Euromaster

Analytical Science at the Interface

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Taught courses at University of Aberdeen

Elemental speciation analysis using elemental and molecular mass spectrometry
(6 hours)

Prof Jörg Feldmann

Chemistry Department, University of Aberdeen
AB24 3UE Scotland
j.feldmann@abdn.ac.uk
Tel: +44-1224-272911

This course gives an overview of how elemental speciation analysis in biological and environmental samples is conducted. It covers the basic fundamentals of inductively-coupled plasma mass spectrometry (ICP-MS) and electrospray mass spectrometry (ES-MS), the design and function of instruments, and the applications of the techniques to problems of environmental and biological/chemical interest.

Assumed knowledge: undergraduate analytical chemistry. The course is usually given as 6 one hour lectures, but that is flexible.

Isotope analysis for biochemical cycling and provenance studies – the use of isotope fractionation patterns
(6 hours)

Dr. Eva M Krupp

Chemistry Department, University of Aberdeen
AB24 3UE Scotland
e.krupp@abdn.ac.uk
Tel: +44-1224-272901

Content of this course will be the introduction into the concept of isotope fractionation in nature. The course will cover aspects of precise and accurate isotope ratio measurements using modern mass spectrometric methods, along with applications in the geochemical and biological field.

Assumed knowledge: undergraduate analytical chemistry. The course is usually given as 6 one hour lectures, but that is flexible.

Surface Analysis

(6 hours)

Prof Russell Howe

Chemistry Department, University of Aberdeen
AB24 3UE Scotland
r.howe@abdn.ac.uk
Tel: +44-1224-272948

This course gives an overview of how X-ray electron spectroscopy and Auger electron spectroscopy are used to analyse the surface composition of materials. It covers the basic physics of the techniques, the design and function of instruments, and the applications of the techniques to problems of chemical interest.

Assumed knowledge: undergraduate physical chemistry and surface chemistry. The course is usually given as 6 one hour lectures, but that is flexible.

Organic Structure Analysis using NMR and MS

(2 x 5 hours)

Prof Marcel Jaspars & Dr Rainer Ebel

Chemistry Department, University of Aberdeen

AB24 3UE Scotland

m.jaspars@abdn.ac.uk,

Tel:+44-1224-272895

Aims: To introduce the elements of multidimensional NMR spectroscopy and how to combine these to elucidate the structure of complex organic compounds.

- Introduction to 2D NMR spectroscopy:
  - What is a 2D experiment?
  - Types of 2D experiment - autocorrelated/cross correlated
  - Autocorrelated experiments COSY, TOCSY, NOESY, ROESY, INADEQUATE
  - Cross correlated experiments ^{13}C detected HETCOR
  - Cross correlated experiments ^{1}H detected HSQC, HMQC, HMBC.
  - 3D experiments, HSQC-TOCSY, HSQC-NOESY
- Experimental considerations:
  - Sample requirements and time requirements versus resolution.
  - General procedure to acquire data and work-up of experiments.
- Strategy for structure determination:
  - Determining molecular formulae using MS and NMR data
  - Assignment of ^{1}H-^{13}C direct correlations using HSQC data
  - Using COSY/TOCSY data to assemble substructures
  - Combining substructures using long-range data
  - Testing working structures using a combination of data and literature databases to make a structural proposal.
  - Methods to confirm the structural proposal.
- Modern tools to aid structure determination:
  - Structural databases
  - Chemical shift databases
  - Computer aided structure elucidation.

Taught Courses at Gdansk University Of Technology

Surface topography

(6h)

Helena Janik

Gdansk University of Technology
Narutowicza 11/12, 80-952 Gdańsk, PL
janik@urethan.chem.pg.gda.pl
tel. 48 58 347 2634

This course gives an overview of methods, like electron microscopy (different techniques), atomic force microscopy and prophilometry used to estimate the surface topography of different solid-state materials. It covers the background to understand the relationship between chemistry and physics of surface analysis. The practical application of those methods are included (paintings, coatings, implants…).

Assumed knowledge: undergraduate physical chemistry, physics, chemistry

Environmental monitoring with electron microscopy

(8-10h)

Helena Janik

Gdansk University of Technology
Narutowicza 11/12, 80-952 Gdańsk, PL
janik@urethan.chem.pg.gda.pl
tel. 48 58 347 2634

This course gives an overview of techniques of electron microscopy used to monitor the quality of water, air and soil. It covers the basic fundamentals of electron microscopy and modern approach to overspread the application of that method in environmental monitoring with practical case studies like bioindicators, air particles PM10, morphology of different soils etc.

Assumed knowledge: undergraduate physical chemistry, physics, chemistry

Ellipsometry techniques in analysis of properties of surface layers

(10h)

Jacek Ryl, Kazimierz Darowicki

Department of Electrochemistry, Corrosion and Materials Engineering,
Chemical Faculty, Gdansk University of Technology
Tel +48 58 3471977
jacekr@chem.pg.gda.pl

Ellipsometry is a powerful technique used for an investigation of physico-chemical properties of surface as well as dielectric properties and thickness of thin layers. In the end of XIX century Drude has discovered that the phase difference between the polarization components depends on the material. He called this technique ellipsometry after most general polarization state.

Ellipsometry measures a change of polarization of light as it is reflected or transmitted from a material surface. This change of polarization state is represented by the phase difference Δ and an amplitude ratio Ψ and depends on the refractive index and thickness of individual materials. In general the measured values of Δ and Ψ cannot be directly converted into optical constants of the sample. An analysis of optical model has to be performed. Unknown optical constants and/or thickness are estimated on the basis of this optical model.

- Fundamentals of ellipsometry: historical background, propagation of electromagnetic wave, types of polarization, Snellius law, Fresnel coefficients, Delta and Psi
- Optical parameters of investigated materials: the complex refractive index, absorption coefficient, maximum thickness of measured layers, optical model, Delta and Psi
- Single-wavelength vs. spectroscopic ellipsometry: ellipsometer components, types of ellipsometer source of light
- Quantitative analysis of layers and surfaces: effect of angle of incidence and wavelength of laser source, selection of optical model, fitting procedure, determination of thickness for very thin films
- Qualitative analysis of layers and surfaces: determination of refractive indices and constitution, Bruggemann EMA approximation, MSE error function, specific sample measurements

Sustainable energy from solar hydrogen

(6h)

Marcin Janczarek

Department of Chemical Technology
Chemical Faculty, Gdansk University of Technology
mjancz@chem.pg.gda.pl

Technological advancement and a growing world economy during the past few decades have led to major improvements in the living conditions of people in the developed world. However, these improvements have affected essentially on environmental area, especially because of very high usage of energy from non-renewable sources based on coal. Hydrogen is very promising candidate for the fuel of the future. Hydrogen is not a primary source of energy, rather it is an energy carrier much like electricity. Therefore, energy is required to extract hydrogen from substances like natural gas, water, coal, or any other hydrocarbon. Utilization of solar energy in connection with thermal and photosynthetic energy can be very promising alternative to extract hydrogen from non-coal source as water.

