ANX-PR/CL/001-01

LEARNING GUIDE

SUBJECT

93001316 - Computational Laboratory Of Photovoltaic Materials

DEGREE PROGRAMME

09BP - Master Universitario En Energia Solar Fotovoltaica

ACADEMIC YEAR & SEMESTER

2022/23 - Semester 2

Index

Learning guide

1. Description

1.1. Subject details

Name of the subject	93001316 - Computational Laboratory Of Photovoltaic Materials
No of credits	3 ECTS
Type	Optional
Academic year ot the programme	First year
Semester of tuition	Semester 2
Tuition period	February-June
Tuition languages	English
Degree programme	09BP - Master Universitario en Energia Solar Fotovoltaica
Centre	09 - Escuela Tecnica Superior De Ingenieros De Telecomunicacion
Academic year	2022-23

2. Faculty

2.1. Faculty members with subject teaching role

Name and surname	Office/Room	Email	Tutoring hours *
Pablo Sanchez-Palencia Vallejo	A-034	p.sanchez-palencia@upm.es	Sin horario.
Pablo Palacios Clemente (Subject coordinator)	A-034	pablo.palacios@upm.es	Sin horario.
Gregorio Jose Garcia Moreno	A-034	g.garcia@upm.es	Sin horario.

* The tutoring schedule is indicative and subject to possible changes. Please check tutoring times with the faculty member in charge.

3. Skills and learning outcomes *

3.1. Skills to be learned

CB10 - 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.

CB6 - Poseer y comprender conocimientos que aporten una base u oportunidad de ser originales en el desarrollo y/o aplicación de ideas, a menudo en un contexto de investigación

CB7 - 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 - 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 juicios

CE2 - Conocimiento, anÃ¡lisis y propuestas de nuevos conceptos, mÃ©todos o dispositivos para la conversiÃ³n fotovoltaica.

CE6 - Aplicar metodologÃas de diseÃ±o e implementaciÃ³n de tÃ©cnicas de aprendizaje y clasificaciÃ³n automÃ¡ticos para una gestiÃ³n inteligente del conocimiento

CG5 - GestiÃ³n de la informaciÃ³n: buscar y gestionar recursos bibliogrÃ¡ficos adecuados con eficiencia, aprender a continuar los estudios de manera ampliamente autÃ³noma como base para la futura actividad de investigaciÃ³n e innovaciÃ³n

CG7 - Trabajo en contextos internacionales: Llevar a cabo un proceso sustancial de investigaciÃ³n con seriedad e integridad acadÃ©micas, integrado en un grupo de I+D+i con proyecciÃ³n internacional

CG8 - Aplicar metodologÃas, procedimientos, herramientas y normas del estado del arte para la creaciÃ³n de nuevos componentes tecnolÃ³gicos; Construir nuevas hipÃ³tesis y modelos, evaluarlos y aplicarlos a la resoluciÃ³n de problemas

CG9 - Comunicar juicios, y conocimientos a audiencias especializadas y no especializadas, de una manera razonada, clara y sin ambigÃ¿edades

CT3 - Uso de la lengua inglesa: comprender los contenidos de clases magistrales, conferencias y seminarios en lengua inglesa; redactar en inglÃ©s informes y artÃculos cientÃfico-tÃ©cnicos usando herramientas informÃ¡ticas; realizar exposiciones pÃºblicas en inglÃ©s de trabajos, resultados y conclusiones de investigaciÃ³n, por ejemplo, en las asignaturas del MÃ¡ster o en congresos de carÃ¡cter mayoritariamente internacional o en estancias en centros extranjeros, todo ello con la ayuda de medios informÃ¡ticos audiovisuales

3.2. Learning outcomes

RA32 - RA24 - Formación en los aspectos teóricos y prácticos del diseño usando primeros principios

RA31 - RA25 - Capacidad de relacionar los resultados con la aplicación a materiales fotovoltaicos

* The Learning Guides should reflect the Skills and Learning Outcomes in the same way as indicated in the Degree Verification Memory. For this reason, they have not been translated into English and appear in Spanish.

4. Brief description of the subject and syllabus

4.1. Brief description of the subject

Introduction to material properties from a computational and simulation point of view using first principles. Use of free distribution programs that allow the design and characterization of system properties (Molecules, Surfaces and Bulks)

Classes and practices will be taught in English and Spanish. Documentation in Spanish and English. Work and projects may be submitted in Spanish or English

The objective is to train students in the theoretical and practical aspects of first principles material design and focused in materials used as solar cells.

Theoretical and mainly practices classes will be taught. In practices clasess we will use free simulation programs. The theoretical classes will give an approach to the theoretical models on which these programs are based. Students will receive different examples of the different theoretical approaches that exist and the degree of accuracy of each of them. They will be recive exercise problems that they can perform on their own with the free distribution programs and the results will be analyzed in the practical classes where they will perform more complex exercises under the guidance of the teachers.

