UNIVERSITÉ TOULOUSE III PAUL SABATIER

Faculté Sciences et Ingénierie

PÉRIODE D'ACCRÉDITATION : 2022 / 2026

UNIVERSITÉ PAUL SABATIER

SYLLABUS MASTER

Mention Chimie

Master 2 EM Theoritical Chemistry and Computational Modeling

http://www.fsi.univ-tlse3.fr/
https://www.univ-tlse3.fr/master-mention-chimie

2024 / 2025

20 JUILLET 2024

SUMMARY OF THE CONTENT

PRESENTATION

PRESENTATION OF DISCIPLINE AND SPECIALTY

DISCIPLINE CHIMIE

The master in chemistry offers four specialties : green chemistry, analytical chemistry, chemistry for health, theoretical chemistry and also offers training towards careers in teaching.
The objective is to train students into chemists executives for academic positions or positions in companies covering various business sectors such as the pharmaceutical, cosmetics, chemicals and food industry, materials and instrumentation.
The training also helps develop important transversal skills for employability such as : autonomy, communication, project management, ...
The master in chemistry proposes a progressive orientation in the chosen specialty.
The first year includes a significant share of core courses and specific courses in the chosen specialty.
The second year is rather strongly focused on the specialty.
Internships are included in the training (minimum 8 weeks in M1, 5 to 6 months in M2).

SPECIALITY

The European Master's Degree in Theoretical Chemistry and Computational Modelling (TCCM) offers you the opportunity to acquire the knowledge necessary for theoretical simulations which are very important today in all branches of chemistry and molecular physics. Applications include the design of new drugs in the pharmaceutical industry, new materials and nanodevices in applied physics or the prediction of properties and reactivity of new chemical compounds needed in the chemical industry.

PRESENTATION OF THE YEAR OF MASTER 2 EM THEORITICAL CHEMISTRY AND COMPUTATIONAL MODELING

During the Master's programme we will teach you the fundamentals of quantum chemistry, which is at the heart of the most accurate techniques in theoretical chemistry, but we will also give you the skills to use and modify the most advanced software codes used to perform simulations of real systems. You will also learn to simulate complex systems by combining quantum mechanical techniques with classical molecular dynamics techniques.
The courses take the form of intensive weeks organised alternately by the different universities of the TCCM consortium. Geographical mobility is compulsory, as students must complete 30ECTS of a semester in a country other than the one in which they are registered. This mobility can take place either during the first semester of M2 or, and this is the most frequent case, during the second semester when an internship in a research laboratory is carried out.

CONTACTS SECTION

CONTACT INFORMATION CONCERNING THE SPECIALTY

PERSON IN CHARGE OF TEACHING AFFAIRS OF MASTER 2 EM THEORITICAL CHEMISTRY AND COMPUTATIONAL MODELING

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SECRETARY OF STUDENT AFFAIRS OF