The content of the course will be as follows:

1) From hydrocarbons to hydrogen - towards a sustainable future
2) Electrolysis of water – principles
3) The review of most important methods for solar hydrogen generation:
   - thermochemical and thermal/photo hybrid solar water splitting
   - irradiated semiconductor-liquid interfaces
   - photobiological methods
   - complex systems of hydrogen generation
4) Future perspectives

Materials for energy storage and conversion devices

(10h)

Anna Lisowska–Oleksiak

Department of Chemical Technology
Chemical Faculty, Gdansk University of Technology
alo@chem.pg.gda.pl

The lecture course is addressed to students from chemical, physical and material sciences interested in novel devices, especially energy storage and conversion devices such as rechargeable lithium batteries, electrochemical capacitors and low temperature fuel cells. Both, electrode and electrolyte materials in respect to their physicochemical properties are in the scope. Charge transport phenomena and electrode / electrolyte interfacial properties in are of our interest and based in general on solid state electrochemistry.

Surface investigation with scanning probe microscopy techniques

(10h)

Michał Szociński, Kazimierz Darowicki

Department of Electrochemistry, Corrosion and Materials Engineering,
Chemical Faculty, Gdansk University of Technology
Tel +48 58 3471044
micszoci@chem.pg.gda.pl

Performance of any material relies not only upon its bulk properties but also on its surface ones. It is the surface that contacts service environment and interacts with the surroundings. A scope of the course engulfs presentation of a group of investigation techniques devoted to surface characterization, known under the common name of scanning probe microscopy (SPM) methods. An unique feature of them is provision of an outstanding measurement resolution of nanometer or even atomic order. Thus they are ideally fitted for identification of nanoscale phenomena and processes, also at their very onset, yielding valuable information about materials properties, performance and susceptibility to degradation. Such abundance of measurement possibilities made it possible for the SPM techniques to enter new fields of research and evolve into routine surface characterization tools. In the two decades since the invention in the 80s of the last century, probe microscopies in general have made a dramatic impact in fields as diverse as materials science, semiconductor physics, electrochemistry, tribology, medicine, micromechanics, electronics, corrosion etc. The SPM group includes two basic techniques: the atomic force microscopy (AFM) and the scanning tunneling microscopy (STM) operating on the basis of sensing an interaction between the measurement tip and investigated sample. The interaction can be of different character – atomic force, electric, magnetic or optical interactions being the most commonly utilized. There are numerous modes of measurement with these techniques including contact mode, non-contact mode, constant high or constant current mode in case of the STM, constant height or constant force mode in the AFM and many other. The principles of each technique and measurement mode as well as their advantages and drawbacks will be taught in details, including information about selection and optimization of measurement parameters, image processing operation as well as interpretation. These will be supported by numerous examples of the SPM implementation in different research fields. A cooperation between the SPM techniques and other classic ones will also be shown.

Environmental applications of heterogeneous photocatalysis

(6h)

Adriana Zaleska

Department of Chemical Technology,
Gdansk University of Technology
azal@chem.pg.gda.pl
Tel.: +48-58-3472437

The course will cover aspects from the fundamentals of photocatalysis to its applications in environmental protection:

- introduction on the basic of heterogeneous photocatalysis: mechanism of semiconductor photocatalysis, formation of reactive oxygen species, reaction rates, surface interactions and quantum efficiencies
- photochemical transformation of specific compounds: inorganic and organic compounds
- photochemical reactors: gas-phase and water treatment system
- photo-induced superhydrophilicity and self-cleaning materials
- novel photocatalytic materials more active than the conventional materials under both UV and visible light: metal nanoparticles modified TiO2 and (b) non-metal doped TiO_2

Noble metals application in various field of human activity

(5h)

Ewa Kowalska

Department of Chemical Technology,
Gdansk University of Technology
Tel.: +48-58-3472437

Physicochemical properties of noble metals and various possibilities of their application will be discussed.

Brief historical review of their use from ancient time (jewelry, decoration, antiseptic) till nowadays (cosmetics, bio- and chemo- sensors, electronics, fuel cells, surface Raman scattering, lithography, near-field magneto-optical microscopy, antiseptics). Latest progress in noble metal chemistry, such as catalysis (when noble metals are not noble) and phenomenon of localized surface plasmon resonance (LSPR).

Generation of different forms of noble metal, such as colloids, clusters, nanoparticles, films and composites. The change of properties and possible applications during nanoparticle preparation (shape and size dependency) and supporting on various materials.

Laboratory data, commercial products and future perspectives of noble metals application.

Atmospheric chemistry and monitoring

(8-10h)

Waldemar Wardencki

Department of Analytical Chemistry, Chemical Faculty, Technical University of Gdansk
ul. Narutowicza 11/12, 80-952 Gdańsk, Poland
Phone: +48 58 347 22 94
E-mail: wawar@chem.pg.gga.pl

The course will cover following topics:

- Global atmosphere (structure, physical and chemical parameters of the atmosphere);
- Biogeochemical cycles (carbon, nitrogen, sulphur, perturbations);
- Air pollution (classification, emissions, effects);
- Atmospheric aerosols (particles, aerosols and clouds);
- Photochemistry in the atmosphere (solar energy, photolysis, photooxidation);
- Tropospheric ozone chemistry;
- Stratospheric ozone chemistry;
- Atmospheric chemistry of VOCs and $NO_{x;}$
- Degradation of CFCs and HCFCs.

- Environmental monitoring strategies;
- Sampling techniques for atmospheric samples;
- Analytical techniques for identification and quantification of reactants and reaction products;
- Measurements of atmospheric trace gases;
- Application of biological methods in analysis of atmospheric air pollution;
- Total parameters for studies of atmospheric air;
- Remote sensing of pollutants.

Assumed knowledge: undergraduate physics, chemistry and physical and analytical chemistry.

Instrumental techniques in food aroma analysis

(6-8h)

Waldemar Wardencki, Beata Plutowska

Department of Analytical Chemistry, Chemical Faculty, Technical University of Gdansk
ul. Narutowicza 11/12, 80-952 Gdańsk, Poland
Phone: +48 58 347 22 94
E-mail: wawar@chem.pg.gda.pl, marcelinaszpak@interia.pl

Aroma is an important part of organoleptic quality of food products. The aroma of most food products is the result of a huge number of reactions occurring between their components taking place in food production and processing and depends mainly on the presence, contents and composition of volatile substances which are present in raw materials, come into being intentionally or unintended during the technological process and are created during storage of food products.

