



3 credits

22.5 h + 7.5 h

Q1

Teacher(s)	Hautier Geoffroy ;
Language :	French
Place of the course	Louvain-la-Neuve
Main themes	Introduction to the formalism of quantum chemistry. Presentation of mono and multi configuration methods followed by their use in the computation of structural, electronic and energetic molecular properties, including the search of reaction mechanisms.
Aims	<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. It is not limited to formal teaching, but includes an introduction to the practice of the discipline by discussing some carefully chosen examples.</p> <p>-----</p> <p><i>The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".</i></p>
Content	<p>Content - Concepts and methods of current use in molecular and chemical modelling are presented: A short introduction to the formalism is given. Keywords: Orbital model; Hartree-Fock method; Roothaan LCAO-SCF MO expansion, Configuration Interaction, Molecular properties. - Applications: Potential energy surfaces are discussed and analysed in relation to the molecular structure of isolated molecules. Discovering isomers, conformers and other stationary points on the surface leads to evaluate the relative energies and transition barriers involved by structural changes of a molecule. A reaction pathway can be deduced from considering interacting molecules. - A selected example is explicitly studied with the aid of quantum chemical computation software: Keywords: Obtaining a structure; analysing the electron distribution and charge population; imaging electron densities and their reorganisation;</p>
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	Aims
Master [60] in Chemistry	CHIM2M1	3		
Master [120] in Chemistry	CHIM2M	3		
Additional module in Chemistry	LCHIM100P	3		