



## Teaching Guide

Identifying Data					2022/23
Subject (*)	Thermodynamics: Equilibrium and Phases		Code	610G04018	
Study programme	Grao en Nanociencia e Nanotecnoloxía				
Descriptors					
Cycle	Period	Year	Type	Credits	
Graduate	2nd four-month period	Second	Obligatory	6	
Language	Spanish				
Teaching method	Face-to-face				
Prerequisites					
Department	Química				
Coordinador	Sastre De Vicente, Manuel Esteban	E-mail	manuel.sastre@udc.es		
Lecturers	Sastre De Vicente, Manuel Esteban	E-mail	manuel.sastre@udc.es		
Web					
General description	<p>The basic principles and some applications of thermodynamics necessary to address the study and understanding of the effect of the size of the thermodynamic system on its properties, are described. At the same time, it is intended to conceptually frame the study of Nanothermodynamics and nanoscopic systems.</p>				

## Study programme competences / results

Code	Study programme competences / results
A1	CE1 - Comprender los conceptos, principios, teorías y hechos fundamentales relacionados con la Nanociencia y Nanotecnología.
A2	CE2 - Aplicar los conceptos, principios, teorías y hechos fundamentales relacionados con la Nanociencia y Nanotecnología a la resolución de problemas de naturaleza cuantitativa o cualitativa.
A3	CE3 - Reconocer y analizar problemas físicos, químicos, matemáticos, biológicos en el ámbito de la Nanociencia y Nanotecnología, así como plantear respuestas o trabajos adecuados para su resolución, incluyendo el uso de fuentes bibliográficas.
A7	CE7 - Interpretar los datos obtenidos mediante medidas experimentales y simulaciones, incluyendo el uso de herramientas informáticas, identificar su significado y relacionarlos con las teorías químicas, físicas o biológicas apropiadas.
B2	CB2 - Que los estudiantes sepan aplicar sus conocimientos a su trabajo o vocación de una forma profesional y posean las competencias que suelen demostrarse por medio de la elaboración y defensa de argumentos y la resolución de problemas dentro de su área de estudio
B3	CB3 - Que los estudiantes tengan la capacidad de reunir e interpretar datos relevantes (normalmente dentro de su área de estudio) para emitir juicios que incluyan una reflexión sobre temas relevantes de índole social, científica o ética
B6	CG1 - Aprender a aprender
B7	CG2 - Resolver problemas de forma efectiva.
B8	CG3 - Aplicar un pensamiento crítico, lógico y creativo.
C1	CT1 - Expresarse correctamente, tanto de forma oral como escrita, en las lenguas oficiales de la comunidad autónoma
C4	CT4 - Desarrollarse para el ejercicio de una ciudadanía respetuosa con la cultura democrática, los derechos humanos y la perspectiva de género

## Learning outcomes

Learning outcomes	Study programme competences / results		
Understand the principles of Thermodynamics and be able to apply them.	A1	B2	C1
	A2	B3	C4
	A3	B6	
	A7	B7	
		B8	



Understand the equilibrium condition and be able to apply it.	A1 A2 A3	B2 B6 B7 B8	C1 C4
Be able to perform basic thermodynamic calculations.	A1 A2 A3	B2 B3 B6 B7 B8	C1 C4
Understand phase equilibria and be able to use them to solve simple problems.	A1 A2 A3 A7	B2 B3 B6 B7 B8	C1 C4
Understand the fundamentals of surface thermodynamics.	A1 A2 A3 A7	B2 B3 B6 B7 B8	C1 C4

Contents	
Topic	Sub-topic
Unit 1.- Basic concepts	1.1.- Object and limitations of Thermodynamics. 1.2.-Thermodynamic systems and states. 1.3.-Thermodynamic variables. 1.4.-Reversible and irreversible processes. 1.5.-Nanothermodynamics
Unit 2.-Principles of Thermodynamics.	2.1.-Principle of energy conservation. First principle of thermodynamics. Internal energy and enthalpy. 2.2.-Energy properties of a thermodynamic system. Calorimetric coefficients and calorific capacities. 2.3.-Limitations of the First Principle. 2.4.-Formulation of the Second Principle. The function of the entropy state. Clausius inequality. Entropy changes in closed and isolated systems. Entropy production. 2.5.-Equações Tds. 2.6.-Third principle of Thermodynamics. Nernst's claim. Absolute entropies
Unit 3. Thermodynamic potentials and evolution evolution of thermodynamic systems.	3.1.-Principles of maximum and minimum in nature. 3.2.-Hemholtz energy and maximum work. 3.3.-Gibbs energy and useful work. 3.4.-General thermodynamic relations:Maxwell Relations.. Hemholtz equation. Gibbs-Hemholtz equation. 3.5.-Thermodynamics of variable composition systems. Concept of chemical potential. Gibbs-Duhem equation 3.6.- Chemical potential of ideal and real gases. Concept of fugacity. 3.7.-Partial molar magnitudes. 3.8.-Equilibrium conditions. Phase equilibrium and chemical equilibrium.



