VIRT&L-COMM.9.2016.1

KU Leuven

Faculty of Science

ERASMUS MUNDUS MASTER OF SCIENCE IN THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

SELF-EVALUATION REPORT

9 December 2015

ISSN: 2279-8773

VIRT&L-COMM.9.2016.1

ISSN: 2279-8773

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Acronyms

ADS	Arenberg Doctoral School
ATP	Administratief en Technisch Personeel (KU Leuven)
CU	Course Unit
DLO	Discipline-specific Learning Outcome
DOWB	Dienst Onderwijsbeleid – Education Policy Department
EACEA	Education, Audiovisual and culture Executive Agency, European Commission.
ECTNA	European Chemistry Thematic Network Association
ECTS	European Credit Transfer and Accumulation System
EMM	European Erasmus Mundus Master
IC	Intensive Course
ISC	International Steering Committee
LO	Learning Outcome
OLA	Onderwijsleeractiviteit – Educational Activity
PLO	Program-specific Learning Outcome
POC	Permanente Onderwijscommissie (permanent education commission, KU Leuven)
QCPC	Division of Quantum Chemistry and Physical Chemistry, KU Leuven
RI	Research Internship
TCCM	Theoretical Chemistry and Computational Modelling
Y1	First master year
Y2	Second master year
ZER/SER	Zelfevaluatierapport – Self-Evaluation Report

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Chapter 1 Introduction

1.1. Preparation of the Self-Evaluation Report

In September 2014, Prof. De Feyter, Chairman of the Chemistry department, appointed a committee to prepare for the Spring 2016 an external evaluation by the Flemish Council for Universities and Colleges (VLUHR) of the Erasmus Mundus Master of Science in Theoretical Chemistry and Computational Modelling (EMM-TCCM). This committee was in particular charged with preparing the associated self-evaluation report (SER). Some preliminary work had been carried out from April 2014 by the departmental Program Director (chairman of the permanente onderwijscommissie, POC) and the Faculty Coordinator. The TCCM SER committee is chaired by the Faculty Coordinator, and is mainly composed of faculty and staff members of the Division of Quantum Chemistry and Physical Chemistry (QCPC) involved in this education program. Also included are two former EMM-TCCM students who are now doctoral candidates, one current second-year master (Y2) student, and one current first-year master (Y1) student. Finally, two staff members from the Educational Policy units of KU Leuven and the Faculty of Science provided expert advices. The list of all members is given in Annex AdA1.

As part of preparing the SER, the committee analyzed in biweekly meetings the results of surveys of students, and also coordinated a number of new ones. The full set of surveys includes:

i. A September 2014 survey of Y1 students participating in the Intensive Course (IC) for EMM-TCCM students in Toulouse, France, with responses from 16 out of 22 students taken by Prof. Arnout Ceulemans (electronic annex ElA1);
ii. A hearing of four former EMM-TCCM students and present doctoral students, carried out by Mrs. Iris Peeters (report) and Mrs. Inge Groeninckx, the two expert staff members of the committee, in December 2014 (cf. electronic annex ElA2);
iii. A hearing of five EMM-TCCM students spending three-months in Leuven as part of their master thesis research, carried out by Mrs. Iris Peeters and Mrs. Inge Serdons (report), the two expert members of the committee, in April 2015 (see electronic annex ElA3); and

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iv. A survey of all TCCM alumni, carried out by the central Educational Policy Department of KU Leuven (Data management Unit), providing 44 replies (see electronic annex ElA4 for an analysis);

The main outcomes of surveys i. and ii. were presented to the International Steering Committee (ISC) of TCCM consortium during its meeting held in Madrid on 21 March 2015.

The present SER is the result of a collective endeavour encompassing the opinion of all actors taking part in this educational program which places the student at the center of its activities.

1.2. Historical Context and Aims of the Study Program

In November 2003 representatives of over 40 European Universities met at El Escorial near Madrid to discuss organizing a European Master program in Theoretical and Computational Chemistry, following a suggestion by Prof. Manuel Yanez from Universidad Autónoma de Madrid. Acknowledging that theoretical and computational chemistry had become a major scientific tool in chemistry, physics and biology, they argued that there was a pressing need to train experts with a wide knowledge in the field of modelling and computation of molecular matter and materials. It was also important to establish a European standard for studies in TCCM. Given the critical mass needed, and the Bologna reorganization of higher education in Europe this goal would be best met by joining efforts between research universities. As a precursor, a Spanish theoretical chemistry master, had shown that joint master programs were feasible.

