CHEMISTRY

Beidh léachtaí le fáil i nGaeilge agus i mBéarla ar na cúrsaí seo leanas:-

First Year

Course No.: CH101/CH103
Course Name: Chemistry
ECTS Credits: 15 ECTS Credits
Load (Hrs): 72L + 69P

Introduction, Atomic Structure, Chemical Bonding, Molecular Structure.

Units: Seven basic S.I. units. Derived units of force, pressure, energy and volume. Chemical symbols and equations. Elements, compounds. Empirical formula. Molar quantities. **Gases:** Ideal gases. Mixture of gases. Gas Laws. Nonideality of gases. Kinetic theory and derivation of Gas Laws. **Solutions:** Solubility. Solubility product; principle and application in the laboratory. **Periodicity of Properti**es: Periodic Table. Historic development (Mendeleev). First 20 elements.

Atomic Structure: Bohr particle theory of the electron. De Broglie equation and the wavelength of the electron. One dimensional Schrodinger equation for standing waves. s, and p orbitals.

Electronic Structure of Elements: Ionization potentials, covalent and van der Waals atomic radii. Electron affinity. Trends in the Periodic Table. **Chemical Bonding**: Ionic, covalent and polar covalent bonds. Bond energies. Electronegativity. Dipole moments. **Hydrogen:** Molecular Orbital Theory (MOT) of the H2 molecule. Preparation, properties and uses. MOT of diatomic molecules of first period. σ, σ*, π* orbitals. **Water:** MOT and Valence Shell Electron Pair Repulsion Theory (VSEPRT) of the water molecule. Hydrogen bonding. Structure of water liquid and ice. Polymorphs of ice. **Molecular Geometrical Structures and Electronic Structures:** VSEPRT and MOT of ABn molecules with n = 2-6.

Inorganic Chemistry

The periodic table, periodicity of properties, metals, non-metals, semi-metals, compound formation, electronic configuration, orbitals, valence shell, Lewis representation, reactivity, molecular structure.
Alkali metals, halogens, oxy acids, group IV, transition metals.
Chemical reactions and chemical equations.
Occurrence, properties, and extraction of the elements.
Nuclear power, fission, fusion, isotopes.
Redox chemistry, valence, oxidation number, disproportionation, electrode potential.
Structural chemistry; metals, alloys, non-metallic elements, ionic solids, covalent molecules, diamond, graphite, fullerenes, oxides, silica, silicates
Uses of the elements and their compounds; batteries, glass making, depression, soaps, detergents, surfactants, bleaches, plastics, insecticides, pesticides, DDT, freons, cutting, polishing, conductors, lubricants, soot, carbon black, inks, textiles, fibres, semiconductors, p-n junctions.
Environmental issues; hardness of water, acid rain, water quality, pollutants, ozone layer, biological oxygen demand.Common chemicals and chemical processes; home, health, earth, atmosphere, hydrosphere, energy sources, nitrogen fixation, weathering, pollution, water quality, water treatment, eutrophication.

Physical Chemistry

Equilibrium Principle of Le Chatelier, equilibrium law, equilibrium constants and calculations. **Reactions in solution** Electrolytes, acids and bases, precipitation reactions, redox reactions, oxidation numbers, redox titrations. **Acids and bases** Definitions, acid/base strength, pH concept, buffers, acid-base titrations, indicators. **Thermodynamics** 1st law, expansion work, calorimetry, enthalpy changes, Hess's law, bond energies, 2nd law & entropy, 3rd law, Gibbs free energy. **Gases, solids and liquids** Real gases, condensed states, intermolecular forces, properties of liquids and solids, phase changes, phase diagrams. **Solutions** Like dissolves like, heats of solution, Henry's law, colligative properties of solutions. **Kinetics** Rate laws & reaction order, half-life of first and second order reactions, transition-state theory, catalysts. **Electrochemistry** Cell voltages, Nernst equation, applications of galvanic & electrolytic cells.

