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| Subject | COMPUTATIONAL LABORATORY OF PHOTOVOLTAIC MATERIALS |
| Credits | 3 ECTS (1T+2P) |
| Character | Elective |
| Semester | 2nd |
| Language | English |

## Competences

CG3 - Creativity: To conceive, develop and validate new systems that can increase the quality of life of people; to carry out, inacademic and professional contexts, innovations or technological advances that can advance the state of the art.

CG5 - Information management: to search for and manage appropriate bibliographic resources efficiently, to learn to continue studies in a largelyautonomous way as a basis for future research and innovation activity.

CG7 - Work in international contexts: To carry out asubstantial research process with academic seriousness and integrity, integrated in an R+D+i group with international projection.

CG8 - Apply methodologies,procedures, tools and state-of-the-art standards for the creation of new technological components; build new hypotheses andmodels, evaluate them and apply them to problem solving.

CG9 - Communicate judgments and knowledge to specialized and non-specialized audiences in a reasoned, clear and unambiguous manner.

CB6 - Possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context

CB7 - Students should be able to apply their acquired knowledge and problem-solving skills in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their area of study.

CB8 - Students are able to integrate knowledge and face the complexity of making judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities related to the application of their knowledge and judgments.

CB10 - That students possess the learning skills that will enable them to continue studying in a manner that will be largely self-directed or autonomous..

CT3 - Use of the English language: understand the contents of lectures, conferences and seminars in English; write reports and scientific-technical articles in English using computer tools; make public presentations in English of research work, results and conclusions,for example, in the subjects of the Master or in congresses of a mostly international nature or in stays in foreign centers, all with thehelp of audiovisual computer media

CE2 - Knowledge, analysis and proposals of new concepts, methods or devices for photovoltaic conversion.

CE6 - Apply design methodologies and implementation of automatic learning and classification techniquesfor intelligent knowledge management.

## Outcomes

RA04 - Ability to analyze results

RA05 - Relating basic principles to practical aspects

RA06 - Training in the theoretical and practical aspects of design using "first principles".

RA36 - Knowledge of the physical effects that enable the use of solar energy

RA38 - Applied training in materials physics

RA56 - Training in quantum physics and thermodynamics as applied to solar cells

## Description and syllabus

Introduction to material properties from a computational and simulation point of view using first principles. Use of freely available programs that allow the design and characterization of system properties (Molecular, Chains, Surfaces and Volume). The objective is to train students in the theoretical and practical aspects of first principles design of materials used in the fabrication of various types of solar cells.

This course is divided into lectures and practicals using freely available simulation software. The lectures provide an introduction to the theoretical models on which these programs are based. The students will receive different examples of the different theoretical approaches that exist and the degree of accuracy of each one of them. They will be given exercises that they can carry out on their own with the freely distributed programs and the results will be analyzed in the practical classes where they will carry out more complex exercises under the guidance of the professors.

Schematically, the syllabus includes:

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

II. Use and learning of computer programs

III. Theoretical calculation of molecules: Organic solar cells.

IV. Simulation of hybrid materials in solar cells.

V. Simulation of volumetric materials in solar cells.

VI. Applications to semiconductors: Si, III-V, new materials. Structural and defect characterization of their band spectra, absorptions, etc.