A classic approach to the evaluation of organoleptic quality of food is based on the exploitation of sensoric analysis, i.e. analysis employing the use of taste, flavour, vision and touch senses, carried out by a group of properly trained estimators. Sensoric analysis can be a perfect tool in carrying out marketing tests of consumer preferences, but because of great human participation, it contains many limitations. Because of these deficiencies of sensoric analysis methods, a perfect complement in the evaluation of organoleptic food quality is instrumental analysis. Appropriate instrumental techniques allow a detailed and complex qualitative and quantitative analysis of volatile components, which shape the flavour compositions of food products.

The aim of these lectures is to give an overview of analytical methods used in food aroma analysis. The following subjects will be presented:

- the origin of the flavour components in food products
- analytical techniques used in the determination of odorous substances in food products (electronic noses and gas chromatographic profiling with various detection methods – conventional and olfactometric detection)
- sample preparation methods applied in the determination of volatile compounds (solvent extraction, continuous liquid-liquid extraction, steam distillation, simultaneous distillation and solvent extraction, solid phase extraction, supercritical fluid extraction, headspace analysis techniques: static and dynamic, solid phase microextraction)
- application of the instrumental techniques in the valuation of food quality.

Application of gas chromatography–olfactometry (GC–O) in analysis and quality assessment of food products and beverages

(4-6h)

Waldemar Wardencki, Beata Plutowska

Department of Analytical Chemistry, Chemical Faculty, Technical University of Gdansk
ul. Narutowicza 11/12, 80-952 Gdańsk, Poland
Phone: +48 58 347 22 94
E-mail: wawar@chem.pg.gda.pl, marcelinaszpak@interia.pl

In the recent years extensive studies have been performed concerning aroma active components of food products and relations between the aroma and chemical composition of the volatile fraction of these products, using gas chromatography-olfactometry (GC-O) technique. GC-O enables sensory assessment of the eluate from a GC column, what more for each particular compound eluting from the column there is a possibility for qualitative and quantitative analysis due to the presence of a sniffing-port in place or in addition to the conventional GC detector.

Appearance of olfactograms and their usefulness depend on the assay method, particularly on the extraction step and quantitative method used. In this course the most often applied sample preparation methods, including solvent and solventless extraction and also quantitative methods, such as: detection frequency methods, dilution to threshold methods and direct intensity methods will be described and compared.

Special emphasis will be placed on application of the GC-O technique in analysis and quality assessment of food products. A great number of examples of studies undertaken in order to establish the relations between the contents of volatile compounds and organoleptic properties of such products as: meat products, cheeses and other dairy products, fruits, non-alcoholic and alcoholic beverages etc. and also identification and comparison of the bouquet volatiles or unwanted off-odors in different foodstuffs will be presented.

The new and fast analytical techniques in food quality analysis

(6h)

Waldemar Wardencki, Justyna Gromadzka

Department of Analytical Chemistry, Chemical Faculty, Gdansk University of Technology

Ul.G.Narutowicza 11/12, 80-952 Gdańsk, Poland

wawar@chem.pg.gda.pl

tel. +48 58 347 22 94

This course gives an overview of how chromatographic techniques are used to analysis the quality of different food products from alcoholic beverages through edible oils and honeys. It covers different sample preparation and detection techniques (mass spectrometry, olfactometry, flame ionization). It shows how to develop a new analytical methods and its applications to problems of chemical interest.

Assumed knowledge: undergraduate analytical chemistry and food chemistry. The course is usually given as one 6 hours lecture, but that is flexible.

Gas chromatography with different detection systems – an indispensable tool in environmental trace analysis

(12h)

Bogdan Zygmunt

Analytical Chemistry Department, Chemical Faculty,
Gdansk University of Technology
80-952 Gdańsk, Poland
zygmuntb@chem.pg.gda.pl
Tel. +48 58 3472394

The course gives the principles of gas chromatography including history, theory of retention, theory of band broadening, describes separation columns with special emphasis on selection of stationary phases for separation of particular classes of organic and inorganic compounds, and detection systems to selectively detect some groups of environmental pollutants. Gas chromatography- mass spectrometry coupled system is comprehensively described. The stress is put on selection of those types of ionisation sources and analysers, and modes of operations which can allow identification and quantification of ultra-trace organic pollutants in very complex environmental matrices.

Examples of analysis of environmental samples for the content of target and non-target pollutants are given.

Course length – at best 20 hours but that is flexible

Assumed knowledge: undergraduate analytical chemistry and physical chemistry

Strategy of collecting and handling samples from aquatic environment – a critical step in producing quality results on pollution of water bodies

(8h)

Bogdan Zygmunt

Analytical Chemistry Department, Chemical Faculty,
Gdansk University of Technology
80-952 Gdańsk, Poland
zygmuntb@chem.pg.gda.pl
Tel. +48 58 3472394

The course gives description of principles of environmental sampling. Selection of sampling location and sampling sites, sample volume, and the number of samples to get reliable information on the water body studied is discussed. Equipment to take samples of ground water and surface water at different depth for determination of particular organic and inorganic pollutants is described. Sediments constitute an integral part of most of aquatic environments, therefore, they also are taken into consideration.

Advantages and limitations of sampling approaches and equipment are discussed with students, too.

Sample preservation methods and storage conditions to maintain sample integrity are also included in the course .

Course length – at best 8 hours but that is flexible

Assumed knowledge: undergraduate analytical chemistry and physical chemistry, some aspects of environmental chemistry

Hydration of biomolecules and simple model systems from the physical chemistry point of view

(6h)

Maciej Śmiechowski, Janusz Stangret

Department of Physical Chemistry, Chemical Faculty, Gdańsk University of Technology
Narutowicza 11/12, 80-952 Gdańsk, Poland
Phone: (+4858) 347 1283
e-mail: stangret@chem.pg.gda.pl, msmiech@chem.pg.gda.pl

The proposed lecture will address the following issues important for understanding the behaviour of biological macromolecules in their natural aqueous environment:

- introduction to exceptional physical properties of water, making it the ultimate environment for living organisms, the unique nature of hydrogen bond;
- definition of the types of macromolecules encountered in living organisms: proteins, nucleic acids, lipid bilayers;
- introduction of simple model systems used to mimic the contribution of different functional groups to overall interactions with water: amides and N-alkyl amides, carboxylic acids, alkyl phosphates, amino acids and their certain derivatives, oligopeptides, etc.;
- the interaction of water with the above-mentioned model compounds studied with different experimental and computational techniques;
- hydrophobicity in aqueous solutions: the case of hydrophobic hydration and hydrophobic interactions, amphiphiles, micelle formation, etc.;
- proteins in aqueous solutions: protein folding and stability;
- osmolytes in action: examples of osmolyte molecules, reinforcement or rupture of the native state of proteins due to their addition.

