Molecular nano- and bio-photonics for telecommunications and biotechnologies (MONABIPHOT)

Coordinator : Ecole Normale Supérieure de Cachan, Institut d'Alembert
61 avenue du Président Wilson – 94235 – Cachan - France

Outline of the Master Course

(in parentheses, number of ECTS)

Starred courses are mandatory

ENS Cachan

Contact persons : Isabelle Ledoux, Professor, e-mail : ledoux@lpqm.ens-cachan.fr
Joseph Zyss, Professor, Head of Institut d'Alembert, e-mail : zyss@lpqm.ens-cachan.fr

Fundamentals in Photonics (3)*

Fundamentals in Biology (3)*

Light-matter interactions in molecular media (5)*

- molecular spectroscopy and its implications in molecular symmetries
- nonlinear optics : a quantum mechanical approach of multiphotonic processes
- nonlinear optics : propagation aspects, phase matching, parametric and Pockels effects
- orientation processes in molecular materials : electric- and optical field poling processes.

Confinement of light : waveguided optics, microcavities, photonic crystals in molecular media (5)

- Waveguided and integrated optics : propagation aspects, interferometers, couplers
- Microcavities and Distributed Feedback structures : applications to microlaser and filtering technologies
- Photonic crystals: analogy with solid-state band theory. Applications

Molecular Nanophotonics (5)*

- Nanostructures for Photonics : description and elaboration techniques
- The Nanoscale Physics : quantum confinement, implications on optical properties
- Single molecule spectroscopy
- The tools in Nanophotonics : structural and optical microscopy methods ; optical tweezers ; applications in biology.

Molecules and Materials for Electronics, Photonics and Biophotonics (5)

- Molecular and Material Engineering
- Conducting polymers
- Liquids crystals
- Organic Electroluminescent Diodes
- Molecular Magnetism
- Single molecule electronics, single electron gating
- Molecular recognition ; applications to chem- and biosensors.

Biophotonics : theoretical and practical aspects of fluorescence in Biology (5)

- Introduction to the various photonic phenomena involved in Biophotonics
- Instrumentation for fluorescence spectroscopy and imaging
- Experimental investigation of molecular complexes in solutions : protein/protein, protein/DNA…
- Cell imaging of protein/protein complexes

- Proteins-metal ions interactions

Biosensors (5)

- Recognition : molecular interactions, conformational effects, ligand immobilisation
- Data acquisition
- Bioengineering

Polymer-based device technology for optical telecommunications (5)

- Description of the various functionalities in integrated optics
- Modelling and calculation methods in waveguided optics
- Device fabrication
- Device characterization

Microfluidics : fundamentals and applications (2)

- Microhydrodynamics
- Diffusion processes, applications to mixing and particle separation in Microsystems
- Electrohydrodynamics : electro-osmosis, electrophoresis, electrokinetics
- Examples of microfluidic circuits and devices

Photonics and microwaves (5)

- Introduction of optical telecommunications
- Microwave physics and technology
- Applications (laboratory studies) : impedance matching, network analyzer

Conducting Polymers and OLED's (3)

- Information theory and encoding methods
- Multiplexing
- Classical and Quantum Cryptography

French/English/Spanish Courses (3/3/3)*

Complutense University, Madrid

Contact person : Prof. Mercedes Cano(e-mail : mmcano@quim.ucm.es)

Department of Inorganic Chemistry,

Head of Department: Prof. José M. González-Calbet

ELECTRIC AND MAGNETIC MOLECULAR MATERIALS (3 ECTS)*

1. Introduction to the molecular materials.
2. Molecular materials design with electric properties.
3. Molecular conductor and superconductors based on coordination chemistry approach, on charge transfer salts with donor and acceptor molecules, …
4. Magnetic behaviour. Matter interaction with the magnetic field: magnetic interactions.
5. Magnetic behaviour of mononuclear species: Interpretation of magnetic behaviour. Zero field splitting. Spin-orbit coupling. Magnetic behaviour of d^1 – d^9 ions.
6. Magnetic exchange: susceptibility in dimers and clusters. Interpretation of the long range interactions. Low dimensionality compounds.
7. Hybrid molecular materials: multifunctional materials and hybrid polymers. Molecular nanostructures.
8. Practical experiments.

X-RAY DIFFRACTION AND SOLUTION OF CRYSTAL STRUCTURES (5 ECTS)

1. X-Ray diffraction: Geometry, symmetry and structure factors.
2. Data collection: Diffractometers.
3. Solving crystal structures: Patterson and direct methods.
4. Refinement of crystal structures: Problematic cases.
5. Interpretation and presentation of results.
6. Solution and refinement in polycrystalline samples.
7. Practical cases.

