).

Contents:

The course aims at outlining the fundamental steps which characterize the colloidal synthesis of nanocrystals. In details, it will first describe the kinetics and the thermodynamics of the nucleation and growth of nanocrystals and how to control them. At the same time, the course will deal with the surface energy of the nanocrystals, which ultimately determines their shape. Eventually, it will describe one of the most studied post-synthesis strategies that are currently employed in order to finely "modify" colloidal nanocrystals: the cation exchange reaction. This chemical tool allows for exchanging the cations of pre-formed nanocrystals with new desired cations, while retaining the original anion framework. Thanks to this technique, it is possible either to completely change the composition of colloidal nanocrystals, accessing new nanomaterials, or to engineer them, by partial cation exchange, producing alloyed or heterostructured nanoparticles.

Advanced electron microscopy for materials science (1 CFU)

Teachers: Dr. Rosaria Brescia, Dr. Giorgio Divitini, Dr. Iurii Ivanov (IIT, Electron Microscopy).

Contents:

This course aims to provide basic concepts in electron microscopy (EM) as well as an overview of advanced EM-based techniques, precious both for the use of basic techniques and for an approach to EM-based investigations in materials science and life-science and a correct interpretation of the outputs. The course will focus mainly on transmission EM (TEM). A brief introduction will be provided to the main concepts in EM, starting from electron sources, electron optics and electron-specimen interactions. The main signals and operation modes of interest for imaging in scanning and transmission EM (SEM, TEM) will be treated, together with analytical EM techniques. Insights in high-resolution TEM imaging and in-situ TEM will be provided, particularly interesting for materials science. Moreover, the course will provide an introduction to the peculiar aspects of EM in biology and to the more advanced and complex preparation and data elaboration/analysis involved in cryo-EM and electron tomography.

PROGRAMS TYPE "B" COURSES – 2025 (TO BE CONFIRMED)

Crystalline solids: electronic correlations, instabilities and order (2 CFU)

Teacher: Dr. Sergey Artyukhin (IIT, Quantum Materials Theory).

Contents:

Interactions between electrons in narrow orbitals of transition metal ions give rise to fascinating effects beyond band theory of solids. They give rise to instabilities towards new states of matter and complex orders. Effects such as Mott metal-insulator transition, valence fluctuations in f elements, Kondo physics are not described by conventional band theory or by standard density functional theory, and require advanced treatment based on embedding and quantum Monte Carlo impurity solvers. This course covers some of the basics of this exciting field.

Design and synthesis of protein–kinase inhibitors as anticancer agents (2 CFU)

Teacher: Prof. Silvia Schenone, Prof. Michele Tonelli (UniGe, Dipartimento di Farmacia).

Contents:

The first part of this course is an introduction on biochemical pathways involving tyrosine and serine–threonine kinases and on the main pathologies in which these enzymes are overexpressed or hyperactivated. The second part deals with the rational design and the synthesis of kinase inhibitors, focusing on type I and II ATP competitive inhibitors, allosteric inhibitors, irreversible inhibitors. In particular, some VEGFR, mTOR, Bcr–Abl and SFK inhibitors are reported. The last part regards the kinase inhibitors approved for clinical use.

DNA nanotechnology (2 CFU)

Teacher: Dr. Denis Garoli (IIT, Optoelectronics).

Contents:

- DNA: Brief history about the discovery of the structure of DNA, concept of DNA helix, structural features of DNA and its distinction with RNA, basic concept of gel electrophoresis, DNA amplification and ligation.
- Structural DNA nanotechnology: four arm junction, double crossovers, DNA arrays and Lattices, 3D structure-cube, tetrahedron, dodecahedron octahedron, pyramid, DNA origami.
- Dynamic DNA nanotechnology: reconfigurable DNA based structures, DNA nanomechanical devices, DNA nanomotors, DNA aptamers, DNA walker, DNA Tweezer, DNAzyme – structure function and applications, DNA nanotransport device, molecular cages.
- DNA based logic gates: AND, OR, NOT, XOR, NAND gates, single and multiple input DNA logic gates, circular logic gates, DNA Circuits, DNA computing.
- DNA directed assembly of metal, semiconductor nanoparticles and nanoclusters. DNA scaffolding, DNA nanorobot, application of DNA assembled structure in chemical, biological and molecular sensing, DNA-based drug and gene delivery, future applications.

