Course Module Information

CH313: Physical Chemistry

Semester 2 | Credits: 5

This course comprises lectures and tutorials, and expands upon the fundamentals of physical chemistry covered in years 1 and 2. Chemistry of molecular interactions, gas-solid interactions, thermodynamics of phase transitions, chemical kinetics, basic principles of electrode kinetics, spectroscopy and quantum chemistry are covered.The course emphasizes chemistry of interest to modern day chemists.
(Language of instruction: English)

Learning Outcomes

1. Discuss the potential energy of interaction between closed-shell molecules, (i) charge/charge, (ii) charge/dipole, (iii) dipole/dipole, (iv) London (dispersion) interactions.
2. Explain the kinetics associated with reactors, understand the dependence of kinetics on thermodynamics of reactants and products and how the rate constant of a reaction varies with temperature.
3. Discuss thermodynamics of phase transitions of pure substances, understand from thermodynamics why homogeneous mixing of gases and ideal solutions occurs spontaneously and describe the phase diagrams of simple mixtures, focusing on temperature-composition diagrams, azeotropes and eutectics and their applications.
4. Understand the basic principles of electrode kinetics and be able to use the Butler-Volmer and Tafel equations to compute overvoltage values, transfer coefficients and the equilibrium exchange current density.

5. Understand the importance of gas-solid interactions and be able to use and manipulate the various isotherms that are used to describe these interactions. The importance of surface tension, surfactants and the Gibbs adsorption isotherm should also be known.
6. Understand how the molar mass of polymers influence their properties, in particular their mechanical and thermal properties and be able to describe methods used to measure this mass. The influence of crystallinity on polymer properties should also be understood.
7. Explain the selection rules governing and fundamental theory underpinning Rotational and Vibrational (NIR, MIR, & Raman) spectroscopies. Calculate anharmonicity constants, the energies and populations of spectroscopic energy levels.
8. Explain the evidence for quantum theory and the De Broglie Relationship. Explain the Schrodinger Wave Equation (SWE), nature of wavefunctions, Born Interpretation, uncertainty principle. Be able to solve SWE for several simple 1D, 2D, and 3D cases related to spectroscopy and materials science. Be able to use the solutions of the SWE to calculate energy levels in simple systems.

Assessments

ℹ This module's usual assessment procedures, outlined below, may be affected by COVID-19 countermeasures. Current students should check Blackboard for up-to-date assessment information.

- Written Assessment (100%)

Module Director

- HENRY CURRAN: Research Profile | Email

Lecturers / Tutors

- JUDY BUCKLEY: Research Profile
- HENRY CURRAN: Research Profile
- KAREN KELLY: Research Profile
- DONAL LEECH: Research Profile
- YURY ROCHEV: Research Profile
- ALAN RYDER: Research Profile

- DAVID CHEUNG: Research Profile

Reading List

1. ""“Elements of Physical Chemistry" by Atkins and De Paula.

The above information outlines module CH313: "Physical Chemistry" and is valid from 2015 onwards.

Note: Module offerings and details may be subject to change.

ABOUT NUI GALWAY

Founded in 1845, we've been inspiring students for 175 years. NUI Galway has earned international recognition as a research-led university with a commitment to top quality teaching.

Ireland's European Structural and Investment Funds Programmes 2014-2020

Co-funded by the Irish Government and the European Union

EUROPEAN REGIONAL DEVELOPMENT FUND

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