MOLECULAR MATERIALS TOWARDS LIQUID CRYSTAL (LC) OR NON-LINEAR OPTICAL (NLO) PROPERTIES (3 ECTS)*

A. NLO MATERIALS

1. Fundamentals and concepts of NLO: Second-order non-linear processes. Third-order non-linear processes. Experimental techniques.
2. Organometallic/metallorganic compounds for NLO: The organometallic chemistry in NLO. Dipolar and multipolar molecular. Second and third-order NLO materials.
3. Organometallic/metallorganic materials for optical telecommunications: Materials in telecommunications. Optical devices. Material performance.

B. LC MATERIALS

4. Liquid crystals. Basic principles: Introduction and background. Thermotropic and lyotropic LC.
5. Physical properties of LC: Refraction indices. Linear polarizability. Dielectric permitivity. Diamagnetism. Other properties.
6. Mesophases characterization: Polarized optical microscopy. Differential scanning calorimetry. X-Ray diffraction at low angles.
7. Coordination and organometallic compounds as basis of LC molecular materials. Metallomesogens: Design. Synthetic strategies. Physical properties. Applications.
8. Practical work.

Department of Organic Chemistry

(Co-ordinator: Prof. Guillermo Orellana, Department Chair)

ADVANCED POLYMERS:

PREPARATION, CHARACTERIZATION AND APPLICATIONS (ECTS = 3)

1. Introduction to Macromolecular Chemistry.
2. Novel Radical Polymerisation Processes.
3. Ionic Polymerisation
4. Copolymerisation
5. Stereospecific Polymerisation: Last Generation Catalysts for Polyolefin Synthesis.
6. Polymer Biomaterials: Advanced Developments.
7. Polycondensation.
8. Condensation Polymerisation Techniques.
9. Membrane-Forming Polymers. Applications.
10. High-Modulus Fibers.
11. Thermally Stable Polymers.
12. Polymers in Microelectronics.
13. Modern Techniques for Polymer Characterisation.
14. Conjugated Polymers. Introduction.
15. Conjugated Polymers. Synthesis.
16. Optical and Electronic Properties of Conjugated Polymers.
17. Applications of Conjugated Polymers.

CHEMICAL SENSORS AND BIOSENSORS (7)*

Lectures :

1. Chemical sensors: their role in analytical chemistry
2. Recognition elements in sensors
3. Immobilization procedures
4. Electrochemical sensors
5. Optical sensors
6. Thermo sensors
7. Mass sensors
8. Integrated devices

Practical Classes

1. Obtaining and application of catalytic non-enzymatic electrochemical sensors.
2. Obtaining procedures of enzymatic electrochemical sensors. Use of redox mediators. Comparative application to the determination of an analyte of interest.
3. Development of optical pH sensors using different indicators and immobilization techniques.
4. Obtaining and application of ion selective optical sensors based on the use of PVC membranes.
5. Experimental work with an optical biosensor based on surface plasmon resonance using immobilization techniques and immunological detection.
6. Experimental introduction of two types of nanotechnological biosensors: microcantilevers and interferometers.

ORGANIC MOLECULAR MATERIALS (ECTS = 3)

1. New organic Materials
2. Organic materials for electricity conduction (1) : conducting polymers
3. Organic materials for electricity conduction (2) : phthalocyanines
4. Organic materials for electricity conduction (3)
5. Liquid crystals (LC)
6. Self-organization of amphiphilic molecules: Monolayers, multilayers and vesicles
7. Non-linear optics (NLO)
8. Fullerenes. Applications to novel materials
9. Superconducting organic compounds
10. Molecular devices

APPLICATIONS OF ORGANIC PHOTOCHEMISTRY (ECTS = 3)*

1. - Introduction: Photochemistry as a pluridisciplinary area with applications in Chemistry, Biology, Medicine, Environment, Materials and Sensors.

2. - Applications of Photochemistry in Organic Synthesis. Main reactions with preparative interest. Regio- and estereo-selectivity control. Enantioselective reactions. Synthesis of natural products. New photochemical reactions promoted by intermolecular electron transfer.

3. - Laser kinetic spectrometry for the study of photochemical processes. Monitoring deactivation of excited states. Kinetics of molecular deactivation: electron transfer and energy transfer. Identification of photochemical intermediates: absorption spectroscopy of transient species. Application of Photochemistry to chemical optosensor development for environmental monitoring and process control.

