Corso di Laurea in
# SCIENZA E TECNOLOGIA DEI MATERIALI

Triennale – L30

| **General information** | |
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| Academic subject | ***Physical Chemistry*** |
| Degree course | *Materials Science and Technology* |
| Academic Year | *2021-2022* |
| European Credit Transfer and Accumulation System (ECTS) | 6 |
| Language | *Italian* |
| Academic calendar (starting and ending date) | *According to teaching calendar* |
| Attendance | *Compulsory on site for the laboratory activities* |

| **Professor/ Lecturer** | |
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| Virtual headquarters | *AA 2021-22 - Chimica-Fisica <ba9ee226.uniba.it@emea.teams.ms>* |
| Tutoring (time and day) | *From Monday to Friday 9.00-13.00 and 16.00-19.00*<br>*By appointment fixed by email*<br>• *In presence: Office - room 132 – 1st floor at Chemistry Department*<br>*Online: Microsoft Teams Web Site* |

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| ***Syllabus*** | |
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| **Learning Objectives** | *Knowledge of the laws of Thermodynamics applied to the properties of materials and to the transformations of matter.* |
| **Course prerequisites** | *Fundamentals of mathematical analysis and differential calculus. Fundamentals of programming and calculation in Matlab* |
| **Contents** | ***Introduction to the fundamentals of Classical Thermodynamics***.<br>*Thermodynamic system, state quantities, thermodynamic equilibrium and equation of state, state transformations, state functions and exact differentials. Equation of state of the Ideal Gas. Ideal gas mixtures: Dalton's law. Real gases: deviations from ideal behavior. Van der Waals equation. Andrew's diagram and critical parameters.*<br>***The First and the Zero Principle***.<br>*Exchanges of energy between system and environment: heat and work, conventions. Zero principle of thermodynamics. Thermometers: gas and liquid. Thermal capacities and specific heats. The first principle of thermodynamics: internal energy E and heat and work equivalence. Conservation of energy. Limits of the first principle. Enthalpy function of state. Relationship between Cp and Cv. Mayer's report.*<br>***Joule-Thomson coefficient and partial molar volumes.***<br>*Free expansion of a gas. Internal energy and enthalpy of an ideal gas. Real gases: Joule-Thompson coefficient. Intensive and extensive quantities. Partial molar volumes.*<br>***Thermochemistry***. |

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| | *Heat of reaction and thermochemical equations. Reaction enthalpy and Reaction energy. Calorimetry. Calculation of the $\Delta H_R$. Standard state. Standard enthalpies of formation $\Delta H^\circ f$ tabulated. Hess's law. Kirchhoff's law.*<br>***The Second and Third Principles**.*<br>*Entropy as a function of state. Spontaneous processes and entropy variation: Clausius inequality. Thermal machines and the Kelvin-Plank statement. The Third Law of Thermodynamics. Calculation of the standard entropies S of pure substances under standard conditions. Enthalpy of reaction ⍰SR. Variation of ⍰SR with temperature.*<br>***Free Energy**.*<br>*Free energy of Helmholtz and Gibbs: principles of spontaneity and balance. Enthalpy and entropic contribution to the $\Delta G_R$ for spontaneous reactions in standard and non-standard conditions.*<br>***Legendre transformations and equilibrium constant.***<br>*Fundamental equation of thermodynamics. Transformations of Legendre. Maxwell's equations. Variation of G with pressure and temperature. Gibbs-Helmholtz equation. Thermodynamic quotient and constant of equilibrium. Activity of chemical species. Van't Hoff equation.*<br>***Chemical potential.***<br>*Chemical potential and molar free energy G°. Gibbs-Duhem equation. Change of the chemical potentiasl as a criterion of spontaneity and equilibrium. Chemical potential of an ideal and real gas. Activity coefficient. Equilibrium constant as a function of the activities for heterogeneous equilibria.*<br>***State diagrams.***<br>*States of matter and phase transformations. The solid state, liquid state and gaseous state. Thermal analysis and thermogram. P-T and p-V state diagram of pure substances. Heterogeneous systems and phases. Clapeyron equation. Equilibrium condition in a heterogeneous system with several components.*<br>***The Solutions**.*<br>*Passage in solution and enthalpy of mixing. Saturation and solubility. Ideal solutions. Vapor pressure of a pure liquid component. Raoult's law. Colligative properties.*<br>***Chemical Kinetics: introduction***<br>*Chemical reactions and conservation of mass. Reaction mechanism and elementary reactions. Formal analysis and empirical analysis. Rate of reaction: order of reaction and molecularity. Mass law of action. Reversible elementary reactions and equilibrium constant. Arrhenius law and activation energy.*<br>***Chemical Kinetics: formal analysis***<br>*Kinetic mechanism and system of differential equations. Use of mass conservation equations. System of kinetic differential equations: analytical solution for simple mechanisms.*<br>***Chemical Kinetics: empirical analysis and catalysis***<br>*Methods for determining the order of reaction by reaction rate. Principles of chemical catalysis and activation energy. Enzymatic catalysis: Brown's mechanism. Michaelis-Menten equations.*<br>***Laboratory***<br>*• Determination of the enthalpy of evaporation of water.*<br>*• Determination of the heat of combustion of sucrose.*<br>*• Determination of the cryoscopic lowering of non-volatile solute solutions.* |

