Course: NUMERICAL MODELING OF MATERIALS AND SOLID STATE PHYSICS	**Teaching Language:** English	
SSD (Subject Areas): Module 1: CHEM-04/A Module 2: PHYS-04/A		**CREDITS:** **12** Module 1: NUMERICAL MODELING OF MATERIALS 6 credits
		Module 2: SOLID STATE PHYSICS 6 credits
Course year: I	**Type of Educational Activity: C**	
Teaching Methods: In person		

Contents extracted from the SSD declaratory consistent with the training objectives of the course:

Module 1:

The disciplinary scientific sector is interested in scientific and educational - training activities in the field of science and technology for the sustainable industrial development of products, materials, chemicals processes and energy, through the definition of the principles and the study of thermodynamic, kinetic, catalytic and technological aspects related to them. The sector deals also with the chemical and technological properties of polymeric materials, their characterization and the understanding of relationships between structure and properties of polymeric materials.

In this frame, the course gives an introduction to numerical simulations methods aimed to understand the behaviour, the relationship between structure and properties and the thermodynamic properties of materials with special emphasis of polymeric and more in general soft materials. The main numerical techniques related to molecular simulations methods will be introduced. A list of the main topics is reported below:

-Introduction to thermodynamics and to the main features of polymeric materials
-Basics of Statistical Mechanics for Molecular Simulations
-Introduction to Molecular Simulations
-Molecular Dynamics and Monte-Carlo
-Force Fields
-Hands on Tutorials
-Some example applications
-Coarse-Graining Models

Module 2:

Research activities characterize the scientific-disciplinary sector scientific and educational-training regarding theoretical investigation e computational knowledge of dynamic, thermodynamic and statistical phenomena of matter in all its states of aggregation, in conditions of equilibrium and non-equilibrium; the treatment of the properties of propagation and interaction of radiation and particle beams with matter; the knowledge necessary for the development of models theoretical, mathematical methods and numerical techniques, including first-principles and multiscale simulations; the study of aspects mathematical physicists of artificial intelligence and the development of algorithms of machine learning motivated by physics problems of the matter with its related applications, even in different fields interdisciplinary. The skills of the sector concern: mechanics quantum theory and its foundations, quantum information and computation quantum physics, classical and quantum statistical mechanics, phenomena critical and phase transitions, atomic and molecular physics, states liquid and solid, metallic, magnetic and strongly correlated systems, semiconductors and insulators, macroscopic quantum states, disordered systems, materials science, low systems dimensionality, nanosciences and nanotechnologies, conversion and energy storage, thermomechanical properties, been diluted, gases, plasmas, as well as soft matter, active and biological. The sector's activities also include the theoretical study of acoustics, classical and quantum optics, photonics, quantum electronics and optoelectronics, quantum technologies, open systems, statistical, quantum and topological properties of matter, as well as non-linear physics, statistics and complex systems. Finally, sector expertise includes development of teaching and learning methodologies of matter physics, quantum mechanics, statistical mechanics, and their applications. In addition to that relating to the specialist disciplines congruent with this declaration, the teaching activity of those belonging to the sector extends to all institutional aspects relating to the teaching of general physics and basic classical and quantum physics, with the exception of experimental physics laboratory courses.

Objectives:

Module 1:

The student will be familiar with the main techniques utilized in the field of molecular simulations and will have the basis to choose appropriate description of soft materials using these techniques.

Module 2:

Fundamental aspects of solid-state physics. Phenomenological and microscopic description of metals and semiconductors. Transport, thermodynamic and dielectric properties of solids.

Propaedeuticities:

Is a propaedeuticity for:

Types of examinations and other tests:

Report of a project and its oral presentation/Written and oral examination.