UCLouvain

lchm1353

2023

Quantum Chemistry

3.00 credits	22.5 h + 7.5 h	Q1

Teacher(s)	Champagne Benoît ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	*The prerequisite(s) for this Teaching Unit (Unité d'enseignement – UE) for the programmes/courses that offer this Teaching Unit are specified at the end of this sheet.*
Main themes	The course offers an introduction to quantum chemistry, i.e. the use of quantum mechanical principles to calculate the properties of molecules and solids. The course presents the most important theories of the field starting from Hartree-Fock and extending to more modern approaches (post-Hartree-Fock and density functional theory (DFT)). The course also gives an introduction to the use of modern quantum chemistry software by the student.
Learning outcomes	**At the end of this learning unit, the student is able to :** 1 This course aims to initiate the chemistry students to the essential of quantum chemistry and its application to theoretical and/or model chemistry. It is not limited to formal teaching, but includes an introduction to the practice of the discipline by discussing some carefully chosen examples.
Evaluation methods	Students are evaluated through a project to be carried out during the year and for which they must submit a report. An oral exam evaluates the student's theoretical and practical knowledge through questions on the project and on all the subjects covered.
Content	The course mixes theory and computer exercises (using modern quantum chemistry software). An introduction to the use of Linux is also provided. We start with a reminder on Hartree-Fock followed by the presentation of modern post-Hartree-Fock methods (configuration interaction, coupled cluster,...) and end with the density functional theory (DFT). Beside the theoretical concepts, examples of quantum chemical quantities (energies, structures, energy barriers, ...) will be given. The aim of the course is to expose not only the important theories but also to provide a minimum of practical basis for the student to perform quantum chemical calculations by evaluating their quality and remaining critical about the results.
Inline resources	Moodle site available: https://moodle.uclouvain.be/
Other infos	**Background :** - General chemistry and basics in molecular physical chemistry (CHM1252). - Evaluation: written exam. Documents: detailed plan of the course and reference books.
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)

Program title	Acronym	Credits	Prerequisite	Learning outcomes
Master [120] in Chemistry	CHIM2M	3		🔍
Additionnal module in Chemistry	APPCHIM	3	LPHY1203	🔍
Master [60] in Chemistry	CHIM2M1	3		🔍