Universidad Carlos III de Madrid

COURSE: SIMULATION TECHNIQUES IN MATERIALS		
MÁSTER: MASTER IN MATERIALS SCIENCE AND ENGINEERING **Professors: Jon Molina Aldareguia / Lucas Viani**	**ECTS: 3**	**TERM: 2**

WEEKLY PLANING								
WEEK	**LECTURE**	**DESCRIPTION**	**GROUPS (mark X)**		**SPECIAL ROOM FOR SESSION (Computer class room, audio-visual class room)**	**WEEKLY PROGRAMMING FOR STUDENT**		
			1	**2**		**DESCRIPTION**	**CLASS HOURS**	HOMEWORK HOURS (Max. 7h week)
1	1	**1. Introduction to simulation in materials science and engineering.** 1.1. Principles of integrated computational materials engineering (ICME) 1.2 Scales in the structure and behavior of materials 1.3 Simulation techniques at the atomic scale 1.4 Simulation techniques at the mesoscale 1.5 Simulation techniques at the continuum scale 1.6 Multiscale simulations 1.7 Application examples in materials engineering				Review of contents delivered in class	1.5	2
	2	**Part 1**: **Introduction to atomistic simulations , including Monte Carlo and Molecular Dynamics** 2. Introduction to atomistic simulations 2.1 Computational methods 2.2 Quantum vs. Classical Mechanics. 2.3 QM/MM method. 2.3 Finite systems and periodic boundary conditions.				Review of contents delivered in class	1.5	2
2	3	3. Monte Carlo methods and applications in materials engineering. 4. Molecular mechanics 4.1 Interatomic and molecular potentials 4.2 Geometry optimization				Review of contents delivered in class	1.5	2

	4	5. Molecular dynamics: 5.1 Integration of the equations of motion 5.2 Temperature and pressure control, neighbors, etc. 5.3 Determination of physical properties.				Review of contents delivered in class		2
3	5	6. Introduction to computational thermodynamics 6.1. Thermodynamics. Gibbs free energy and models 6.2. Phase equilibrium in heterogenous media 6.3. Experimental data for thermodynamics modelling 6.4. CALPHAD method 6.5. Case study and examples				Review of contents delivered in class	1.5	2
	6	**Computer practice**: Evaluation of the energy of a solid			Computer Lab	Analysis of computer practice. Evaluation report	1.5	4
4	7	**Computer practice**: Setting up a MD simulation: volume generation, geometry optimization, temperature, etc.			Computer Lab	Analysis of computer practice.	1.5	3
	8	**Computer practice**: Case study in MD: melting of a solid.			Computer Lab	Analysis of computer practice. Evaluation report	1.5	4
5	9	**Part 2**: **Introduction to continuum micromechanics** 6. Introduction. 6.1 Mean field approaches.				Review of contents delivered in class	1.5	2
	10	6.2 Bounding methods 6.3. Periodic microfield approaches 6.4. RVEs				Review of contents delivered in class	1.5	2
6	11	**Computer practice**. Setting up a RVE in a finite element model: geometry, meshing, boundary conditions, material properties. Composites.			Computer Lab	Analysis of computer practice. Evaluation report	1.5	3

	12	7. Numerical solving methods. Introduction to the finite element method. Principles. Spatial discretization and numerical integration. Time discretization. Boundary conditions.				Review of contents delivered in class	1.5	2
7	13	**Computer practice**. Elastic properties of composite materials. Comparison with homogenization theories.			Computer Lab	Analysis of computer practice. Evaluation report	1.5	3
	14	**Computer practice**. Plastic properties. Local stress fields.			Computer Lab	Analysis of computer practice. Evaluation report. Preparation of final exam.	1.5	4
TOTAL HOURS							21	37