COURSES

- Lectures will be held during the period June – September. The Teaching Timetable will be furnished individually by each teacher.

- Examinations must be completed within **October, 10th,**

SUPRAMOLECULAR CHEMISTRY

Prof. G. Arena

Introduction. Brief overview of basic concepts. Analytical Aspects
Methods to check guest and host purity. Thermal analysis, potentiometry, NMR
Techniques and methods employed to evaluate the stability of a supramolecular assembly. ^{1}H NMR, Potentiometry, Titration Calorimetry. Applicability. Advantages and disadvantages of each method.

ARCHAEOMATERIALS

Prof. E. Ciliberto

Ceramics: fillosilicates and natural clay. Technology of furnace processes. Equivalent temperature of firing. Decoration of the pottery, Egyptian faiences, Attic vases, majolica.
Glasses: ores and technologies of glasses. Former oxides, modifiers oxides, chromatic elements and particles.
Metal and alloys: copper, bronze, brass and steel, ores and early technologies.
Mortar and concretes: lime, technologies and hardening process. Hydraulic limes: technologies and uses.

MOLECULAR DYNAMICS SIMULATION

Prof. C. La Rosa

The Aims of Molecular Dynamics.
Classical Mechanics, Quantum Mechanics and Statistical Thermodynamics.
Molecular Interactions: Non-bonded Interactions, Bonding Potentials, Force Calculation.
The MD Algorithm: The Verlet Algorithm, Constraints and Restrain.
Time Dependence: Propagators and the Verlet Algorithm, Multiple Time-steps.
Rigid Molecule Rotation and Harmonic Oscillator.
Molecular Dynamics in Different Ensembles
Explicit and Implicit Solvent
Force Field: CFF and CHARMM
Program: NAMD and VMD

Molecular Dynamics and Steered Molecular Dynamics: from simulations to thermodynamic functions.Computer tutorials

SURFACE MASS SPECTROMETRIES

Prof. A. Licciardello

Aim of the course is to provide a survey on surface mass spectrometries, namely Secondary Ion Mass Spectrometry (SIMS), Sputtered Neutrals Mass Spectrometry (SNMS) an Glow-Discharge Mass Spectrometry (GD-MS).

The first part of the course will provide the necessary background of ion-matter and plasma-matter interaction.

The second part of the course will deal with the application of such techniques in the study of inorganic and organic surfaces and thin films, and their impact in different fields of materials science and life science.

CHEMICAL NANOTECHNOLOGIES

Prof. G. Marletta

The Course will provide a synthesis of current advances in Nanotechnologies, merging a synthetic view of fundamental approaches with applications to specific case studies.

As to the fundamental approaches, the course will deal with three well-focused topics:

1) Patterning strategies at nanoscale,
2) Advances in self-organisation processes,
3a) Current trends in nanoscale molecular electronics.

As to the applications, the following case studies will be dealed with:

A) Nanobiotechnologies: cell and biomolecule response to nanosystems,
B) Nanosystems for molecular sensing and biosensing,
C) Carbon-based nanosystems: Nano-Micro integration: nanosystems for microscale platforms.

The applications will be discussed in view of understanding limits and advantages of nanotechnologies.

AN INTRODUCTION TO LARGE-SCALE MATHEMATICAL MODELS IN CHEMISTRY AND BIOLOGY

Prof. A. Raudino

Mathematical tools: Ordinary Differential Equations, Partial Differential Equations, Initial and Boundary Conditions, Eigenvalue Problems, Fourier Analysis.

Applications: Electrolytes, poly-electrolytes, gels and charged Membranes models. Theory of patterns formation and evolution, nucleation and growth of a new phase, Stability analysis of thin fluid films.

FABRICATION AND PHYSICO-CHEMICAL CHARACTERIZATION OF FUNCTIONAL BIOLOGICAL INTERFACES

Prof. C. Satriano

Preparation and characterization of functional surfaces for specific interactions with bio-systems, in vivo and in vitro. Studies of the molecular and kinetic processes occurring at such interfaces, ranging from small molecule and biomolecular interactions, to cell adhesion, differentiation and tissue formation at the interface. Case studies of biomimetic surface platforms, biomembrane and supramolecular materials, nanotechnology applications.

CATALYSIS FOR ENERGY PRODUCTION AND ENVIRONMENTAL PROTECTION

Prof. S. Sciré

Principles and objectives of Green Chemistry. Atom and energy efficient processes. Catalytic processes with low environmental impact.

Catalysis for environmental protection. Clean-up of emissions from industry. Catalytic abatement of NOx, SOx, VOCs, CFCs, particulate matter.

Catalysis and automotion. Gasoline, diesel, electric and hybrid engines. Clean-up of emissions from cars. Catalytic converters. Catalytic removal of diesel particulate.

Catalysis for hydrogen production. Fuel Cells Technologies.

Catalytic processes for fuel production and improvement.

Principles and applications of photocatalysis.

PHOTOCHEMISTRY: FROM BASIC PRINCIPLES TO PRACTICAL APPLICATIONS

Prof. S. Sortino

The aim of the course is twofold. In a first introductory part the basic principles of photochemical and photophysical processes will be provided. In a second part, the role of photochemistry as multidisciplinary science will be highlighted. In particular it will be shown the importance of the processes initiated and/or controlled by light in multifaceted applications in different fields, encompassing optoelectronics, environment, biology and medicine.

