From Quantum to Molecule (X_420545)

Medische Natuurwetenschappen (MNW) BSc program

Study Guide 2019-2020

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1 Introduction

The *From Quantum to Molecule* course is part of the second year of the *Medische Natuurwetenschappen* (MNW) Bachelor program offered by the Faculty of Science at the VU Amsterdam. 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 medical science. On the other hand, this formalism allows us to translate quantum mechanical concepts into measurable quantities that can be used for medical applications, such as positron therapy or magnetic nuclear resonance (MNR).

Specifically, the course starts with a introduction to the quantum world, relevant for the description of small objects like atoms, molecules, and electrons. This will require introducing the basic principles of quantum mechanics and presenting important concepts such as the wave-particle duality, the De Broglie relations, and the Heisenberg uncertainty principle. We will then move to present the fundamental equation of motion of quantum theory, namely the Schroedinger 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 explore next how quantum theory allows describing the binding mechanisms between atoms that lead to the formation of molecules, describing in particular the valence bond theory, the molecular orbital theory, the concepts of hybridization and molecular interactions, hydrogen bridges, and then Huckel theory. The last part of the course will consider molecular spectroscopy, with emphasis on its medical applications, and we will end up describing the underlying physics of one of the most popular tools in medical imaging, namely nuclear magnetic resonance, illustrating the deep connection between the quantum description of nature and recent breakthroughs in medical science and tools.

2 Lecturer and Teaching Assistants

The course coordinator and instructor of the course is

Dr. Juan Rojo
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The tutorial sessions (*werkcolleges*) will be supervised by three teaching assistants (TAs):

- Nova Jansen (nova.a.jansen@gmail.com)
- Ryan Pollitt (ryanpollitt1998@gmail.com)
- Pepijn Schoutens (pepijn.sch@gmail.com)

The instruction language of the course and of the associated course materials will be English. Students have also the possibility to communicate with the course coordinator in Dutch if they prefer so (including in exams and written homework). The tutorial sessions will take place in Dutch.

3 Textbook and course materials

The material covered in this course follows mostly the content of the course textbook, **Atkins' Physical Chemistry** by Atkins & De Paula & Keeler (**11th edition**, Oxford University Press). Note that other editions have a different chapter structure and content, so we recommend the students to use this specific edition. The textbook can for example be acquired at the VU bookshop. Below we indicate the chapters of the course textbook that will be covered in each of the lectures.

In addition to the textbook, the lecture notes, slides, and other course material for each of the lectures will be posted on the Canvas page of the course:

`https://canvas.vu.nl/courses/42487`

together with the tutorial exercises and their solutions. All students registered in the course should automatically have access to this Canvas page. Through this page you will also receive the notifications that will be sent by the course instructors and the TAs. We strongly recommend that you subscribe to the Canvas notifications and that you check these regularly during term time.

4 Course schedule

The course schedule, including the division between lectures (*hoorcolleges*) and tutorial sessions (*werkcolleges*), is indicated in Table 1. There we indicate the date and time where the lecture will take place, as well as the names of the instructors. The dates of the intermediate and final exams are also listed here (see below for more information about the course assessment).

The specific lecture and exam rooms can be found by logging into the Rooster page at `http://rooster.vu.nl`. In the case of last-minute cancellations or modifications of the course schedule, students will be notified via Canvas.

In addition to the lectures and tutorials listed in Table 1, we will also schedule extra times for revision and discussion, about the contents of the lectures and the exercises, between the lecturer and small groups of students. We will have two of these: on **Thursday January 30th** (to prepare the midterm exam) and on **Thursday March 19th** (to prepare the final exam). More details about these extra revision and discussion slots will be announced via Canvas.

5 Course assessment I: partial and final exam

The assessment of the course is divided into two separate parts: (i) two exams, one halfway of the course and the second at the end of the course, and (ii) the participation in the tutorial sessions with the teaching assistants. We present here the details of these examinations, and in the next section we discuss how the tutorial sessions will be organized.

