PROPOSTA DIDATTICA 2018-2019

Modern Applications of Chiroptical Spectroscopies

Prof. Gennaro Pescitelli, Dott. Francesco Zinna

The course aims to furnish the basic knowledge of the major chiroptical spectroscopies and discuss their modern applications to the study of different kinds of systems.

The course is organized into four units (approximately 2h each) covering the following topics:

(1) basic introduction to electronic circular dichroism (ECD) and vibrational circular dichroism (VCD) spectroscopy; ECD and VCD equipment; major factors determining ECD spectra; applications of ECD and VCD spectroscopies;

(2) chiral supramolecular systems and use of ECD as a privileged means for their study: detection, quantification, assessment of supramolecular helicity, structure determination;

(3) ECD and VCD calculations as a modern tool to assign absolute configuration of chiral molecules;

(4) basic introduction to circularly polarized luminescence (CPL) technique; CPL equipment; examples of applications of CPL: small organic chiral molecules, chiral lanthanide complexes, chiral macromolecules, (bio)-analyte sensing; circularly polarized emitters in OLED technology

[May 2019]

Synchrotron radiation-based methods of imaging and (micro)analysis

Koen Janssens (Department of Chemistry, Faculty of Science, University of Antwerp)

The course will discuss the use of synchrotron radiation (micro) beams for non-destructive materials analysis. Synopsis:

1. X-ray (Synchrotron) sources, X-ray optics and X-ray based methods of non-destructive analysis
2. Spectroscopy and spectroscopic-imaging in 2D and 3D at different length scales
3. Applications I: Localized metal speciation in catalytic, environmental and biological materials
4. Applications II: Degradation studies and imaging of cultural heritage materials

For a detailed presentation of the course see here.

[June 2019]

Self-assembly as nanofabrication tool

Enrico Dalcanale (Dipartimento di Chimica, della Vita e della Sostenibilità Ambientale, Università di Parma)

Self-assembly has its roots in biology and in supramolecular chemistry. Biology has been and still is the major source of inspiration for designing functional self-assembled systems. Supramolecular chemistry has given to the field the basic rules for manipulating noncovalent interactions at the molecular level. Examples from both sides will be provided following the silver line of function through organization.

Self-assembly is rapidly emerging as the most promising tool for nanofabrication technology, being one of the few practical ways for making organized large ensembles of molecules. The thermodynamic constraints for self-assembled systems will be discussed, as well as the concepts of allosteric and chelate cooperativity, this last one in the context of surface self-assembly.

This course will cover the subject by defining the term self-assembly in each context and by discussing selected examples taken from different fields like crystal engineering, liquid crystals, supramolecular catalysis, surface manipulation, mesoporous materials, DNA origami, etc.. Rules to control metal-directed self-assembly and H-bonding will be provided, discussing the successful strategies emerged so far, some typical mistakes to avoid and perspectives for future work.

[February 2019]

Application of Speciation Analysis to Real Systems: from Theory to Practice

Prof. Demetrio Milea (Università di Messina)

Chemical Speciation (CS), as defined by IUPAC, is the "distribution of an element amongst defined chemical species in a system". Since the chemical and physical properties of any elements of compounds are strictly related to the species in which they occur in particular conditions, CS studies are of outmost importance to evaluate their impact, activity and/or performances in real systems of environmental, biological and technological/industrial interest.

One of the most effective ways to perform Speciation Analysis is through computer modelling based on thermodynamic equilibrium data. Several real systems (e.g., seawater, estuarine and fresh waters, biological fluids, process and/or waste waters) are, from a chemical point of view, multi-electrolyte aqueous solutions in which many elements and compounds are simultaneously present in a wide range of conditions.

Starting from the basic concepts regarding the chemical speciation of real aqueous systems, lectures will then focus on: i) the evaluation of the most critical aspects related to the experimental determination of thermodynamic parameters in multicomponent aqueous solutions; ii) their modelling as a function of chemical and physical variables like composition, ionic strength and temperature; iii) the use of computer tools and calculation approaches for data elaboration and speciation analysis; iv) examples and applications od speciation studies.

[December 2018]

Tecniche di Laboratorio in Elettrochimica

Dr.ssa Tiziana Funaioli (Università di Pisa)

Il corso è una introduzione all'uso di alcune tecniche elettrochimiche con lo scopo di:

- Determinare se una molecola è redox-attiva
- Misurare il potenziale di elettrodo a cui gli eventuali processi redox hanno luogo
- Stabilire se i processi redox portano a specie stabili
- In caso di composti che si degradano in seguito a processi di trasferimento elettronico, misurare la velocità dei cammini di degradazione, eventualmente suggerendo tecniche che possano aiutare nell'identificazione dei prodotti intermedi
- Suggerire gli opportuni reagenti chimici per processi redox su larga scala
- Fare luce su cammini redox attraverso meccanismi di elettrodo basati su ben documentate evidenze sperimentali
- Segnalare eventuali dinamiche molecolari causate da processi di trasferimento elettronico.

Sarà oggetto del corso anche una elettrochimica non tradizionale che combina misure spettroscopiche ai metodi elettrochimici, conosciuta come spettroelettrochimica (SEC). Abbinando l'opportuna tecnica spettroscopica all'esperimento elettrochimico, l'analisi in situ permette una più completa analisi dei processi di trasferimento elettronico e di reazioni redox complesse, rendendo possibile lo studio anche di specie che hanno una vita breve.

[data da stabilire, contattare il docente]