# Corsi di Dottorato in Scienze Chimiche
# A. A. 2018-2019

**(1) Prof. Assunta MARROCCHI**
***Chemical risk.***
The course will be given in December 2018 (see calendar of courses).

Program:
Introduction.
The industrial chemical risk and the risk of "relevant accidents". Reference legislation.
The legislative decree 81/2008 and the chemical risk. The chemical risk in the research labs; definition of chemical agent; definition of hazardous chemical agents; hazard categories; the concept of exposure to hazardous chemicals; the threshold limit value (TLV).
The CLP regulation. Hazard communication; hazard categories and concentration of mixtures; incompatible chemical agents; labeling of substances and mixtures; safety data sheets (SDSs); common issues with SDSs; examples and critical discussion for the interpretation of SDSs.
REACh Regulation.
Routes of absorption of chemical agents. Parameters which influence the absorption.
Devices for individual and collective protection.
The chemical risk assessment. Algorithms. Monitoring of chemical exposure in the workplace. Management of chemical waste.

**(2) Prof. Gabriele CRUCIANI**
***Artificial intelligence and deep learning in chemistry*.**
The course will be given in February 2019 (see calendar of courses).

Program:
1 - Machine learning and Linear discriminant models (LDA)
2 - Application of LDA in chemistry/ pharmaceutical research
3 - Patter recognition and algorithms
4 - Applications of patter recognition in chemistry/pharmaceutical research
5 - Support vector machine, regression methods and projection to latent structures
6 - Examples in chemical and -omics arena
7 - Deep learning with practical examples

**(3) Prof. Paola SASSI**
***Raman micro-spectroscopy: theory and applications.***
The course will be given in February 2019 (see calendar of courses).

Program:
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.

**(4) Proff. Filippo DE ANGELIS, Paola BELANZONI, Francesca NUNZI, Drs. Leonardo BELPASSI, Simona FANTACCI, Edoardo MOSCONI, Daniele MEGGIOLARO**

***Advanced electronic structure and dynamics methods for molecules and materials*.**

The course will be given in February 2019 (see calendar of courses).

Program:

1) Electronic structure calculation methods: Hartree-Fock, post Hartree-Fock, DFT.
2) Relativistic effects in electronic structure: Dirac equation and spin-orbit coupling.
3) Time-dependent DFT. UV-vis spectra and nonlinear optical properties.
4) Calculations of molecular properties: IR, EPR, UV-vis spectra.
5) Relativistic effects: observations and applications to molecular and material properties (IR, UV-vis spectra).
6) Ab initio molecular dynamics methods. Car-Parrinello method. Applications (examples).
7) Applications to materials and processes for energy.

**(5) Prof. Cristiano ZUCCACCIA**

***Advanced NMR techniques for investigating the molecular and supramolecular structures in solution.***

The course will be given in June 2019 (see calendar of courses).

Program:

The course is separated into two modules. In the first part 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 application of diffusion NMR experiments (PGSE and DOSY) will be presented. In the second part, a series of practical exercises will be carried out, including 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.

**(6) Prof. Pier Luigi GENTILI**

***Investigation into Complex Systems.***

The course will be given in June 2019 (see calendar of courses).

Program:

Despite significant achievements in science and technology, humankind still needs to win compelling challenges. We must defeat diseases that are still incurable; we are unable to predict catastrophic events, such as earthquakes and volcanic eruptions, which often cause many deaths; we struggle to avoid global warming; we want to exploit the energy and food resources without deteriorating the natural ecosystems and their biodiversity; we would like to, at least, predict the unavoidable financial and economic crises; we make efforts to guarantee stability in our societies. Whenever we face these challenges, we deal with Complex Systems. Complex Systems are natural systems that science is unable to describe exhaustively. Examples of Complex Systems are both unicellular and multicellular living beings; human brains; human immune systems; ecosystems; human societies; the global economy; the climate and geology of our planet. By using the fundamental principles of physical chemistry, in particular, the Second Law of Thermodynamics that describes the spontaneous evolution of our universe, and the tools of Nonlinear dynamics, this course analyzes the properties of the Complex Systems. It will be shown that Complex Systems are networks that work in very-far-from equilibrium conditions. They exhibit emergent properties such as the power of self-organizing in time and space. Moreover, Complex Systems can show chaotic dynamics. The chaos in time originates fractal structures. The content of this course will be interdisciplinary. In fact, subjects regarding chemistry, biology, physics, economy, and philosophy will be presented. This course intends to give the Ph.D. students new tools and ideas to face their specific research.