Week	Day	Date	Time	HC/WC	Lecturer	Info
2	Wed	8-1	11:00	HC1	JR	
2	Fri	10-1	09.00	HC2	JR	
3	Mon	13-1	13:30	WC1	NJ/RP/PS	
3	Wed	15-1	11:00	HC3	JR	
3	Fri	17-1	09:00	HC4	JR	
4	Mon	20-1	13:30	WC2	NJ/RP/PS	
4	Wed	22-1	11:00	HC5	JR	
4	Fri	24-1	09.00	HC6	JR	
5	Mon	27-1	13:30	WC3	NJ/RP/PS	
6	**Fri**	**7-2**	**09:00**	**Exam**		**Partial Exam**
7	Wed	12-2	13.30	WC4	NJ/RP/PS	
7	Fri	14-2	09:00	HC7	JR	
8	Wed	19-2	13:30	WC5	NJ/RP/PS	
8	Fri	21-2	09:00	HC8	JR	
9	Wed	26-2	13:30	WC6	NJ/RP/PS	
9	Fri	28-2	09:00	HC9	JR	
10	Wed	4-3	13:30	WC7	NJ/RP/PS	
10	Fr	6-3	09:00	HC10	JR	
11	Wed	11-3	13:30	WC8	NJ/RP/PS	
11	Fri	13-3	09:00	HC11	JR	
12	Wed	18-3	13:30	WC9	NJ/RP/PS	
12	Fri	20-3	09:00	HC12	JR	**Preparation exam**
13	**Tue**	**24-3**	**08:30-11:15**	**Exam**		**Final Exam**

Figure 1: Course schedule. For each lecture, we indicate the year week, the date and time of the lecture, the type of lecture, and the name of the instructor. The dates and times of the intermediate and final exams are also listed. Students should always check `rooster.vu.nl` for updated information as well as for the information about the specific lecture rooms.

- There will be first an intermediate (midterm) examination after the first six lectures, followed by a final test at the end of the course.

- The material that will be covered in the midterm exam includes everything from the start to the course to the topics covered in HC6, inclusive (see Table 1 and the detailed course syllabus below).

- The final exam will cover all the topics between HC1 and HC11 inclusive. The contents of HC12 (Magnetic Nuclear Resonance Imaging) will not enter in the final exam.
- The midterm exam corresponds to **25% of the final grade** of the course while the final exam to **75% of the final grade**. If the mark of the final exam is higher than the weighted sum of the midterm and final exams, then the former will be taken as final mark of the course. In other words the mark of the course will be computed as:

$$\max\left(0.75 \times \text{FinalExamMark} + 0.25 \times \text{MidtermExamMark},\, \text{FinalExamMark}\right) \tag{5.1}$$

Note that both during the partial and the final exams the use of any external material such as textbooks or lecture notes is not allowed. Furthermore, the use of scientific programmable calculators is not allowed: students are allowed to bring only a simple calculator without capability for symbolic manipulation or function plotting. A list of all required physical formulae, constants, and mathematical expressions will be provided together with the exam and posted on Canvas before the exam.

6 Course assessment II: tutorial sessions

The second part of the course assessment is based on the tutorial sessions (*werkcolleges*). An important part of the course is the active participation of all the students in these sessions. In total there will be 9 of such tutorial sessions.

In order to take the most profit of these tutorial sessions, it is very important that you prepare in advance the tutorial work for each session, taking into account the following guidelines:

- Read the corresponding chapters in the textbook and the lecture notes in advance, in order to become familiar with the basic concepts underlying the problems that will be carried out during the tutorial session.
- The exercises corresponding to each tutorial session will be announced in advance by the teaching assistants. If you have questions, you can also contact them via email either before or after the specific tutorial session. As for all the course communications, these announcements will be send through the Canvas page of the course.
- You might want to self-organise yourselves in groups of three or four students to prepare beforehand the tutorial work for each session.
- Note that it is possible to submit specific questions by email about the exercises to the TAs at any point during the course, including about problems covered in previous tutorial sessions.

