# Approches computationnelles des états de la matière

**Lecturers**
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**Course mnemonic**
CHIM-F443

**ECTS credits**
5 credits

**Language(s) of instruction**
French

**Course period**
First term

## Course content

Content: introduction to chemometrics (experimental design, multivariate and principal components analysis, QSAR) and to computational chemistry (molecular mechanics, Hartree-Fock and post-Hartree-Fock methods, density functional theory)

## Objectives (and/or specific learning outcomes)

Goal: introduction to computer techniques for analyzing chemical data and for modelizing molecules and molecular reactivity. Preparation to reading research papers in computational chemistry

## Teaching method and learning activities

Teaching Method: Ex cathedra lectures illustrated by examples from the literature and by on line computer applications. Exercises consisting in the analysis of research papers.

## References, bibliography and recommended reading

Biblio: Leach, Prentice Hall 2001; Brereton, Wiley 2003

## Other information

### Contact(s)

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## Evaluation method(s)

Other

## Programmes

### Programmes proposing this course at the faculty of Sciences

MA-BINF | Master in Bio-informatics and Modelling | finalité Research/unit 2, MA-CHIM | Master in Chemistry | finalité Research/unit 1, finalité Teaching/unit 1, finalité Teaching/unit 2 and finalité Professional/unit 1 and MA-IRBC | Master in Chemistry and Bio-industries Bioengineering | finalité Professional/unit 2

### Programmes proposing this course at the Brussels School of Engineering

MA-IRBC | Master in Chemistry and Bio-industries Bioengineering | finalité Professional/unit 2 and MS-NATE | Specialized Master in Nanotechnology | unit U