COURSE OF STUDY *Physics (LM-17)*

ACADEMIC YEAR *2023-2024*

ACADEMIC SUBJECT *Spectroscopy and Computer Modeling of Molecular Systems*

General information	
Year of the course	1st
Academic calendar (starting and ending date)	2nd semester: March - May 2024
Credits (CFU/ECTS):	6
SSD	CHIM/03
Language	English
Mode of attendance	Recommended, not compulsory

Professor/ Lecturer	
Name and Surname	Savino Longo
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Telephone	080 5442088
Department and address	Dipartimento di Chimica, Via E. Orabona 4, 70125 Bari (BA)
Virtual room	
Office Hours (and modalities: e.g., by appointment, on line, etc.)	Wednesday 15:00-19:00; it is recommended to contact carla.coppola@uniba.it to be sure of the professor's availability

Work schedule			
Hours			
Total	Lectures	Hands-on (laboratory, workshops, working groups, seminars, field trips)	Out-of-class study hours/ Self-study hours
150	40	15	95
CFU/ECTS			
6	5	1	

Learning Objectives	Introduction to spectroscopy methods used in chemistry but adapted for use by physicists. Calculation methods that can be used in the simulation of the structure, dynamics and spectroscopy of the different phases of matter, from gaseous to biological, mainly with the use of tools accessible directly via browser.
Course prerequisites	Background knowledge on chemistry and quantum physics at the level of bachelor degree in physics.

Teaching strategies	Lessons with proposal of cases of study. Hands-on computer codes. Discussion of real cases.
Expected learning outcomes in terms of	
Knowledge and understanding on:	o Understand the scientific method, the nature, and the methods of research in Physics o Knowledge of spectroscopic methods in different energy ranges o Using computer modeling and quantum mechanics to understand the properties of chemical systems in many applications
Applying knowledge and understanding on:	o Ability to identify the essential elements of a phenomenon o Ability to use analogy to apply known solutions to new problems (problem solving)

	o Ability to design and implement experimental or theoretical procedures to solve problems in academic and industrial research or to improve existing results o Ability to use analytical and numerical mathematical computation tools o The student is able to apply physical theories to molecular systems / crystals / biomolecules / materials, knows the modern methods available to use computers to model the dynamics of molecular system
Soft skills	● **Making informed judgments and choices** o Ability to work with increasing levels of autonomy, including taking responsibility in project planning and managing facilities o Students are encouraged to choose personal solutions for the proposed problems and to propose interesting study cases that can be the essential part of the exam interview. ● **Communicating knowledge and understanding** o Competence in communication in Italian and English in advanced fields of Physics o Know how to expose the particularities of case studies and propose solution techniques, discussion in the classroom is encouraged ● **Capacities to continue learning** o Acquisition of basic knowledge tools for continuous learning and knowledge updates o Know how to extract operational information for real case studies from formal texts, using computer codes, advanced mathematical techniques, artificial intelligence
Syllabus	
Content knowledge	**Molecular modeling**: Classical molecular dynamics. Quantum treatment of the electrons in molecules. **Molecular spectroscopy**: Electronic transitions in pi systems. Vibrational spectroscopy, vibration modes and group frequencies. Notes on NMR spectroscopy. Use of spectroscopic techniques for the recognition of molecular structures. **Physical understanding and modeling of biological systems**: The molecular nature of enzymes. Dynamics and use of energy in biological systems. Some examples of complex molecular systems. Theories and models for computer simulation. **Hands-on**: Use of various software for the construction of molecular models and the analysis of delocalized pi systems. Coding and molecular construction in the SMILES language. **Introduction to the techniques of artificial intelligence (AI)** applied to molecular systems.
Texts and readings	Harris, Daniel C., and Michael D. Bertolucci. *Symmetry and spectroscopy: an introduction to vibrational and electronic spectroscopy*. Dover Cartwright H.M.: *Applications of artificial intelligence in chemistry, Oxford* *Goodsell, D. S. The machinery of life. Springer.* Scientific papers are used for special applications.
Notes, additional materials	Selected chapters.
Repository	

Assessment	
Assessment methods	Oral examination, based on student's seminar on a case study agreed with the teacher, using a powerpoint presentation and computer code.
Assessment criteria	Knowing how to apply theory to the discussion of real molecular spectra.

	Being able to propose a specific computer modelling technique for a real problem involving molecules and/or surface in the context of a real application. Being able to use actual programs to obtain useful information.
Final exam and grading criteria	Oral exam (100%)
Further information	
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