MASTER'S DEGREE IN CHEMISTRY AT THE UNIVERSITY OF PARMA

(2-year programme, 120 Credits)

The Master's Degree Programme in Chemistry at the University of Parma consists of 12 compulsory courses (75 credits) and two elective ones (12 credits). The Programme is divided into two curricula: i) Biomolecular Chemistry or ii) Material Chemistry which differ by five subject (30 credits).

At the end of the programme the student must undertake an internship on a research project. This internship may be splitted into two modules, part A and B, of 20+10 credits which on average require 6 months. The internship may be carried out in a research group within the University of Parma or in external companies/research structures, either in Italy or abroad. The Master's degree programme is completed with the final exam (Esame di Laurea - 3 credits) where the student will be awarded the Master's Degree title in Chemistry. For detailed information on each of the subjects and on the curricula, please check out the relevant syllabus for the academic year 2018/2019 (information provided may be subject to change, year by year).

This Master's Degree Programme is offered by the Department of Chemistry, Life Sciences and Environmental Sustainability, a Department that has been awarded the title of "Department of Excellence" by the Italian Ministry of Education specifically funded for the 2018-2022 five-year period.

Where not indicated, lectures are given in Italian. Book Exams* are available for all subjects. The experimental thesis internship work is held in English. For the academic year 2018/2019, two courses of this programme will be given in English, but a student can possibly choose another subject in English from the Master in Chemistry (Functional Materials). The offer of subjects in English is going to be expanded in the academic year 2019/2020.

*Book Exams means that the lectures are held in Italian but the lecturer gives the student the necessary study material in English and the exams are held in English.

- first term: October - February
- second term: March - June.

Common subjects	Year 1			
	I Term	**ECTS**	**II Term**	**ECTS**
	ANALYTICAL TECHNIQUES AND METHODOLOGIES IN MASS SPECTROMETRY	6	STRUCTURAL CHEMISTRY	6
	COMPUTATIONAL CHEMISTRY	6	MOLECULAR SPECTROSCOPY	6
	METALORGANIC CHEMISTRY	6		
	SUPERIOR ORGANIC CHEMISTRY	6		
	ENGLISH B2	3		

CURRICULUM Biomolecular Chemistry

Biomolecularn Chemistry	Year 1	
	II Term	**ECTS**
	BIOINORGANIC CHEMISTRY (in English)	6
	ORGANIC CHEMISTRY OF BIOMOLECULES	6
	PHYSICAL METHODS IN ORGANIC CHEMISTRY AND LABORATORY	6
	Year 2	
	I Term	
	SENSORS AND SCREENING METHODS	6
	MOLECULAR PHOTONICS	6

CURRICULUM Material Chemistry

Chemistry of the Materials	Year 1	
	II Term	**ECTS**
	PHYSICAL CHEMISTRY OF MOLECULAR MATERIALS	6
	SOLID STATE CHEMISTRY (in English)	6
	LABORATORY OF CHEMISTRY OF INORGANIC MATERIALS	6
	Year 2	
	I Term	
	ANALYTICAL CHEMISTRY OF SURFACES AND INTERPHASES	6
	ORGANIC CHEMISTRY OF MATERIALS	6

Common subjects	Year 2			
	I Term	**ECTS**	**II Term**	**ECTS**
	SUPRAMOLECULAR CHEMISTRY	6	EXPERIMENTAL THESIS – PART A	20
			EXPERIMENTAL THESIS – PART B	10
			FINAL EXAM	3

I YEAR SUBJECTS

METALORGANIC CHEMISTRY (Common Subject)

