



INTERNATIONAL  
CAMPUS OF  
EXCELLENCE

COORDINATION PROCESS OF  
LEARNING ACTIVITIES  
PR/CL/001



E.T.S. de Ingenieros de  
Telecomunicación

# 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

2023/24 - Semester 2

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## 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 of 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	2023-24

## 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.

\* 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, análisis y propuestas de nuevos conceptos, mediante dispositivos para la conversión fotovoltaica.

CE6 - Aplicar metodologías de diseño e implementación de técnicas de aprendizaje y clasificación automática para una gestión inteligente del conocimiento

CG5 - Gestión de la información: buscar y gestionar recursos bibliográficos adecuados con eficiencia, aprender a continuar los estudios de manera ampliamente autónoma como base para la futura actividad de investigación e innovación

CG7 - Trabajo en contextos internacionales: Llevar a cabo un proceso sustancial de investigación con seriedad e integridad académicas, integrado en un grupo de I+D+i con proyección internacional

CG8 - Aplicar metodologías, procedimientos, herramientas y normas del estado del arte para la creación de nuevos componentes tecnológicos; Construir nuevas hipótesis y modelos, evaluarlos y aplicarlos a la resolución de problemas

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

CT3 - Uso de la lengua inglesa: comprender los contenidos de clases magistrales, conferencias y seminarios en lengua inglesa; redactar en inglés informes y artículos científicos usando herramientas informáticas; realizar exposiciones públicas en inglés de trabajos, resultados y conclusiones de investigación, por ejemplo, en las asignaturas del Máster o en congresos de carácter mayoritariamente internacional o en estancias en centros extranjeros, todo ello con la ayuda de medios informáticos 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

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### 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 classes 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 receive 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

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### 5.1. Subject schedule\*

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

12		V. Simulation of hybrid materials Duration: 02:00 Laboratory assignments		
13	VI. Semiconductor applications: Si, III-V, new materials. Duration: 02:00 Lecture			
14	VI. Structural and defect characterization, band spectrum, optical absorptions, etc. Duration: 01:00 Lecture	VI. Structural and defect characterization, band spectrum, optical absorptions, etc. Duration: 01:00 Laboratory assignments		
15		VI. Structural and defect characterization, band spectrum, optical absorptions, etc. Duration: 02:00 Laboratory assignments		
16				Individual Workbooks collection Individual work Continuous assessment Presential Duration: 00:30  Theme V. and VI. evaluation Group presentation Continuous assessment Presential Duration: 01:00
17				Presentation of work about an interest materials similar to the studied in themes III to VI. Individual work 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	Individual presentation	Face-to-face	02:00	20%	0 / 10	CE2 CG8 CG5 CT3
11	Theme III. and IV. evaluation	Group presentation	Face-to-face	01:00	20%	0 / 10	CB10 CG9 CB6 CB8 CT3 CE6 CG7 CB7
16	Individual Workbooks collection	Individual work	Face-to-face	00:30	40%	0 / 10	CG3 CG5 CT3 CE6 CG7 CG8
16	Theme V. and VI. evaluation	Group presentation	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.	Individual work	Face-to-face	01:00	100%	0 / 10	CB10 CG3 CG5 CG9 CB6 CB8 CT3 CE2 CE6 CG7

						CG8 CB7
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### 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.	Individual work	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.