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| | • *MATLAB exercise for the processing of laboratory data*<br>• *Example of drafting the final report* |
| **Books and bibliography** | • *Atkins Chimica Fisica – Zanichelli*<br>• *Lecture notes* |
| **Additional materials** | *The lecture notes are exhaustive on the course contents, while the proposed textbooks can be used for in-depth analysis regarding specific topics together with scientific articles and web contents as indicated by the teacher.* |

| **Work schedule** | | | |
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| Total | Lectures | Hands on (Laboratory, working groups, seminars, field trips) | Self-study hours |
| **Hours** | | | |
| *150* | *32* | *30* | *88* |
| **ECTS** | | | |
| *6* | *4* | *2* | |
| **Teaching strategy** | *Lectures, exercises, laboratory experiments* | | |
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| **Expected learning outcomes** | | | |
| **Knowledge and understanding on:** | *The student must have assimilated the basic concepts and laws of thermodynamics and master the mathematical tools that underlie them.* | | |
| **Applying knowledge and understanding on:** | *• Know the difference between intensive and extensive chemical-physical properties, and the properties of the molar partial sizes.*<br>*• Know the four laws of thermodynamics, the fundamental equation of thermodynamics, the definition of the main state functions: internal energy (E), Enthalpy (H), Gibbs (G) and Helmotz (F) free energy and the of their differentials for systems with variable and constant composition. Master the concept of chemical potential.*<br>*• Master the principles of spontaneity and balance in different operating conditions.*<br>*• To be able, from the tabulated data, to calculate the values of the free Enthalpies and Energy of the reaction under standard conditions at different temperatures and of the equilibrium constant for chemical reactions with known stoichiometry.*<br>*• Know the main differences between the three fundamental states of matter: solid, liquid, gaseous. Knowing the difference between gas and vapor, between a gas with ideal and real behavior.*<br>*• Knowing how to discuss the state diagrams of pure substances and the phase equilibrium laws. Knowing the equilibrium condition for multi-component systems.*<br>*• Obtain the fundamental equations that describe colligative properties and mixing.*<br>*• Knowing how to set up and solve systems of differential equations for simplified kinetic mechanisms. Knowing the Michaelis-Menten equations for enzymatic kinetics* | | |
| **Soft skills** | *Autonomy of judgment:*<br>• *be able to write a laboratory report in a critical way by correctly reporting the measured data and evaluating errors on estimated properties with indirect measurement procedures.*<br>• *be able to evaluate the energy involved in the transformations of matter*<br>*Communication skills:*<br>• *be able to express themselves using appropriate technical language.*<br>*Ability to learn independently*<br>• *be able to solve thermodynamic problems not explicitly addressed during the course of lessons* | | |