Drug Discovery: an introduction to the process leading to new small-molecule drugs (2 CFU)

Teachers: Dr. Andrea Armirotti (IIT, Analytical Chemistry and Translational Pharmacology), Dr. Tiziano Bandiera (IIT, D3 PharmaChemistry), Dr. Fabio Bertozzi (IIT, D3 PharmaChemistry), Dr. Marco De Vivo (IIT, Molecular Modeling and Drug Discovery), Dr. Stefania Girotto (IIT, Computational and Chemical Biology), Dr. Benedetto Grimaldi (IIT, Molecular Medicine), Dr. Debora Russo (IIT, D3 PharmaChemistry), Dr. Rita Scarpelli (IIT, D3 Validation), Dr. Marina Veronesi (IIT, D3 PharmaChemistry).

Contents:

The course will describe the process that leads to the approval of a new chemical entity as a drug. This process develops through three main phases: the discovery phase, the preclinical development, and the clinical development. In turn, each phase consists of a number of subsequent steps where different activities are performed. The successful completion of each of these steps allows one or more molecules or candidate drugs to be progressed to the following ones. The main focus of the course will be on the discovery phase, which consists of four steps: target identification and validation, hit identification, hit to lead, and lead optimization. Each of the four steps will be described. Several topics will be addressed, including biological studies for the validation of a new target, virtual screening, types of assays for compound screening, medicinal chemistry strategies for elucidating the Structure-Activity Relationships of a chemical class, assessment of the drug-like properties of compounds, and optimization of the profile of lead compounds.

Elementary electronic structure of solids (3 CFU)

Teacher: Prof. Liberato Manna (IIT, NanoChemistry).

Contents:

This course presents an overview of the electronic structure of solids from an *analytic* point of view, rather than computational. The properties of solids (and of molecules) are predicted based on a one–electron approximation of electronic states and simple formulas are obtained for various properties, which depend on chemical parameters (for example polarity, covalency, bond lengths, etc.). The methodology is mostly based on a tight–binding approach. It is particularly suited for chemists, who are used to deal with atomic and molecular orbitals. It is additionally extremely useful for physicists, who instead tend to approach solids with the *nearly free electron* approximation, which however does not fully give justice of the underlying "chemical" nature of solids.

INN and IUPAC nomenclature of organic drugs (2 CFU)

Teacher: Prof. Giancarlo Grossi (UniGe, Dipartimento di Farmacia).

Contents:

INN Nomenclature:

WHO and the INN project. Need for drugs INN nomenclature. Criteria for selecting drugs INNs. The use of "stems" to identify a therapeutic class. Making an application for an INN. Examples of the main INNs adopted in the field of synthetic, biotechnological and gene therapy drugs.

IUPAC Nomenclature:

IUPAC and CAS organizations. Monocyclic hydrocarbons. Polycyclic hydrocarbons. Fused polycyclic hydrocarbons. Accepted trivial names. Replacement nomenclature ("a" nomenclature). The Hantzsch–Widman System. Fused heterocyclic systems. Nomenclature of substituted systems.

Introduction to nanofotonics and nanofabrication (3 CFU)

Teacher: Prof. Maria Caterina Giordano (UniGe, Dipartimento di Fisica).

Course Objective:

The objective of this course of study is to give an overview of the fundamental micro and nanofabrication processes which are at the basis of the exceptional technological development in the field of microelectronics and, more recently, in nanotechnology. In the last 50 years, thanks to the capability to control the fabrication process at the nanoscale, the dimensions of the features built into integrated circuits devices have shrunk from 25 μm to 25 nm. This nanofabrication capability has allowed the study novel physical and chemical effect at the nanoscale, opening a variety of applications in nanophotonics, optoelectronics, biosensing, photodetection and photocatalysis. Very recently, materials with atomic dimensions such as two dimensional layers (e.g. graphene) and quantum dots are widely studied for achieving atomic scale active components, giving rise to a host of unique challenges and opportunities in nano– and quantum– technologies.

Contents:

- Introductory concepts: nanoscience & nanotechnology, micro– & nano–electronics.
- Overview of main top-down nanofabrication approaches: Optical Lithography – Electron beam Lithography - Focused Ion Beam lithography – Laser interference Lithography – Scanning Probe Microscopy (SPM) Lithography.
- Technological processes: spin coating, etching, lift off, thin film deposition (thermal metal deposition, RF sputtering, atomic layer deposition).
- Overview of main bottom–up nanofabrication approaches: self–assembly (e.g. Soft Lithography assembling) and self–organization (e.g. defocused Ion Beam Sputtering).
- Morphological nanoscale characterization of nanostructures and nanomaterials by scanning probe microscopy (e.g. atomic force microscopy – AFM) and scanning electron microscopy (SEM).
- Optical characterization of nanostructures and nanomaterials by far–field optical spectroscopy (e.g. optical transmission, reflection) and scanning near–field optical microscopy (SNOM).
- Examples of nanostructures and novel nanoscale two–dimensional materials with application in the field of nanophotonics, biosensing and photodetection.
- Hands on demonstration of Electron Beam lithography and Laser Interference Lithography. Morphological nanoscale characterization of the fabricated nanostructures by AFM and SEM. Optical characterization by far–field spectroscopy.