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CONTACT INFORMATION CONCERNING THE DISCIPLINE

PERSON IN CHARGE OF THE DISCIPLINE CHIMIE

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CONTACT INFORMATION FOR THE DEPARTMENT : FSI.CHIMIE

HEAD OF DEPARTMENT

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DEPARTMENT SECRETARY

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TABLE SUMMARIZING THE MODULES THAT MAKE UP THE TRAINING PROGRAM

page	Code	Title of the module	semestre*	ECTS	Mandatory Optional	Cours	Cours-TD	TD	TP	Stage
First semester										
9	KCHM9AAU	ADVANCED METHODS IN ELECTRONIC STRUCTURE, DYNAMICS AND MOLEC (AMESDM)	I	12	O	40		40		
Choose 3 module among the following 8 modules :										
10	KCHM9ABU	MULTISCALE, MACHINE LEARNING AND QSAR METHODS APPLIED TO BIO (MultiMLQSAR)	I	6	O		30		15	
11	KCHM9ACU	ADVANCED COMPUTATIONAL TECHNIQUE (ACT)	I	6	O		30		15	
12	KCHM9ADU	THEORETICAL METHODS FOR SIMULATION OF MATERIALS (TMSM)	I	6	O		30		15	
13	KCHM9AEU	COMPUTATIONAL CHEMISTRY PROGRAMMING PROJECT (CCPC)	I	6	O		30		15	
14	KCHM9AFU	FROM THEORY TO IMPLEMENTATION : TUTORIALS IN THEORETICAL CHEM (LTTC)	I	6	O		30		15	
15	KCHM9AGU	MODELLING ELECTRONIC STRUCTURE (MES)	I	6	O		30		15	
16	KCHM9AHU	MULTISCALE MODELLING OF COMPLEX MOLECULAR SYSTEMS (MMCMS)	I	6	O		30		15	
17	KCHM9AIU	SURFACE AND INTERFACE CHEMISTRY : EXPERIMENT AND MODELLIN (SICEM)	I	6	O		30		15	
Second semester										
18	KCHMAAAU	STAGE (Stage)	II	30	O					6

* **AN** :year long teaching, **I** : first semester, **II** : second semester

LIST OF THE MODULES

UE	COMPUTATIONAL MODELING AND ML (CMML)	6 ECTS	
KCHM0FAU	Cours : 15h , TP : 25h	Teaching in anglais	Personal work 150 h

[Retour liste de UE]

TEACHER IN CHARGE OF THE MODULE

SUAUD Nicolas
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LEARNING GOALS

See https ://www.emtccm.org/

SUMMARY OF THE CONTENT

See https ://www.emtccm.org/

PREREQUISITES

M2 TCCM students must have validated a first year of TCCM Master of any of the 9 universities of the TCCM consortium

SPECIFICITIES

All courses are in English. They are provided alternatively by a University of the TCCM consortium. Their location change each year.

TARGETED SKILLS

See https ://www.emtccm.org/

REFERENCES

See https ://www.emtccm.org/

KEYWORDS

See https ://www.emtccm.org/

UE	ADVANCED METHODS IN ELECTRONIC STRUCTURE, DYNAMICS AND MOLEC (AMESDM)	12 ECTS	1st semester
KCHM9AAU	Cours : 40h , TD : 40h	Teaching in anglais	Personal work 220 h

[Retour liste de UE]

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LEARNING GOALS

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SPECIFICITIES

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TARGETED SKILLS

See https ://www.emtccm.org/

REFERENCES

See https ://www.emtccm.org/

KEYWORDS

See https ://www.emtccm.org/

UE	MULTISCALE, MACHINE LEARNING AND QSAR METHODS APPLIED TO BIO (MultiML-QSAR)	6 ECTS	1st semester
KCHM9ABU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h
URL	Seehttps://www.emtccm.org/		

[Retour liste de UE]

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SUMMARY OF THE CONTENT

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PREREQUISITES

See https ://www.emtccm.org/

SPECIFICITIES

See https ://www.emtccm.org/

TARGETED SKILLS

See https ://www.emtccm.org/

REFERENCES

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KEYWORDS

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UE	ADVANCED COMPUTATIONAL TECHNIQUE (ACT)	6 ECTS	1st semester
KCHM9ACU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

TEACHER IN CHARGE OF THE MODULE

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

A compléter

SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

A compléter

KEYWORDS

A compléter

UE	THEORETICAL METHODS FOR SIMULATION OF MATERIALS (TMSM)	6 ECTS	1st semester
KCHM9ADU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

A compléter

SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

A compléter

KEYWORDS

A compléter

UE	COMPUTATIONAL CHEMISTRY PROGRAMMING PROJECT (CCPC)	6 ECTS	1st semester
KCHM9AEU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

A compléter

SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

A compléter

KEYWORDS

A compléter

UE	FROM THEORY TO IMPLEMENTATION : TUTORIALS IN THEORETICAL CHEM (LTTC)	6 ECTS	1st semester
KCHM9AFU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

A compléter

SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

A compléter

KEYWORDS

A compléter

UE	MODELLING ELECTRONIC STRUCTURE (MES)	6 ECTS	1st semester
KCHM9AGU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

A compléter

SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

A compléter

KEYWORDS

A compléter

UE	MULTISCALE MODELLING OF COMPLEX MOLECULAR SYSTEMS (MMCMS)	6 ECTS	1st semester
KCHM9AHU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