Review of some basic knowledge of coordination chemistry (metal-ligand bonding, coordination geometries, chelation). Metal-carbon interaction based on the type of C-ligand (sigma-donor, sigma-donor/pi-acceptor, pi-donor/pi-acceptor), 18e rule. Organometallic chemistry of some s and p-blocks metals: organolithium compounds, organomagnesium compounds, organoalluminium compounds, organisilicon compounds, organophosphorious compounds. Systematic study of the main classes of C-based ligands for transition metals: alkyls and aryls, carbonyls, monoolefins, dienes, allens, alkynes, cyclopentadienyls, arenes, carbenes, isonitriles. Agostic interactions, beta-elimination, alfa-elimination. Substitution reaction is octahedral and square-planar complexes. Nucleophilic and electrophilic addition reactions to coordinated ligands. Oxidative addition, migratory insertion, reductive elimination. Organometallic catalysis: main differences between homogeneous and heterogeneous catalysis, role played by an organometallic catalyst (ligand and metal effect), efficiency of a catalyst. Homogeneous hydrogenation, hydrogen transfer reaction, coupling reactions (Heck, Suzuki, Sonogashira, Negishi), nucleophilic addition to coordinated allenes.

ANALYTICAL TECHNIQUES AND METHODS IN MASS SPECTROMETRY (Common Subject)

Introduction to mass spectrometry and general principles. Description of the essential components of a mass spectrometer. LC-MS, GC-MS and CE-MS. Ion sources. Hard and soft ionization techniques in GC-MS and LC-MS. CE-MS coupling. Source for laser-assisted laser desorption / ionization (MALDI) and SELDI (Surface Enhanced Laser Desorption / ionization). Mass analyzers. Fourier transform mass spectrometry. Detectors and data acquisition. Tandem mass spectrometry. Interpretation of mass spectra. Applications and quantitative analysis. Application of mass spectrometry techniques to the study of biomolecules. Proteomics. Laboratory activities: i) Search in NIST library of mass spectra for the identification of unknown compounds (criteria for the comparison of the unknown spectra with those of the library); ii) Determination of acrylamide in samples of foods subjected to different cooking processes; iii) Determination of oligosaccharides of prebiotic interest by high-performance anion exchange chromatography with pulsed electrochemical detection (HPAEC-PED)

COMPUTATIONAL CHEMISTRY (Common Subject)

Introduction to computational chemistry. The Hartree-Fock method. One-electron properties. Basis Sets for expansion of molecular orbitals. Geometry optimization. Electron correlation methods. Density Functional theory. Molecular response properties. Statistical thermodynamics and transition state theory. Solvation models. Practices on a molecular modelling suite.

SUPERIOR ORGANIC CHEMISTRY (Common Subject)

Organic stereochemistry and molecular chirality. Atropoisomerism. Chirooptical methods: polarimetry; circular dicroism (CD) and its application in conformational and configurational studies. Study of dynamic phenomena by NMR spectroscopy. Determination of the enantiomeric composition by chromatographic and NMR methods. Stereoselective and stereospecific reactions. 1,2-Concerted rearrangements involving C, O and N atoms. Diastereo- and enantioselective syntheses. Aldolic condensations and Diels-Alder reactions. Pericyclic reactions. Epoxidation reactions and use of Sharpless as well as Jacobsen-Katsuki chiral catalysts. Chirality amplification. Protective groups. Cycloaddition reactions. Heterogeneous catalysts for enantioselective reactions. Supported catalysts. Sustainable development and eco-compatibility of chemical processes. The twelve principles of the Green Chemistry. New reaction media: water, supercritical fluids, ionic liquids. Heterogeneous catalysis. Examples of environmental friendly industrial processes and comparison with traditional ones.

STRUCTURAL CHEMISTRY (Common Subject)

Nature of intermolecular interactions. Close packing principle and symmetry for molecular crystals. Kitaigorodski's aufbau principle for rationalizing structural patterns. Analysis of the main intermolecular interactions responsible for structural organization: electrostatic interactions, conventional hydrogen bond, weak hydrogen bond, p-p interactions, metallophylic interactions, halogen-halogen interactions, aromatic interdigitation. Definition of supramolecular synthons. Classification and exemplification of common structural patterns for solid state organic/inorganic hybrid compounds: networks of hydrogen bond assembled coordination compounds, diamontoid networks, inorganic helices, coordination polymers, porous networks. Illustration of stereochemical requirements for designing supramolecular coordination compounds as polyhedral aggregates, monodimensional, bidimensional, and tridimensional polymers. Exercitations: analysis of structural patterns by using the Cambridge Crystallographic Database software. Single crystal structure determination by X-ray diffraction.

