5CI209	***Multiscale Modeling of complex molecular systems*** Keywords : ***Link between theory and experiment, Molecular simulations, Mesoscopic simulations***								
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ECTS 6	*Cours* 30	*TD* 10	*TP* 4	*Tutorat* 16	*Ecrit* 40	*CC* 30	*TP*	*Oral* 30	*Eval. répartie* non

Description of the coursee

The aim of this course is to present the various possible levels of description of a physico-chemical system, be it a biological medium, a complex liquid or a material of industrial or environmental interest. Each description of a phenomenon at one scale will be related to the other scales. On this basis, the various analytical or numerical methods for modeling complex molecular systems will be covered for these different scales, from the atom to the continuous medium.
The course is aimed both at students interested in theoretical aspects and at students from a wide range of backgrounds who wish to use simulations to interpret experimental results.

Learning objectives

At the end of this course, students will be able to:

- Find their way around the different worlds - microscopic, mesoscopic and macroscopic - in order to determine which theoretical approach to use for a given experimental problem.
- Analyze a chemical system and choose an appropriate level of description for simulation.
- Compare the advantages and disadvantages of molecular simulation methods.
- Implement a simple machine-learning method
- Relate macroscopic phenomena to their microscopic origin

Prerequisites

Thermochemistry, kinetics and electrochemistry:

- First and second principles
- Free enthalpy of reaction
- Laws of diffusion
- Transition state

Point mechanics

- Newton's equation
- Kinetic energy, potential energy and mechanical energy

Fundamentals of statistical equilibrium mechanics :

- Microscopic definition of entropy, entropy and free energy, partition functions.
- Intermolecular interactions.

Language	*Course, TD, TP*	*Documents*	*Bibliographie*
	English	English	English

How the EU operates

The course consists of lectures and tutorials. The aim of the tutorial is to study a few articles describing an application of simulation to a physico-chemical problem. These articles are chosen by the teachers to introduce a simulation method not seen in class. The aim is to understand this technique so as to be in a position to explain it to the rest of the group, and then to illustrate its value in understanding a problem. This tutorial will result in a five-page report and a 20-minute oral presentation.

The themes covered in the course are

I- General introduction (Teacher: Rodolphe Vuilleumier)

1. Scales

Different length and time scales, orders of magnitude, links with different experimental approaches to physical chemistry.

2. Statistical mechanics

Fundamental principles, statistical sets, fluctuations and response coefficients.

II- Microscopic modeling: statistical mechanics of liquids (Teacher: Rodolphe Vuilleumier and Jean-Philip Piquemal)

1. Molecular modeling

a) Principles of molecular dynamics, periodic edge conditions

b) Force fields

Intermolecular and intramolecular terms, treatment of coulombic forces, Ewald sums

c) Verlet algorithm for molecular dynamics

d) Monte-Carlo and Metropolis methods

Principle and demonstration, transition probability calculation.

e) Ab initio molecular dynamics, hybrid QM/MM methods, advanced algorithms for simulations

2. Fluctuations and linear response

a) Average quantities and fluctuations, correlation functions, Brownian motion, size effects at the nanoscale

b) Temporal response to mechanical perturbation

Response function, impulse response, relaxation, response to sinusoidal disturbance, Susceptibility

c) Expression of the response function within the framework of statistical mechanics

Correlation functions, fluctuation-dissipation theorem

d) Response to a thermal disturbance - Transport coefficients

Diffusion and viscosity coefficients, link with mesoscopic and hydrodynamic descriptions

3. Reactivity

a) Mean force potentials

b) Free energy of reaction: thermodynamic integration

c) Free energy surfaces, order parameters, Landau free energy

d) Advanced free energy surface exploration methods

III- Dimensional reduction in physicochemical simulations (Teacher: Guillaume Jeanmairet)

1. Interest and examples

Classical examples of reduction in the number of degrees of freedom: coarse-grained electrolyte models, continuous solvent model, reaction coordinates, mechanistic reduction.

2. Reminders of statistical physics and effective potential

Notions of mean force and mean force potential. Factorization of the partition function. Practical application

3. Coarse-grain models for electrolytes.

Debye-Hückel and Poisson-Boltzmann theory.

4. Coarse-grain models for biochemistry.

General presentation. Historical approach. Physical and knowledge-based models. MARTINI and ROSETTA models: principles, applications, limitations.

5. Integral equation theory, continuous solvent model and classical DFT

1) Presentation of the Ornstein-Zernike equation and the main closure relations.

2) Interest. Presentation of an example using the polarizable continuum model. A more advanced model: 3DRISM.

3) Introduction to classical DFT. Demonstration of the variational principle for high potential and density. Construction of the excess functional from direct correlation functions.

4) Current approximations to the excess functional: homogeneous reference fluid approximation and Fundamental Measure Theory.

IV- Macroscopic modeling (Teacher: Benjamin Rotenberg)

1. Hydrodynamics

a) Reminders

Macroscopic description of a fluid, conservation of matter and momentum, hydrodynamic regimes, Poiseuille flow, Couette cell

b) Hydrodynamic effects on a solute

Frictional forces, hydrodynamic interactions

c) Microscopic approach

Green-Kubo formula for viscosity, notions of kinetic theory, "long-time tails" of correlation functions

d) Simulation methods for hydrodynamics

Computational Fluid Dynamics, molecular simulations, coarse-grained simulations (Dissipative Particle Dynamics), multiparticle Collision Dynamics (Stochastic Rotation Dynamics), lattice models: Lattice-Boltzmann, continuous solvent models.

2. Electrokinetic phenomena

a) Classification

Definition, electro-osmosis, electrophoresis, flow potential, sedimentation potential

b) Electro-osmosis

Microscopic origin, Helmholtz-Smoluchowski theory

c) Electrophoresis

Limit of small double layers and general case

d) Flow potential

V- Introduction to Machine Learning methods for molecular simulations (Teacher: Arthur France-Lanord)

This part is accompanied by 4h of computer science practical work

1. Introduction. Supervised and unsupervised learning
2. Artificial neural networks
3. Interatomic potentials using machine learning