General agreement was obtained on a title and the program structure: a two-year European Master on Theoretical Chemistry and Computational Modelling (EM on TCCM); the first master year (Y1) would be organized locally in one of the participating universities and give students the necessary background in theoretical chemistry, whereas the second master year (Y2) would have a pronounced international character, and would start with a joint intensive course (IC) to bring together all the participants during four weeks.

In the following years this proposal gradually came to realization, following criteria laid out by EU Erasmus Mundus Program, which aims to enhance the quality and attractiveness of higher education in Europe, by promoting joint programs. The Erasmus Mundus model required to

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establish criteria of excellence and to procure a general quality assurance for all participants. As a result the originally considered very broad partnership was abandoned in favor of a workable consortium of seven key universities:

1. Universidad Autónoma de Madrid, Spain (coordinating institution)
2. Rijksuniversiteit Groningen, The Netherlands
3. Universita degli Studi di Perugia, Italy
4. Universidade do Porto, Portugal
5. Université Paul Sabatier - Toulouse III, France
6. Universitat de Valencia, Spain
7. KU Leuven, Belgium.

The EMM-TCCM came into existence some ten years ago, with the first IC taking place in Perugia in 2006. In 2007 the program acquired the "European Master" label from the European Chemistry Thematic Network Association (ECTNA), and in 2009 it was recognized – and funded – by the European Erasmus Mundus Master (EMM) program, with the first students with EMM scholarships starting in September 2010. At KU Leuven the program was approved in May 2010 and installed as a separate master program in the Faculty of Science. The chemistry POC was assigned as its program committee. In 2015, the EMM-TCCM Award was renewed by the European Commission for three more editions.

Information on the EMM-TCCM program in KU Leuven and in the partner institutions can be found on following websites:

1. Central webpage:

   https://emtccm.qui.uam.es/

2. KU Leuven:

http://www.kuleuven.be/toekomstigestudenten/publicaties/Wts/ChemistryComputational.pdf

https://onderwijsaanbod.kuleuven.be/opleidingen/e/CQ_51186233.htm

3. Universidad Autónoma de Madrid, Spain:

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http://www.uam.es/ss/Satellite/es/1242670751438/1242662106159/masteroficial/masterOficia/Master_Universitario_en_Quimica_Teorica_y_Modelizacion_Computacional.htm

4. Université Toulouse III - Paul Sabatier, France:

http://www.univ-tlse3.fr/m2r-chimie-specialite-chimie-theorique-erasmus-mundus--357710.kjsp?RH=1237305346255

5. Rijksuniversiteit Groningen, The Netherlands:

http://theochem.chem.rug.nl/TCCM program
https://www.rug.nl/ocasys/fwn/vak/showpos?opleiding=5706

6. Universitat de València, Spain:

http://www.uv.es/uvweb/universidad/es/estudios-postgrado/masteres-oficiales/master-1285848941532/Titulacio.html?id=1285874232271

7. Università Degli Studi di Perugia, Italy:

http://www.dcbb.unipg.it/titoli-europei?lang=it

1.3. Organizational and Administrative Context of the Study Program

For an organizational chart of EMM-TCCM implying KU Leuven, see Annex A1. The TCCM program at KU Leuven follows both European and local regulations and duties. The organization is monitored by an ISC, with one representative for each consortium university, and which meets annually. It has full responsibility regarding the admission policy and selection of students. The selection criteria of the consortium are given in Annex AdA2.

The task of ISC also involves analysis of student feedback, organization of ICs, and quality review reports to the EACEA. The grants are managed by the international coordinator. Fixed points on the annual ISC agenda include the ranking of student applications and distribution of scholarships, selection of EM Scholars, feedback of the past and organization of the next IC, and verification of mobility criteria for master theses. Additional items are publication initiatives (for TCCM textbook series of Springer), organization of winter schools, etc. The coordination between partner institutions which is essential for the selection of students, organization of IC and master theses, is thus regularly done through the ISC.

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On regular occasions the ISC initiated small changes to the program to meet requirements of EACEA and to take feedback of students into account.