MOLECULAR SPECTROSCOPY (Common Subject)

Basic concepts: Electromagnetic spectrum, absorbance, Fourier transforms. Elettromagnetic radiation: classic and quantistic description; radiation-matter interaction. Time-dependent perturbation theory: general discussion; absorbance and emission of monochromatic radiation; electric dipole approximation; absorbance, spontaneous and stimulated emission. Linear response theory: responce and susceptibility functions; steady-state and time-resolved experiments; density matrix: pure and mixed states, populations and coherences, thermodynamic equilibrium; density matrix temporal evolution; Steady-state experiments: active and passive processes, Kramers-Krönig relations; complex dielectric constant: refractive index and extinction coefficient; microscopic formulation of the response and susceptibility functions; reduced density matrices: relaxation and bandshapes. Optical spectroscopy: the adiabatic approximation; selection rules; vibrational spectroscopy: normal coordinates, internal coordinates, group frequencies, FT-IR and Raman spectroscopies; electronic spectroscopy: absorption, Frank-Condon principle and band-shapes, fluorescence, Kasha rule, fluorescence excitation, phosphorescence. Organic chromophores, solvatochromy: Optical spectroscopy with polarized light: polarizability tensor. ORD and CD spectra. Magnetic spectroscopy: the basic NMR and ESR experiments; solution NMR: chemical shift and J-coupling; FT-NMR: basic experiment and some more refined measurements; systems of many non-interacting spins, density matrices and product operators; systems of many interacting spins, density matrices and product operators; an introduction to 2D-NMR.

ENGLISH B2 (Common Subject)

All the topics for English 1. Present Perfect Simple and Present Perfect Continuous. Second Conditional. The Passive voice. Indirect speech. Modal verbs of deduction. Main conjunctions. Use of prefixes and suffixes to build nouns, adjectives, etc. Expressing opinions.

BIOINORGANIC CHEMISTRY (given in English) (Biomolecular Chemistry Curriculum)

Summary of the main metalloenzymes and metalloproteins studied in the course – Proteins and nucleic acids from a structural perspective – Protein crystallography: preparing crystals, preliminary characterization, reciprocal lattice, data collection, solution of the phase problem, refinement and structure - Protein data bank and use of CHIMERA to display proteins - Roles of metalloproteins in cells: choice, uptake and assembly of metal containing units in biology – Control and use of ion concentration in the cell - Influence of metals in folding and cross linking in biomolecules – Interactions between metal ions and complexes in biomolecules – Electron transport proteins - Nonredox activation mechanisms and interactions with substrates – Atom and atom groups transfer chemistry – Tuning of metal properties by proteins to obtain specific functions Metal protein analysis according to the metal: Iron, Copper, Molybdenum, Cobalt, Zinc and other metals. Metals in medicine.

ORGANIC CHEMISTRY OF BIOMOLECULES (Biomolecular Chemistry Curriculum)

Chemico-physical properties and reactivity of carbohydrates, amino acid and peptides, lipids and nucleic acids. Modification of their structures and synthesis of corresponding oligomers. Artificial mimics. Use as raw material for the production of chemicals. Noncovalent interaction within molecular and macromolecular species. Applications.

PHYSICAL METHODS IN ORGANIC CHEMISTRY AND LABORATORY (Biomolecular Chemistry Curriculum)

Magnetic properties of nuclei: angular momentum and spin angular momentum. The Vector model. Fundamental concepts of 2D NMR spectroscopy. Relaxation processes. The Chemical exchange. The modern NMR spectrometer.
Interpretation of 1D e 2D NMR spectra and determination of the structure of an organic compound.
Laboratory: Synthesis of an organic compound and its structural characterization through advanced NMR techniques.

