INCOMING UTWENTE STUDENTS

The Masters in Chemistry and Industrial Chemistry at Parma University welcome UTwente students willing to earn the Double Degree Title.

These masters are linked to the Department of Chemistry, Life-Sciences and Environmental Sustainability that was awarded (2nd in the ranking of 11 departments funded out of list of 24 departments participating to the selection) a special funding as Italian "Department of Excellence" for the 2018-2022 five-year period.

A 9-month grant of the Erasmus+ project is available for students to partially cover their living expenses in Parma.

Subjects are distributed in two terms:

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

<u>Subjects for this special programme are given in English.</u>
<u>The Experimental thesis work is held in English.</u>

Master in **Chemistry**	
Computational Chemistry (6ECTS)	3rd semester
Solid State Chemistry (6ECTS)	4th semester
Bio-inorganic Chemistry (6ECTS)	4th semester
Functional Materials (9ECTS)	4th semester
Research project – 38 ECTS Starting early in the 3rd semester	8 months

Master in **Industrial Chemistry**	
Computational Chemistry (6ECTS)	3rd semester
Sustainable Technologies and Alternative Sources (6ECTS)	3rd semester
Chemistry and Technology of Glasses (6ECTS)	3rd semester
Functional Materials (9ECTS)	4th semester
Research project – 38 ECTS Starting late in the 3rd semester	8 months

<u>Programmes of the Compulsory Subjects for students subscribing to the Master in Chemistry</u>

COMPUTATIONAL CHEMISTRY (in English) (recommended Statistical Thermo – prof. de Beer and Physical Organic Chemistry – Prof. Huskens)

Theory: 1) The surfaces of molecular potential energy; 2) Concepts and methods of molecular electronic structure; 3) The Hartree-Fock Method; 4) Expansion basis sets for molecular orbitals; 5) Post-SCF methods of electronic correlation; 6) Density functional theory; 7) Electronic properties from Hartree-Fock and DFT calculations; 8) Study of potential energy surfaces (PES); 9) Vibrational frequencies from calculations of molecular electronic structure; 10) Thermochemistry in gas phase from calculations of electronic structure; 11) NMR shielding constants from calculations of molecular electronic structure; 12) Reaction mechanisms and potential energy surfaces; 13) Explicit and implicit models of solvation.

Laboratory: 1) Calculation of Hartree-Fock and DFT equilibrium geometries; 2) Electronic structure and molecular orbitals from Hartree-Fock and DFT calculations; 3) Hartree-Fock and DFT calculations of the molecular electrostatic potential; 4) Hartree-Fock / MP2 / DFT calculations of the dissociation enthalpy of chemical bonds; 5) DFT calculation of chemical shifts in organic compounds; 6) DFT / PCM calculation of the energy profile for a SN2 reaction in gas phase and in solution.

BIOINORGANIC CHEMISTRY (in English)
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 RASMOL 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.

SOLID STATE CHEMISTRY (in English)
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 symmetry. 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. Polymorphism 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.

FUNCTIONAL MATERIALS (in English)

Aim of the course: New materials represent one of the frontiers of chemical research. This course will highlight the working methodology in materials research through the study of three different classes of materials. For each class physical, chemical and application aspects will be discussed in a comprehensive way. Self-assembly: Nanofabrication via self-assembly and self-organization, transfer of the molecular properties to the macroscopic properties. Liquid crystals: Definition, physical properties, types of mesophases, synthesis, structure-property relationship, characterization, electrical and optical properties. LC polymers. Applications: LCD, thermochromism, flat panel TV, etc. Chemical sensors: Working principle of piezoelectric and optical sensors. Sensing materials like ionophores, host-guest compounds, etc. Applications: gas sensors, liquid sensors, artificial olfactory systems. Specialty polymers: Conductive and self-healing polymers. Design, synthesis and functional properties.

Programmes of the Compulsory Subjects for students subscribing to the Master in Industrial Chemistry

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Theory: 1) The surfaces of molecular potential energy; 2) Concepts and methods of molecular electronic structure; 3) The Hartree-Fock Method; 4) Expansion basis sets for molecular orbitals; 5) Post-SCF methods of electronic correlation; 6) Density functional theory; 7) Electronic properties from Hartree-Fock and DFT calculations; 8) Study of potential energy surfaces (PES); 9) Vibrational frequencies from calculations of molecular electronic structure; 10) Thermochemistry in gas phase from calculations of electronic structure; 11) NMR shielding constants from calculations of molecular electronic structure; 12) Reaction mechanisms and potential energy surfaces; 13) Explicit and implicit models of solvation.
Laboratory: 1) Calculation of Hartree-Fock and DFT equilibrium geometries; 2) Electronic structure and molecular orbitals from Hartree-Fock and DFT calculations; 3) Hartree-Fock and DFT calculations of the molecular electrostatic potential; 4) Hartree-Fock / MP2 / DFT calculations of the dissociation enthalpy of chemical bonds; 5) DFT calculation of chemical shifts in organic compounds; 6) DFT / PCM calculation of the energy profile for a SN2 reaction in gas phase and in solution.

SUSTAINABLE TECHNOLOGIES AND ALTERNATIVE SOURCES (in English)

Biomass gasification principles. Bioethanol and ethylene production. Chemicals production from biomasses and their uses in the biofuel production. Bio-oil production and upgrading. Bio-diesel hydrocarbons production from triglycerids. Biodegradable polymers production. Problems in the polymer recycle. Chemical recycle processes of polymers. Thermal depolymerization reactions. Polymer oxidative degradation. Chemical depolymerization reactions. Polymer natural degradation processes. Industrial wastewater and exhaust gases treatments. Wastewater biological treatments. Fuel cells.

CHEMISTRY AND TECHNOLOGY OF GLASSES (in English)

The glassy inorganic materials are at the basis of several technological and traditional applications. The course is intended to provide the fundamentals of glass chemistry with particular attention to the role played by the composition of vitreous state in determining the desired optical physical and chemical properties. Some classes of glassy inorganic materials will be widely described in terms of their microstructure, optical properties, chemical behaviour and bio-activity. A series of experimental characterization procedures will be exposed for the study of the different aspects concerning the glass material. The principal industrial processes of glass fabrication will be discussed.

FUNCTIONAL MATERIALS (in English)

Aim of the course: New materials represent one of the frontiers of chemical research. This course will highlight the working methodology in materials research through the study of three different classes of materials. For each class physical, chemical and application aspects will be discussed in a comprehensive way. Self-assembly: Nanofabrication via self-assembly and self-organization, transfer of the molecular properties to the macroscopic properties. Liquid crystals: Definition, physical properties, types of mesophases, synthesis, structure-property relationship, characterization, electrical and optical properties. LC polymers. Applications: LCD, thermochromism, flat panel TV, etc. Chemical sensors: Working principle of piezoelectric and optical sensors. Sensing materials like ionophores, host-guest compounds, etc. Applications: gas sensors, liquid sensors, artificial olfactory systems. Specialty polymers: Conductive and self-healing polymers. Design, synthesis and functional properties.

For any inquiries, please mail to

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