Molecular markers of food quality and genuineness (2 CFU)

Teachers: Prof. Raffaella Boggia, Prof. Federica Turrini (UniGe, Dipartimento di Farmacia).

Contents:

The course will cover topics such as food quality, particularly focusing on the possibility both to find marker of food quality and genuineness. The course will pay attention to:

- Different processing technologies and their impact on active components in foods, as case studies the dehydration of herbs and the preparation of infant formulas.
- Alternative analytical methods proposed to detect food adulterations, as case studies the adulteration of fruit juices and of high quality extra–virgin olive oils.

Multivariate analysis of chemical data (3 CFU)

Teachers: Prof. Monica Casale, Prof. Cristina Malegori, Prof. Paolo Oliveri (UniGe, Dipartimento di Farmacia).

Contents:

The course presents the fundamentals of chemometrics, with a specific focus on multivariate analysis of chemical data. The main strategies for data mining, pre-processing and processing will be described, including both unsupervised exploratory strategies and supervised methods for qualitative and quantitative data modelling. Concerning unsupervised methods, principal component analysis (PCA) and cluster analysis (CA) will be presented. In the family of supervised methods, a focus will be made on: (i) classification, including k-nearest neighbours (k-NN), linear discriminant analysis (LDA), and quadratic discriminant analysis (QDA); (ii) class-modelling, including unequal class modelling (UNEQ) and soft independent modelling of class analogy (SIMCA); (iii) regression, including principal component regression (PCR) and partial least squares (PLS) regression. Applications in several fields (food sciences, biomedical, environmental, cultural heritage) will be presented. Hands-on-computer sessions will be performed using a freely distributed open-source chemometric package.

Patent and bibliographic databases searching in medicinal chemistry (2 CFU)

Teachers: Prof. Chiara Brullo, Prof. Paola Fossa (UniGe, Dipartimento di Farmacia).

Contents:

Aim of this course is to get a good level of knowledge and expertise in the use of the principal patent and bibliographic research databases in chemistry and medicinal chemistry, thus all resources will be fully described, some search examples will be showed, and students will test their ability during specific hands–on sessions. Main topics will be:

- searching strategies consulting Unige chemistry, medical and medical-pharmaceutical resources (Uno per tutti and related Unige resources);
- particular attention will be deserved to Pubmed, Scifinder and Reaxys platforms; for these databases additional practical exercises will be also performed for each student;
- searching strategies on Scopus, Web of Science, clinical trials and patent office databases;
- searching on cross-linked scientific databases of medical-pharmaceutical interest: PubChem, Protein Data Bank, Uniprot, DrugBank, Aifa database, Natural Compounds database;
- Additional on–line platforms used in patent research and drug design campaigns will be examined and discussed.

A final practical exam, focused of some selected databases, will be performed by each student.

Perspectives on bioinorganic chemistry (2 CFU)

Teacher: Prof. Serena De Negri (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

General principles of bioinorganic chemistry (historical background, occurrence, availability and biological functions of inorganic elements, biological ligands for metal ions). Experimental techniques for the study of bioinorganic compounds, utility of model compounds. Biological functions of the alkaline and alkaline earth metal cations. Biomineralization: the assembly of advanced inorganic materials in biology. Bioinorganic chemistry of transition elements with particular attention to relevant biomolecules of Fe, Co, Ni, Cu and Zn. Uptake, transport and storage of the dioxygen molecule O_2. Biological functions of nonmetallic inorganic elements such as iodine and selenium. Bioinorganic chemistry of the quintessentially toxic metals.

Polymeric nanocomposites (2 CFU)

Teacher: Prof. Orietta Monticelli (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

General features of polymer–based nanostructured materials. Type of nanofillers. Methods used for the preparation of polymer nanocomposites. Layered silicates: structures and properties. Modification of layered silicates. Anionic clay, layered phosphates and sepiolites. Type of nanocomposites. Characterization techniques: X–ray diffraction, transmission electron microscopy (TEM) and atomic force microscopy (AFM). Preparation of nanocomposites based on layered silicates: in–situ polymerization (examples: polyamide 6 and polystyrene) and melt–blending. Nanocomposite properties: permeability (Nielsen's model), mechanical properties (Halpin–Tsai's model), thermal and combustion properties.