These tutorial sessions represent an integral part of the course, and we expect students to take them very seriously. Moreover, these tutorial sessions will **contribute to the final mark of the course**. In selected tutorial sessions, in the last 20 minutes, the TAs will hand out one short problem closely related to those that you will have worked on during this session. Then, individually, you will attempt to solve this problem and then handle your work to the TAs at the end of the session. You can use all available course materials while working on this exercise (but laptops and cell phones are not allowed). Each successfully completed problem will **add 0.2 points to the total course mark**, up to a total of a maximum of 1.4 points. Note that no points will be subtracted for students that fail to solve correctly these problems or that they are not able to attend this specific tutorial session.

The content of the tutorial sessions will be the following:

- **WC1**: exercises corresponding to HC1 and HC2
- **WC2**: exercises corresponding to HC3 and HC4
- **WC3**: exercises corresponding to HC5 and HC6
- **WC4**: discussion of the solutions to the problems in the midterm exam.
- **WC5**: exercises corresponding to HC7
- **WC6**: exercises corresponding to HC8
- **WC7**: exercises corresponding to HC9
- **WC8**: exercises corresponding to HC10
- **WC9**: exercises corresponding to HC11

7 Communications

The main interface for the communications between the students and the instructors is the Canvas page for the course. All the relevant course documents and teaching materials will be make available there. It is important that you familiarize yourselves with Canvas if you have never used it before. You can fine many online tutorials describing the use of Canvas, such as for instance this one:

https://www.youtube.com/watch?v=bHyUPjf37rY

In particular, please take into account the following points concerning the communication of relevant course information:

- All the students registered in the course will receive automatically the course notifications via the Canvas interface. If you have any trouble receiving the emails, please contact the IT help-desk or the Canvas help-desk for assistance.
- The relevant information about the course, tutorial sessions, and evaluations and exams will take place though your VU student email. Therefore, please check regularly your VU email (or another email account to which this is forwarded), at least once per day during term.
- Note that changes in the course schedule such as different lecture rooms will be announced by email, so please be aware of possible last-minute changes.

8 Course learning objectives

At the end of this course, the students should be able to satisfactorily grasp the following set of course objectives:

- Understand why quantum theory is necessary to describe the structure and properties of electrons, atoms and molecules, and in which respect it represents a radical departure with respect to the intuitive concepts of classical physics.
- Understand how experimental observables can be calculated from the quantum wave-function as a solution of the Schrödinger equation with different symmetries and boundary conditions, and perform these calculations in simple systems.
- To able to determine the electronic structure of the hydrogen atom in terms of electronic levels and shells, in particular taking into account the role of angular momentum, by means of solving the Schrödinger equation in systems with rotational symmetry.
- To be able to derive solutions for the Schrödinger equation for multi-electron atoms by means of the orbital approach, and to determine in which respect the resulting electronic structure differs from that of the hydrogen atom.
- To become familiar with the concept of molecular orbital, and to be able to represent it in terms of the underlying probability density. This goal also involves being able to combine electric orbitals from individual atoms into joint molecular orbitals.
- To understand the basic symmetry properties of molecular orbitals, with special emphasis on the role of angular momentum, and to be able to determine the resulting consequences for the electronic structure of important molecules.
- Understanding and applying the basic properties of absorption and emission of electromagnetic radiation in molecules, and being able to determine which specific properties of important molecules we can access which each type of radiative process.
- Understanding and applying the principles of fluorescence and phosphorescence, and being able to compute the rates of different radiative emission processes of relevant molecules.
- Become familiar with the basic principles of Magnetic Resonance Imaging, and understand how the spin of atomic nuclei represents one of the most helpful ingredients of modern medical imaging.