1.4. Current Status at the Partner Institutions

Applications for a five-year EM Master are highly competitive, and are based on extensive reports by international experts. Fewer than 10 % of the applications are approved by EC. Likewise renewal of the program can only be granted after detailed review(s), based on a self-evaluation report, which is examined by a course quality advisory board. An independent survey of all students by the EM Student Association is part of the procedure. In the last call for renewal of the many applications, only 50 were considered eligible, and of those 50 only 19 were approved, including this TCCM program. Criteria for approval are based on relevance, attractiveness, level of integration, and sustainability.

Of all partners, only the Spanish National Accreditation Agency has recognized the values of the screening process by EACEA. According to Royal Decree of 2 July 2010 of Spain, "the EM programmes created by means of international consortia that have been selected in competitive calls by the EACEA and awarded with the Erasmus label of excellence by the EC will obtain the corresponding positive authorization (*ex ante* evaluation) by the Ministry of Education."

In France, Portugal and Italy, accreditation is part of a general evaluation of the whole chemistry curriculum. International recognition of TCCM invariably is considered as an important strength of chemistry programs. In Flanders and the Netherlands, accreditation is organized by the Dutch Flemish Accreditation Organization (NVAO). The TCCM Master at the University of Groningen received accreditation as part of the general chemistry curriculum.

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Chapter 2 Generic Quality Standard 1: Targeted Outcome Level

2.1. Objectives and Profile of the Curriculum

Theoretical and computational chemistry has become a key sub-discipline in chemistry, playing a central role in academic and industrial research, and providing a tool that helps students' understanding of fundamental concepts. To train the many experts who will start careers in this field, there is a growing realization that bespoke university courses are needed. It is within this context that the *Erasmus Mundus Master of Science in Theoretical Chemistry and Computational Modelling* was created, with the objectives:

- To prepare experts in the use and development of computational techniques in molecular sciences, to work with innovative pharmaceutical, petrochemical and new-materials industries.
- To offer to students from a wide range of countries (including non-European ones) a highly qualified title at the master level.
- To establish a European standard for research-oriented studies in TCCM.
- To promote international mobility of research students.
- To prepare students for doctoral studies in Chemistry, Physics, Life or Materials Sciences.

This two-year master program is cross-European, and involves seven European partner institutions. During the first year (Y1), each student follows courses in his/her home institution, whereas in year two (Y2), the whole cohort assembles for a joint international IC. Later, each student carries out a research stay in a laboratory, which must be based outside their home institution and country.

The TCCM has made the choice to teach students about fundamental theory in chemistry, as well as about computational applications. Being able to run calculations using existing methods is an important skill for master graduates in this area. However, getting insight into the underpinning theories guarantees that the training will remain relevant even with further rapid technological change. These factors motivate our choice to focus on both theory and computation.

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2.2. Learning Outcomes

During the development of the program and the (successful) processes of (re)application for EMM status, the intended learning outcomes (LO) of the program have been established and also agreed upon between the partner institutions. These LO documents are attached as Annex A2. Briefly summarized, at the end of the program, the students will have acquired: a deep *knowledge and understanding* of theoretical chemistry and simulation techniques and their applications; the ability to use these in a *professional* setting; the ability to *acquire and use* relevant information; the ability to *communicate* about their field; the ability to *learn independently*; a high motivation and *collaborative and ethical* attitude; and an *international* orientation.

The LOs map naturally onto the program objectives in section 2.1. They relate to the knowledge and understanding of theoretical chemistry and associated simulation methods: the master program prepares *experts* in the field. At the same time, for what is a relatively young field of chemistry, and one with many specialized sub-areas, it also ensures that the students gain an international and polyvalent orientation.

2.3. Assessment of the Learning Outcomes by Alumni and Professionals

The targeted LOs have been assessed both informally and formally by students, alumni and professionals. The TCCM has undergone rigorous formal assessment by professionals during applications for the EM and Erasmus$^+$ funding, and the successful outcome reflects further recognition of the need for a TCCM master. Informally, many academics from institutions outside the consortium have learned about the program by teaching in the IC. Very positive testimonials from these academics were obtained when applying for renewal of the EMM-TCCM. For example, Professor Arvi Rauk from the University of Calgary, Canada, noted that the program "encompassed all areas of modern chemical theory, computation and simulation". As will be discussed in section 2.5, that a number of other related master programs with similar aims have been created in recent years within Europe, demonstrating the relevance of the LOs.

