Course guide
230865 - MSD - Materials Science of Drugs

Last modified: 02/06/2022

Unit in charge: Barcelona School of Telecommunications Engineering
Teaching unit: 748 - FIS - Department of Physics.

Degree: MASTER'S DEGREE IN ENGINEERING PHYSICS (Syllabus 2018). (Optional subject).
ERASMUS MUNDUS MASTER'S DEGREE IN BIO & PHARMACEUTICAL MATERIALS SCIENCE (Syllabus 2021). (Compulsory subject).

Academic year: 2022 **ECTS Credits:** 4.0 **Languages:** English

LECTURER

Coordinating lecturer: Consultar aquí / See here: https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/responsables-assignatura

Others: Consultar aquí / See here: https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/professorat-assignat-idioma

PRIOR SKILLS

Knowledge on fundamental thermodynamics and solid-state physics.

REQUIREMENTS

None.

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Basic:
CB7. (ENG) Que los estudiantes sepan aplicar los conocimientos adquiridos y su capacidad de resolución de problemas en entornos nuevos o poco conocidos dentro de contextos más amplios (o multidisciplinares) relacionados con su área de estudio.
CB8. (ENG) Que los estudiantes sean capaces de integrar conocimientos y enfrentarse a la complejidad de formular juicios a partir de una información que, siendo incompleta o limitada, incluya reflexiones sobre las responsabilidades sociales y éticas vinculadas a la aplicación de sus conocimientos y juicio.
CB9. (ENG) Que los estudiantes sepan comunicar sus conclusiones ¿y los conocimientos y razones últimas que las sustentan a públicos especializados y no especializados de un modo claro y sin ambigüedades
CB10. (ENG) Que los estudiantes posean las habilidades de aprendizaje que les permitan continuar estudiando de un modo que habrá de ser en gran medida autodirigido o autónomo.

TEACHING METHODOLOGY

The subject is given in 3 expositive 2-hour lessons weekly in large group, that combine theory and exercices, plus 2 laboratory sessions in small group.

LEARNING OBJECTIVES OF THE SUBJECT

On successful completion of the course, the students will be able to discuss the crystallographic properties of different polymorphs, the equilibrium conditions for a phase or phase coexistence, draw multiphase and/or binary phase diagrams, and distinguish between different equilibrium, metastable, and unstable states, and their relevance for drug formulations.

STUDY LOAD

Type	Hours	Percentage
Hours large group	30,0	30.00
Hours small group	6,0	6.00
Self study	64,0	64.00

Total learning time: 100 h

CONTENTS

Basics concepts of crystallography

Description:
Translational order, unit cell, Bravais lattices. Point groups, space groups, crystal systems. Crystallographic planes, reciprocal lattice, Miller indices. From crystal system to molecular structure and geometry: crystals with a base and molecular crystals. Calculation and modelling of diffraction patterns from atomic and structure scattering factors. Solid-state polymorphism of drugs and other organic molecules. Second harmonic generation.

Specific objectives:
The student will learn to distinguish and characterize the different structural phases based on their symmetries and the relationships between them.

Related activities:
Lectures including theory and problems solving

Full-or-part-time: 24h
Theory classes: 8h
Self study : 16h

Phase Equilibrium and phase transitions

Description:
Thermodynamic Potentials for hydrostatic pvT systems; Maxwell relations; TdS equations; General conditions for equilibrium; Fluctuations; Le Châtelier principle.

Specific objectives:
The student will acquire the basic thermodynamics needed to be able to understand more advanced and specific concepts in later topics.

Related activities:
Lectures including theory and problems solving

Full-or-part-time: 18h
Theory classes: 6h
Self study : 12h

Phase transitions and topological pressure-temperature phase diagram

Description:
Equilibrium conditions for hydrostatic pvT systems; First-order phase transitions: Clausius-Clapeyron equation. Stability and metastability domains; High-order phase transitions. Group-subgroup phase transitions.; Critical and triple points; Topological P-T phase diagram. Calorimetry techniques.