9 Textbook chapters for the exam

The following chapters of the course textbook (*Physical Chemistry*, Atkins and De Paula, 11th edition) contain material that is relevant for the questions in the **intermediate midterm exam**:

- **7A.2**: *Wave-particle duality.*
- **7B.1**: *The Schroedinger equation.*

- **7B.2**: *The Born interpretation of the wave function.*
- **7B.3**: *The probability density.*
- **7C.1**: *Operators.*
- **7C.2**: *Superpositions and expectation values.*
- **7C.3**: *The uncertainty principle.*
- **8A.1**: *Free motion in one dimension.*
- **8A.2**: *Confined motion in one dimension.*
- **8A.3** *Confined motion in two or more dimensions.*
- **8A.4**: *Tunneling.*
- **8B.1**: *The harmonic oscillator.*
- **8B.2**: *The properties of oscillators*
- **8C.1**: *Rotation in two dimensions.*
- **8C.2**: *Rotation in three dimensions.*
- **9A.1**: *The structure of hydrogenic atoms.*
- **9A.2**: *Atomic orbitals and their energies.*
- **9B.1**: *The orbital approximation.*
- **9B.2**: *The building-up principle.*

In addition, the following textbook chapters are relevant for the **final exam**:

- **10A.1**: *Diatomic molecules.*
- **10A.2**: *Polyatomic molecules.*
- **10B.1**: *Linear combination of atomic orbitals.*
- **10B.2**: *Orbital notation.*
- **10C.1**: *Electron configurations.*
- **10C.2**: *Photoelectron spectroscopy.*
- **10D.1**: *Polar bonds.*
- **10D.2**: *The variation principle.*
- **10E.1**: *The Huckel approximation.*

- **10E.2**: *Applications.*
- **12A.1**: *The absorption and emission of radiation.*
- **12B.2**: *The rotational energy levels.*
- **12C.1**: *Microwave spectroscopy.*
- **12C.2**: *Rotational Raman spectroscopy.*
- **12D.1**: *Vibrational motion.*
- **12D.2**: *Infrared spectroscopy.*
- **12D.3**: *Anharmonicity.*
- **12D.4**: *Vibration-rotation spectra.*
- **12E.1**: *Normal modes.*
- **12E.2**: *infrared absorption spectra.*
- **12E.3**: *Vibrational Raman spectra.*
- **13A.1**: *Diatomic molecules.*
- **13B.1**: *Fluorescence and phosphorescence.*
- **13C.1**: *Population inversion.*
- **14A.1**: *Nuclear magnetic resonance.*
- **14B.1**: *The chemical shifts.*
- **14B.2**: *The origin of shielding constants.*
- **14C.1**: *The magnetisation vector.*

10 Course syllabus

Here we present the specific detailed syllabus of the course. As indicated in Table 1, the course is divided into 12 *hoorcolleges* (HCs), each one corresponding to a 1.45h lecture (with a 10 minute break in the middle). For each HC, we present a general overview of the topics that will be covered and the specific **learning goals** of each lecture. We also indicate the corresponding chapters in the course textbook that will be covered in each lecture.

The 12 *hoorcolleges* of the course will cover the following topics:

- HC1: Introduction to quantum theory: basic formalism and principles.
- HC2: The quantum wave-function and the Schroedinger equation.
- HC3: Quantum mechanics of simple systems.

- HC4: The Schroedinger equation for systems with rotational symmetry.
- HC5: The hydrogen atom.
- HC6: Multi-electron atoms and orbital theory.
- HC7: Molecular structure.
- HC8: Molecular Orbital theory and hybridization.
- HC9: Huckel theory.
- HC10: Molecular and vibrational spectroscopy.
- HC11: Molecular spectroscopy and electronic transitions.
- HC12: Magnetic nuclear resonance (*does not enter in the final exam*)

In the following, we detail the contents of each of these HCs in turn.

HC1: Introduction to Quantum Theory: basic formalism. In this first lecture we provide a general introduction to the main concepts underlying the formulation of quantum mechanics, and present some of the most important concepts in quantum theory such as the intrinsic duality between waves and particles. We discuss the differences and similarities between the classical and quantum description of nature. We will also review some mathematical tools that will be necessary to solve problems involving quantum mechanics.

Learning goals of the lecture:

(a) Understand the the conceptual similarities and differences between the classical and quantum description of nature.

(b) Familiarise with the mathematical tools required to described quantum systems.

(c) Understand that both matter particles and light have a dual wave/particle character, with different behaviour arising in different situations.