As mentioned in Section 1.1, focus groups of current students and alumni considered the program in general, and the LOs in particular, during preparation of the SER (cf. Electronic Annexes ElA1, ElA2, ElA3 and ElA4). To the alumni, the LOs were considered to be in line

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with the expectations of the professional field. It was noted that education about ethics and environment skills was not explicitly included for these students, and that relatively little programming training is provided. Also, there was some debate about the importance of training in communication skills, and about whether provision in this area was adequate.

Current students were also generally positive about the LOs. Here too, there was some debate, e.g. about whether the LOs are too ambitious for some of the students at least. A broader group of alumni were consulted via a questionnaire which partly addressed the LOs. On a scale from 1 = Strongly Disagree to 6 = Strongly Agree, questions such as “In the […] programme, I have learned […] a sound knowledge of the fundamentals and methodology of theoretical chemistry and simulation techniques”, relating to LO-1a, received a mean response of 4.93, and related questions on other LOs also received mean responses above 4.5 (and often over 5.0). In questions concerning the importance of these LOs to their professional practice, very high mean scores were obtained (Electronic Annex ElA4).

2.4. The Relation with Discipline-Specific Learning Outcomes

In consultation with VLUHR, the set of discipline-specific learning outcomes (DLO) as drafted in Annex A3 were submitted to the NVAO and subsequently validated. The DLO’s reflect the core targeted LOs that would be a feature of any program in the general area. The program-specific learning outcomes (PLO) fully cover these more fundamental aims (Annex A2). Annex A4 displays the interconnections between both the DLO’s and PLO’s. The largest added value of the EMM-TCCM with respect to the general DLO’s concerns its inherent international aspect. The international dimension of the program is specifically highlighted in learning outcome 7 (Annex A2). The students learn working in international teams, making networks and living in different countries.

In the TCCM area, there are no other master programs in Flanders or the Netherlands. However, as discussed below in Section 2.5, the LOs for the present program overlap very well with those of the comparable programs run in other countries (international benchmark). Also, the LOs align closely where appropriate with those of the master in chemistry at KU Leuven. Two key areas of difference concern the subject area and the international character. On the first of these aspects, unlike the Master in Chemistry at KU Leuven, EMM-TCCM focuses on theoretical and computational chemistry, with students being able to follow a small number of

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courses on cognate areas of experimental chemistry. In this sense, EMM-TCCM is a more specialized form of a chemistry master, and is also accessible to students with Bachelor degrees in other related areas such as physics, engineering or life sciences. The second aspect is discussed below.

It should be stressed that theoretical and computational chemistry is a broad field in which few institutions have expertise across the whole range. Single institutions can hardly host the *critical mass*, both in numbers of students and staff that is required by the high specificity of EMM-TCCM. The model used here, as reflected in the PLO, is international and multi-institutional, with the students being offered a unique international experience through the IC with its external lecturers on the one hand, and the student mobility for theses on the other hand. This has advantages such as the broader range of experts involved in the teaching than would be available in a single institution, the ability to participate in determining a 'standard' for master teaching in the field within Europe, and the educational benefits in terms of broadening of horizons for students. At the same time, disadvantages in terms of costs and organizational overhead are mitigated by EM funding, and the existence of a network of colleagues with close connections to one another.

2.5. A Comparison with Similar Curricula in Belgium and Europe

In Flanders

As mentioned above, there are no other Masters in the area of theoretical chemistry in Flanders at present. The natural reference point within Flanders is Masters of Chemistry courses, and especially for us, the KU Leuven "Master in de Chemie" and "Master of Chemistry". Like the EMM-TCCM, these are two years long and involve 120 ECTS. However:

- While the "Master in de Chemie" to some extent, and in particular the "Master of Chemistry" programs are tailored for education of more experiment or synthesis orientated chemists,[1] TCCM program is focused towards theoretical and computational aspects of the field.

[1]This, however, does not prevent a "Master in de Chemie" student from composing an individual program of optional courses as an adequate preparation for conducting research in the broad field of quantum chemistry.

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- An important part of EMM-TCCM consists of courses that are also part of the master of chemistry program. Other courses were taken from the master of nanoscience and nanotechnology, master of biophysics, biochemistry and biotechnology, and master of physics. From these programs a selection of courses has been distilled that focus on theoretical concepts, computational methodologies and physico-chemical techniques for molecules, biomolecules, molecular materials and solid state.[2] In addition, the TCCM master program contains two modules that were specifically designed for this program, namely the "Module II: Computational Techniques" (Y1) and the IC (Y2).
- The TCCM is accessible for students with a broader range of bachelor degrees than the master of chemistry program (e.g. physics, chemical engineering, materials science, biology, bio- and biomedical engineering…). This is enabled inter alia through the presence of two levelling courses, which allow starting TCCM students to acquire sufficient fundamental knowledge of quantum chemistry.