Process Intensification (3 CFU)

Teacher: Prof. Alberto Servida (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

Process Intensification (PI) has become an effective approach for improving productive capacity and updating outdated batch processes without the need for large civil engineering investment. The methodology is well established and often it allows to achieve significant yield improvements and waste reductions.

The course provides the basics of Process Intensification by discussing specifications for the selection and operation of PI equipment. Emphasis will be put on the pivotal role of chemistry, heat and mass transfer for the identification of an effective PI program. The key features of PI methodology will be illustrated along with the tools (based on laboratory and process plant knowledge) useful for PI implementation.

The course breakdown:

- Process Intensification overview (origin, advantages, obstacles);
- Technologies for PI (intensified heat and mass transfer; electrically intensified processes; microfluids).
- Overview of the most relevant equipment for intensified unit operations: compact and micro–heat exchangers; reactors (spinning disc reactors, oscillatory baffled reactors; micro–reactors); separation units (distillation, membranes, drying, crystallization); mixing.

Course material:

[1] Lecture slides.

[2] Reay, D.; Ramshaw, C; Harvey, A. Process Intensification Engineering for efficiency, sustainability and flexibility. Butterworth–Heinemann, 2008.

Science at Large Scale Facilities: Neutron and Synchrotron Light sources (2 CFU)

Teacher: Dr. Alberto Martinelli (CNR-SPIN, SuPerconducting and other INnovative materials and devices institute).

Contents:

The course illustrates the use of synchrotron X-ray and neutron radiation (techniques and applications) for the determination of materials' structures and properties in physics, chemistry, biology and related disciplines such as archaeology and environmental science. The following subjects are presented:

- Introduction to synchrotron radiation and fundamentals of the interaction of X-ray with matter.
- Introduction to neutron scattering.
- Diffraction Techniques: X-ray diffraction; neutron diffraction and magnetic scattering; pair distribution function.
- Spectroscopic Techniques: XANES and EXAFS.
- Application for beam time: how to write and submit a proposal.

Single crystal diffraction at work (2 CFU)

Teacher: Prof. Pavlo Solokha (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

The aim of this course is to provide the basic principles of single crystal X-ray diffraction and guide the students through a typical experiment, from sample selection to crystal structure solution. The following subjects are presented:

- Introduction to single crystal diffraction (crystal systems, space groups, X-ray diffraction theory).
- Overview of instrument hardware and software.
- Techniques for selection and mounting of specimens for X-ray analysis.
- Discussion of data collection techniques and strategies.
- Instruction and practice with APEX4 software package:
    - Structure determination and refinement - use of SHELXTL software package;
    - preparation of final reports, tables, diagrams and CIF files.
- Visualization of different types of crystal structures.
- Use of Cambridge Crystallographic Database.

The Rietveld method: fundamentals and applications (2 CFU)

Teacher: Prof. Cristina Artini (UniGe, Dipartimento di Chimica e Chimica Industriale).

Contents:

The course aims at providing students with the basic knowledge of the Rietveld method for the refinement of powder diffraction data.

Theoretical part:

General introduction on the Rietveld method: historical outline and benefits of the method. Information obtainable from a diffraction spectrum and contributions to the calculated intensity; profile functions. Minimization function and nonlinear least squares method. Refinable parameters and refinement strategies. Correlation among parameters, treatment of data deriving from polyphasic samples; treatment of data containing microstructural information. Agreement factors. Preparation of the input file.

Hands–on sessions:

Students will individually perform refinements by means of the FullProf software on x–ray diffraction spectra collected by synchrotron radiation or by a laboratory powder diffractometer, with the aim to become familiar with different cases: diffraction spectra of oxides will be supplied, as well as of alloys, of polyphasic samples, of samples showing non negligible microstructural effects.

Water soluble nanoparticles (2 CFU)

Teacher: Dr. Teresa Pellegrino (IIT, Nanomaterials for Biomedical Applications).

Contents:

- An introduction to inorganic nanoparticles in biomedical applications: exploiting photoluminescence, magnetic and metallic properties at the nanoscale for accomplish to biomedical needs.
- An overview of water transfer strategies of inorganic nanoparticles: from ligand exchanges and polymer coating protocols to more advances in situ polymer and silica growth approaches.
- Surface functionalization of nanoparticles with biomolecules.
- An overview of characterization techniques suitable for investigating aqueous stabilized nanoparticles.
- Cytotoxicity of nanoparticles: analysis of nanoparticle toxicity as a function of size, shape and composition and methods to evaluate cytotoxicity.
- Degradation of nanoparticles: biological transformations of inorganic nanoparticles into living cells.