HC2: The quantum wave-function and Schroedinger equation. In this lecture we present the mathematical framework of quantum theory, where the main entity is the *quantum wave-function*, and the dynamical equation that this wave-function must obey, the Schroedinger equation. We also introduce a number of mathematical tools which are required in the quantum formalism. We discuss Heisenberg's uncertainty principle, and show that it entails a fundamental limitation about the physical knowledge that we can have about quantum systems.

Learning goals of the lecture:

(a) Understand that the state of a quantum system is described by the quantum wave-function, which is a solution of the Schroedinger equation.

(b) Understand and apply the mathematical description of quantum physics, including Hermitian operators, eigenvalue, orthogonality

(c) Understand how experimental observables can be calculated from the wave-function, and perform these calculations in simple systems.

(d) Understand the Copenhagen interpretation of the physical meaning of the wave-function.

(e) Understand and apply Heisenberg's uncertainty principle in different situations, in its two versions between position and velocity and between energy and time.

Chapters in textbook

- **7A.2**: Wave-particle duality.
- **7B.1**: The Schroedinger equation.
- **7B.2**: The Born interpretation of the wave function.
- **7B.3**: The probability density.
- **7C.1**: Operators.
- **7C.2**: Superpositions and expectation values.
- **7C.3**: The uncertainty principle.
- **8A.1**: Free motion in one dimension.

HC3: Quantum mechanics of simple systems. In this lecture we discuss quantum mechanics applied to relatively simple systems such as the particle in a confining box and the quantum harmonic oscillator. We will study some remarkable phenomena that appear in these systems that do hot have an analog in classical mechanics, such as that the *the quantization of energies* and the *quantum tunneling*. For instance, we will show how a quantum particle can cross an energy barrier even if its energy is smaller than that of the barrier. You will also start to carry out simple calculations that will train you for the more difficult calculations in the following sections. Note that this lecture assumes the knowledge of ordinary and partial differential equations.

The **learning goals** of this lecture are:

(a) Solving the Schroedinger equation for simple quantum systems.

(b) Understanding that confinement of a quantum particle in space leads to the quantization of its energy levels, with an non-vanishing energy for the ground state.

(c) Interpret the physical content of the wave-functions from the solutions of the Schroedinger equation.

(d) Understanding and applying the mathematical technique of separation of variables.

(e) Understanding and applying the phenomenon of quantum tunneling.

Chapters in textbook

- **8A.2**: Confined motion in one dimension.
- **8A.3** Confined motion in two or more dimensions.
- **8A.4**: Tunneling.
- **8B.1**: The harmonic oscillator.
- **8B.2**: The properties of oscillators

HC4: The Schroedinger equation for systems with rotational symmetry. In this lecture we continue with the applications of the Schroedinger equation for important physical systems, in this case in the presence of rotational symmetry such as a particle moving on a ring or on the surface of a sphere. We will also introduce the concept of intrinsic angular momentum of a particle, known as *spin*. Learning how to solve the Schroedinger equation in these systems will allow us then in the next lectures to compute the structure of electronic levels in atoms and molecules.

The **learning goals** of this lecture are:

- To be able to solve the Schroedinger equation for a rotating particle, specifically in the two-dimensional (particle on a ring) and three-dimensional (particle on a sphere) cases.
- To understand the mechanism by means of which rotational symmetry leads to the quantization of of the physically allowed energy levels.
- To interpret the solutions of Schroedinger equation for a rotating particle.
- To become familiar with the concept of *spin* (intrinsic angular momentum) in quantum mechanics.

Chapters in textbook

- **8C.1**: Rotation in two dimensions.
- **8C.2**: Rotation in three dimensions.

HC5: The hydrogen atom. In this lecture we will study in some detail the solutions of the Schroedinger equation applied to the hydrogen atom, and display the connection with the empirical assumptions of Bohr's atomic model. We will show how important features of the electronic structure of atoms can be modeled by this system, in particular the classification of electronic levels in terms of energy and angular momentum quantum numbers. The understanding of the electronic structure of the hydrogen atom will allow us to describe multi-electron atoms and then in describe the electronic structure of molecules.

