MASTER

Chimie

SCIENCES SORBONNE UNIVERSITÉ

5CI208	**Chimie Quantique** Méthode Hartree-Fock et post-HF, Fonctionnelle de la densité et TD-DFT, Modélisation des propriétés électroniques et structurales moléculaires et du solide.
Responsable, Coordinateur	MARKOVITS Alexis, Pr., Laboratoire de Chimie Théorique, UPMC

ECTS	*Cours*	*TD*	*TP*	*Tutorat*	*Ecrit*	*CC*	*TP*	*Oral*	*Eval. répartie*
6	20 h	0 h	16 h	non	0	100			oui

Descriptif de l'UE

This course aims at providing an advanced description of the electronic structure at the molecular or solid scale, and its consequences on certain properties (structure, energy and optical spectroscopies). It combines lectures with examples to present the fundamental principles and practical exercises to better understand the implication of these principles on examples. The manipulation of the fundamental formalisms, which allow a better understanding of the associated concepts, will be approached during practical work allowing the student an autonomous acquisition adapted to his previous training. Both traditional and more elaborate methods are examined. This course is not only intended for those wishing to continue their studies in molecular modelling, but also for experimentalists who will interact with quantitative chemists (organic and inorganic chemistry, spectroscopy).

Objectifs d'apprentissage

The learning is divided into three levels. On the one hand, the student will know the different quantum methodologies of representation of molecular and periodic systems and will be able to associate to each of them the current physico-chemical interpretations and to deduce the applicability domain of these methods. Furthermore, the student will be able to manipulate quantum equations and formalisms. Finally, he will be able to apply and interpret these methods in the context of simple concrete problems.

Langue)	*Cours, TD, TP*	*Documents*	*Bibliographie*
	Anglais	Anglais	Anglais

Thèmes abordés

Course on quantum chemistry wave-function methods

- Introduction to the quantum many-electron problem
- Hartree-Fock (HF) method
- Overview of post-HF methods for electron correlation
- Configuration interaction
- Perturbation theory
- Coupled cluster theory

Course on quantum chemistry Density Functional method

The course is aimed to give a general overview of the Density Functional Theory (aka DFT), starting from early developments and ending to some of the most recent developments. Together with the theorems giving a rigorous theoretical framework, some examples will be discussed in order to illustrate the advantages and limitations of DFT approaches in Chemistry.

Practical work

Concerning practical exercices, a series of hands-on problems with the accompanying theory will be proposed.

This part will be subdivided in four largely independent sub-sections:

- Introduction to basic quantum chemical computations using Gaussian on a Linux terminal.
- Fundamentals of the characterisation of Potential Energy Surfaces: algorithms and basic implementation.
- Advanced techniques for the optimisation and characterisation of Transition States
- Introduction to multiconfigurational methods: Symmetry, electronic transitions and spectra.

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