Unit 4. Phase balance.	4.1.-Phase equilibria in systems of a component. Rule of phases. Clapeyron and Clausius-Clapeyron equation. Phase diagrams. 4.2.-Phase equilibria in two-component systems. Ideal and real solutions. Activity concept. Solubility and other properties. 4.3.- Other phase equilibria.
Unit 5. Thermodynamics and size of the system: surfaces and systems of "small size",	5.1.-Surface tension. Laplace equation. Capillary ascent. Contact angle. 5.2.-Thermodynamic properties and size. Solubility, Melting point, Nucleation? 5.3.-Nanothermodynamics. Hill's formulation of the general equation of thermodynamics (Gibbs equation).
Unit 6. Introduction to the thermodynamics of irreversible processes.	6.1.-Production of entropy. 6.2.-Generalized forces and flows. Linear and nonlinear thermodynamics. 6.3.-Heat transmission processes: conduction, convection and radiation.

**Planning**

Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student's personal work hours	Total hours
Problem solving	A1 A2 A3 A7 B2 B3 B6 B7 B8 C1 C4	16	30.4	46.4
Mixed objective/subjective test	A1 A2 A3 A7 B2 B3 B6 B7 B8 C1 C4	3	0	3
Document analysis	A1 A2 A3 A7 B2 B3 B6 B7 B8 C1 C4	0.6	1	1.6
Guest lecture / keynote speech	A1 A2 A3 A7 B2 B3 B6 B8 C1 C4	32	64	96
Personalized attention		3	0	3

(\*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

**Methodologies**

Methodologies	Description
Problem solving	The problem seminars will be dedicated to reinforcing the understanding of the contents taught in the master sessions by solving conceptual questions and numerical problems. Part of the resolved questions/problems may deal with research/dissemination articles directly related to the contents of the subject. Said articles will be provided to all students of the course through Moodle, email for their reading!
Mixed objective/subjective test	It can integrate different types of questions and/or problems: test, multiple choice, ordering, short answer, discrimination, completion or association.  Two tests will be carried out during the course, which will be set in the calendar.  In the two tests carried out, one of the questions/questions may deal with the topic analyzed in one of the outreach/research articles that have been provided to the students in the problem seminars as a documentary source.
Document analysis	Students will be given the necessary keys for the proper search, reading and interpretation of different research/dissemination articles in the field of Thermodynamics.
Guest lecture / keynote speech	The master lines and fundamental contents of the subject are described.

**Personalized attention**

Methodologies	Description
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Problem solving	The student is recommended to resolve all their doubts by contacting the teacher through tutoring, email.
Document analysis	Part-time students or students with academic exemption will have face-to-face tutorials or by email whenever they need it.

Assessment			
Methodologies	Competencies / Results	Description	Qualification
Mixed objective/subjective test	A1 A2 A3 A7 B2 B3 B6 B7 B8 C1 C4	Two tests will be carried out: The first one will be partial with a value of 30% of the final grade. The second will be the final exam on the whole subject, a score greater than 4 out of 10 must be obtained and weights 70%.	90
Document analysis	A1 A2 A3 A7 B2 B3 B6 B7 B8 C1 C4	Analysis of documentary sources The student will deliver, throughout the course, a summary that synthesizes the most relevant aspects of the article/s read that will have previously been delivered with sufficient time and precise indications for its reading.	10

Assessment comments
Students on a part-time or academic basis will have tutorials in person or by e-mail whenever they need it.

Sources of information	
<b>Basic</b>	- LEVINE, I N (). Physical Chemistry (different editions). Mc Graw Hill - (). .
<b>Complementary</b>	- (). . - KONDEPUDI DILIP (2008-2014). INTRODUCTION TO MODERN THERMODYNAMICS. WILEY - AGUILAR PERIS (1981). CURSO DE TERMODINÁMICA. ALHAMBRA - ATKINS P.W (). QUÍMICA-FÍSICA (distintas ediciones). - CALLEN H.B (1981). TERMODINÁMICA. AC - DENBIGH K (1985). EQUILIBRIO QUÍMICO. AC - TERRELL L.HILL (2001). Perspective:Nanothermodynamics. Nano Lett , 1:111-112 - TERRELL L.HILL (2001). A different Approach to Nanothermodynamics. Nano Lett , 1:273-275 - TERRELL L.HILL (1994). THERMODYNAMICS OF SMALL SYSTEMS. DOVER

Recommendations
<b>Subjects that it is recommended to have taken before</b>
Chemistry: Equilibrium and Change/610G04008 Fundamentals of Mathematics/610G04001 Physics: Mechanics and Waves/610G04002
<b>Subjects that are recommended to be taken simultaneously</b>
<b>Subjects that continue the syllabus</b>
Surface Science/610G04021
<b>Other comments</b>

(\*The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.