The lecture will be concluded with highlights from recent state-of-the-art research and visualization of perspectives for future studies in the field.

Taught courses at University of Oviedo

The use of novel nanomaterials in chemical analysis: organically modified quantum dots and molecularly imprinted polymers

(7 h)

José Manuel Costa Fernández

Department of Physical and Analytical Chemistry, University of Oviedo
C/ Julian Claveria, 8. 33006 Oviedo. Spain
jcostafe@uniovi.es
Phone: +34-985102970

Fluorescence spectroscopy has become an invaluable analytical tool for bioanalytical research. However, its applicability in biochemical analysis is very often limited by photobleaching processes, short fluorescence lifetimes or poor selectivity of the conventional organic indicators.

Recent investigations suggested that the special photophysical properties of semiconductor nanocrystals, known as "quantum dots" (QDs), can offer highly valuable solutions to the typical problems associated with conventional organic dyes. In fact, only few years after biocompatible QDs were described they have been applied in an increasing number of bioanalytical assays and imaging applications, and the variety of new applications of QDs in chemical analysis is expanding quickly. On the other hand, the design of molecularly imprinted materials (organic polymers and sol-gels) has emerged as an exciting new tool to improve the selectivity of the luminescence-based methodologies.

This course will cover some basic aspects of the use and applications of novel functionalized nanomaterials to develop novel photoluminescence methodologies. Topics that will be covered include:

- Advantages of quantum dots as novel "visualization tools" (fluorescent labels) for luminescence-based applications (0.5 h)
- Synthesis and surface modification of quantum dots (1)
- Quantum dots in chemical analysis: strategies (2 h.)
- The use of molecularly imprinted polymeric materials in photoluminescence sensing and bio-sensing (1 h)
- Synthesis and characterization of the imprinted polymers (1 h.)
- Immobilization of dyes and luminescent indicators: applications (1.5 h)

Trace elements in biology and medicine: analytical tools for speciation in living systems and heteroatom(isotope)-tagged proteomics

(7 h)

Alfredo Sanz-Medel

Department of Physical and Analytical Chemistry. University of Oviedo.
c/Julián Clavería, 8; 33006 Oviedo (Spain)
Email: asm@uniovi.es
Phone: +(34) 985 103474

To understand the role of trace and ultratrace elements in health and disease very sensitive and selective detectors must be employed. Although photon-based techniques (e.g. atomic absorption, emission or fluorescence) can be used, inductively-coupled plasma-mass spectrometry (ICP-MS) plays today a major role for trace and ultratrace total determinations and for speciation analysis as well.

For speciation analysis, hybrid techniques (consisting of coupling a powerful separation to ICP-MS) have proved most effective for speciation analysis in real life biological samples.

Such tools and applications have paved the way to the study of proteins in biological systems following the possible heteroatoms (isotopes) present in those biomolecules by ICP-MS detection. Such element-driven proteins research has been coined as "heteroatom(isotope)-tagged proteomics".

Techniques used and applications for multiscreening of (semi)metals in proteins previously separated will be explained, particularly in the context of milk nutrients distribution. "Absolute" quantitative strategies to determine proteins by using hybrid techniques with ICP-MS detection (internal standard and isotope dilution approaches) will also be discussed in detail to solve present clinical problems.

Schedule

1h. Trace elements importance in Biology and Medicine.
1h. Trace elements speciation concept, importance and tools
1h. Heteroatom-tagged Proteomics for screening
2h. "Absolute" quantification of metalloproteins via ICP-MS (quantitative heteroatom-tagged proteomics).
2h. "Absolute" quantification of phosphoproteins and "artificial" heteroatom(isotope)-tagged proteomics.

The Use of Isotopes in Quantitative Protein Analysis

(6-10 h)

Jörg Bettmer

Universidad de Oviedo,
Departamento de Química Física y Analítica,
C/ Julián Clavería 8, E-33006 Oviedo
bettmerjorg@uniovi.es,
phone: +34-985-103069

Quantitative protein analysis has become an important task in many fields of biochemical research and clinical application. Besides the qualitative characterisation of the proteom or subproteom in a specific tissue or body fluid quantitative aspects have been identified to be relevant for a better understanding of biological processes on the protein and/or peptide level. Different mass spectrometric techniques have served as useful tools for quantitative protein studies, especially since isotopically labelled compounds have been discovered for this purpose.

This course will provide an overview on the strategies and techniques using *stable isotopes* for quantitative protein analyses. It will be divided into two main parts: 1) strategies based on mass spectrometric techniques with soft-ionisation sources like *electrospray ionisation* (ESI) and *matrix-assisted laser desorption and ionisation* (MALDI). Herein, typical methods to be discussed are e.g. *isotope coded affinity tags* (ICAT) and *stable isotope labelling by amino acids in cell culture* (SILAC), 2) strategies based on the application of *inductively coupled plasma-mass spectrometry* (ICP-MS). Here, mainly two different quantification strategies based on *isotope dilution analysis* (IDA) will be discussed for its current and future potential in quantitative protein analysis, but also other purposes will be presented related to this field.

Schedule

1 h	Introduction to Quantitative Protein Analysis
1 h	Molecular Mass Spectrometry: ESI-MS and MALDI-MS
2 h	Isotope Labelling Strategies in Molecular MS
1 h	Elemental Mass Spectrometry: ICP-MS
1.5 h	Isotope Dilution Analysis
1.5 h	Applications of ICP-MS to Quantitative Protein Analysis

$\sum$ 8 h

Inorganic mass spectrometric methods for direct solid analysis

(6 h)

Jorge Pisonero Castro

Departamento de Física, Universidad de Oviedo
C/ Calvo Sotelo s/n, 33007 Oviedo, Spain
pisonerojorge@uniovi,es,
phone: +34-985102896/3476

Inorganic mass spectrometric methods for direct solid analysis are widely required to obtain valuable information about the multi-elemental spatial distribution (surface and/or bulk measurements with lateral and/or in-depth resolution) in a great variety of materials (technical, geological, biological, and environmental). For instance, this information is demanded more and more in production control and quality assurance in industry and material science. This course discusses the capabilities and controversy points of three remarkable and promising inorganic mass spectrometric techniques used for the direct characterisation of solids, including: glow discharge mass spectrometry (GD-MS), laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), and secondary ion (neutral) mass spectrometry (SIMS / SNMS).

