Corso di Laurea in
**SCIENZA E TECNOLOGIA DEI MATERIALI**

Triennale – L30

| **General information** | | |
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| Academic subject | Physical Chemistry of Materials | |
| Degree course | *Materials Science and Technologies* | |
| Academic Year | *Third* | |
| European Credit Transfer and Accumulation System (ECTS) | | 5 |
| Language | *Italian* | |
| Academic calendar (starting and ending date) | *As academic calendar* | |
| Attendance | *Strongly reccomended* | |

| **Professor/ Lecturer** | |
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| Name and Surname | Giuseppe Colafemmina |
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| Telephone | 0805442040 |
| Department and address | *Chemistry department - via Orabona, 4 - 70125 BARI* |
| Virtual headquarters | *https://teams.microsoft.com/l/channel/19%3ae6be8865fd9348a8a46ec6c75eb39bb8%40thread.tacv2/Generale?groupId=fb033635-8153-42dc-819f-960acf7d2a7a&tenantId=c6328dc3-afdf-40ce-846d-326eead86d49* |
| Tutoring (time and day) | Mon-Fri: 15-18, by mail or telephone |

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| ***Syllabus*** | |
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| **Learning Objectives** | Acquire knowledge of the chemical structure of solid, liquid and gaseous materials through the use of common spectroscopic techniques. Basic knowledge of the theoretical and instrumental aspects underlying the techniques studied |
| **Course prerequisites** | Knowledge of general chemistry and physical chemistry.<br>Ability to represent experimental data |
| **Contents** | Historical remarks and the electromagnetic spectrum.<br>Emission and absorption of a radiation, theory of time-dependent perturbations. Lambert-Beer law and dipolar moment of transition. Line width.<br>Fourier Transform - General aspects with examples of Fourier Transform spectroscopies (NMR and IR).<br>Born-Oppenheimer principle: separation of nuclear from electronic motions<br>Rotational Spectroscopy<br>Rotational energy levels, selection rules and level degeneration; centrifugal distortion and spectrum of a linear rotator.<br>Vibrational Spectroscopy<br>Roto-vibrational spectra, selection rules and measurement of rotational constants, centrifugal and vibrational distortion. Measurement of bond lengths.<br>Polyatomic molecules: introduction of normal coordinates<br>Molecular spectroscopy<br>LCAO molecular orbital method for diatomic molecules, vibronic transitions. Franck-Condon principle, Fate of excited states. Triplet and singlet states.<br>Block illustration of spectrophotometers and spectrofluorimeters; operation of their components.<br>NMR Spectroscopy<br>General aspects, Vector model, Bulk magnetization, obtaining a spectrum, chemical shift. Fourier Transform and data processing. NMR instrumentation. |

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| | Nuclear interactions, chemical shift, dipole-dipole, scalar and quadrupolar coupling<br>Solid State NMR<br>General aspects and essential techniques: MAS, Cross-Polarization and decoupling techniques.<br>Laboratory Experiments<br>1) Analysis of the IR spectra in gas phase of CO and HCl diatomic molecules for the measurement of the roto-vibrational constants relative to the two molecules in an anharmonic potential.<br>2) Quantitative analysis of an unknown sample of bromo-benzene by means of a calibration line,<br>3) Determination of average lengths of conjugated bonds in dienes and dyes. Measurement of the 0-0' transition through fluorescence measurements. |
| **Books and bibliography** | SPECTRA OF ATOMS AND MOLECULES<br>P. F. Bernath 2nd *ed.* Oxford (2005)<br>MODERN SPECTROSCOPY<br>J. Michael Hollas 4th Ed. – Wiley (2004)<br>SOLID STATE NMR BASIC PRINCPLES AND PRACTICE – D C Apperley, R K Harris, P Hodgkinson – Momentum Press (2012)<br>Some chapters o Section of the books |
| **Additional materials** | *Slides of the lessons* |

| **Work schedule** | | | |
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| Total | Lectures | Hands on (Laboratory, working groups, seminars, field trips) | Out-of-class study hours/ Self-study hours |
| **Hours** | | | |
| 125 | *24* | *30* | *71* |
| **ECTS** | | | |
| *5* | *3* | *2* | |

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| **Teaching strategy** | Lectures with slides provided to students before the lesson; group work within the laboratory experiences accompanied by procedures to be followed; at least two ongoing tests not agreed, during the class. |
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| **Expected learning outcomes** | |
| **Knowledge and understanding on:** | Understanding and knowledge of the basic concepts of quantum mechanics and spectroscopy related to the different materials. |
| **Applying knowledge and understanding on:** | Ability to process and present experimental datab obtained in lab |
| **Soft skills** | • *Making informed judgments and choices*<br>Ability to identify the most effective techniques fpr the characterizing the material under investigation, ability to autonomously carry out simple experiments and to process experimental molecular spectroscopy data.<br>• *Communicating knowledge and understanding*<br>Correct Italian language in the use of written and oral presentation of the results;<br>Computer skills respect to the elaboration and presentation of a simple experimental dataset; |

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| | Drafting of reports on the laboratory activities carried out. Graphical presentation of the experimental data obtained. |

| **Assessment and feedback** | |
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| Methods of assessment | |
| Evaluation criteria | Knowledge of the principles underlying spectroscopy;<br>Knowledge of the fundamental equations that describe the energetic and spectroscopic states, the selection rules in order to explain the different spectra;<br>Knowledge of the common chemical equipment of a laboratory and use of simple procedures in use in a chemical laboratory;<br>Estimate the errors of a measurement and graph the experimental data correctly;<br>knowing how to write a laboratory report;<br>be able to effectively present the results of an experiment in written and oral form. |
| Criteria for assessment and attribution of the final mark | o Evaluation of the learned contents<br>o Exposure assessment<br>o Evaluation of the results obtained in the laboratory.<br>Final mark is obtained:<br>Laboratory report evaluation (40%),<br>Oral exam (60%), Speed incentive (+ 2/30);<br>Partial exam without notice during the class. |
| **Additional information** | |
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