The **learning goals** of this lecture are:

- To determine a suitable coordinate system to express the Schrödinger equation applied to the hydrogen atom in a physically transparent way.
- To learn how to solve the Schrödinger equation for the hydrogen atom.
- To be able to provide a physical interpretation of the radial and angular wave functions of the hydrogen atoms in terms of probability densities.
- The understand how these solutions lead to the electronic structure of the hydrogen atom in terms of electronic levels and shells.

Chapters in textbook

- **9A.1**: The structure of hydrogenic atoms.
- **9A.2**: Atomic orbitals and their energies.

HC6: Multi-electron atoms and orbital theory. Building on the experience with the hydrogen atoms acquired in the previous lecture, here we take a step forward and move to solving the Schroedinger equation for atoms characterized by more than one electron, the so-called *multi-electron atoms*. This will require introducing a number of important concepts that were absent in the description of the hydrogen atom such as the idea of shielding, the Pauli and Aufbau principles, and the ideas behind how to combine the spin states of two particles.

The **learning goals** of this lecture are:

- To learn how to derive solutions for the Schrödinger equation for multi-electron atoms by means of the orbital approach.
- Understand a number of important concepts in multi-electron atoms such as shielding, the Pauli principle, and the Aufbau-principle.
- To become familiar with the concept of spin combination, in particular with the ideas of *singlet* and *triplet* states for a pair of particles with spin.

Chapters in textbook

- **9B.1**: *The orbital approximation.*
- **9B.2**: *The building-up principle.*

HC7: Molecular structure. This is the first of three lectures dealing with molecular structure, that is, aiming to understand the allowed energy levels that electrons can occupy in molecules composed by two or more atoms, as compared to the electronic levels of individual atoms described in the previous two lectures. We will present in this context the valence bond theory, based on the overlapping of individual atomic orbitals. We will also discuss the Born–Oppenheimer (BO) approximation, namely the idea that the motion of the electrons within a molecule takes place at a much higher speed than that of the atomic nuclear and that thus is becomes effectively decoupled from the latter.

The **learning goals** of this lecture are:

- To understand and be able to apply the valence-bond theory to homonuclear diatomic molecules as well as to multi-atomic molecules composed by more than two atoms.
- To become familiar with the concept of molecular orbital and to be able to represent it in terms of the underlying probability density.
- To understand the Born–Oppenheimer approach and to be able to use it in different configurations.
- To be able to graphically represent the concept of hybrid molecular orbital.

Chapters in textbook

- **10A.1**: *Diatomic molecules.*
- **10A.2**: *Polyatomic molecules.*
- **10B.1**: *Linear combination of atomic orbitals.*

HC8: Molecular Orbital theory and hybridization. In this lecture we continue our study of the electronic structure of molecules by presenting the Molecular Orbital theory, a method that allows to determine the molecular electronic structure where electrons are not assigned to individual bonds between atoms, but are rather treated as moving under the influence of the nuclei in the whole molecule. This will also leads us to the important concept of hybridization, describing the rules that govern how electronic orbitals in individual atoms can merge among them to give rise of molecular orbitals.

The **learning goals** of this lecture are:

- To understand and be able to apply the molecular orbital theory, based on the method of linear combinations of atomic orbital, to simple diatomic molecules.
- To be able to predict whether a specific molecular configuration will lead to orbital bonding or instead to anti-bonding.
- To manage to to draw up a molecular orbital energy diagram for homonuclear diatomic molecules.
- To understand the basic symmetry properties of molecular orbitals, with special emphasis on the role of angular momentum.

Chapters in textbook

- **10A.2**: *Polyatomic molecules.*
- **10B.2**: *Orbital notation.*
- **10C.1**: *Electron configurations.*
- **10D.1**: *Polar bonds.*
- **10D.2**: *The variation principle.*

HC9: Huckel theory. This lecture completes the part of the course describing molecular structure, and is focused on the formulation of the so-called Huckel theory. This is a method based on the linear combination of atomic and molecular orbitals (LCAO MO) which allows to determine the energy levels of π electrons in conjugated hydrocarbon systems and other related molecules. Using Huckel methods, it is possible to derive the energies of some of molecular levels in important cases such as the butadiene molecule.

