



Exchange programme Vrije Universiteit

Vrije Universiteit Amsterdam - Exchange programme Vrije Universiteit - 2022-2023

Exchange

Vrije Universiteit Amsterdam offers many English-taught courses in a variety of subjects, ranging from arts & culture and social sciences, neurosciences and computer science, to economics and business administration.

The International Office is responsible for course approval and course registration for exchange students. For details about course registration, requirements, credits, semesters and so on, please [visit the exchange programmes webpages](#).

From Quantum to Molecule

Course Code	X_420545
Credits	6.00
Period	P4
Course Level	200
Language Of Tuition	English
Faculty	Faculty of Science
Course Coordinator	prof. dr. ir. E.J.G. Peterman
Examiner	prof. dr. ir. E.J.G. Peterman
Teaching Staff	prof. dr. ir. E.J.G. Peterman
Teaching method(s)	Partial Exam, Lecture, Seminar

Course Objective

The overall aim of this course is to introduce the students to the basic mathematical language required to describe atoms, electrons, and molecules by means of the quantum mechanical description of matter. On the one hand, the topics covered in the course are required to gain a better understanding of the physical basis of important chemical properties and physical reactions that appear frequently in a medical context. On the other hand, this formalism also allows us to translate quantum mechanical concepts into measurable quantities that can then be used for medical applications, such as positron therapy or magnetic nuclear resonance. In this course, we will therefore cover a number of topics which range from fundamental quantum mechanics to the corresponding applications in medical sciences.

Course Content

The contents of the course are the following:

- It starts with an introduction to the quantum world, relevant for the description of small objects like atoms, molecules, and electrons. This involves presenting important concepts such as the wave-particle duality, the De Broglie relations, and the Heisenberg uncertainty principle of quantum mechanics.
- We will then move to present the fundamental equation of motion of quantum theory, namely the Schrodinger equation, and apply it to a number of important systems such as the particle in a box, the hydrogen atom, the harmonic oscillator, and the hydrogen atom.
- The course will then explore next how quantum theory allows describing the binding mechanisms between atoms that lead to the formation of molecules. In this context, we will study the valence bond theory, the molecular orbital theory, the concepts of hybridization in molecular interactions, hydrogen bridges, and then Huckel theory for the description of pi-bonds in polyatomic molecules.
- In the last part of the course we will consider the phenomena associated to light-matter interactions in molecules, known as molecular spectroscopy. We study vibrational modes in molecules, and how we can characterise them, as well as the mechanism underlying phosphorescence and photoluminescence. We emphasise their medical applications, such as Photosensitive Therapy and Magnetic Nuclear Resonance.

Additional Information Teaching Methods

Lectures and tutorials

Method of Assessment

Final Exam and short assessments (mini-test) during the werkcolleges.

Entry Requirements

Fysica en Medische Fysica 1/2
Thermodynamica
Calculus
Mathematische methoden

Literature

Physical Chemistry, 11th edition (Oxford University Press), by P. Atkins, J. De Paula, J. Keeler.
(The 12th edition appears on its way, that one will also be okay)

Additional Information Target Audience

2MNW