Course unit : MOLECULAR MODELLING (28h – 3 ECTS – compulsory)

Content

This module introduces the principal methods used to simulate structure and dynamics in clay systems on the atomic scale. After a reminder of the main concepts of statistical thermodynamics necessary to understand atomic-level simulations (thermodynamic ensembles, ensemble averages etc.), Monte Carlo and Molecular Dynamics simulation techniques are presented, followed by numerous examples concerning clays. Lastly, comparison of simulated structural and dynamic data with that obtained by scattering techniques (X-ray and neutrons) is given. About a half of the module is dedicated to practical work, where the student becomes familiar with the basics of programming and the general structure and use of a simulation code.

Learning outcomes

To understand the general outline of a simulation code, with the specificities related to clay systems.
To be able to analyse the simulation output and deduce/calculate the corresponding physical properties of the clay system.

Horary

Lecture : **14 h**
Supervised works : **2 h**
Practical works : **12 h**

Evaluation

Final examination : 50% of the grade
Evaluation during the teaching period : 50% of the grade

Teaching staff

Virginie Marry (University of Paris VI)
Natalie Malikova, (CEA-CNRS, Saclay)
Benjamin Rotenberg, (University of Paris VI)