Specific objectives:
The student will go deep into first-order phase transitions and the notion of relative stability and will know how to construct topological phase diagrams. The student will acquire the experimental capability to characterize a phase transition and the temperature-pressure phase diagram.

Related activities:
Lectures including theory and problems solving
Lab session 1: Characterization of phase transitions and temperature-pressure phase diagram via calorimetry.

Full-or-part-time: 20h
Theory classes: 6h
Practical classes: 2h
Self study : 12h

Landau theory for phase transitions

Description:
Landau Theory. Order Parameter. Ferroic phase transitions. Long-range anisotropic interactions. Self-accommodation. Structural phase transitions. Mechanistic and kinetic classification of phase transitions.

Specific objectives:
The student will be introduced to Landau's theory for phase transitions, and how it can be used to understand the origin of microstructural textures and domains, giving rise to cycles of hysteresis and other phenomena.

Related activities:
Lectures including theory and problems solving

Full-or-part-time: 18h
Theory classes: 6h
Self study : 12h

Phases out of equilibrium

Description:
Glass state and glass transition; dynamics and structural relation in the glass state; pressure dependence of the glass transition temperature; non-equilibrium phases and mesophases of drugs. Dielectric spectroscopy.

Specific objectives:
The student will learn the concept of glass state and glass transition and their characteristics, and experimental techniques to characterize them.

Related activities:
Lab session 2: Characterization of relaxation dynamics and glass transition via dielectric spectroscopy and calorimetry.

Full-or-part-time: 11h
Theory classes: 3h
Practical classes: 2h
Self study : 6h

Binary systems

Description:
Thermodynamics of mixing, thermodynamic potential; types of binary phase diagrams: eutectic, metatectic and peritectic; solubility and miscibility; metastable and unstable states; nucleation vs spinoidal decomposition.

Specific objectives:
The student will learn the concepts related to the thermodynamics of binary systems.

Related activities:
Lectures including theory and problems solving

Full-or-part-time: 9h
Theory classes: 3h
Self study : 6h

GRADING SYSTEM

Problems solved autonomously concerning Topic 1: 20%
Problems solved autonomously concerning Topic 2-3: 25%
Problems solved autonomously concerning Topic 4: 15%
Problems solved autonomously concerning Topic 6: 10%
Laboratory reports 30%
Reevaluation tasks will not be performed.

EXAMINATION RULES.

Problems will be performed individually
Laboratory reports will be performed in group.

BIBLIOGRAPHY

Basic:
- Giacovazzo, C., Monaco, H.L., Viterbo, D., Scordari, F., Gilli G., Zanotti, G., Catti, M. . Fundamentals of Crystallography. Bath (Gran Bretanya): Oxford University Press, 1995. ISBN 0198555792.
- Cuevas-Diarte, Miquel Àngel; Oonk, Harry A. J.. Molecular mixed crystals [on line]. Switzerland: Springer, 2021 [Consultation: 19/10/2021]. Available on: https://ebookcentral.proquest.com/lib/upcatalunya-ebooks/detail.action?docID=6629023. ISBN 9783030687274.
- Papon, P.; Leblond, J; Meijer, P.H.E. Physique des transitions de phases : concepts et applications : cours avec exercices corrigés. 2e éd. Paris: Dunod, 2002. ISBN 2100065513.
- Descamps, M. Disordered pharmaceutical materials [on line]. Lille (France): Wiley-VCH, 2016 [Consultation: 19/10/2021]. Available on: https://onlinelibrary-wiley-com/doi/book/10.1002/9783527652693. ISBN 9783527652693.
- Ashcroft, N.W.; Mermin, N. D.; Wei, D. Solid state physics. Singapore: Cengage Learning, 2016. ISBN 9789814369893.

Complementary:
- Saleh, B.E. A; Teich, M.C. Fundamentals of photonics. 3rd ed. Hoboken: John Wiley & Sons, 2019. ISBN 9781119506874.

RESOURCES

Other resources:
Information about Crystallography:
https://www.ccdc.cam.ac.uk/solutions/csd-core/components/csd/
https://www.cryst.ehu.es/