



3.00 credits

22.5 h + 7.5 h

Q1

Teacher(s)	Champagne Benoît (compensates Hautier Geoffroy) ;Hautier Geoffroy ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	<i>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.</i>
Main themes	<p>The course offers an introduction to quantum chemistry, i.e. the use of quantum mechanical principles to calculate the properties of molecules and solids.</p> <p>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)).</p> <p>The course also gives an introduction to the use of modern quantum chemistry software by the student.</p>
Learning outcomes	<p>At the end of this learning unit, the student is able to :</p> <p>1 This course aims to initiate the chemistry students to the essential of quantum chemistry and its application to theoretical and/or model chemistry.</p> <p>It is not limited to formal teaching, but includes an introduction to the practice of the discipline by discussing some carefully chosen examples.</p>
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	<p>The course mixes theory and computer exercises (using modern quantum chemistry software).</p> <p>An introduction to the use of Linux is also provided.</p> <p>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).</p> <p>Beside the theoretical concepts, examples of quantum chemical quantities (energies, structures, energy barriers, ...) will be given.</p> <p>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.</p>
Inline resources	<p>Moodle site available:</p> <p>https://moodle.uclouvain.be/</p>
Other infos	<p>Background :</p> <ul style="list-style-type: none"> - General chemistry and basics in molecular physical chemistry (CHM1252). - Evaluation: written exam. <p>Documents: detailed plan of the course and reference books.</p>
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		
Additional module in Chemistry	APPCHIM	3	LPHY1203	
Master [60] in Chemistry	CHIM2M1	3		