PHYSICAL CHEMISTRY OF MOLECULAR MATERIALS (Chemistry of the Materials Curriculum)

Classification of materials. Basic notions of solid state: the crystals and their symmetry properties. Symmetry and phase transitions. Vibrations (phonons) in crystals: investigation methods and properties connected to the phononic structure. Electronic states of crystals. Optical spectroscopy of crystals. Dynamics of electrons: charge transport in metals and semiconductors. Superconductivity. Molecular Materials. Molecular crystals: intermolecular forces. Optical spectroscopy of molecular crystals. Organic semiconductors. Charge transfer crystals: the organic metals. Organic superconductors. Electroluminescence and photovoltaic effect.

SOLID STATE CHEMISTRY (given in English) (Chemistry of the Materials Curriculum)

The crystal state. Origin of 3D-periodicity. Crystallization. Nucleation and growth. Amorphous materials and glasses. Bravais lattice and crystal lattice. Symmetry classification. Point symmetry. Point groups of Bravais lattices: the 7 crystallographic systems. Point group of crystal lattices: the 32 crystallographic classes. Symmetry operation involving translation. Space groups of crystal lattices. X-rays. Scattering process: Thompson and Compton. Atomic scattering factor. Scattering from ordered systems: the diffraction process. Bragg's law and Laue's equations. Reciprocal lattice. Ewald sphere. Structure factor and equation of the electron density. Relationships between diffraction and lattice simmetry. The phase problem in crystallography and its possible solution. Practical aspects of X-ray diffraction. Single crystal and powder diffraction. Crystallographic data bases. Classification of crystal structures. Close packing and eutectic models. Principal types of binary and ternary structures. Polymorphismus and phase transitions. Kinetic and thermodynamic classifications. Continuous phase transitions. Crystallographic trends in phase transitions. Solid solutions: interstitial and substitutional. Heterovalent substitutions and charge compensation mechanisms. Reactivity of solid. Solid state reactions. Principles and mechanisms. Experimental aspects. Sintering and ceramic materials.

LABORATORY OF CHEMISTRY OF INORGANIC MATERIALS (Chemistry of the Materials Curriculum)
Chemistry of the SolGel process: preparation of siliceous xerogel, preparation of hybrid organic-inorganic xerogels and their use for the purification of solutions of metals. Preparation and stabilization of metal nanoparticles and oxides. Use of water soluble organic polymers for the separation of nanoparticles from solution. Preparation of colored films based on metal oxides. Preparation of conducting glass based on tin oxide. Functionalization of a surface of silver with an organic monomolecular layer. Ferrofluids based on magnetite. Construction of a photovoltaic DSSC cell .
Formation of electrochromic films based on iron cyanometalates.

II YEAR SUBJECTS

SUPRAMOLECULAR CHEMISTRY (Common Subject)
Introduction to Supramolecular Chemistry. Molecular recognition. Intermolecular forces. Methods for the determination of the stoichiometries of the complexes and of the complexation constants via different techniques (NMR, UV-vis, fluorescence, calorimetry, potentiometry). General methodologies for the synthesis of macrocyclic compounds (crown, aza-crown, calixarenes, resorcarenes, cyclodextrins). Synthetic modifications of the macrocycles.
Cation complexation with crown-ethers, cryptands, spherands and ciclophanes. Applications in the field of imaging (MRI, luminescent probes, radiolabelling), of radiotherapeutics, of metal detoxification and of the treatment of radioactive and heavy metals waste. Neutral molecules complexation with crown-ethers, cyclodextrins and cyclophanes: studies on the complexes, thermodynamic and kinetic parameters, effect of the structure of the guest and of the solvent: the hydrophobic effect. Anion complexation by natural and synthetic receptors. Self-assembly. Supramolecular catalysis. Cavitands from cyclotriveratrylene, resorcarenes and calixarenes in molecular recognition. Discussion on some applications in the field of Supramolecular Science: Ionselective Electrodes (ISE), ion-selective membranes, chromoionophores, piezoelectric and fluorescence sensors.