TEACHER IN CHARGE OF THE MODULE

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

A compléter

SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

A compléter

KEYWORDS

A compléter

UE	SURFACE AND INTERFACE CHEMISTRY : EXPERIMENT AND MODELLIN (SICEM)	6 ECTS	1st semester
KCHM9AIU	Cours-TD : 30h , TP : 15h	Teaching in anglais	Personal work 105 h

[Retour liste de UE]

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LEARNING GOALS

A compléter

SUMMARY OF THE CONTENT

A compléter

PREREQUISITES

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SPECIFICITIES

A compléter

TARGETED SKILLS

A compléter

REFERENCES

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KEYWORDS

A compléter

UE	STAGE (Stage)	30 ECTS	2nd semester
KCHMAAAU	Stage : 6 mois	Teaching in anglais	Personal work 750 h

[Retour liste de UE]

TEACHER IN CHARGE OF THE MODULE

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LEARNING GOALS

The internship is dedicated to apply knowledges.

SUMMARY OF THE CONTENT

Minimum 4 months.

PREREQUISITES

TCCM M1 and M2 courses

SPECIFICITIES

The choice of the lab or firm must fulfill the mobility rules

TARGETED SKILLS

Be able to adapt to working conditions

GLOSSARY

GENERAL TERMS

DEPARTMENT

The departments are teaching structures within components (or faculties). They group together teachers lecturing in one or more disciplines.

MODULE

A semester is structured into modules that may be mandatory, elective (when there is a choice) or optional (extra). A module corresponds to a coherent teaching unit whose sucessful completion leads to the award of ECTS credits.

ECTS: EUROPEAN CREDITS TRANSFER SYSTEM

The ECTS is a common unit of measure of undergraduate and postgraduate university courses within Europe, created in 1989. Each validated module is thus assigned a certain number of of ECTS (30 per teaching semester). The number of ECTS depends on the total workload (lectures, tutorials, practicals, etc.) including individual work. The ECTS system aims to facilitate student mobility as well as the recognition of degrees throughout Europe.

TERMS ASSOCIATED WITH DEGREES

Degrees have associated domains, disciplines and specialities.

DOMAIN

The domain corresponds to a set of degrees from the same scientific or professional field. Most of our degrees correspond to the domain Science, Technology and Health.

DISCIPLINE

The discipline corresponds to a branch of knowledge. Most of the time a discipline consists of several specialities.

SPECIALITY

The speciality constitutes a particular thematic orientation of a discipline chosen by a student and organised as a specific trajectory with specialised modules.

TERMS ASSOCIATED WITH TEACHING

LECTURES

Lectures given to a large group of students (for instance all students of the same year group) in lecture theatres. Apart from the presence of a large number of students, lectures are characterized by the fact they are given by a teacher who defines the structure and the teaching method. Although its content is the result of a collaboration between the teacher and the rest of the educational team, each lecture reflects the view of the teacher giving it.

TD : TUTORIALS

Tutorials are work sessions in smaller groups (from 25 to 40 students depending on the department) led by a teacher. They illustrate the lectures and allow students to explore the topics deeper.

TP : PRACTICALS

Teaching methods allowing the students to acquire hands-on experience concerning the knowledge learned during lectures and tutorials, achieved through experiments. Practical classes are composed of 16 to 20 students. Some practicals may be partially supervised or unsupervised. On the other hand, certain practicals, for safety reasons, need to be closely supervised (up to one teacher for four students).

PROJECT

A project involves putting into practice in an autonomous or semi-autonomous way knowledge acquired by the student at the university. It allows the verification of the acquisition of competences.

FIELD CLASS

Field classes are a supervised teaching method consisting of putting into practice knowledge acquired outside of the university.

INTERNSHIPS

Internships are opportunities enabling students to enrich their education with hands-on experience and to apply lessons learned in the classroom to professional settings, either in industry or in research laboratories. Internships are strongly regulated and the law requires, in particular, a formal internship convention established between the student, the hosting structure and the university.

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