| **Assessment and feedback** | |
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| Methods of assessment | *Oral examination and Laboratory reports*<br>*The evaluation method is through a final oral exam with discussion of the laboratory reports.*<br>*The oral exam is divided into the discussion of one topic chosen by the student + 3 topics chosen by the teacher, plus the discussion of laboratory reports. In order for the exam to be considered passed, the student must have satisfactorily exposed all 4 topics under examination. In case of insufficient discussion of one or more topics, the teacher can, at his sole discretion, proceed with the selection of further topics to verify the student's preparation.*<br>*The three laboratory reports must be submitted in paper format and discussed during the examination. They can also be delivered at least 15 days before the date of the exam and discussed / corrected with the teacher. In this case the corrected version of the reports must be presented during the examination and the discussion of the reports will be considered outdated.*<br>*During the course, 2 tests will be carried out in Itinere with voluntary participation.*<br>*• I test in itinere: Lessons I-V*<br>*• II test in itinere: Lessons VI-X* |
| Evaluation criteria | *• Knowledge and understanding:*<br>*- Minimum level:*<br>*knowing how to correctly frame the problem with respect to the question / problem addressed*<br>*- Intermediate level:*<br>*knowing how to give a correct answer to the question / problem faced with the appropriate terminology*<br>*- Upper level:*<br>*knowing how to mathematically formalize the answer to the question / problem faced correctly and master the calculation methods*<br>*• Applied knowledge and understanding*<br>*- Minimum level:*<br>*know the main laws of thermodynamics and their meaning and know how to correctly set the calculation of thermodynamic properties of interest from tabulated data*<br>*- Intermediate level:*<br>*ability to independently calculate the thermodynamic properties of interest in standard to non-standard conditions from the tabulated data*<br>*- Upper level:*<br>*ability to mathematically derive thermodynamic properties from fundamental laws*<br>*• Autonomy of judgment*<br>*- Minimum level:*<br>*show during the oral exam to be aware of own level of preparation,*<br>*have delivered the reports on the laboratory experiences following the format of a scientific article by completing the different sections adequately*<br>*- Intermediate level:*<br>*show during the oral exam to be aware of own shortcomings in preparation,*<br>*have critically introduced the problem of determining the thermodynamic property at stake and correctly reported the data in the laboratory reports*<br>*- Upper level:* |

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| | *show during the oral exam to be aware of how to improve own level of preparation.*<br>*have correctly calculated the errors, reported the data with the correct number of significant figures and critically discussed the results obtained on the basis of the estimation of errors in the laboratory reports.*<br>*• Communication skills*<br>*- Minimum level:*<br>*clarity in the presentation even in the absence of an appropriate use of technical-scientific terminology*<br>*- Intermediate level:*<br>*clarity of presentation and appropriate use of technical-scientific terminology*<br>*- Upper level:*<br>*ability to critically deal with natural phenomena with clarity and terminological rigor, even if not explicitly dealt with during the course*<br>*• Ability to learn*<br>*- Minimum level:*<br>*having understood the meaning of the main fundamental laws of thermodynamics and having participated carefully in the lectures and laboratory experiences.*<br>*- Intermediate level:*<br>*have understood the use of mathematical methods of chemical thermodynamics and have actively participated in lectures and laboratory experiences by asking relevant questions.*<br>*- Upper level:*<br>*mastering the calculation methods of thermodynamics by applying them also to problems not explicitly addressed, having participated in lectures and laboratory experiences with a critical spirit by asking non-trivial questions and responding in a pertinent way to the verification questions posed by the teacher.* |
| Criteria for assessment and attribution of the final mark | *For each in itinere test passed with a score higher than 18, one of the three questions available to the teacher will be considered passed with a score equal to that achieved in the in itinere test. In any case, the student may not use the result of one or more tests in Itinere to answer a question on the corresponding part of the program. The final mark will be given by the average of the exam mark (from 40 to 80%) with the marks of the passing tests (from 0 to 40%) plus the laboratory reports (20%)* |
| **Additional information** | |
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