Universidad de Navarra

Statistical Thermodynamics, Transport (F.Ciencias)

Teaching guide 2023-24

INTRODUCTION

Course description: The microscopic world of atoms and molecules, which is studied by Quantum Mechanics (*PChem II*), and the macroscopic systems, governed by the Laws of Thermodynamics (*PChem I*), can be connected through Statistics. In this course (***PChem III***) we will see how, starting from the properties of molecules, the behaviour of bulk matter systems can be predicted. After the introduction of Statistical Thermodynamics, we use the molecular-kinetic theory to study transport phenomena. The foundations of Physical Chemistry are completed with the study of interfaces. Finally, all previous knowledge will be applied in several physicochemical fields of interest: molecular dynamics, catalysis, electrode kinetics, polymers and colloids.

- **Degree**: CHEMISTRY, CHEM+BIOCHEM.
- **Module in the Degree Program**: Module II, Theoretical Foundations of Chemistry
- **Number of credits**: 6 ECTS
- **Year**: Third, 2nd semester
- **Type of course**: Required
- **Instructors**: José R. Isasi
- **Language**: English
- **Lecture schedule**: Tuesdays at 10h, Thursdays at 11h, Fridays 11h-13h

COMPETENCIES

General and basic competencies

- **CB1.** Students have demonstrated knowledge and understanding in an area of study that starts from the foundations of general secondary education, and is usually at a level that, while supported by advanced textbooks, also includes some aspects that involve knowledge from the cutting edge of their field of study.
- **CB2.** That students know how to apply their knowledge to their work or vocation in a professional way and have the skills that are usually demonstrated through the development and defense of arguments and problem solving within their area of study.
- **CB3.** That students have the ability to gather and interpret relevant data (usually within their area of study) to make judgments that include reflection on relevant issues of a social, scientific or ethical nature.
- **CB4.** That students can transmit information, ideas, problems and solutions to both a specialized and non-specialized audience.
- **CG1.** Plan and organize time and manage one's own continuous training, updating knowledge of innovations in the scientific field and knowing how to analyze future trends.
- **CG2.** Think in an integrated way and approach problems from different perspectives. Have critical reasoning. Provide solutions to problems in the scientific field.
- **CG3.** Work in a team, select and choose the work methodology and distribution of functions. Know how to listen and make use of the word with positive and constructive interventions.
- **CG6.** Use the induction method correctly. Being able to generalize the knowledge obtained on one occasion to other cases or similar occasions that may arise in the future.

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Specific competencies

- **CE1.** Analyze and solve qualitative and quantitative problems according to previously developed models, as well as recognize new problems and plan strategies for their resolution.
- **CE2.** Process, compute, evaluate, interpret and synthesize chemical data and information.
- **CE9**. Know the characteristics of the states of matter.
- **CE11.** Analyze the principles of various disciplines such as thermodynamics, quantum mechanics, spectroscopy and electrochemistry. Know its applications in Chemistry, its role in the description of the structure and properties of atoms and molecules or its function in analytical or structural research techniques.
- **CE12.** Know the most relevant materials, their properties, based on their chemical composition and structure. Identify the various analysis and structural determination techniques.

PROGRAM

(A) Lectures

FOUNDATIONS OF STATISTICAL MECHANICS

1. **Probability.** Basic probability theory. Stirling's approximation. Probability distribution functions.
2. **The Boltzmann Distribution.** Microstates and configurations. Derivation of the Boltzmann distribution. Physical meaning of the Boltzmann distribution law. The definition of *beta*.
3. **Ensemble and Molecular Partition Functions.** The canonical ensemble. Relating canonical to molecular partition functions. Molecular energy levels. Partition functions: translational, rotational, vibrational and electronic. The equipartition theorem.
4. **Statistical Thermodynamics.** Energy. Heat capacity. Entropy. Other thermodynamic functions.

KINETIC THEORY OF GASES AND TRANSPORT PROCESSES

1. **Kinetic-Molecular Theory of Gases.** Pressure of an ideal gas. Kinetic energy and temperature. Distribution of molecular speeds in an ideal gas. Collisions with a wall and effusion. Molecular collisions and mean free path.
2. **Transport Processes. Thermal conductivity.** Heat transfer and Fourier's law. Kinetic theory of thermal conductivity of gases.
3. **Viscosity.** Newton's law of viscosity. Flow rate of fluids. Measurement of viscosity. Kinetic theory of gas viscosity. Viscosity of polymer solutions.
4. **Diffusion and Sedimentation.** Fick's first law and diffusion coefficients. Net displacement of diffusing molecules. Theory of diffusion in liquids. Kinetic theory of diffusion in gases. Sedimentation of macromolecules in solution.
5. **Electrical Conductivity.** Electric current and conductivity. Electrical conductivity of electrolyte solutions. Electric mobilities and electrophoresis. Transport numbers. Molar conductivities of ions. Applications of conductivity.

SURFACE AND COLLOID CHEMISTRY

1. **The Interphase Region.** Surface tension and interfacial tension. Curved interfaces and the measurement of surface tension. Thermodynamics of surfaces. The Gibbs adsorption isotherm. The gas-liquid interface.
2. **Adsorption.** The gas-solid interface. Chemisorption and physical adsorption. Adsorption isotherms. Enthalpy of adsorption.
3. **Macromolecules and Colloids.** Determination of size and shape. Structure and dynamics. The electrical double layer. Colloidal dispersions.