4. - Applications in photochemistry of polymers. Photopolymerization and photocross-linking. Photodegradation and photostabilization of polymers. Applications in electrical transport and microelectronics, printing, coatings, optics, holography and stereolithography. Other applications.

SUPRAMOLECULAR CHEMISTRY (ECTS = 3)

1. General concepts. Definition and development of Supramolecular Chemistry.
2. Chiral recognition.
3. Supramolecular chemistry of anions.
4. Model systems: An approximation to the study of relevant interactions in Bioorganic chemistry.
5. Molecular recognition in the solid state.
6. Crystal engineering.

ELECTRON MICROSCOPY AND ASSOCIATED TECHNIQUES (ECTS = 4)

1. Interactions between electrons and matter : the transmission electron microscope.
2. Electron diffraction : geometry, techniques : selected area diffraction and microdiffraction.
3. Image formation : contrast transfer function. High resolution.
4. Simulation and process of images : selected examples.
5. Scanning electron microscope.
6. Analysis by electron microscopy : WDS, EDS, EELS

NANOMATERIALS (ECTS = 4)*

1. Nanotechnology : concepts, different perceptions of nanotechnology. Bottom-up versus top-down. Tools for nanosynthesis
2. Nanomaterial design : clusters, nanoparticles, nanowires, nanotubes
3. Synthesis in confined areas
4. Mesoporous solids : synthesis and properties. Guest-host chemistry. Applications in catalysis. Design of matrices for controlled drug delivery.
5. Hybrid Materials. Functionnalization.
6. Electronic transport in nanostructures. Mesoscopic systems.
7. New systems useful in nanoelectronics : carbon nanotubes, molecules, DNA…
8. Metallic nanocontacts : conductance histograms.
9. Near-field microscopy : AFM, STM.

BIOMATERIALS (ECTS = 4)*

1. Introduction and definitions
2. Cellular biology
3. Tissue reaction on biomaterials
4. Biomechanics principles applied to biomaterials
5. General properties of the main synthetic biomaterials : metallic materials. Polymer materials. Ceramic materials.
6. General properties of the main natural biomaterials.
7. Clinical applications.
8. Research in biomaterials.

Wroclaw University of Technology

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Pr. Andrzej Miniewicz (e-mail : andrzej.miniewicz@pwr.wroc.pl)

COURSE TITLE	Person in charge	Lecture (hours)	Laboratory	Seminar	Evaluation	ECTS
Theoretical modelling of the nonlinear optical properties of molecules and clusters	W. Bartkowiak	30			Project	6
Introduction to optical telecommunications	K. Abramski	22	8		Exam, Lab report	6
Nanoscale physics*	J. Misiewicz	20	10		Exam, Lab report	6
Liquid crystals in photonics	A. Miniewicz	22	8		Exam, Lab report	6
Molecular electronic materials*	J. Sworakowski	22	8		Essay	6
Micro- and nanophotonics Devices, technology and applications	S. Patela	22	8		Exam, Lab report	6
Monte-Carlo-based modelling of photonic processes in liquid crystals and azo-polymers	A.C. Mitus	15	15		Exam Project	6
Introduction to quantum information processing and quantum cryptography	L. Jacak	30			Exam	6
Fluorescence microscopy and imaging in life sciences	M. Langner	22		8	Exam, Lab report	6
Bioorganic chemistry with elements of biochemistry	P. Kafarski	30	15		Exam Discussion	6
Genetic engineering as a tool for bio-based technology*	A. Ozyhar	30			Exam	6
Bioorganic chemistry for photonics	P. Mlynarz	30		15	Exam, Discussion	6
Methods of structural investigations in physics, chemistry and biology	R. Latajka	30		15	Exam Discussion	6

University of Wroclaw

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Prof. Jan Baran, e-mail : j.baran@int.pan.wroc.pl

-Bioinorganic chemistry*

Prof. Henryk Kozłowski, DSc.

4.0 ECTS

Lecture: 30 hours

Essential and toxic metals, general properties of metal ions, co-ordination chemistry of essential metals in bioinorganic systems. The interactions of metal ions with proteins and their subunits, nucleic acids and nucleotides. Natural and synthetic chelating agents. Biological functions of Na, K, Mg, Ca. Non-redox metaloenzymes, proteins involved in dioxygen transport, heme proteins. Red-ox proteins. Metal ion transport in biological systems. Inorganic drugs. Toxicology of metal ions (Cr and Al).

Seminar: 15 hours

Students prepare short talks (30 min.) on selected by them subject concerning biological chemistry. All students discuss the talk.

Bioorganic chemistry*

Dr Piotr Stefanowicz, PhD.

