

Corsi specifici per gli studenti della Scuola nel 2011

**Ph. D. School in
Chemical and Pharmaceutical Sciences and Technologies
University of Trieste (Italy)**

Specific Courses for the Ph D students in 2011

- Title:** Quantum Mechanics 2
Lecturer: prof. Piero Decleva (DSCF, decleva@univ.trieste.it, 040 5583946)
Aim and contents: The purpose of the course is to integrate important topics in Quantum Mechanics which are not taught within the Chemistry courses, in particular the following topics will be treated: Review of the postulates, Continuous spectrum, Density Matrices, Temporal evolution, Scattering theory.
Length: ca. 20 h
Schedule: interested students should contact Prof. Decleva well in advance for agreeing on date and time, that will be officially communicated to the Director of the School.
Reference textbooks: C. Cohen-Tannoudji et al. "Quantum Mechanics", available in the library of DSCF
- Title:** Experimental design and optimization
Lecturer: prof. Cynthia Ebert (DSCF, ebert@units.it, 040 5583103)
Contents: Chemometrics. Multivariate analysis; Experimental planning and analysis; Sequential and simultaneous methods; Screening design and optimization design; Factorial analysis. Main effects and interaction effects; Evaluation of effects of variables, validation; Fractional factorial design. structure, construction, resolution; Response surface methods; Sequential methods: Steepest Ascent Methods, Gradient, Simplex.
Length: 8 h
Schedule: Dates to be agreed with the lecturer.
- Title:** Rheology of Complex Systems
Lecturer: Prof. Romano Lapasin (DI3, ROMANO.LAPASIN@dicamp.units.it, 040 558 3434)
Contents: Introduction to rheology. Types of flows and relevant material functions. Shear-dependent and time-dependent behaviours. Rheological models. Rheology of polymeric systems (from ordinary and crystalline solutions to physical gels). Rheology of dispersions (from emulsions and suspensions to colloidal systems and nanodispersions).
Length: 20 h
Schedule: Dates to be agreed with the lecturer
Reference textbooks: H.A. Barnes, J.F. Hutton, K. Walters, Introduction to rheology, Elsevier, 1989.
R. Lapasin, S. Pricl, Rheology of Industrial polysaccharides: Theory and Applications, Chapman&Hall, 1995.
M. Grassi; G. Grassi; R. Lapasin; I. Colombo, Understanding Drug Release and Absorption Mechanisms: A Physical and Mathematical Approach, Chapter 3, CRC Press, 2007.
Additional information: Course slides in ppt format available from the lecturer.

4. **Title:** Validation of analytical methods and applications in environmental sciences (VAM11).
Lecturer: Prof. Gianpiero Adami (DSCF, gadami@units.it; 040 5583996)
Contents: Importance of analytical quality management and quality assurance in industry, academia and research projects. Method validation for analytical measurements. Worked examples of analytical quality concepts. Experiments as tools to demonstrate principles of quality assurance. Applications to environmental chemistry analysis.
Length: 20 h (including 6 h of practices).
Schedule: Dates to be agreed with the lecturer
Reference textbooks: B. Neidhart, W. Wegscheider, eds. "Quality in Chemical Measurements", Springer, Heidelberg, 2001.
The Fitness for Purpose of Analytical Methods A Laboratory Guide to Method Validation and Related Topics, LGC, Eurachem, 1998.
E. Desimoni e B. Brunetti, "Assicurazione di qualità nel laboratorio chimico", CLUEB (Bologna-2003).
5. **Title:** Mathematical Modelling in bio-pharmaceutics
Lecturer: Prof. Mario Grassi (DI3, mariog@dicamp.units.it; 040 5583435)
Contents: Relation between Chemical Engineering and Pharmaceutics. The concept of fitting and related statistics. The concept of mathematical model. Mass conservation law. Diffusion coefficient: definitions and methods for its measurement. Effect of initial and boundary conditions on release kinetics. Matrices for controlled drug release: topology and structure. Release mechanisms. Matrix loading: mechanochemical activation. Skin and intestine absorption.
Length: 12 – 16 h (depending on student's background and requests).
Schedule: Interested students are kindly requested to contact prof Mario Grassi in order to exactly define the time schedule.
Reference textbooks: "Understanding drug release and absorption mechanisms: a physical and mathematical approach", M. Grassi, G. Grassi, R. Lapasin, I. Colombo, CRC Press, Boca Raton (FL, USA), 2007, 1-627. This book is also available at the "Biblioteca Tecnico-scientifica" of the University.
6. **Title:** Biocatalysis and enzymatic technologies in the chemical and pharmaceutical industry
Lecturer: Prof. Lucia Gardossi (DSCF, gardossi@units.it; 040 5583110)
Contents: Introduction to activity stability of enzymes. Enzyme kinetics. Biocatalysts for industrial applications. Enzyme selectivity and resolution of racemates. Selected examples of industrial applications of enzymes: peptide synthesis, antibiotics synthesis. Solid phase biocatalysis. Enzyme immobilization. Application of computational methods to the rational planning of biocatalyzed processes.
Length: 6 h.
Schedule: Interested students are kindly requested to contact prof Gardossi well in advance in order to exactly define the time schedule.
7. **Title:** The crystallography in the chemistry and biochemistry of vitamin B₁₂: *from models to macromolecules... to compounds socially useful*.
Lecturer: Prof. Lucio Randaccio (DSCF, lrandaccio@units.it; 040 5583935)
Contents: Brief history of vitamin B₁₂ (cobalamins). Vitamin B₁₂ in mammals. A simple B₁₂ model: cobaloximes and their structural properties. Structural aspects of cobalamins. cis and trans Influence in octahedral Co(III) complexes. Structure and function of B₁₂ enzymes: methionine synthase. Structure and function of B₁₂ enzymes: mutases and eliminases. Structure and function of B₁₂ transport proteins. B₁₂ bioconjugates.