ADVANCED KINETICS

1. **Molecular Kinetics.** Hard-sphere collision theory. Potential-energy surfaces. Molecular reaction dynamics. Transition-state theory for ideal gas reactions. Reactions in solution.
2. **Catalysis.** Enzyme catalysis. Heterogeneous catalysis.
3. **Electrode Kinetics.** Rate of charge transfer.
4. **Polymer synthesis.** Step-growth and Chain polymerization. Copolymerization.

(B) Practical sessions

1. Computing heat capacities.
2. Computing populations of energy levels.
3. Equations of state and kinetic theory calculations.
4. Transport properties.
5. Adsorption phenomena.

EDUCATIONAL ACTIVITIES

Classroom activities

1. LECTURES. 46 Hours (1.84 ECTS)

- Methodology: lectures in the classroom for all the students, in which interactive and participative training will be encouraged. The fundamental concepts for each lesson will be presented.
- Acquired competencies: the students will learn the basic aspects of the subject and how to apply them to problem solving.

2. PRACTICALS. 10 Hours (0.4 ECTS)

- Methodology: practical sessions, seminars and/or computer lab workshops; students will solve practical cases including computational calculations. The corresponding reports are due one week after the sessions.
- Acquired competencies: the students will consolidate computational skills acquired in previous courses in order to apply them to solve complex problems in Physical Chemistry.

3. EXAMINATIONS. 6 Hours (0.25 ECTS)

- Methodology: the students must assimilate the core contents of the course and demonstrate their skills solving theoretical/practical exercises and problems.
- Acquired competencies: once the course contents have been studied and the corresponding related exercises have been solved, the essential knowledge and skills are acquired in order to achieve the course goals and objectives.

4. TUTORING. 3 Hours (0.12 ECTS)

- Methodology: students are encouraged to speak with their instructor for individual or group tutoring to get help with the most difficult parts of the subject.
- Acquired competencies: the students will learn to apply the acquired knowledge to problem solving, in order to improve their comprehension of the subject.

Out of classroom activities

1. SOLVING PROPOSED EXERCISES. 35 Hours (1.4 ECTS)

- Methodology: after lecturing, the students are prompted to carry out an activity that involves solving some related exercise. Although students are encouraged to work with these activities (and to seek help when needed), they are not mandatory.
- Acquired competencies: students develop the ability to apply the acquired knowledge to solve problems.

2. PERSONAL AND/OR GROUP STUDY. 50 Hours (2 ECTS)

- Methodology: students must study the material discussed in class, with particular emphasis on solving the proposed exercises.
- Acquired competencies: after studying the theoretical concepts and solving the related exercises, the skills necessary to achieve the objectives of the course are set.

ASSESSMENT

ORDINARY CALL (May)

- Weekly quizzes will be taken along the course during class. Those students who do not prefer this continuous assessment may respond to an extra section in the final exam. The course grade will correspond to a weighted average of the best ten quiz scores (**20%**), the final exam grade (**65%**) plus the practicals reports (**15%** , due on the final exam date). Student participation during lectures is encouraged and could be rewarded with extra points.
- Quizzes are open-book exams. The final examination will consist of a set of short questions, exercises and problems. One double-sided formula sheet will be allowed for the final exam. A minimum score of **40/100** in the final exam is required to consider the other scores and pass the course.

EXTRAORDINARY CALL (June)

- Those students unable to pass the course with a score over 50/100 in May will have to retake the final exam in June. The quizzes and reports scores will be considered in case this improves the final average score.

OFFICE HOURS

Dr J.R. Isasi (jrisasi@unav.es)

- Despacho 0110. Edificio de Investigación. Planta 0.

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- Horario de tutoría: Thursdays, 9:00 to 11:00 and 16:00 to 18:00, or by appointment.

BIBLIOGRAPHY AND RESOURCES

Recommended textbooks: (Find them in the Library)

Main textbooks:

- Levine, I.N. "Physical Chemistry". 6th edition. Mc Graw-Hill, 2009. Find it in the Library
- Engel, T.; Reid, P. "Physical Chemistry". 3rd edition. Pearson, 2014. Find it in the Library
- Kontogeorgis, G.M.; Kiil, S. "Introduction to Applied Colloid and Surface Chemistry". Wiley, 2016. Find it in the library

Additional reference textbooks:

- Atkins, P.W.; de Paula, J. "Physical Chemistry". 2nd edition. Oxford University Press, 2011. Find it in the Library
- Barnes, G.T.; Gentle, I.R. "Interfacial Science: An Introduction". 2nd edition. Oxford University Press, 2011. Localízalo en la Biblioteca

Spanish versions of the textbooks:

- Levine, I.N. "Fisicoquímica" 5ª edición. Ed. Mc Graw-Hill, 2013. Localízalo en la Biblioteca
- Engel, T.; Reid, P. "Química Física". Pearson, 2006. (Libro electrónico) Localízalo en la Biblioteca
- Atkins, P.W. "Química Física". 8ª edición. Ed. Médica Panamericana, 2008. Localízalo en la Biblioteca