Organic Chemistry

- Introduction & Alkanes. Empirical, molecular and structural formula. Structure of methane and ethane; sp3 hybridisation. Structure, names and isolation of alkane isomers up to C6. Homolysis and heterolysis of covalent bonds. Homolytic chlorination of methane and propane.
- Alkyl Halides. Preparation of alkyl halides and conversion to alcohols, amines, nitriles and ethers: SN1 and SN2 reactions. E1 and E2 elimination reactions. Grignard reagent preparation, structure and reaction with aldehydes, ketones and carbon dioxide.
- Alcohols, Ethers & Amines. Alcohols: structure and names up to C4; industrial preparation of methanol and ethanol; preparation, physical properties and reactions. Ethers: preparation and properties. Amines: preparation, nomenclature and properties/reactions of aliphatic amines.
- Alkenes. Structure of ethene; sp2 hybridisation. *cis*- and *trans*-2-butene. Preparation of ethene from ethanol. Addition to alkenes of hydrogen, bromine, and water. Addition of hydrogen halides to propene. Oxidation of alkenes with potassium permanganate and ozone.

- Carbonyl Chemistry. Electronic structure of the carbonyl group. Preparation of carbonyl compounds. Oxidation and reduction of carbonyl compounds. Addition to carbonyl group of hydrogen cyanide and amines/hydrazines. Silver mirror test for aldehydes.
- Carboxylic Acids. Preparation and properties of carboxylic acids. Reactions of carboxylic acids; reduction; decarboxylation; preparation & reactions of acid chlorides, amides and esters.
- Alkynes & Nitriles. Alkynes: structure and preparation of ethyne; oxidation and reduction of alkynes; preparation of *cis*- and *trans*-2-butene; reactions of the ethylene hydrogen in ethyne. Nitriles: preparation & reactions.
- Stereochemistry. Definition and importance of chirality and enantiomers.
- Aromatic Chemistry. Aromaticity and electrophilic aromatic substitution. Conversion of benzene to toluene, chlorobenzene, nitrobenzene, benzene sulfonic acid and acetophenone. Preparation & properties of benzoic acid, phenol and aniline; diazonium salts and their reactions.

Uimhir Chúrsa: CH107
Course Name: Ceimic
ECTS Credits: 15 ECTS Credits
Load (Hrs): 72L + 69P

An Cheimic Fhisiciúil

Na haonaid bhunúsacha. Dlús, fórsa, brú, toirt, teocht, fuinneamh, toilleadh teasa. Teoiric adamhach Dalton, siombail na ndúl. Dlí Gay-Lussac. Fóshuíomh agus tairismheach Avogadro. Dúile, comhdhúile, móilíní, an mól, foirmlí empiriceacha, iomoibrithe agus cudromóidí ceimice.
An stáid ghásach. Na príomh-gháisdlíthe, dlús na ngás agus na ngal, an gás idéalach agus an teoiric chinéiteach, an chudromóid idéalach stáide, idir- agus eis-leathadh, mais mhóilíneach, na gáisdlíthe agus stóicioméadracht, páirtbhrú agus dlí Dalton, dlí Henry.
An struchtúr adamhach. An leictreon, proton, neutron, raidighníomhacht, leath-shaol, dátú radiocheimiceach, an iarmhairt fotóleictreach. Teoiric chuantamach, teoiric Bohr do'n adamh hidrigine. Tonn-thréithe an leictreoin.
Teirmidionaimic. An chéad dlí, sainmhínithe ar chórais ionchúlaithe (ionchasta), toilleadh teasa, feidhmeanna stáide, fuinneamh inmheánach, eintealpai, obair, nasc-fhuinneamh, eintreopai, próiséis neamh-ionchasta agus ΔS. Fuinneamh saor.
Leictricheimic. Tualaingí dí-ocsaoidiúcháin, leath-chealla agus cealla leictricheimiceacha, leictriliú, cudromóid Nernst. Tairismheach Faraday, prionsabal an pH méadar.
Cothromaíocht. Tairismheacha cothromaíochta, Kp agus Kc, Prionsabal le Chatelier.
Pás-léaráidí. An córas uisce agus déocsaoid carbóine, pás-athrú agus eintreopai, Dlí Raoult,
Gásanna Réadacha. Diallais ó na gáisdlithe, cudromóid Van der Waals, treastómhas móilíneach.

