# COURSE OUTLINE

## (1) GENERAL

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|---|---|---|---|---|
| **SCHOOL** | SCHOOL OF SCIENCES | | | |
| **ACADEMIC UNIT** | PHYSICS DEPARTMENT | | | |
| **LEVEL OF STUDIES** | UNDERGRADUATE | | | |
| **COURSE CODE** | **202** | **SEMESTER** | **6,8** | |
| **COURSE TITLE** | MOLECULAR PHYSICS | | | |
| **INDEPENDENT TEACHING ACTIVITIES** *if credits are awarded for separate components of the course, e.g. lectures, laboratory exercises, etc. If the credits are awarded for the whole of the course, give the weekly teaching hours and the total credits* | | | **WEEKLY TEACHING HOURS** | **CREDITS** |
| | | | **4** | **5** |
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| *Add rows if necessary. The organisation of teaching and the teaching methods used are described in detail at (d).* | | | | |
| **COURSE TYPE** *general background, special background, specialised general knowledge, skills development* | Special background/skills development | | | |
| **PREREQUISITE COURSES:** | | | | |
| **LANGUAGE OF INSTRUCTION and EXAMINATIONS:** | Greek | | | |
| **IS THE COURSE OFFERED TO ERASMUS STUDENTS** | Yes (Greek) | | | |
| **COURSE WEBSITE (URL)** | The associated webpage in the E-course platform of the University of Ioannina | | | |

## (2) LEARNING OUTCOMES

**Learning outcomes**

*The course learning outcomes, specific knowledge, skills and competences of an appropriate level, which the students will acquire with the successful completion of the course are described.*

*Consult Appendix A*

- *Description of the level of learning outcomes for each qualifications cycle, according to the Qualifications Framework of the European Higher Education Area*
- *Descriptors for Levels 6, 7 & 8 of the European Qualifications Framework for Lifelong Learning and Appendix B*
- *Guidelines for writing Learning Outcomes*

The aim of this course is to provide students with the knowledge of fundamental aspects of Molecular Physics and the interaction of molecules with electromagnetic radiation. Introducing the appropriate approximations (Born- Oppenheimer), the electronic motion, the eigenstates and the corresponding wave functions (molecular orbitals) are discussed in terms of quantum mechanics. In particular, the nature of the chemical bond is described in a comparative way in terms of the Valence Bond & the Molecular Orbital quantum Theories. The module starts with a detailed description of the molecular bond starting from the simplest case of $H_2^+$ towards molecular systems of increasing complexity: diatomic, polyatomic ones and the use of hybrid orbitals for the latter case. Similarly, the nuclear motion is described by taking into account the rigid rotator and the non-rotating harmonic oscillator approximations, and the corresponding vibrational and rotational states (energies and eigenfunctions) are introduced. Special emphasis is placed on the interaction of molecules with photons in different wavelength regions (from UV to Visible to mid-infrared to microwaves), the selection rules and the information on the Molecular structure, which can be drawn by using the associated Spectroscopic techniques.

Upon the successful completion of the course the student:

- Should have a consolidated knowledge for the order of magnitude for a series of fundamental quantities in the field of Molecular Physics: size, bond strength, the energy of the electronic-vibrational-rotational states, the corresponding timescales of electronic and nuclear motion.
- He/She will be able to apply the Variation Theory and the Molecular Orbital Theory to calculate the bond dissociation energy, the equilibrium bond length and the distribution of the electronic charge for the case of $H_2^+$.
- He/She should be able to use apply the Molecular orbital Theory on the description of the electronic structure of diatomic molecules: the bonding or non-bonding character of the molecular states, their symmetry, the corresponding molecular term symbol.
- He/She should be aware of the dependence of nuclear motion on the characteristics of the molecular orbitals (qualitative features of electronic distribution, shape of the Morse potential) and the physical mechanisms leading to the mixing of vibrational and rotational spectra.
- He/She should be able to use Molecular Spectra (Absorption-Emission-Raman) and search for the required information in the available literature to draw qualitative conclusions about the properties of the molecular sample.

**General Competences**

*Taking into consideration the general competences that the degree-holder must acquire (as these appear in the Diploma Supplement and appear below), at which of the following does the course aim?*

| | |
|---|---|
| *Search for, analysis and synthesis of data and information, with the use of the necessary technology* | *Project planning and management* |
| *Adapting to new situations* | *Respect for difference and multiculturalism* |
| *Decision-making* | *Respect for the natural environment* |
| *Working independently* | *Showing social, professional and ethical responsibility and sensitivity to gender issues* |
| *Team work* | *Criticism and self-criticism* |
| *Working in an international environment* | *Production of free, creative and inductive thinking* |
| *Working in an interdisciplinary environment* | *……* |
| *Production of new research ideas* | *Others…* |
| | *…….* |

Team work, Working independently, Decision-making.

## (3) SYLLABUS

• Molecular properties: Shape, size, molecular bond, dipole moment, polarizability.
• Molecular symmetry. The Schrödinger equation-Born Oppenheimer approximation, electronic states, Molecular orbitals, Morse Potential.
• Nuclear motion – vibrational & rotational states, examples of molecules and the corresponding timescales, energies, absorption wavelengths
- Rotational motion _ states – transitions – spectra – isotopic labeling
- Vibrational motion _ states – transitions – spectra
- Interaction of Vibrational & rotational motion, molecular states of mixed character – the molecular vibrational/rotational spectra.
• Electronic transitions - Franck-Condon factors, selection rules, emission (Fluorescence, Phosphorescence, non-radiative relaxation, bond dissociation, Multiphoton absorption and ionization.

## (4) TEACHING and LEARNING METHODS - EVALUATION

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|---|---|
| **DELIVERY**<br>*Face-to-face, Distance learning, etc.* | Face-to-face |
| **USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY**<br>*Use of ICT in teaching, laboratory education, communication with students* | The ppt presentations and the notes used by the tutor during the lectures are available in the Molecular Physics webpage in the E-course online platform of the University of Ioannina |
| **TEACHING METHODS**<br>*The manner and methods of teaching are described in detail.*<br>*Lectures, seminars, laboratory practice, fieldwork, study and analysis of bibliography, tutorials, placements, clinical practice, art workshop, interactive teaching, educational visits, project, essay writing, artistic creativity, etc.*<br><br>*The student's study hours for each learning activity are given as well as the hours of non-directed study according to the principles of the ECTS* | |

| ***Activity*** | ***Semester workload*** |
|---|---|
| Lectures (Theory) | 39 |
| tuition | 13 |
| Study & analysis of bibliography | 55 |
| Essay writing | 15 |
| Exams | 3 |
| | |
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| Course total | **125** |

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| **STUDENT PERFORMANCE EVALUATION**<br>*Description of the evaluation procedure*<br><br>*Language of evaluation, methods of evaluation, summative or conclusive, multiple choice questionnaires, short-answer questions, open-ended questions, problem solving, written work, essay/report, oral examination, public presentation, laboratory work, clinical examination of patient, art interpretation, other*<br><br>*Specifically-defined evaluation criteria are given, and if and where they are accessible to students.* | Written Exam (100%). |

## (5) ATTACHED BIBLIOGRAPHY

- Suggested bibliography:


- *Physical Chemistry, Peter Atkins, J. De Paula (2014)*
- *Molecular quantum mechanics, Peter Atkins, Rional Freidman (Oxford University Press)*