SYLLABUS MASTER

Mention Chimie

Master 2 EM Theoretical Chemistry and Computational Modeling

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

2023 / 2024

29 MARS 2024
SUMMARY OF THE CONTENT

PRESENTATION ................................................. 3

PRESENTATION OF DISCIPLINE AND SPECIALTY ................. 3
  Discipline Chimie ........................................ 3
  Speciality ......................................................... 3

PRESENTATION OF THE YEAR OF Master 2 EM Theoritical Chemistry and
  Computational Modeling ........................................... 3
  List of recommended courses : .............................. 3

CONTACTS SECTION ........................................ 4
  CONTACT INFORMATION CONCERNING THE SPECIALTY ........ 4
  CONTACT INFORMATION CONCERNING THE DISCIPLINE ........ 4
  CONTACT INFORMATION FOR THE DEPARTMENT : FSI.Chimie .... 4

Table summarizing the modules that make up the training program . 5

LIST OF THE MODULES ........................................... 7

GLOSSARY ......................................................... 23
  GENERAL TERMS .............................................. 23
  TERMS ASSOCIATED WITH DEGREES ........................... 23
  TERMS ASSOCIATED WITH TEACHING ......................... 23
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.

LIST OF RECOMMENDED COURSES:

M1 CHI TCCM EM
CONTACT INFORMATION CONCERNING THE SPECIALTY

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

EVANGELISTI Stefano
Email: stefano@irsamc.ups-tlse.fr

SORTAIS Jean-Baptiste
Email: jean-baptiste.sortais@lcc-toulouse.fr

SUAUD Nicolas
Email: suaud@irsamc.ups-tlse.fr
Téléphone: 05 61 55 65 48

SECRETARY OF STUDENT AFFAIRS OF

BOURREL Céline
Email: celine.bourrel@univ-tlse3.fr
Téléphone: 05.61.55.65.37

Université Paul Sabatier
U2 rdc porte 26
118 route de Narbonne
31062 TOULOUSE cedex 9

CONTACT INFORMATION CONCERNING THE DISCIPLINE

PERSON IN CHARGE OF THE DISCIPLINE CHIMIE

SORTAIS Jean-Baptiste
Email: jean-baptiste.sortais@lcc-toulouse.fr

CONTACT INFORMATION FOR THE DEPARTMENT : FSI.CHIMIE

HEAD OF DEPARTMENT

JOLIBOIS Franck
Email: franck.jolibois@univ-tlse3.fr
Téléphone: 0561559638

DEPARTMENT SECRETARY

TEDESCO Christine
Email: christine.teesco@univ-tlse3.fr
Téléphone: +33 561557800
<table>
<thead>
<tr>
<th>page</th>
<th>Code</th>
<th>Title of the module</th>
<th>semestre</th>
<th>ECTS</th>
<th>Mandatory</th>
<th>Optional</th>
<th>Cours</th>
<th>Cours-TD</th>
<th>TD</th>
<th>TP</th>
<th>Stage</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td><strong>First semester</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>KCHM9AAU</td>
<td>ADVANCED METHODS IN ELECTRONIC STRUCTURE, DYNAMICS AND MOLEC (AMESDM)</td>
<td>I</td>
<td>12</td>
<td>O</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>Choose 3 module among the following 8 modules :</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>KCHM9ABU</td>
<td>MULTISCALE, MACHINE LEARNING AND QSAR METHODS APPLIED TO BIO (MultiMLQSAR)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>KCHM9ACU</td>
<td>ADVANCED COMPUTATIONAL TECHNIQUE (ACT)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>KCHM9ADU</td>
<td>THEORETICAL METHODS FOR SIMULATION OF MATERIALS (TMSM)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>KCHM9AEU</td>
<td>COMPUTATIONAL CHEMISTRY PROGRAMMING PROJECT (CCPC)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>KCHM9AFU</td>
<td>FROM THEORY TO IMPLEMENTATION : TUTORIALS IN THEORETICAL CHEM (LTTC)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>KCHM9AGU</td>
<td>MODELLING ELECTRONIC STRUCTURE (MES)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>KCHM9AHU</td>
<td>MULTISCALE MODELLING OF COMPLEX MOLECULAR SYSTEMS (MMCMS)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>KCHM9AIU</td>
<td>SURFACE AND INTERFACE CHEMISTRY : EXPERIMENT AND MODELLIN (SICEM)</td>
<td>I</td>
<td>6</td>
<td>O</td>
<td>30</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>Second semester</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>KCHMAAAU</td>
<td>STAGE (Stage)</td>
<td>II</td>
<td>30</td>
<td>O</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6</td>
</tr>
</tbody>
</table>