4.2. Syllabus

1. I. Introduction to theoretical methodologies for the study of materials

2. II. Use and learning of computer programs

3. III. Theoretical calculation of molecules: Organic solar cells

4. IV. Simulation of bulk materials in solar cells

5. V. Simulation of hybrid materials in solar cells

6. VI. Semiconductor applications: Silicon, III-V, new materials. Structural and defect characterization, band spectrum, optical absorptions, etc.

5. Schedule

5.1. Subject schedule*

Week	Classroom activities	Laboratory activities	Distant / On-line	Assessment activities
1	**I. Introduction to theoretical methodologies** Duration: 02:00			
2	**I. Introduction to theoretical methodologies.** Duration: 01:00	**I. Introduction to theoretical methodologies** Duration: 01:00		
3	**II. Use and learning of computer programs** Duration: 01:00	**II. Use and learning of computer programs** Duration: 01:00		
4		**II. Use and learning of computer programs** Duration: 02:00		
5		**II. Use and learning of computer programs** Duration: 02:00		
6				**Theme I. and II. evaluation** Continuous assessment Presential Duration: 02:00
7	**III. Theoretical calculation of molecules** Duration: 02:00			
8		**III.Theoretical calculations of molecules** Duration: 02:00		
9	**IV. Simulation of bulk materials** Duration: 01:00	**IV.Simulation of bulk materials** Duration: 01:00		
10	**V.Simulation of hybrid materials** Duration: 01:00	**V.Simulation of hybrid materials** Duration: 01:00		
11				**Theme III. and IV. evaluation** Continuous assessment Presential Duration: 01:00

12		**V.Simulation of hybrid materials** Duration: 02:00		
13	**VI. Semiconductor applications: Si, III-V, new materials.** Duration: 02:00			
14	**VI. Structural and defect characterization, band sprectrum, optical absorptions, etc.** Duration: 01:00	**VI. Structural and defect characterization, band sprectrum, optical absorptions, etc.** Duration: 01:00		
15		**VI. Structural and defect characterization, band sprectrum, optical absorptions, etc.** Duration: 02:00		
16				**Individual Workbooks collection** Continuous assessment Presential Duration: 00:30 **Theme V. and VI. evaluation** Continuous assessment Presential Duration: 01:00
17				**Presentation of work about an interest materials similar to the studied in themes III to VI.** Final examination Presential Duration: 01:00

Depending on the programme study plan, total values will be calculated according to the ECTS credit unit as 26/27 hours of student face-to-face contact and independent study time.

* The schedule is based on an a priori planning of the subject; it might be modified during the academic year, especially considering the COVID19 evolution.

6. Activities and assessment criteria

6.1. Assessment activities

6.1.1. Assessment

Week	Description	Modality	Type	Duration	Weight	Minimum grade	Evaluated skills
6	Theme I. and II. evaluation		Face-to-face	02:00	20%	0 / 10	CE2 CG8 CG5 CT3
11	Theme III. and IV. evaluation		Face-to-face	01:00	20%	0 / 10	CB10 CG9 CB6 CB8 CT3 CE6 CG7 CB7
16	Individual Workbooks collection		Face-to-face	00:30	40%	0 / 10	CG3 CG5 CT3 CE6 CG7 CG8
16	Theme V. and VI. evaluation		Face-to-face	01:00	20%	0 / 10	CB10 CG9 CB6 CB8 CT3 CG7 CB7

6.1.2. Global examination

Week	Description	Modality	Type	Duration	Weight	Minimum grade	Evaluated skills
17	Presentation of work about an interest materials similar to the studied in themes III to VI.		Face-to-face	01:00	100%	0 / 10	CB10 CG3 CG5 CG9 CB6 CB8 CT3 CE2 CE6 CG7

							CG8 CB7

6.1.3. Referred (re-sit) examination

Description	Modality	Type	Duration	Weight	Minimum grade	Evaluated skills
Presentation of work about an interest materials similar to the studied in themes III to VI.		Face-to-face	01:00	100%	0 / 10	CB10 CG3 CG5 CG9 CB6 CB8 CT3 CE2 CE6 CG7 CG8 CB7

6.2. Assessment criteria

Students will have to make a laboratory workbook in which the carried out practices and the results obtained are described. (40%)

They will also have to make presentations about what they have learned in the practices. (60%)

7. Teaching resources

7.1. Teaching resources for the subject

Name	Type	Notes
Introduction to solid state physics	Bibliography	C. Kittel, Ed. Wiley, 8th ed., 2013
Basic Semiconductor Physics	Bibliography	C. Hamaguchi, Springer 2001
Electronic Structure, Basic Theory and Practical Method	Bibliography	R. M. Martin, Cambridge, 2005
Calculation codes	Others	Manuals of the programs
Research papers	Web resource	Papers related with the subject themes

8. Other information

8.1. Other information about the subject

The subject has been designed for a preferably face-to-face teaching.

Communication:

Face-to-face communication with the teacher will be carried out in the teacher's office during the hours of tutoring by previous appointment.

Communication with the teacher electronically will preferably be carried out using the e- mail .

Teachers will respond to students within 48 hours

Change of modality for health reasons:

In case of need for health reasons, all teaching activities in the classroom and evaluation programmed as face-to-face would take place online.