Course Title	Course Code	Number of Study Hours				Year	Level	Prerequisites
		Theo.	Lab.	Credit	ECTS			
Computational Physics	PHYS610	2	2	3	11	1st/ 2nd	2nd/ 3rd	-

Student's workload			
In-class activities	Contact Hours	Self-learning/study	Hours
Lectures	30	Preparation for classes	90
Laboratory	30	Case studies	-
Exams and quizzes	5	Working on lab experiment	126
Lab demo	-	HW/Assignments	12
		Study for exam	25
Total	65	Total	253
Total Learning Hours = 318		Equivalent ECTS points = Total LH/28 = 11	

BRIEF COURSE DESCRIPTION

- The course is designed to use the computer as a powerful tool to solve and understand some physical problems as well as in other related fields using both numerical methods. Numerical methods such as Fortran language and MATLAB software will be applied. Also, the simulation and modeling programs (as free NWChem package and free Hyper Chem modeler) are used to model, and predict the properties of real materials at different energy levels: Density-functional theory, Hartree-Fock, Monte Carlo sampling and molecular dynamics simulations.

COURSE OBJECTIVES

The main objectives of this course are focused on the following:

1. Investigate some physical phenomena using numerical program language such as Fortran language.
2. Investigate some physical phenomena using numerical program software such as MATLAB software.
3. Apply modeling program to solve some physical problems.
4. Apply simulation program to solve some physical problems.
5. Obtain and Predict properties of some real materials.

COURSE CONTENTS

- **Theoretical part**
- Review on basic numerical methods; Interpolation and extrapolation, numerical integration and differentiation, Random numbers, Ordinary differential equations.
- Introduction to numerical methods (Fortran language and MATLAB software).
- Introduction to modelling and simulation programs (as free NWChem and free Hyper Chem modeler).
- **Simulation part**
- Apply numerical methods (Fortran language and MATLAB software) to solve some physical problems such as non-linear equation, eigenvalues problems and ordinary differential equation.
- Apply modeling and simulation programs (as free NWChem package and free Hyper Chem modeler) at different levels of theories (Density-functional theory, Hartree- Fock, Monte Carlo and Molecular dynamics simulations) to obtain some physical properties as energy gap, transition states, density of states.

ASSESSMENT CRITERIA

- Mid -Term exam and Quizzes: 20 %
- Assignments and classroom activities: 10%
- Laboratory Work: 20%
- Final Exam: 50%

COURSE TEACHING STRATEGIES

- Lectures, Discussion, Tutorial, Expository and Discovery, and Interactive Discussions.

TEXT BOOK

- B. A. Stickler and E. Schachinger, Basic Concepts in Computational Physics, 2ndedition, (Springer 2016).

REFERENCE BOOKS

- J. M. Thijssen, Computational Physics, 2nd edition, (Cambridge University Press, 2007).
- W. H. Press et. al., Numerical Recipes, The Art of Scientific Computing, 3rd edition, (Cambridge University Press, 2007)
- H. Gould, J. Tobocnik, and W. Christian, Introduction to Computer Simulation Methods, (Addison Wesley 2007).