Schedule:

1.- Introduction to Glow Discharge Mass Spectrometry: theoretical background, limitations and applications. (2 h)
2.- Introduction to Laser Ablation Inductively Coupled Plasma Mass Spectrometry: theoretical background, limitations and applications. (3 h)
3.- Introduction to Secondary Ionization Mass Spectrometry: theoretical background, limitations and applications. (1 h)

Species quantification using Elemental Mass Spectrometry: Isotope dilution analysis and species-independent calibration

(6 h)

Jorge Ruiz Encinar

Departamento de Química Física y Analítica, Universidad de Oviedo
C/ Julián Clavería 8, 33006 Oviedo, Spain
ruizjorge@uniovi.es,
phone: +34-985103069

In the last 15 years elemental mass spectrometry (ICPMS) has become an indispensable quantitative tool for speciation analysis. Two exceptional features of the ICPMS are responsible for such boom: (i) the elemental response obtained by ICPMS when operated under certain conditions could be directly proportional to the absolute amount of the ICP-detectable element present and completely independent of the structure of the species and (ii) ICPMS provides the isotopic information required to develop isotope dilution strategies.
In this course students will be provided with the theoretical background behind the two quantitative approaches. Advantages, limitations and potential fields of application for each approach will be critically discussed.

Schedule:

1.- Unique features of the ICPMS for species quantification (0.5 h)
2.- Isotope dilution: theoretical background (0.5 h)
3.- Isotope dilution for elemental speciation: measurement of isotope ratios in transient signals (1 h)
4.- Species-unspecific isotope dilution analysis: basis, advantages, limitations and applications (1 h)
5.- Species-specific isotope dilution analysis: basis, advantages, limitations and application to correct for species degradations (1.5 h)
6.- Species-independent calibration: requirements, applicability, advantages and potential fields of application (1.5 h)

Spectral Interferences in Inductively Coupled Plasma Mass Spectrometry: High Resolution and Collision and Reaction Cells.

(6 h)

Juan-Manuel Marchante-Gayón

Department of Physical and Analytical Chemistry.
Faculty of Chemistry.
University of Oviedo. Julián Clavería 8.
33006-Oviedo. Spain.
marchant@uniovi.es
Phone:. +34-985109574

Nowadays, Quadrupole (Q) mass analyzer is the most popular mass filter in Inductively Coupled Plasma Mass Spectrometry (ICP-MS) owing to their relatively low cost and easy handling. However, the main limitation of these instruments is their low resolution power and consequently the presence of spectral interferences caused by ions having the same nominal mass as the isotope monitored. There are several approaches to overcome these interferences: a) mathematical corrections, b) solvent or matrix elimination, c) changes in the plasma conditions, d) used of Collision and Reaction Cells (CRC), and e) use of High Resolution (HR) instruments. Although the technique of choice depends on the type and severity of the interference, CRC and HR are general approaches to tackle the problem of spectral interferences. In this course the students will learn:

1) The fundamentals of HR and CRC (3 hours).
2) Main applications of HR and CRC (3 hours).

ICP-MS: Fundamentals and Applications

Mariella Moldovan

Department of Physical and Analytical Chemistry,
University of Oviedo
Julián Clavería 8,
33006 Oviedo, Spain
e-mail: moldovanmariella@uniovi.es;
phone: +34-985103069

Inductively coupled plasma mass spectrometry (ICP-MS) has become the analytical technique of choice for the determination of trace, minor and major elements in almost every analytical field owing to its multi-element and multi-isotope capability, low detection limits (down to ng L^{-1} level), good precision and high sample throughput.

The aim of this course is to provide general knowledge on:

- Fundamentals of ICP-MS: overview of major components
- Control of interferences in ICP-MS
- Sample preparation and contamination control
- Hyphenated ICP-MS
- Applications of ICP-MS

Enriched Stable Isotopes in Chemical Metrology

José Ignacio García Alonso

Department of Physical and Analytical Chemistry,
University of Oviedo
Julián Clavería 8,
33006 Oviedo, Spain
e-mail: jiga@uniovi.es;
phone: +34-985103484

Mass Spectrometry has established itself as a reference analytical technique in different scientific fields ranging from environmental analysis and food quality to qualitative and quantitative proteomics and chemical metrology. Mass Spectrometry can provide qualitative, quantitative and isotopic information. The use of this isotopic information will be addressed in the course.

The actual and future use of enriched isotopes in Mass Spectrometry is not restricted to applications in environmental analysis (using ^{13}C and ^{2}H labelled compounds), but includes also trace element metabolism, elemental analysis and speciation and traceability studies. A new mathematical technique, Isotope pattern deconvolution, which can be applied to solve all these problems, will be discussed

This course will explore also new applications of the use of enriched stable isotopes in Chemical Metrology. Therefore, the synthesis of isotopically labelled compounds and the development of analytical methodologies and instrumentation, based on isotope dilution analysis, for the improvement in the quality of measurements performed by clinical, testing and industrial laboratories in any analytical field but, particularly, in clinical chemistry will be presented and discussed.

Taught courses at University of Pau

Analytical methods applied to the characterization of polymers (6 h)

Maud Save

IPREM - UMR 5254 - Equipe Physique et Chimie des Polymères (EPCP)
Bureau N202,
Hélioparc - 2 Av Pierre Angot
64053 PAU cedex 9

Tél : +33 (0)5 40 17 50 14
Fax : +33 (0)5 59 40 76 22

maud.save@univ-pau.fr

Polymer is a class of materials commonly used for numerous applications such as for example paints, adhesives, plastics, inks, resins for surface coating, technical sport's wears, contact lenses or drug delivery devices. A widerange of natural polymers could also be found in the environment such as the cellulose and hemicellulose forming wood's fibers. Polymers are formed of macromolecules with a distribution of molar masses and a distribution of various topologies (linear, branched or cross-linked macromolecules). In comparison with organic molecules, polymers are not pure products and the intrinsic distribution of their properties influences their mechanical properties. For these reasons, the characterization of these materials is a very important point to better understand their intrinsic properties.

The aim of this course is to present the specific use of the classical analytical techniques for the characterization of polymers.

The content of the course will be as follows:

- Short introduction to the basis of polymer chemistry: chemical structures of the macromolecules, basic and more complex microstructures (linear, block, branched, cross-linked, presence of a tacticity….), nature of chain ends.

- Presentation of the basic principles of the analytical techniques commonly used for the characterization of polymers: Size Exclusion Chromatography (SEC), Infra-Red spectroscopy (FTIR), Nuclear Magnetic Resonance (NMR), Mass spectrometry (MALDI-TOF) and Gaz Chromatography (GC).

- Details of the interesting points provided by each technique for the specific characterization of polymers. Concrete examples will be given for illustration.

The course duration will be 6 h.

Evaluation of the transport and fate of pollutants in the environment

(5-8 h)

David Amouroux

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel: +33 - (0)559 407 756

david.amouroux@univ-pau.fr

This course intends to provide basic principles and practical applications for chemists to investigate the transport and fate of contaminants in the environment. Through various chemical/physical principles and "real life" examples, and beside the available analytical technologies, we will see how to set an environmental case study, choose the best sampling strategy and better interprete or formulate the obtained results.