MOLECULAR BASES OF PHARMACOLOGICAL ACTIVITY

Prof. C. Tringali

Introduction to Medicinal Chemistry - Drug Discovery and Drug Development – Natural Products and Drug Discovery – Lead Compounds

- Pharmacokinetics and Pharmacodynamics – Structure-activity relationships (SAR) – Lipophylicity (Log P).
Receptors, Enzymes and Drugs. – Agonists and Antagonists – Enzyme inhibitors – Xenobiotics – Phase I and Phase II Enzymes – Cytochrome P 450 – Conjugates – Drug metabolism.
Cancer chemoprevention: anticarcinogenic, antiproliferative and pro-apoptotic agents.

POTENTIALITIES OF CHEMOINFORMATICS IN DRUG DESIGN AND DATA MINING

Prof. Giuseppe Musumarra

Multivariate analysis. Classification and regression methods. Principal component analysis. The SIMCA method. Latent variables: the PLS method. Partial and global molecular descriptors. Principal properties. Selection of informative molecules in drug design. Pharmacokinetic profiles and ADME properties. Multivariate methods for data mining and applications in genome-based cancer research.

Biosensors

Prof. Giuseppe Spoto

Basic features of biosensors. Biological receptors: Their classification; surface immobilization/entrapment of receptors; side effects (e.g. non-specific interactions), surface geometry design. Transducers: Optical, electrochemical, piezoelectric.
Assay design, sample requirement and manipulation, biosensor specifications. Microfluidics basic principles and use in biosensing.

STEREOCHEMISTRY OF COORDINATION COMPOUNDS

Prof. Roberto Purrello

Aim of this course is to present an overview of a part of stereochemistry usually not presented during the studies leading to Laurea, to give to the Ph.D. students a thorough vision of stereochemistry.The emergence and role of stereochemistry of coordination compounds; basic concepts: structure, geometry, symmetry; methods for the elucidation of the stereochemistry of coordination compounds, general concepts: the classification of ligands, isomerism, nomenclature; mononuclear and polynuclear coordination units.

A BIOINORGANIC APPROACH TO NEURODEGENERATIVE DISEASES

Prof. Giuseppe Grasso

Brief overview of neurodegenerative diseases: a bioinorganic point of view. Alzheimer's disease. Parkinson disease. Prion diseases. Catabolism of aggregation-prone proteins. Aβ, α-synuclein and prion

protein. Protein-metal ions binding. Chemical factors regulating the clearance of proteins by metalloproteases: oxidative stress, small molecules and metal ions. Metal ions and metalloproteases at physiological conditions and in neurodegeneration. Some of the most commonly used experimental techniques to study metal binding to proteins.

PROTEIN (MIS)FOLDING AND AMYLOID AGGREGATION: CLASSICAL PRINCIPLES AND EMERGING APPROACHES IN THE THERAPY OF NEURODEGENERATIVE DISORDERS

Dr. Danilo Milardi

The protein folding energy landscape. Sequence-based prediction of protein behavior. The amyloid phenomenon and its significance in human diseases. The kinetics and mechanisms of amyloid formation. Amyloid structures at the atomic level: insights from crystallography. Pathways of amyloid formation. Fibrillar Polymorphism. Structural and compositional information about pre-amyloid oligomers. Fluorescence spectroscopy and Statistical Differential Scanning Calorimetry: two tools to characterize amyloid and to probe folding/unfolding ensembles. Inhibitors of Amyloid and Oligomer Formation. Functional Amyloids. A study case: the role of Aβ in Alzheimer's Disease.

CHEMOINFORMATIC IN DRUG DESIGN

Dr. Cosimo G. Fortuna

SOSPESO PER QUEST'ANNO

Computational Organic Chemistry

Prof. Rescifina

Course Aims

Molecular modelling is a collection of computer based techniques for deriving, representing and manipulating the structures and reactions of molecules, and those properties that are dependent on these three dimensional structures. This lecture course aims to introduce in a simple way the hierarchy of computational modelling methods used nowadays as standard tools by organic chemists for searching for, rationalising and predicting structure and reactivity of organic, bio-organic and organometallic molecules. The emphasis will be on helping to develop a feel for the correct "tool" to use in the context of a typical problem in structure, activity or reactivity, by describing the limitations and strengths of each method.

The Synopsis and Syllabus will be provided after the eventual approval

Metodi di calcolo quantomeccanici: teoria ed applicazioni
Dott. Forte Giuseppe

Il corso si occuperà di fornire i principi basilari su cui si fondano i metodi di calcoli quantomeccanici, partendo dal metodo Hartree Fock ed estendendolo a metodi molto più avanzati in grado di stimare accuratamente l'energia di correlazione, proseguendo infine con la teoria del funzionale densità (DFT) ad oggi tra gli approcci computazionali più utilizzati in campo chimico.

Le applicazioni dei metodi teorici a varie problematiche di carattere chimico verranno presentate durante il corso insieme alla presentazione dei migliori software oggi disponibili per il calcolo e la visualizzazione.