A special characteristic of TCCM, distinctly different from the master in chemistry, is its *international character*. This is manifested by:

- The IC (24 ECTS): This is taught every year in August / September at a different university of the consortium, and brings all TCCM Y2 students together. It allows them to acquire additional specialized knowledge about chemical theory and computations compared to the courses taught at their home university.
- Part of the master thesis (at least 18 ECTS) is carried out at one of the other universities involved in the program.[3]
- Belgian students enrolled in the program have to study abroad for a total of 60 credits, which can either be done in Y1 or Y2.

In Europe

Internationally, there are several masters programs in the general area of theoretical and computational chemistry (see a list below), though there are many fewer masters in this sub-field

[2] The TCCM program at KU Leuven is flexible enough to include various kinds of courses in connection with the student's specific interests, which might be both theoretical and experimental.

[3] To improve their knowledge of a second European language, the TCCM master programs also includes a language course.

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than e.g. in chemistry. It should however be pointed out again that TCCM is quite a broad and not a "traditional" academic subject. Therefore it is possible to make different choices about the range of topics chosen for a master. There can be an emphasis either on underpinning theory, on computational methods, on their applications, on new methodology, on programming and high-performance computing, on related fields in physics, biochemistry, or indeed some combination of all of these. The EMM-TCCM makes the choice to focus on fundamental theory as well as its computational applications.

As each institution, particularly smaller ones, will only have a small number of academics with expertise in TCCM, it is natural that a number of other benchmark master programs involve some collaboration between institutes in several countries. The strong international dimension of our TCCM program is almost unparalleled though.

The related programs are (all being two-year, 120-ECTS, unless mentioned otherwise):

- Nordic Master Program in Computational Chemistry and Physics. This is a bit broader (physics as well as chemistry) than EMM-TCCM, but otherwise has rather similar LOs, and also involves multiple institutions.
- Chemistry: Molecular Simulation and Photonics, M. Sc. in Chemistry at Universiteit van Amsterdam (The Netherlands). It has an (to an outsider) unusual combination of allowing students to focus either on computational chemistry *or* molecular photonics (with some courses on both topics in core material).
- M. Sc. in Molecular Modeling, UC London (UK). 12-month, 90 ECTS course. It focuses mainly on materials modelling.
- Atomic Scale Modeling of Chemical, Physical and Biological Systems (ATOSIM). As the Nordic program, this is quite broad covering condensed matter and statistical physics, chemistry, materials science, and theoretical biomolecular science. Courses are divided between Amsterdam (UvA and VUA), Lyon (ENS) and Rome (La Sapienza), with research projects also possible in one of 21 partner universities or companies. This program has EM status.

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- Masters in Modeling Molecules and Nanosystems (MoMoNano) (Helsinki, Finland). Joint between chemistry and physics, with courses on computational methods and their applications to chemistry, physics, nanoscience and biological systems.
- M. Sc. in Molecular Modeling and Bioinformatics, Birkbeck College London (UK). This 1-year 60 ECST program is oriented towards biomolecular modelling and bioinformatics.

As can be seen, some of the programs are more specialized, while others cover more of chemical physics as well as chemistry. Not all of these programs exist with an EM funding. In summary, the international character of EMM-TCCM emerges as a crucial part, and is a highly valuable perspective that make the present master program unique.

2.6. Critical Reflection and Future Perspectives

The preparation of this SER encouraged us to investigate the content and practice of similar programs elsewhere in Flanders and Europe. This clearly shows us that the program offers a valuable distinctive focus on TCCM in an international framework. The inherently international character of the program constitutes a strength of the program.

- Consulting with current students and alumni of the TCCM program concerning the LOs and other aspects led to a number of comments and suggestions (cf. Electronic Annexes ElA1-ElA4). One aspect that will lead to immediate development concerns the LO on ethical and environmental impacts. In fact, the LO on ethical issues has recently been discussed within the ISC and it was decided to incorporate a special session in this year IC (organized by us in September 2015, the course on ethical issues was given in the IC in Groningen).

