

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
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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)	<p><b>Knowledge and understanding:</b> Using the concepts of group theory, computer modeling and quantum mechanics to understand the properties of chemical systems in many applications.</p> <p><b>Applied knowledge and understanding:</b> The student is able to apply the theory of symmetry to molecular systems / crystals / biomolecules / materials, knows the modern methods available to use computers to model the dynamics of molecular system.</p> <p><b>Judging autonomy:</b> 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.</p> <p><b>Communicative Skills:</b> Know how to expose the particularities of case studies and propose solution techniques, discussion in the classroom is encouraged</p> <p><b>Learning Skills:</b> Know how to extract operational information for real</p>

	case studies from formal texts, using computer codes, advanced mathematical techniques, artificial intelligence.
Course contents summary	Structural, electronic, vibrational, optical and transport properties of condensed matter.
<b>detailed syllabus</b>	<p><b>Bonding and structure in molecules.</b> Short review of VSEPR, Molecular Orbital (MO) Method and the Huckel method.</p> <p><b>Symmetry and spectroscopy.</b> Groups of symmetry operations. Representations of point groups and character tables. Application to orbitals, vibrations and spectroscopy. Discussion of real IR/Raman spectra. Applications of computational tools to spectroscopy.</p> <p><b>Molecular modeling.</b> Classical molecular dynamics. Quantum treatment of the electrons in molecules. Hands-on modeling. Application to selected molecular systems from microelectronics, biotechnology, material production.</p> <p><b>Introduction to the techniques of artificial intelligence (AI)</b> applied to molecular systems.</p>
books	<p>Harris, Daniel C., and Michael D. Bertolucci. <i>Symmetry and spectroscopy: an introduction to vibrational and electronic spectroscopy</i>. Dover</p> <p>Jensen, J. H. <i>Molecular modeling basics</i>. CRC Press.</p> <p>Cartwright H.M.: <i>Applications of artificial intelligence in chemistry</i>, Oxford</p>
notes	Selected chapters
Teaching methods	Lessons with proposal of cases of study. Hands-on computer codes. Discussion of real cases.
<b>Assessment</b> % 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	<p>Knowing how to apply symmetry theory to the discussion of real molecular spectra.</p> <p>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.</p> <p>Being able to use actual programs to obtain useful information.</p>