MASTER

Chimie

SCIENCES SORBONNE UNIVERSITÉ

5CI359	**Statistical Mechanics for Complex Chemical and Biochemical Systems** Keywords: statistical mechanics, theoretical chemistry, numerical simulations								
Responsable	Damien Laage, DR CNRS / Prof attaché ENS, UMR PASTEUR, ENS								
ECTS 4	*Cours (h)* 16	*TD (h)* 16	*TP (h)*	*Tutorat (h)*	*Ecrit (%)* 100	*CC (%)*	*TP (%)*	*Oral (%)*	*Eval. répartie* non

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.

Objectifs d'apprentissage

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

Prérequis

This course requires a background in physical chemistry (L2/L3), statistical thermodynamics (L3) and chemical kinetics (L3).

Langue[1]	*Cours, TD, TP*	*Documents*	*Bibliographie*
Anglais			