MU5CI359	**Statistical Mechanics and Simulations for Chemical and Biochemical Systems** Keywords: statistical mechanics, theoretical chemistry, numerical simulations
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ECTS	*Cours*	*TD*	*TP*	*Tutorat*	*Ecrit*	*CC*	*TP*	*Oral*	*Eval. répartie*
6	20h	12h		12h	50%	20%	30%		

Descriptif de l'UE:

This course is aimed at both experimentalists and theoreticians. Its main focus is the molecular description of the dynamics of complex chemical and biochemical systems. It will cover both fundamental theoretical concepts in statistical mechanics and numerical simulation methods. Their applications to a broad range of questions and systems will be discussed, ranging from chemical kinetics and diffusion to vibrational spectroscopy, biomolecular conformational dynamics and protein folding.

The course includes a simulation project which will provide students with an opportunity to apply the concepts and the tools presented in class by performing molecular dynamics simulations and analyzing the trajectories. This project is tutored and the results presented in a short written report.

Objectifs d'apprentissage

After this class, the students will master the essential concepts of nonequilibrium statistical mechanics and molecular dynamics simulations, and they will be able to apply them to key chemical and biochemical systems.

Prérequis

Physical chemistry (L2/L3)
- Hamiltonian
- Fick's law of diffusion

Statistical thermodynamics (L3)
- Microcanonical and canonical ensembles
- Phase space, ensemble averages
- Central limit theorem
- Equipartition of energy

Chemical kinetics (L3)
- Transition State Theory
- First order kinetics

Quantum Mechanics (L3)
- Harmonic oscillator
- Time-dependent perturbation theory
- Schrödinger and Heisenberg pictures

Langue(1)	*Cours, TD, TP*	*Documents*	*Bibliographie*
Anglais			

Bibliography

- M.E. Tuckerman, Statistical mechanics theory and molecular simulation, Oxford University Press
- D. Frenkel and B. Smit, Understanding molecular simulation, Academic press
- D. Chandler, Introduction to modern statistical mechanics, Oxford University Press
- R. Zwanzig, Nonequilibrium statistical mechanics, Oxford University Press

Detailed description

I. Basic concepts of statistichal mechanics (G. Stirnemann)

- From Newton's formulation to the Lagrangian
- Hamiltonian approach
- Phase space motion, Liouville equation.

II. Molecular modeling (D. Laage)

II.A. Introduction to molecular dynamics

- Molecular dynamics simulations
- Calculating energies and forces
- Integrating the equations of motion
- Simulations in different ensembles
- Monte Carlo simulations
- Applications

II.B. Advanced simulation techniques

- Free energy calculations: perturbation theory, thermodynamic integration, umbrella sampling, metadynamics, parallel tempering
- Describing chemical reactions: ab initio molecular dynamics, QM/MM
- Simulating very long times: multiple time steps, coarse graining

III. Time-dependent processes and kinetics (D. Laage)

III. A. Classical time-correlation functions

- Non-equilibrium statistical mechanics
- Definition of time-correlation functions
- Properties of time correlation functions
- Examples of time correlation functions
- Application to diffusion coefficient: Einstein and Green-Kubo relations
- Time-correlation functions from molecular dynamics simulations

III.B. Rate theories

- Rate laws and time correlations
- Transition state theory
- Corrections to transition state theory: Kramers and Grote-Hynes theories

III.C. Quantum time-dependent statistical mechanics: application to spectroscopy

- Time-dependent perturbation theory
- Time-correlation function and frequency spectra
- Application to Förster resonant energy transfer
- Optical absorption coefficient
- Kubo's stochastic lineshape theory

IV. Diffusion processes (G. Stirnemann)

IV.A. Introduction to diffusion
- Historical perspective
- Einstein theory
- Langevin equation: solutions, applications, limitations

IV.B. The generalized Langevin equation
- Model of a system in a bath
- Derivation
- Dynamic friction kernel
- Limit cases

IV.C. Stochastic approaches
- Fokker-Planck equation
- Smoluchowski equation
- Determination of mean-first passage times
- Demonstration of Kramers theory

V. Introduction to deep learning approaches to chemical and biophysical processes (Damien Laage and Guillaume Stirnemann)
- Basic concepts of machine learning
- Deep neural networks
- Variational autoencoders
- Application to reactivity
- Applications to phase space exploration