4.0 ECTS

Lecture: 30 hours.

The lecture presents the mutual influences of organic chemistry and current biology. There will be provided information on modern peptide synthesis, protein properties determined by their amino acid composition and 3D structure, introduction to enzymology. The theory is illustrated by examples such as drug designing, abzymes, enzyme inhibitors, ion channels, chemical modifications of anibiotics. Some negative examples of the scientific progress as war gases and non-biodegradable chemicals (DDT, dioxins) are also included.

Laboratory: 30 hours

The experimental part of the *Bioorganic Chemistry* course allows students to explore advanced methods of preparation, separation and determination of natural products.
Organic compounds isolated from biological sources. Chemical and spectroscopic characterisation. Chromatography methods: TLC, gel filtration, HPLC. Peptide chemistry: synthesis and sequentional analysis. Enzymes in organic chemistry.

Spectroscopic techniques*

Prof. Jerzy Hawranek, DSc.

ECTS : 4

Lecture: 30 hours; examination.

Computer laboratory: 90 hours;

Seminar: 30 hours;

Orthogonal polynomials and their properties. Analysis of trend, smoothing and differentiation of experimental data with the use of Gram polynomials. Statistical analysis of experimental data. Fourier transforms, their properties and computation. The FFT method. Experimental data processing with the use of Fourier transforms. The Fourier Self - Deconvolution method. Spectroscopic and chromatographic band models and their integrals. Simulation of spectra. Correlation functions and their use in chemistry. Methods of two - dimensional correlation analysis in spectroscopy. Quantitative analysis of multicomponent systems. Multivariate calibration. Eigenvalues and eigenvectors. Principal Factor Analysis and its application in Chemistry and Natural Sciences. Linear and nonlinear regression. Optimization methods and their application. Pattern recognition methods in chemistry.

Application of electron spectroscopy in studies on the structure of lanthanide compounds and materials

Prof. J. Legendziewicz, DSc.

4 ECTS

Lecture: 45 hours

Classification of electron transitions according to the selection rule. Mechanisms of intraconfigurational f-f transitions. Application of spectroscopic effects (changes of intensity, nepheloauxetic effect, splitting of levels, charge-transfer transitions) in studies on structure of solutions and in solids. Theory of radiative and non-radiative transitions. Life times of excited states, quantum yields, structural aspects. Electron-phonon coupling in luminescence and absorption spectra. Mechanisms of vibronic transitions. Processes of energy transfer, structural aspects of these processes. Cooperative interactions.

Computer design methods of new materials on biological importance and others*

prof. dr hab. Zdzisław Latajka

Lecture: 30 hours, 4 ECTS

1. Introduction to theoretical methods of modelling: molecular mechanics methods, Hartree-Fock method, semiempirical methods, ab initio methods, electron correlations methods, density functional theory methods.
2. Modelling of structure and properties of molecular systems in the gas phase.
3. Modelling of structure and properties of molecular systems in environment – continuum models.
4. Modelling of structure and properties of periodic systems. Plane wave, Bloch functions. Periodic Hartree-Fock methods. Calculations of band structures and density of states. Polymers: organic conductors, biopolymers and crystals. Theoretical design of new materials for nonlinear optics.
5. Modelling of surface processes. Activation of molecules on catalyst surface. Modelling of corrosion processes.
6. Modelling of structure and properties of condensed systems on base of statistical physics methods:
   - Monte Carlo method. Microcanonical and canonical ensemble. Grand ensemble. Isothermal-isobaric ensemble. Boundary condition.
   - Molecular dynamics methods. Classical molecular dynamics methods. Ab initio molecular dynamics methods. Application of molecular dynamics methods to clusters, biological systems (modelling enzymatic reactions) and solid state (superconductors, conductors, semiconductors and insulators).

Laboratory: 60 hours.

Laboratory work with computers is strictly related to the lecture. Particularly, following topics will be considered:

- determination of geometrical structure and properties of antibiotics in the gas phase and in water,
- determination of a band structure of simple organic conductors and design of new conductors,
- studies of a band structure and density of states of insulators and conductors,
- materials for nonlinear optics - calculations of hyperpolarizability,
- application of the Monte Carlo method to study of biological systems (structure of simple polipeptide),
- modelling of enzymatic reactions by mean of molecular dynamics methods,
- work on own project.

Molecular interactions*

Prof. A. Koll, DSc.; Prof. M. Rospenk, DSc.

4.0 ECTS

Lectures: 30 hours.

