Approches computationnelles des états de la matière

Lecturers
Nathalie VAECK (Coordinator), Antoine Aerts, Emilie CAUET and Martine PREVOST

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