  At KU Leuven, the scientific integrity is now taught for starting PhD's (http://www.kuleuven.be/research/integrity/culture/phd_lecture.html), but not for master students yet. Accordingly, this lecture empowers starting researchers 'to understand the difference between what is and is not acceptable, and prevent them from making mistakes they would later regret because of the adverse consequences for others, for science and for their own career'. In the following years, TCCM master students could attend this course.

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- The relative paucity of training in communication skills was also noted. Given the very diverse background of EMM-TCCM students, this is a point of attention for future improvements, with remediation within the plan of research internships and master theses.

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Chapter 3 Generic Quality Standard 2: Educational Learning Environment

While admission to the EMM-TCCM program is centralized, each student is enrolled in one of the universities of the consortium, their home institution, and follow courses there for Y1. In Y2, the whole cohort is assembled for an IC, and students then pursue research projects in preparation for their master thesis in one or more of the partner universities.

The general structure of the program is organized around seven *modules* (I to VII), defined on the central TCCM webpage: http://emtccm.qui.uam.es. In terms of the general philosophy, cohesion and practicability of the curriculum, the idea is that Y1 serves to bring bachelor graduates from a variety of related disciplines to a good basic knowledge of theoretical and computational chemistry and its applications. This is done through the use of general backgrounds and applications courses, as well as levelling courses. Then, the students, who are by now at a fairly homogeneous level, take part in the common IC of module VI, and deepen their knowledge through research training (module VII).

Y1:

Module I. General backgrounds, covering e. g. fundamentals of quantum mechanics and statistical mechanics (Y1, 14 ECTS).

Module II. Computational techniques: introduction to programming and computation (Y1, 6 ECTS).

Module III. Basic applications, including spectroscopies and chemical reactivities (Y1, 10 ECTS).

Module IV. Levelling courses and other elective courses. Students can take courses that complement those followed during the Bachelors, and/or courses in related areas of chemistry (Y1, 30 ECTS).

Module V. Foreign language (Y1, 5 ECTS).

Y2:

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Module VI. International IC on advanced topics in theoretical and computational chemistry, delivered jointly to the whole cohort, and including subsequent self-study (Y2, 24 ECTS).

Module VII. Research training including the master thesis (Y2, 36 ECTS), which is carried out at more than one university.

Due to the need to fit in with local institutional and national rules and frameworks, the exact nature of the courses making up each module is slightly different for each institution, especially for Y1. For example, the indicated number of ECTS credits is subject to small deviations, and the denomination of the courses entering into each module can also vary. The full list of ECST credits at KU Leuven are given in the following webpage:

https://onderwijsaanbod.kuleuven.be/opleidingen/e/SC_51186236.htm

3.1. Realization of the Learning Outcome in the Curriculum

The curriculum is designed based on the LOs described in Chapter 2, with the relationship discussed in more detail in this section. To take into account the multi-institutional nature of the masters, the discussion is structured around the modules described above, since they are common to all institutions. In the text below, detail is given about the individual courses that make up these modules, and the mapping of the PLOs onto those of the courses. Also, information is provided about the course structure in other institutions.

3.1.1. Mapping of the individual learning outcomes onto the curriculum

The mapping between the intended LOs and the curriculum is summarized in the matrix shown in Annex A5. The LOs are labeled as in Annex A2. Before discussing the curriculum mapping in detail for each module, some general comments may be useful.

First, each LO is mapped to at least one module. Some LOs are mapped to many modules. This reflects the fact that the LOs are rather heterogeneous in nature, with e.g. the core traditional “knowledge and understanding” LOs mapping onto many of the traditional CUs within the modules, whereas the more generic skills represented e.g. by the LOs on Motivation and Attitudes, and International Orientation are associated only with the broader type of training provided by the internships or the Master Thesis. It can also be noted that some of the LOs are attitudes that the students acquire throughout their study program. As such, these LOs are

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perhaps not ideally suited as LOs in the strong sense of measurable outcomes that can be positively taught and evaluated. They have been included as the consortium feels they are important aims of the master program.

3.1.2. Details of the Curriculum Mapping: KU Leuven

A more detailed discussion of the mapping between the PLOs and the modules is provided here, based on the detailed learning objectives and content description provided for each course within KU Leuven.