An Cheimic Neamhorgánach

An Tábla Peiriadach, Dlí Peiriadach na nDúl, Obair Lothar Meyer agus Mendéelef.
Cumraíochtaí Leictreonacha na nDúl, Prionsabal Auf-bau, Poitéinsil Ianúcháin, Leictreonfhíníocht agus Leictridhiúltacht na nDúl.
Nascanna Ceimiceacha, an Nasc Ianach, an Nasc Comhfhiúsach, Fórsa Van der Waals agus an H-nasc.
Ullmhú na nGásanna atá Feichithe Cheana ins an Saotharlainn.
Uisce, Ibhuisce agus Truailliú, Bogadh Uisce, Galúnach agus Glantacha. Struchtúr Uisce i nGal Uisce, Uisce Leachtach agus Uisce Soladach.
Iantoradh Uisce, Aigéid agus Bunnanna. Obair Arrhenius, Brønsted agus Lewis. Neart Aigéid agus Bunanna agus Maoláin. Tuaslagáin agus an Toradh Tuaslagachta.
Struchtúir de Mhóilíní Comhfhiúsacha, leis an foirmle ABn, de Réir an TEDLSF.
Stáid Ocsaídeach, Cothromóidí Ceimiceacha Á Mheá agus Toirtmheascadh.
An Tionscal Ceimiceach, Táirgeadh Aigéad Niotrach, Aigéad Sulfarach agus Amóinia. Leasú Talúin, Táirgeadh Iarann agus Cruach.
Áiríonna Ceimiceacha Grúpaí 1 agus 2.
Áiríonna Ceimiceacha Grúpaí 13, 14, 15, 16 agus 17.

An Cheimic Orgánach

- **Ceimic na Dúile Carbón**
- **Na hAlcáin (Carbóin Teitrihéadrach) –** Híbridiú sp3, struchtúir móilíneach; isiméireacht; córas ainmniúcháin IUPAC; imoibríocht ceimiceach
- **Sintéis Cheimiceach ó Hailídí Orgánacha**. **Imoibrithe SN** – Meicníochtaí SN1, SN2; gníomhaíocht optúil agus isiméireacht spás–déanamh; sintéis le comhdhúil orgánaímhiotail.
- **An Nasc Dúbailte > C = C < ; > C = O ; > C = N-** ; Struchtúr, híbridiú sp2; giniúint nasc dúbailte
- **Na hAilcéiní -** Imoibrithe suimiúcháin leictrifíleach; féin-suimiú, poiliméirí; ocsaídiú
- **Nasc Dúbailte: >C=O (Carbóin plánach) -** Aildéid, Céatóin agus Aigéadaí carbocsaileacha; struchtúr agus iompair ceimiceach.
- **An Nasc Triarach – C ≡ C –; – C ≡ N: -** hibridiú sp, struchtúr.

- **Beinséin: Ceimic Aramatach –** Struchtúr fisiceach agus leictreonach; Athshondas; Ionadaíocht leictrifíleach; feanól;
  anailín; aspirin agus paracetamol; salainn déasónium; sintéis aramátacha, iompair arail-X vs. alcail-X.

First year laboratory work

Students attend one three-hour laboratory session per week.

Second Year
Course **CH201** covers **Physical, Inorganic** and **Organic Chemistry** and **Analytical and Environmental Chemistry** comprising **20 ECTS Credits.**
Module: CH202
Name: Organic Chemistry 2
Load (hrs): First Semester 24L + 5P + 4T
Pre-requisite: First Year Chemistry
Co-requisites: CH203, CH204, CH205
Marks: 100
Examination: First Semester, One 2 hour exam
Examination Paper: 1 paper
Staff Member: Professor R.N. Butler (ext. 2460)
Course Content: Structure and reactions of Hydrocarbons: alkanes, alkenes and alkynes. Substitution Reactions (SN), synthesis and mechanism. Functional Groups: hydroxy, ether, carbonyl, carboxylic acid, amine and Grignard reagents. Aromatic compounds: benzene, naphthalene, electrophilic substitution. Introduction to stereochemistry and natural products: Sugars, amino acids, peptides, proteins, optical isomerism and resolution of racemates. Cycloalkanes, conformations and Baeyer strain theory. The laboratory practical course consists of five four-hour sessions which will start in week 2 of Semester I. Registration for these practicals will take place in week 1 of Semester I. Laboratory notebooks must be handed in for marking when required.

