Erasmus Mundus Joint Master GREENANO

SYLLABUS

Semester 2

COURSE NAME:	**Nanoscale Materials Modelling**
HOSTING UNIVERSITY:	Tor Vergata University of Rome

SEMESTER:	**NUMBER OF ECTS:**	**PILLAR:**
2	6	1

DISTRIBUTION OF HOURS

Lectures	*Seminars*	*Lab work*	*Individual student work*
20	2	24	104 (including 20 hrs project)

PROFESSOR:	Dr. Conor Hogan
LEARNING AND TEACHING METHODS:	The course will be delivered in three parts: 1. Formal instruction on fundamental theory will be conducted through classroom lectures using computer-prepared slides integrated by on-board explanations; 2. Practical laboratories will consist of exercises using open-source codes focused on nanoscale systems and experimental simulations of relevance to other GREENANO courses; exercises will be prepared on a wiki to allow self-paced tutoring 3. A loosely-supervised practical project carried out by each student independently.
PREREQUISITES:	Basic principles in solid state physics and organic chemistry: (a) fundamentals of quantum mechanics; Bloch theorem, crystals, band structure, Born-Oppenheimer approximation, magnetism; (should be provided in 1st Semester Solid State Physics) (b) atomic orbitals and hybridization, Lewis structures; (provided when? Other TV courses also request basic chemistry) (c) basic surface physics and chemistry; surface reconstructions (should be provided at start of 2nd Semester) Students must possess a notebook with adequate computational power to install and run the practical labs via virtual machine.
OBJECTIVES OF THE COURSE:	1. Provide the student with a solid theoretical basis in first principles materials modeling, in particular in density functional theory and molecular dynamics 2. Provide students with practical skills in using diverse atomistic software (quantum-ESPRESSO, Orca, Gromacs) for treating nanoscale systems of different physical and chemical character, dimension, and scale, including those studied in the other 2nd Semester courses; 3. Enable students to simulate selected experimental probes relevant to GREENANO and interpret the results 4. Introduce students to modern initiatives and methods in computational material science

CONTENT OF THE COURSE:	**Theory lectures (20 hours + assessment)** 1. Introduction to atomistic computational material science: atomistic methods (TB/DFT/QC) vs multiscale approaches, modern initiatives (high-throughput, genetic algorithms, crystal structure prediction, online databases) 2. Fundamentals of density functional theory: Hohenberg Kohn theorem; Kohn-Sham equations; XC potential, LDA, GGA, meta-GGA, hybrids; Hartree-Fock and overview of quantum chemistry methods 3. DFT in practice: crystal representation; plane waves and Gaussian orbital schemes; pseudopotentials; energetics (IE/EA/WF); supercells for defects, surfaces, and molecules; 4. Geometrical optimization: forces; Hellmann-Feynmann theorem; vdW interactions; transition state theory; 5. Electronic and optical properties: KS eigenvalues, gap problem in DFT, band structure, DOS/LDOS, linear response 6. Classical molecular dynamics for biophysical applications **Seminars (2 hours)** GREENANO@Tor Vergata special topics (invited lectures): from STM/STS, XPS, Raman, NEXAFS/XANES, etc; **Practical (lab) lessons (24 hrs)** 1. Unix for comp. mat. sci (basics + bash scripting; parallel/cluster usage) [4-6 hrs] 2. Quantum-ESPRESSO: Basic concepts for tackling molecules, nanostructures, and 3D systems; convergence testing [6 hrs] 3. QE & ORCA (quantum chemistry): Focus on Organic molecules: energy levels, binding energy, dipoles, orbital projections, Bader charges, chemical reactions [4 hrs] 4. QE: Focus on carbon based 1D/2D systems: electronic properties, phase transitions; [2 hrs] 5. QE: Surface/interfaces: adsorption, diffusion, thermodynamics, reflectivity [2-4 hrs] 6. GROMACS (molecular dynamics) [4-6 hrs] **Project work (10-20 hrs, loose supervision, + assessment)** Semi-independent case-work connected to GREENANO topics, e.g. Molecular self-assembly; Carbon nanowires/nanotubes; Microscopy/spectroscopy of a relevant surface; molecular dynamics for bioplastics/sensors/epitaxial growth
INTENDED LEARNING OUTCOMES:	Following completion of this course, the student should be able to: 1. identify the optimal and appropriate approach for treating a nanoscale system of interest to the wider GREENANO using atomistic computational methods; 2. perform quantitatively correct simulations of real-world experiments and be able to identify appropriate technical and physical approximations for tackling challenging systems 3. understand the underlying physical and chemical concepts and methodologies
FORM OF ASSESSMENT:	Each student will be required to carry out a loosely-supervised computational investigation of a system or technique of relevance to the wider GREENANO objectives, and present the results in a “mini-thesis” and oral presentation; Fundamentals will be evaluated via an oral examination.