The course presents a basic information on the nature of molecular interactions and is an introductory to use of the modern physico-chemical methods in study the stoichiometry of complexes their structure, properties, thermodynamics of complexation and proton-transfer reaction.

Content of the lecture

The course presents a basic information on the nature of molecular interactions and is an introductory to use of the modern physico-chemical methods in study the stoichiometry of complexes, their structure, properties, thermodynamics of complexation and proton-transfer reaction.

Experimental evidences on molecular interactions, nature, the ways of description. Dispersive interactions. Potentials for molecular non-specific interaction. Reproduction of the properties of real gases.

Specific interactions. Hydrogen bonding as acid-base interactions according to Brönsted theory. Types of complexes. Macroscopic consequences of molecular interactions.

Methods of stoichiometry and structure of complexes determination. Evaluation of physico-chemical parameters and structure of the complexes as well as their thermodynamic characteristics. Spectroscopy of interacting molecules - vibrational spectra, electronic spectra, NMR spectroscopy. Isotopic effects. Dielectric properties of complexes.

Solvent influence on the strength and character of interactions. Proton transfer reaction. Potential for the proton movement. Types of dependence of various parameters of complexes on the acid-base characteristics of the

components of complexes. Specificity of intramolecular interactions. Blue shifted hydrogen bonds. Theoretical: MM semiempirical, DFT and *ab initio* description of hydrogen bond.
Electron-donor-acceptor interactions as acid-base interactions according to Lewis theory.
Interacting components. Nature of interactions; quantum-mechanical description. Electronic spectra, charge transfer transitions. Dielectric and spectroscopic characteristics of interactions. Structure of complexes.

Laboratory: 6 hours,
Groups of students will use different experimental and theoretical methods to characterise of selected interacting systems.

- The IR bands shift as a measure of interactions, the effects of concentration change.
- The ν(X-H)intensity increase upon the complexation.
- Force field. Redistribution of normal coordinates upon the complex formation. Anharmonicity.
- Experimental and theoretical NMR studies of molecular interactions.
- Polarity of hydrogen bonded complexes.
- Determination of proton-transfer degree by electronic spectra.
- Influence of temperature on the proton-transfer equilibrium. Thermodynamic data.
- Determination of the average molecular weight of solute by using the vapour pressure method (VPO).
- Determination of the formation constants and dipole moments of complexes.
- Theoretical studies on the potential of Van der Waals interactions.
- Determination of the structure of complexes by using semiempirical methods of quantum chemistry.
- Application of CT bands in determination of thermodynamic characteristics of EDA complexes
- Investigation of the structure of biologically important systems by spectroscopic methods.

Photoinduced electron transfer

Anna Szemik-Hojniak PhD.

4 ECTS

Lecture: 30 hours, examination.
The course on "Photoinduced Electron Transfer-(ET)" for students of Chemistry, Biochemistry, Biology and Physics as well for all with a general background in Chemistry being interested in the field f Photochemistry is forseen for the summer semester 1997/98. The " ET" course is meant as primary and secondary knowledge in advanced Photochemistry both at undergraduate and graduate level. The following problems are included in:

- Basic principles and terminology of Photochemistry.
- Rehm-Weller equation and the role of energetics (Excited-State Ionization Potentials and Electron Affinities,Excited - State Redox Potentials).
- Properties of Ion-Pairs and Exciplexes with experimental procedures to study them.
- Photoinduced Electron Transfer in reactions of organic substrates.
- Intramolecular (TICT-systems,Twisted Intramolecular Charge Transfer) and Supramolecular Photoinduced ET.
- Classical and nonclassical theories of ET (Marcus theory, Dynamic Solvent Effect, Electron tunnelling).

Molecular magnetism

prof. Jerzy Mroziński DSc, Maria Korabik, PhD.

4 ECTS

Lecture 15 h, examination
The aim of the lecture is to get acquainted with magnetic phenomena in biology from both experimental and theoretical perspectives.
Topics:
Essence of magnetic phenomena in living organisms. Magnetic research methods as physico-chemical methods of analysis of compounds. Influence of a magnetic field upon living organisms.

Laboratory 15 h
Exploration of the magnetic properties of d-electron metal complex compounds. Biologically active complex compounds. Magnetism of models of systems occurring in living organisms.

Conversional seminar 15 h.
Determination of the molecular structure of complexes on the basis of magnetic studies. Coordination compounds of d-electron metal ions with drugs. High- and low-spin complexes. Dimer - monomer magnetic equilibria. Living organisms in strong and weak magnetic fields. Application of magnetic methods in studies of electron transfer. Magnetic super-exchange as a function of the distance of interacting metal ions.