1-Basic physico-chemical principles

2-Water, atmosphere, soils and environmental pollution

3-Evaluation of the transport of pollutants in the environment

4-Evaluation of the fate of pollutants in the environments

Speciation analysis by hyphenated techniques

Dirk Schaumlöffel

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

dirk.Schaumloeffel@univ-pau.fr

Elemental speciation dealing with the specific chemical forms of an element has become a challenging part of analytical chemistry during the last 20 to 30 years. Technological and methodological achievements in recent years have considerable increased the possibilities of speciation analysis. More and more sensitive analytical techniques have reached a detection power limited only by contamination problems. At the same time, the risk of contamination has been drastically reduced by on-line coupling of separation and detection techniques. For these coupling systems the term "hyphenated techniques" was coined in the early eighties. Separation techniques such as gas chromatography, liquid chromatography and electrophoresis enable high resolution separation of the target species, while modern mass spectrometric techniques allow collecting atomic and molecular information on element species. Among these techniques inductively coupled mass spectrometry (ICP MS) has been turned out to be the most versatile and sensitive element-specific detector.

Hyphenated techniques have been successfully applied in many cases to speciation analysis in environmental and biological matrices. In the past elemental speciation analysis dealt mainly with the analysis of anthropogenic contaminants such as tributyl tin or As(III) in the environment. In recent years the analysis of endogenous element species in biological systems (metallobiomolecules) came more and more in the focus of research. In this context the application of organic mass spectrometry (electrospray and MALDI MS) has become an important technique for the identification and structural characterisation of unknown element species.

The lectures intend to give an overview of modern speciation analysis by hyphenated techniques from the basics to hot topics of recent research. The following fields of this scientific discipline will be discussed:

- Elemental speciation and speciation analysis
- Analytical techniques for speciation analysis
- Elemental mass spectrometry (ICP MS)
- Hyphenated techniques: GC-, HPLC-, and CZE- couplings with ICP MS
- Downscaling the dimensions: capillary- and nano-HPLC in speciation analysis
- From speciation analysis to metallomics: analysis of endogenous metallobiomolecules
- Electrospray and MALDI MS for structural characterisation of unknown species
- Quantification strategies by isotope dilution analysis
- Application examples from the research in our laboratory

Application of UV Photoelectron Spectroscopy to Study of Electronic Structure of Organic and Organometallic Molecules
(5 - 8 h)

Anna Chrostowska

Institut Pluridisciplinaire de Recherche sur l'Environnement et les Matériaux, UMR 5254, Université de Pau et des Pays de l'Adour, Hélioparc Pau Pyrénées, 2 avenue du Président Angot, 64053 PAU cedex 9, France.

Tel. 0559407580,
Fax 0559407451

anna.chrostowska@univ-pau.fr

Knowledge of the electronic structure of molecules is absolutely essential to progress in any chemical research. Examples include organic or organometallic synthesis, material sciences or analytical chemistry. Ultraviolet photoelectron spectroscopy (UV-PES) is a well-established technique that can provide ionization potentials of molecules in gas phase. Ionization potentials allow a better appreciation of the “nature of the chemical bond” and predict many interesting properties. Flash vacuum thermolysis (FVT) or vacuum gas-solid reactions (VGSR) coupled with UV-PES prove to be especially suited to generate and analyze small quantities of short-lived species in real time. These experimental data supported by quantum calculations for the consistency of the assignments of PE spectra provide fundamental information about electronic structure and bonding that cannot be obtained by any other technique. Representative examples to illustrate the advantages and wide applicability of these techniques will be chosen exclusively from our research in the field of the reactivity of organic and organometallic molecules in gas phase. In particular, the effects of electron deficiency, σ- and π-interactions, electron pair delocalization, and substituent effect or geometry perturbations, will be presented and discussed with the aim of shedding light on the intrinsic “personality” of molecules.

Quality assurance for chemical analysis
(6 h)

F. Pannier

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel +33 (0)5 59 40 76 73, Fax + 33 (0)5 59 40 76 74,
florence.pannier@univ-pau.f

The aim of the courses is to give an overview of QA & QC in chemical analysis and to illustrate the sources of errors which could occur during the different steps of analysis.

The Need for QA/QC of Analysis
Metrology and traceability
Analysis : Preparation and measurement
QA of Sampling
QA of Sample Treatment and Measurement
Method validation
Reference Materials

Surface Characterization of solids
(8h)

Hervé Martinez

University of Pau / IPREM CNRS UMR 5254 /
Helioparc, 2 Avenue du president Angot
64053 PAU

Tel: +33 (0)5 59 40 75 99

herve.martinez@univ-pau.fr

Surface characterization is gaining increasing use and applications in a wide variety of fields (catalysis, microelectronic, adhesion, composite materials, thin film deposit, modification and surface treatment, corrosion, ageing of polymers…) .

The XPS technique can fill the following objectives related to surface analysis : elemental analysis, trace analysis, chemical speciation, structural and molecular structure analyses, quantitative analysis and finally analytical imagery. Used for all solids under all conditions (mass, films, fibres, powder), it can also analyse the liquids. Not aggressive, it proves very interesting for fragile materials such as organic materials, polymers or biological samples for example.

The objectives of this course are: 1° Define what we mean by surfaces and exhibit their importance in an industrial and technological point of view. 2° Compared XPS with others surface techniques, 3° Present the main analytical characteristics of the techniques, its limitations and the instrumental part, 4° illustrate with appropriate examples the importance of surface analysis for the environment and industrial applications.

The general objectives of this courses is open a wide audience and aims at helping analyst to characterize a surface. It will also provide the attendees with a complete review and start of the art in this domain and hands on solutions.

From speciation analysis to metalomics: the importance of trace metal analysis
(6 h)

Brice Bouyssiere, Sandra Mounicou, Ryszard Lobinski, Joanna Szpunar

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel: +33 (0)559 407 752

brice.bouyssiere@univ-pau.fr, sandra.mounicou@univ-pau.fr, ryszard.lobinski@univ-pau.fr, joanna.szpunar@univ-pau.fr

The advances in trace element analysis with the introduction of the inductively coupled plasma mass spectrometry stimulated the development of a new research field of analytical sciences: "speciation analysis". This course will present, after a short introduction on mass spectrometry, the evolution of speciation analysis based on some specific applications. New trends related to metallomics research will also be highlighted.