* **AN**: year long teaching, **I**: first semester, **II**: second semester
LIST OF THE MODULES
<table>
<thead>
<tr>
<th>UE</th>
<th>VAE : M2 CHI TCCM EM</th>
<th>ECTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sous UE</td>
<td>VAE Phase 1 - Avis de faisabilité : M2 CHI TCCM EM</td>
<td></td>
</tr>
<tr>
<td>K5CHMV1E</td>
<td>VAE : 1h</td>
<td>Teaching in anglais</td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]
<table>
<thead>
<tr>
<th>UE</th>
<th>VAE : M2 CHI TCCM EM</th>
<th>ECTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sous UE</td>
<td>VAE Phase 2 - Accompagnement : M2 CHI TCCM EM</td>
<td></td>
</tr>
<tr>
<td>K5CHMV2E</td>
<td>VAE : 4h</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Teaching in anglais</td>
<td>0 h</td>
</tr>
<tr>
<td></td>
<td>Personal work</td>
<td></td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]
<table>
<thead>
<tr>
<th>UE</th>
<th>VAE : M2 CHI TCCM EM</th>
<th>ECTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sous UE</td>
<td>VAE Phase 3 - Participation à un jury : M2 CHI TCCM EM</td>
<td></td>
</tr>
<tr>
<td>K5CHMV3E</td>
<td>VAE : 8h</td>
<td>Teaching in anglais</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Personal work 0 h</td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]
<table>
<thead>
<tr>
<th>UE</th>
<th>VAE : M2 CHI TCCM EM</th>
<th>ECTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sous UE</td>
<td>VAE Phase 4 - Accomp suivant les prescriptions du jury : M2 CHI TCCM EM</td>
<td></td>
</tr>
<tr>
<td>K5CHMV4E</td>
<td>VAE : 6h</td>
<td></td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]
TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email: suaud@irsamc.ups-tlse.fr

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 ]

TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

LEARNING GOALS
See https ://www.emtccm.org/

SUMMARY OF THE CONTENT
See https ://www.emtccm.org/

PREREQUISITES
See https ://www.emtccm.org/

SPECIFICITIES
See https ://www.emtccm.org/

TARGETED SKILLS
See https ://www.emtccm.org/

REFERENCES
See https ://www.emtccm.org/

KEYWORDS
See https ://www.emtccm.org/
<table>
<thead>
<tr>
<th>UE</th>
<th>MULTISCALE, MACHINE LEARNING AND QSAR METHODS APPLIED TO BIO (MultiML-QSAR)</th>
<th>6 ECTS</th>
<th>1st semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCHM9ABU</td>
<td>Cours-TD : 30h , TP : 15h</td>
<td>Teaching in anglais</td>
<td>Personal work 105 h</td>
</tr>
<tr>
<td>URL</td>
<td>See <a href="https://www.emtccm.org/">https://www.emtccm.org/</a></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[Retour liste de UE]

TEACHER IN CHARGE OF THE MODULE

SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

LEARNING GOALS

See https://www.emtccm.org/

SUMMARY OF THE CONTENT

See https://www.emtccm.org/

PREREQUISITES

See https://www.emtccm.org/

SPECIFICITIES

See https://www.emtccm.org/

TARGETED SKILLS

See https://www.emtccm.org/

REFERENCES

See https://www.emtccm.org/

KEYWORDS

See https://www.emtccm.org/
<table>
<thead>
<tr>
<th>UE</th>
<th>ADVANCED COMPUTATIONAL TECHNIQUE (ACT)</th>
<th>6 ECTS</th>
<th>1st semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCHM9ACU</td>
<td>Cours-TD : 30h , TP : 15h</td>
<td></td>
<td>Teaching in anglais</td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]

TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

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 ]

TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

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

TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

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
<table>
<thead>
<tr>
<th>UE</th>
<th>FROM THEORY TO IMPLEMENTATION : TUTORIALS IN THEORETICAL CHEM (LTTC)</th>
<th>6 ECTS</th>
<th>1st semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCHM9AFU</td>
<td>Cours-TD : 30h , TP : 15h</td>
<td>Teaching in anglais</td>
<td>Personal work 105 h</td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]

TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

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)

<table>
<thead>
<tr>
<th>UE</th>
<th>6 ECTS</th>
<th>1st semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCHM9AGU</td>
<td>Cours-TD : 30h, TP : 15h</td>
<td>Teaching in anglais</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Personal work 105 h</td>
</tr>
</tbody>
</table>

[Retour liste de UE]

**TEACHER IN CHARGE OF THE MODULE**

SUAUD Nicolas  
Email: suaud@irsamc.ups-tlse.fr

**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
MULTISCALE MODELLING OF COMPLEX MOLECULAR SYSTEMS (MMCMS)

KCHM9AHU  |  Cours-TD : 30h , TP : 15h  |  Teaching in anglais  |  Personal work 105 h

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
<table>
<thead>
<tr>
<th>UE</th>
<th>SURFACE AND INTERFACE CHEMISTRY : EXPERIMENT AND MODELLING (SICEM)</th>
<th>6 ECTS</th>
<th>1st semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCHM9AIU</td>
<td>Cours-TD : 30h , TP : 15h</td>
<td>Teaching in anglais</td>
<td>Personal work 105 h</td>
</tr>
</tbody>
</table>

[ Retour liste de UE ]

TEACHER IN CHARGE OF THE MODULE
SUAUD Nicolas
Email : suaud@irsamc.ups-tlse.fr

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
**TEACHER IN CHARGE OF THE MODULE**

SUAUD Nicolas  
Email: suaud@irsamc.ups-tlse.fr

**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
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 successful 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 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.