Basic/Essential Course Information	
Course title	Spectroscopy and Computer Modeling of Molecular Systems
Degree Course title	Physics
ECTS	6
Compulsory attendance	No
Course teaching language	ENGLISH

Teacher	Savino Longo	Savino.longo@uniba.it

ECTS Details	Disciplinary area/broad field:	SSD	ECTS
		CHIM/03	6

Time management and teaching activity type	Period	Year	lesson type
	2 st semester	1st	Lessons (40h) Laboratory (15h)

Time management,	Total hours	in-class/in-lab study hours	out-of-class study hours
	150	55	95

Course calendar	Starting date	Ending date
	First week of March	End of May

Syllabus	
Prerequisites	Background knowledge on chemistry and quantum physics at the level of bachelor degree in physics.
Expected learning outcomes (according to Dublin Descriptors)	**Knowledge and understanding**: Using computer modeling and quantum mechanics to understand the properties of chemical systems in many applications. **Applied knowledge and understanding:** 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. **Judging autonomy:** 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. **Communicative Skills:** Know how to expose the particularities of case studies and propose solution techniques, discussion in the classroom is encouraged

	Learning Skills: Know how to extract operational information for real case studies from formal texts, using computer codes, advanced mathematical techniques, artificial intelligence.
Course contents summary	Introduction to the calculation methods that can be used in the simulation of the structure, dynamics and spectroscopy of different phases of matter, from gaseous to biological, mainly with the use of calculation tools directly accessible via browser.
detailed syllabus	**Molecular modeling**: Classical molecular dynamics. Quantum treatment of the electrons in molecules. **Molecular spectroscopy**: Electronic transitions in pi-greek systems. Vibrational spectroscopy, vibration modes and group frequencies. **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.
books	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	Selected chapters.
Teaching methods	Lessons with proposal of cases of study. Hands-on computer codes. Discussion of real cases.
Assessment % of final mark	Oral examination, based on student's seminar on a case study agreed with the teacher, using a powerpoint presentation and computer code.
Evaluation 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.