Module: CH203
Name: Physical Chemistry 2
Load (hrs): First Semester 24L + 6P + 4 T
Pre-requisite: First Year Chemistry
Co-requisites: CH202, CH204, CH205
Marks: 100
Examination: First Semester, One 2 hour exam
Examination Paper: 1 paper
Staff Member: Dr. D. Leech (ext. 3563)
Course Content: Gaseous State, Thermodynamics, Equilibria and Phases, Ions in Solution, Electrode Processes, Introduction to Spectroscopy and Chemical Kinetics. Considerable emphasis is placed on the solution of numerical problems in physical chemistry. The laboratory practical course consists of five four-hour sessions, commencing on week seven of Semester 1. Laboratory notebooks must be handed in for marking and an oral examination on the subject material of the experiments will be held at the end of the course.

Module: CH204
Name: Inorganic Chemistry 2
Load (hrs): Second Semester 24L + 8P + 6T
Pre-requisite: First Year Chemistry
Co-requisites: CH202, CH203, CH205
Marks: 100
Examination: Second Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Professor P. McArdle (ext. 2487)
Course Content: Molecular structure (application of VSEPRT) and chemical bonding theory. Structure in the solid state. Co-ordination compounds of the transition metals:Ligand types, crystal field splitting and d-d transitions. Comparative chemistry of the elements: deduction of trends in chemical properties in the main groups of the periodic table based on the trends in ionisation potential, electron affinity and bond energies. The laboratory practical course consists of five four-hour sessions and these will commence in week 1 of Semester II. Laboratory notebooks must be handed in for marking when required and an oral examination on the subject material of the experiments will be held at the end of the course.

Module: CH205
Name: Analytical and Environmental Chemistry
Load (hrs): Second Semester 24L
Pre-requisite: First Year Chemistry
Co-requisites: CH202, CH203, CH204
Marks: 100

Examination: Second Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Professor M.J. Hynes (ext. 2488)
Course Content: While chemistry is frequently blamed for many environmental problems, it frequently passes unrecognised that most of the environmental problems of past decades and centuries are being solved by the application of science, in particular chemistry. Environmental and analytical chemistry are closely connected for it is only by the application of modern analytical chemistry techniques that it is possible to study environmental problems. The course covers; Environmental Chemistry, Atmospheric Chemistry, Water Treatment, EcoToxicology, Analytical Chemistry, Spectroscopy, Separation Techniques, Atomic Absorption Spectrometry, Electrochemistry. The laboratory practical course consists of six four-hour sessions

Third Year
Course **CH301** covers **Physical, Inorganic and Organic Chemistry** and **Molecular Structure Determination** comprising **24 ECTS Credits**
Module: CH307
Name: Inorganic Chemistry 3
Load (hrs): First Semester 36L + 8P + 5T
Pre-requisites: CH201
Co-requisites: CH308, CH311, CH313
Marks: 100
Examination: First Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Professor P. McArdle (ext. 2487)
Course Content: Structure and bonding of transition-metal complexes. Introduction to organometallic chemistry and the complexes of pi-bonding ligands. The eighteen electron rule and electron counting in low oxidation state systems. Kinetics and mechanism of inorganic reactions. Application of point group theory to vibrational spectroscopy and molecular orbital theory. Biological function of metals. The laboratory practical course consists of eight four-hour sessions over a period of seven weeks. Laboratory notebooks must be handed in for marking when required and an oral examination on the subject material of the experiments will be held at the end of the course.

Module: CH308
Name: Determination of Molecular Structure
Load (hrs): First Semester 36L + 5T
Pre-requisites: CH201
Co-requisites: CH307, CH311, CH313
Marks: 100
Examination: First Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Professor P. McArdle (ext. 2487)
Course Content: Introduction to point group theory, symmetry operations and character tables. Principles and application of nuclear magnetic resonance spectroscopy (NMR) in organic chemistry, proton carbon-13 and heteronuclear NMR. Pulsed FT and high-field NMR, 2D spectra and the use of shift reagents. Available methods for polymer characterisation and the relationship between polymer structure and physical properties. Crystal symmetry and x-ray diffraction. Principles and applications of mass spectrometry.

Module: CH311
Name: Organic Chemistry 3
Load (hrs): Second Semester 36L + 8P + 5T
Pre-requisites: CH201
Co-requisites: CH307, CH308, CH313
Marks: 100
Examination: Second Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Professor R.N. Butler (ext. 2460)
Course Content: Heterocyclic Chemistry: Synthesis structure and reactions of five and six membered rings with one heteroatom. Diels-Alder reactions. Laboratory and industrial photochemistry. Organic synthesis and stereochemistry. Natural product chemistry, carbohydrates, peptides and proteins, terpenes and steroids.. Physical organic chemistry and mechanistic studies. The laboratory practical course consists of eight four-hour sessions over a period of seven weeks. Laboratory notebooks must be handed in for marking when required.