The **learning goals** of this lecture are:

- To understand and be able to apply the variational principle to an heteronuclear diatomic molecule.
- To become familiar with the mathematics and physics behind the Huckel approach.
- To be able to produce the complete Huckel matrix for a generic, not too large, molecule.

Chapters in textbook

- **10E.1**: The Huckel approximation.
- **10E.2**: Applications.

HC10: Molecular and vibrational spectroscopy. HC10 is the first of the last three lectures of the course. In this final part, we will discuss the *interaction of molecules and nuclei with different types of electromagnetic radiation*. First of all, in HC10 we will discuss the general properties of *molecular spectroscopy and vibrational spectra*, where by *spectroscopy* we understand the study of the interaction between electromagnetic radiation and matter using different experimental techniques. Then in HC11 we will study electronic transitions in molecules. Finally, in HC12 we will illustrate the underpinnings of Nuclear Magnetic Resonance (MNR), highlighting how quantum physics is central to one of the most widely used methods of medical imaging.

The **learning goals** of this lecture are:

- Understanding and applying the basic properties of absorption and emission of electromagnetic radiation in molecules.
- Become familiar with the vibrational states and the corresponding transitions among them for di- and poly-atomic molecules.
- Understand that vibrational transitions lead the interactions with infrared light via Raman scattering, and learn how to exploit this knowledge for practical applications.

Chapters in textbook

- **12A.1**: The absorption and emission of radiation.
- **12B.2**: The rotational energy levels.
- **12C.1**: Microwave spectroscopy.
- **12C.2**: Rotational Raman spectroscopy.
- **12D.1**: Vibrational motion.
- **12D.2**: Infrared spectroscopy.
- **12D.3**: Anharmonicity.

HC11: Molecular spectroscopy and electronic transitions. In this lecture, we will study electronic transitions in *p-electron conjugate systems*, the Franck-Condon principle, the physics underlying the phenomena of *fluorescence* and *phosphorescence*, as well as the basic principles of operation of a *laser*. We will also present an application of these ideas in the medical context, namely the *photo-dynamic therapy* (PDT).

The **learning goals** of this lecture are:

(a) Understanding and applying π-π^* electronic transitions in molecules.

(b) Understanding which electronic transitions can take place for either absorption or emission of a photon while the atomic nuclei are at rest (the Franck-Condon principle), including the mathematical description and implications of absorption and emission spectra.

(c) Understanding and applying the principles of fluorescence and phosphorescence.

(d) Understanding the basic principles that underlie the operation of a laser, such as the concept of population inversion.

Chapters in textbook

- **12D.4**: Vibration-rotation spectra.
- **12E.2**: infrared absorption spectra.
- **12E.3**: Vibrational Raman spectra.
- **13A.1**: Diatomic molecules.
- **13B.1**: Fluorescence and phosphorescence.
- **13C.1**: Population inversion.

HC12: Magnetic Nuclear Resonance. In this final lecture of the course, we will explore the important topic of Magnetic Nuclear Resonance and show it is the basis for one of the most important applications of quantum theory in medical therapy, namely *Magnetic Resonance Imaging*. The contents of this lecture will not enter the final exam.

The **learning goals** of this lecture are:

(a) Understand that the atomic nucleus has a magnetic moment, and that upon interaction with a magnetic field its energy levels split for different values of z component of the nuclear spin.

(b) Understand and be able to interpret Nuclear Magnetic Resonance (NMR) spectra.

(c) Understand how pulse techniques can be employed in order to measure NMR spectra.

(d) Become familiar with the basic principles of Magnetic Resonance Imaging (MRI).

Chapters in textbook

- **14A.1**: Nuclear magnetic resonance.
- **14B.1**: The chemical shifts.
- **14B.2**: The origin of shielding constants.
- **14C.1**: The magnetisation vector.