- Introduction: mass spectrometry – its principles and history
- Speciation analysis: basic concepts and techniques
- Identification of metalobiomolecules: metal complexes, selenoproteins, arsenosugars
- Routine applications: analysis of metallodrugs
- Metallomics

Electronic structure of crystalline surfaces and solids : quantum-mechanical calculations

Isabelle Baraille, Hervé Martinez

IPREM, 2 avenue du président Angot, 64053 Pau cedex 9

isabelle.baraille@univ-pau.fr, herve.martinez@univ-pau.fr

The purpose is to provide an overview of the methods and computational tools currently adopted in the ab initio quantum-mechanical study of the chemical and physical properties of periodic systems, and more specifically to make it easier for non-specialists to find their way in a disconcerting variety of codes (CRYSTAL, SIESTA, WIEN2k, VASP), each characterized by different languages, different approaches and different topical problems.
The use of translational symmetry to calculate the structure and properties of periodic systems is discussed. Particularly, reciprocal space vectors, Brillouin zone, Bloch functions and periodic boundary conditions are introduced. The π bands of graphene are calculated with a model Hamiltonian and used to illustrate the effect of the periodicity on the electronic structure.
Special attention is given to the study of crystalline surfaces (slab model) and of local defects in crystals (supercell model), especially to the analysis of surface and defect states. The (001) surface of titanium disulfide (TiS_2) and interstitial defect are used as examples. Theoretical scanning tunneling microscopy (STM) images of these systems are generated and permit to identify the various defects observed by this technique on the titanium disulfide surface (001).

Practical electronic spectroscopy: avoiding artefacts (9 h)

Patrice Bordat, Sylvie Blanc, Ross Brown

Université de Pau et des Pays de l'Adour
Institut IPREM
UMR 5254 - Equipe de Chimie Physique
Hélioparc - 2 avenue du président Pierre Angot
64053 PAU cedex 9 (FRANCE)

Tel : +33 5 59 40 78 49

patrice.bordat@univ-pau.fr, sylvie.blanc@univ-pau.fr, ross.brown@univ-pau.fr

While electronic spectroscopy (absorption, fluorescence, diffuse reflectance) is one of the most powerful, sensitive and widespread methods of non-destructive analysis (with applications in bioassay and biological samples, dyes and inks, foodstuffs, hybrid organic-inorganic materials), it is subject to various experimental artefacts which are often ignored or underestimated leading to serious errors of interpretation.
These lectures will discuss the principles of the above spectroscopies starting from an overview of experimental apparatus: light sources, dispersive elements, detectors.
We will then discuss quantitatively artefacts due to inner filter, self-absorption, light trapping, scattering, instrumental defects… and how to estimate and avoid them.

Numerous case studies will be provided. A hands-on illustration could be organized with very basic local facilities.

Understanding electronic spectroscopy:

from quantum mechanics to molecular dynamics (9 h)

Patrice Bordat, Didier Bégué, Isabelle Baraille

Université de Pau et des Pays de l'Adour
Institut IPREM
UMR 5254 - Equipe de Chimie Physique
Hélioparc - 2 avenue du président Pierre Angot
64053 PAU cedex 9 (FRANCE)

Tel : +33 5 59 40 78 52

patrice.bordat@univ-pau.fr
didier.begue@univ-pau.fr
isabelle.baraille@univ-pau.fr

Electronic spectroscopy (absorption, fluorescence) is one of the most powerful and sensitive methods of analysis offering non-destructive characterisation from single molecules to dense materials including bioassay and biological samples, dyes and inks, foodstuffs, hybrid organic-inorganic materials …
Moreover, electronic spectra are very sensitive to perturbation by environmental effects. While this sensitivity contributes much to the power of electronic spectroscopy, its practical use requires deeper understanding of the factors determining electronic spectra in solids and liquids. These lectures aim to provide the necessary background:

- how to identify the relevant electronic transitions of a molecule: *ab-initio* quantum mechanical methods (TDDFT, post Hartree-Fock);
- intra-molecular sources of spectral broadening: Franck Condon factors ;
- environmental effects : solvation shift and broadening
  - simple qualitative models
  - quantitative models : polarisable continuum model (PCM), explicit solvent by classical Molecular Dynamics (MD), explicit solvent by QM /MM coupling.

These topics will be illustrated by numerous practical examples.

Modelling the vibrational spectra of molecules (8h)

Claude Pouchan, Didier Bégué, Philippe Carbonnière

University of Pau/ IPREM CNRS UMR 5254
Hélioparc, 2 Avenue du Président Angot
64053 Pau
Tel +33(0)559407850

Claude.pouchan@univ-pau.fr
Didier.begue@univ-pau.fr
Philippe.Carbonniere@univ-pau.fr

The aim of these lectures is to provide an overview of the modern computational methods used to explain, predict and assign the vibrational spectra obtained in laboratory from IR and Raman techniques and to identify bands observed in particular atmosphere.
The contents of the course will be as follows:

- Overview of the experimental techniques to obtain vibrational spectra
- Why modelling a vibrational spectra
- Classical resolution of the vibrational motions in the harmonic approximation
- Quantum Mechanical treatment of the vibrational spectra
- Ab Initio Molecular Dynamic approach
- IR and Raman Intensities
- Examples

Advanced Electronic Structure Theory: Methods and Applications (8h)

Claude Pouchan

University of Pau/ IPREM CNRS UMR 5254
Helioparc, 2 Avenue du Président Angot
64053 Pau
Tel +33 (0)559407850
Claude.pouchan@univ-pau.fr

The purpose of this course is to provide an overview of the methods and computational treatments commonly used to explain and predict the reactivity of some chemical reactions. Special attention will be given to the study of the thermodynamic and kinetic properties from modern computational methods

The lecture aim to provide the backgrounds to understand the reactivity of molecular systems in a given environment.

The content of the course will be as follows:

- Basis and Backgrounds of Advanced Electronic Structure Theory
- Overview of the main methods : ab-initio; semi-empirical ; DFT
- Predictions and Limitations of the methods
- Illustration by examples

Polymer characterization using light scattering and chromatography techniques.

Bruno Grassl

IPREM - UMR 5254 - Equipe Physique et Chimie des Polymères (EPCP)
Bureau N202,
Hélioparc - 2 Av Pierre Angot
64053 PAU cedex 9

Tél : +33 (0)5 40 17 50 14
Fax : +33 (0)5 59 40 76 22

Bruno.grassl@univ-pau.fr

1. Introduction
- molar mass and size of polymers

2. Classic Light Scattering
- The Nature of Light Scattering
- Multi-Angle Light Scattering
- Zimm Equation
- MALLS Instruments
- Applications

3. Dynamic Light Scattering
- Correlation Function
- Diffusion and Radius
- Applications

4. Chromatography techniques
- Separation Principle
- on-line coupling to SEC
- Applications

5. Summary

Air purification by photocatalysis : fundamentals and applications
(7.5 h)

S. Lacombe, T. Pigot

IPREM, Helioparc, 2 Avenue Pierre Angot, 64053 PAU Cedex 9 France

sylvie.lacombe@univ-pau.fr, thierry.pigot@univ-pau.fr

Tel : +33 559 407 579 +33 559 407 433

Photocatalysis belongs to heterogeneous catalysis following the same rules with in particular the occurrence of the chemical reaction in an adsorbed phase. The only difference is that photocatalysis only requires photonic energy to activate solid (TiO_2 in most cases).