Module: CH313
Name: Physical Chemistry 3
Load (hrs): Second Semester 36L + 6P + 5T
Pre-requisites: CH201
Co-requisites: CH307, CH308, CH311
Marks: 100
Examination: Second Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Dr. W. Carroll (ext. 2452)

Course Content: Thermodynamics of Mixtures, Phase Diagrams, Molecular Interactions, Surface Chemistry, Dynamic Electrochemistry, Quantum Chemistry, Spectroscopy, Chemical Kinetics, Macromolecules . Considerable emphasis is placed on the solution of numerical problems in physical chemistry. The laboratory practical course consists of six four-hour sessions over a period of six weeks. Laboratory notebooks must be handed in for marking and an oral examination on the subject material of the experiments will be held at the end of the course.

CH314 is a **12 ECTS Credit** Course
Module: CH314
Name: Cheminformatics & Validation
Load (hrs): Second Semester 36L + 10P
Pre-requisites: CH201
Co-requisites: None
Marks: 100
Examination: Second Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Dr. Henry Curran (ext. 3856)
Course Content:
Cheminformatics is the retrieval and usage of data related to molecules or compounds such as chemical and physical properties, hazard indices, and structure activity relationships. The use of on-line computer searching of chemical formulae (STN) and chemical reactions (Beilstein). The use of computer packages for molecular modelling and spectral simulation. Validation in the chemical and pharmaceutical industries. Validation is the provision of documented evidence that assures, to a high degree of confidence, that a process performs its intended functions accurately and reliably.

CH304 is a **12 ECTS Credit** Course
Module: CH304
Name: Analytical and Industrial Chemistry
Load (hrs): First Semester 36L + 5P
Pre-requisites: CH201
Co-requisites: none
Marks: 100
Examination: First Semester, One 2 hour exam
Examination Paper: 1 Paper
Staff Member: Professor M.J. Hynes (ext. 2488)
Course Content: The aim of this course is to introduce students to: (a) the application of information technology to sourcing and retrieving chemical information; (b) a range of analytical techniques and procedures widely used in the modern chemical laboratory; (c) the economics and practice of large-scale industrial processes. The course covers: Sampling and Analysis, Writing reports, Information retrieval using electronic methods and the internet, Analytical techniques; x-ray methods, gas chromatography, HPLC and thermal analysis. Standards and their preparation and storage. Introduction to laboratory information management systems (LIMS). Structure of the chemical industry, economic factors, reactor types and the use of catalysts.

Fourth Year Honours
Course No.: CH401 (60 ECTS Credits)
Load (Hrs.): 198L
PHYSICAL CHEMISTRY
CP-401 Statistical thermodynamics.
CP-402 Thermodynamics.
CP-403 Heterogeneous catalysis.
CP-404 Surface chemistry.
CP-405 Quantum chemistry.
CP-406 Spectroscopy.
CP-407 Kinetics.
CP-408 Electrochemistry.
INORGANIC CHEMISTRY
CI-401 Descriptive inorganic chemistry.
A. Advanced transition metal and organometallic chemistry.
B. Selected topics in Bioinorganic Chemistry.
CI-402 Electronic spectra and bonding in transition metal complexes.
CI-403 Spectroscopic techniques.
CI-404 Diffraction techniques.
CI-405 Kinetics of complex formation, ligand substitution and electron transfer. Pressure effects.
ORGANIC CHEMISTRY
CO-401 Instrumentation and spectroscopy.
CO-402 Reaction mechanisms and advanced physical organic chemistry.
A. Orbital symmetry in organic synthesis and mechanism.
B. ß-Elimination reactions.
C. Acidity functions and their applications.
D. Rearrangements in Organic chemistry.
CO-403 Advanced heterocyclic chemistry.
CO-404 Advanced natural product chemistry.
A. Alkaloid chemistry.
B. Nucleic Acids.
C. Advanced carbohydrate chemistry.
CO-405 Selected synthetic methods.
CO-406 Photochemistry.
CO-407 Synthetic organic polymers.
Fourth Year Laboratory Work
Each student will carry out a research level project in the area of Physical or Inorganic or Organic Chemistry.
Tutorials
Attendance will be required at tutorials as appropriate to the programme.