SENSORS AND SCREENING TECHNIQUES (Biomolecular Chemistry Curriculum)
Definitions, characterization, quality parameters of the sensors. Transduction mechanisms. Potentiometric Sensors: Basic thermodynamics of electrochemical interphase potentials. ISFET and MOSFET Sensors: “n-p" junctions; diodes and photodiodes; principle of operation of the field effect transistors (FET); combination of FET with ion-selective membranes (ISFET) and with films of metal mixed oxides (MOSFET). Amperometric Sensors: Elements of electrodic thermodynamics and kinetics, mechanisms for mass transport and electronic transfer; reversibility of a response. Biosensors: Properties of bioreceptors as antibodies, enzymes and conjugates haptens; operating principle of competitive and non-competitive immunosensors; immobilization of bioreceptors of nanomaterials for the production of nanobiocomposite substrates; redox mediators, applications in clinical, environmental and food samples. Screening Techniques: General Principles; difference between methods of analysis and screening; immunochemical and immunoenzymatic assays, working principle of the "ELISA" kits (Enzyme Linked Immunosorbent Assay) "Lateral flow" ELISA test on disposable strips; applications and examples in clinical field.

MOLECULAR PHOTONICS (Biomolecular Chemistry Curriculum)
Fluorescence anisotropy; Excitation energy transfer; Electron transfer; Nonlinear optics; Optical microscopy; Time-resolved spectroscopy; Optical Bloch equations and photon echo; Two-dimensional IR spectroscopy.

ANALYTICAL CHEMISTRY OF SURFACES AND INTERPHASES (Chemistry of the Materials Curriculum)
Definition of interphase and surface, bulk and (multi)layers materials. Classification of interphases. Classical and modern methodologies for the interphase characterization: application field and information obtained. Thickness of the interphase region. Application fields: examples of reaction, processes and phenomena that involve the interphase concept. Classification and main properties of interphases. Surface preparation and modification, etching and deposition techniques. Etching techniques. Selective and non-selective chemical etchings. Composition rules for the etching mixtures, ternary composition diagrams, viscosity and temperature effects. Photoactivated chemical etchings.
Deposition techniques. Physical Vapour Deposition and Chemical Vapour Deposition. Characterization. Morphological characterization of interphases: point, surface, localized and extended defects, defect propagation within the interphase. Chemical characterization of interphases: compositional inhomogeneity. Evaluation of functional characteristics. Characterization techniques. Interactions between particle.

ORGANIC CHEMISTRY OF MATERIALS (Chemistry of the Materials Curriculum)
Kinetics in organic reactions and in organic material chemistry. Degradation of organic. Spontaneous and controlled radical reactions. Pyrolysis and related processes. Oxidation, autooxidation and photooxidation of organic materials. Combustion and resistant materials. Organic Photochemistry. Photodegradation and Photostability. Effect of ionizing

radiations. Polar reactions on organic materials. Ractions under acidic and basic conditions. Properties: Optical and Electronic Properties. Intermolecular interactions and properties of rigidity, elasticity, adhesiveness, plasticity, crystallinity and amorphous states. Stereochemical properties of materials. Helicity. Solubility: descriptors and solvent theories. Swelling and gel formation. Biodegradation. Self-repair. Structure: Main classes of organic materials of technological or industrial interest. Common organic materials: wood, paper, textiles. Recall of polymers structure, and focus on some polymers for high-tech applications. Materials that form gels. Organic coatings. Materials Organic-inorganic hybrids. Biomaterials. Biointerphases. Organic Nanomaterials. Carbon-based nanomaterials. Examples of functional materials for advanced applications. Tailored modification. Transformation of bulk material (e.g. biomineralisation, carbon fibres). Surface chemistry and surface treatments. Surface derivatization. Bioconjugation and bio-orthogonal chemistry. Organic reactions on carbon nanomaterials.