For the last decade, photocatalysis have been extensively studied and appeared to be very efficient to chemical and bacteriological decontamination of polluted atmospheres.

The content of the course will be as follows:

- Fundamentals of photocatalysis
- Practical use of photocatalysis : light sources, reactors, photocatalytic media
- Recent industrial applications of photocatalysis : VOC, odour and indoor treatment; self-cleaning and anti-bacterial materials, ….
- Latest research developments : visible light sensitive TiO_2, supported photosensitizers as an alternative way to TiO_2

Chemometrics in Analytical Chemistry
(6 h)

G. Lespes

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel. +33 (0)5 59 40 76 71, Fax +33 (0)5 59 40 76 74

gaetane.lespes@univ-pau.fr

Chemometrics relates to statistical-based methods to plan experimentation and evaluate results with an optimal precision. In analytical chemistry, chemometrics is mainly used to improve, validate and control a procedure.
This course is organised according to:

1- Experimental designs: from factor screening to optimisation
2- Analytical accuracy: evaluation of significance, trueness and precision of a measurement process
3- How to calculate the limits of detection

Its aim is to give basic operational tools and strategies to optimise and evaluate the characteristics of an analytical procedure.

Environmental ecotoxicology in soil- water- plant system
(6 h)

M. Potin-Gautier and G. Lespes

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel. +33 (0)5 59 40 76 69 and 33 (0)5 59 40 76 71

martine.potin@univ-pau.fr, gaetane.lespes@univ-pau.fr

The objectives of this course is to (i) give essential knowledge about sources, transfer, transformation, accumulation and impact of chemical species including persistent organic pollutants (POPs) and trace metals and (2) relate it to analytical needs.
The content is:

1. The main pollutants according to the European legislation
2. Biogeochemical cycles in soil-water-plant system
3. Phytoavailability, uptake and toxicity : assimilated species, mechanisms of transfer and in vivo fate
4. Critical overview of soil-water-plant monitoring

This course is illustrated by different examples concerning organic and metal-based pesticides.

Nanoparticles and colloids: environmental and analytical challenges (6 h)

G. Lespes

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel. +33 (0)5 59 40 76 71, Fax +33 (0)5 59 40 76 74

gaetane.lespes@univ-pau.fr

Nanoparticles and colloids are recognized to play a crucial role towards environmental quality due to their mobility, intrinsic toxicity, reactivity and their capability to transport pollutants. Their impact (including transfer to living organisms) is especially linked to their size, shape and chemical composition. Physico-chemical characterization is of main concern, particularly since the advent of nanotechnologies and the environmental occurrence of anthropogenic nanoparticles. Among the different analytical techniques devoted to nanoparticle and colloid characterization, the on-line separation hyphenated to multi-detection appears as very powerful according to fractionation power and number of complementary physico-chemical information obtained.

The aim of this course is to give an overview of the current size-fractionation methods based on chromatography and ultrafiltration processes and focus on on-line field-flow fractionation (FFF) coupled to multi-detection chain. The content of the course is:

1. Analytical challenges : comparative presentation of the main different techniques of size-fractionation and characterization
2. Field-flow fractionation (FFF) : principle and uses
3. UltraViolet, Multi-angle Laser Light Scattering and Inductively coupled mass spectrometry (UV-MALLS-ICPMS) : advantages and benefits of a multi-detection for qualitative and quantitative analysis

Examples and applications to different case studies

Speciation Concept and methodological approach
(8 h)

M. Potin-Gautier and I. Le Hécho

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

Tel. +33 (0)5 59 40 76 69 and 33 (0)5 59 40 76 72

martine.potin@univ-pau.fr, isabelle.lehecho@univ-pau.fr

The objectives of this course is to (i) give essential knowledge about speciation concept from fractionation to speciation of metal and metalloïds in environment. The importance of the speciation on element transfert, mobility and toxicity will be discussed.

This course is composed of different points:

1) the different compartments of terrestrial ecosystem

2) trace elements in environment: chemical species and distribution between the different phases : solids, liquids, gaseous and colloidal.

3) impact in environment : dose, physico-chemical forms, , lability, liposolubility, biotransformation, bioaccumulation

4) speciation and fractionation definition

5) the different approach to speciation and fractionation
- water complexing capacity
- speciation and fractionation in water (equilibrium calculation, speciation schems,hyphenated methods)
- speciation and fractionation in soils(soft extractions,sequential extractions)

6) the different steps of speciation analysis

Characterisation methods of partially ionised gases (cold plasma)

Franck Clément, Jean-Francis Loiseau

LEGP – IPREM
Technopole Hélioparc
2 avenue du Président Angot
64000 Pau

Tel : +33 (0)559407657

franck.clement@univ-pau.fr, jean-francis.loiseau@univ-pau.fr

Cold plasmas are gaseous environments containing a large variety of elements as electrons, ions, excited neutral particles, neutral particles and photons.
Depending on the experimental conditions, these particles and their formation lead to a complex gaseous chemistry with numerous applications like physical and chemical modifications of solid, liquid and gaseous materials : etching, cleaning, reticulation, functionalisation, grafting, deposition, …
In order to optimize a cold plasma reactor for the wished application often linked with industrial needs, numerous methods are used allowing the qualification and the quantification of these gaseous reactive species.
The aim of this course is to deliver an overview of electrical, spectroscopic and numerical methods commonly used in this area.

Chapter 1 : Definition of a cold plasma and industrial applications
Chapter 2 : Electrical methods of cold plasma characterisation
Chapter 3 : Spectroscopic methods of cold plasma characterisation
Chapter 4 : Numerical methods of cold plasma characterization

Trace element analysis by Inductively Coupled Plasma Spectrometry : Laser ablation to ICPAES and ICPMS.

(5 h)

Christophe Pécheyran

LCABIE IPREM CNRS/UPPA UMR 5254
Hélioparc Pau Pyrénées
2 avenue Pdt Angot
64053 Pau Cedex 9

tel: +33 (5)59 407 757

Christophe.pecheyran@univ-pau.fr,

In this course, I propose a comprehensive approach of ICPMS and ICPAES spectrometry as it is really used in laboratories involved in trace metal and metalloid analysis.
The first section will be dedicated to sample introduction strategies in the spectrometer: pneumatic, concentric, ultrasonic, and micro nebulisers will be described in details as well as their fields of application. Hydride generation and flow injection analysis will be discussed. As an illustration of direct solid analysis, laser ablation (nanosecond and femtosecond) will also be described thoroughly.
In the second section we will consider the use of ICPAES and ICPMS in research and routine laboratories in a *practical* point of view.