Length: 5 h.

Schedule: to be agreed with the lecturer.

8. **Title:** Metals in medicine

Lecturer: Prof. Enzo Alessio (DSCF, alessi@units.it; 040 5583961)

Contents: Introduction and general concepts, MRI contrast agents, Radiopharmaceuticals and radiodiagnostics, Anti-infective agents, Insulin mimetics, Anticancer Pt drugs: history, development, structure-activity relationships, activity, mechanism of action, recent developments, new trends; Other anticancer metal agents (Ru, Au, Bi); Photodynamic therapy, Boron-neutron capture therapy; Cardiovascular system: systems for controlled NO release and for NO scavenging; Gold antiarthritic drugs.

Length: 8 - 10 h.

Schedule: Typically in May – June every year. Dates to be agreed with the lecturer.

9. **Title:** Nanoparticles: synthesis and applications

Lecturer: Prof. Lucia Pasquato (DSCH, lpasquato@units.it; 040 5582406)

Contents: Introduction to nanochemistry. Nanoparticles, definition, variety of materials. Metal Nanoparticles. Synthesis and characterization techniques. Nanoparticles of different shape and size. Quantum Dots. Properties of nanoparticles, optical properties. Applications to material chemistry and applications to biology and medicine.

Length: 8 - 10 h.

Schedule: Typically in June each year (Students are invited to contact the teacher for further informations).

10. **Title:** Electronic spectroscopy

Lecturer: Prof. Giovanna Fronzoni (DSCF, fronzoni@units.it; 040 5583948)

Contents: Brief review of electronic spectroscopy : electronic states of atoms and molecules, absorption and emission processes, notation for electronic states, spin-orbit coupling. Electric dipole selection rules. Introduction to photoelectron spectroscopy (UPS and XPS). Introduction to X-Ray photoabsorption spectroscopy (NEXAFS region). Examples and applications.

Length: 12 h.

Schedule: Lecturer will arrange the timetable of the lessons with the interested students.

11. **Title:** Quantum mechanical methods in chemistry

Lecturer: Prof. Mauro Stener (DSCF, stener@univ.trieste.it, 040 558 3949)

Contents: Quantum mechanics, approximate methods for electronic structure. Hartree Fock (HF) method and Density Functional Theory (DFT). Basis functions. Geometry optimizations. Computer exercises.

The purpose of the course is to support students graduated in non chemistry fields (Farmacy, Biology, CTF) with an overview on principles and simple applications relative to the most diffuse approaches in computational chemistry.

Length: 20 h

Schedule: July 2011: specific dates and timetable will be arranged with interested students.

12. **Title:** Introduction to Impedance Spectroscopy (IS)

Lecturer: Prof. Claudio Tavagnacco (DSCF, tavagnac@units.it, 040 5583942)

Contents: Differences Between Aqueous and Solid State Electrochemistry; The Importance of IS in Interfaces Studies; Physical Models for Equivalent Circuit Elements; Simple RC Circuits; Argand Diagram and Analysis of Simple Impedance Arcs; Conductivity and

Diffusion in Electrolytes; IS Measurement Techniques; Instrumentation and Practical Examples in Simple RC Circuits; Practical Applications.

Length: 10 h.

Schedule: The interested students are invited to contact the lecturer for arranging the schedule of the lessons

13. **Title:** High pressure technology.

Lecturer: Prof. Ireneo Kikic (DI3, ireneo.kikic@dicamp.units.it, 040 558 3433)

Contents: Introduction to phase equilibrium concepts; thermodynamic behaviour of systems at high pressure; modelling phase equilibria at high pressure; supercritical fluid technologies (natural products extraction, pharmaceutical applications..).

Length: 20 h

Reference textbooks: J.M. Prausnitz, R. N. Lichtenthaler, E. G. de Azevedo, "Molecular thermodynamics of fluid-phase equilibria", Prentice Hall, 1999, P. York, U. B. Kompella, "Supercritical fluid technology for drug product development", Marcel Dekker, Hew York (NY, USA) 2004; J.L. Martinez, "Supercritical fluid extraction of nutraceuticals and bioactive compounds", CRC Press, Boca Raton (FL, USA), 2008.

Additional information: Course slides in ppt format available from the lecturer