Module I includes four courses: Quantum Chemistry (QC, 3 ECTS), Density Functional Theory (DFT, 4 ECTS), Electronic Structure of Molecular Materials (ESMM, 3 ECTS) and Reactive Systems (RS, 6 ECTS). These courses cover a range of theoretical topics and their applications, e.g. "*Energy expressions for multi-electron determinant wavefunctions*" and "*Time-dependent Schrödinger equation and perturbation theory*" (QC), "*connection between molecular orbitals and band structure*" (ESMM), "*the Hohenberg-Kohn theorems*" (DFT), and "*Quantum-statistical theories of reaction rates*" (RS). This module thereby clearly serves to support the reaching of LO 1a ("a sound knowledge […] of theoretical chemistry") and 1b ("potential of these techniques in chemistry").

Module II includes the element "Computer Module" within the research internship (RI). In this element, students learn about the UNIX operating system, and programming e.g. in Fortran. This element requires self-study in the pursuit of a set of advanced exercises, and uses continuous assessment. LOs 2b and 2c – on the ability to work autonomously and to apply and develop codes – are thereby supported, and the self-study aspects provide support for LOs 3b and 5.

Module III comprises the courses on "Chemical Aspects of Group Theory" and "Dynamics of Chemical and Biochemical Systems". Both of these courses include fundamental theory as well as extensive applications throughout chemistry and beyond. The first aspect clearly maps onto the LOs "Knowledge and Understanding", LOs 1a and 1b, whereas the broad range of applications also support LO 1c, by providing "advanced and precise knowledge of […] the particular field [… of the] research project".

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Module IV comprises a series of elective courses as well as a six-week internship. The latter is specific to KU Leuven, i.e. it is not included in the general description of the seven modules on the TCCM webpage (see above). Within the series of elective courses, one can further distinguish:

a. two leveling courses “Quantum Physics” (3 ECTS) and “Computational Chemistry” (3 ECTS);

b. a series of courses that are aimed at broadening the student’s knowledge into chemistry and related fields such as molecular physics, material science, and biological chemistry.[4] These courses however need approval of the related POCs, and

c. two specializing courses “Computational Methods in Solid State Physics” (3 ECTS) and “Advanced Computational Chemistry” (3 ECTS).

In Annex A5, module IV is presented as the three submodules IVa, IVb, IVc. Module IVc comprises the RIs, whereas modules IVA and IVB encompass the leveling courses (a) and broadening courses (b) respectively. For the mapping of the LOs the two specializing courses (c) are placed under module I because they best map onto the “Knowledge and Understanding” LOs 1a/1b. The courses in module IVa are optional, and serve to upgrade the student’s background in quantum mechanics and/or computational chemistry to the level needed for the compulsory courses. On the other hand, the elective courses of module IVb serve to broaden the student’s knowledge.

The RI-1, module IVc, offers students the opportunity to familiarize themselves with research work in the areas covered by the different courses of the EMM-TCCM, with a focus on gaining experience with scientific techniques, rather than on solving research problems. As such, it serves as a preparation for the master thesis, module VII, by introducing the students into important aspects of a daily research environment, i.e. obtaining autonomous knowledge from the scientific literature (LO3a), writing scientific projects, and reporting the results of their work, either orally or in written reports (LO 4a and 4b).

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[4] A list of seven courses (36 ECTS in total) is explicitly proposed in the TCCM master program on the KU Leuven website. However, students are also allowed to choose from various other courses offered at KU Leuven, in connection with their specific interests.

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In Module V, students choose one language course intended to improve their knowledge of a second European language, by gaining practice in listening, reading, speaking and writing. Students who do not speak Dutch can choose a basic course in this language (3 ECTS, level A1 of the Common European Framework), which also pays attention to the Flemish culture with guided visits to important towns in Flanders (LO 7b).

Module VI corresponds to the four-week IC run at the beginning of Y2 on a rotating basis among the partners (in Leuven and Groningen in September 2015). This aims to supplement Y1 students with a background necessary for them to pursue Y2 program. The lecturers include both local staff and invited scholars (2 for Leuven in 2015). The list of professors involved in the teaching of an IC should be approved by ISC. As for an example, the program of IC 2015 in Leuven and Groningen is given in Annex AdA3.

Module VII mainly comprises the *Research Internship* RI-2 (Y2, 6 ECTS) and *Master Thesis* (Y2, 30 ECTS). RI-2 is followed during the first semester of Y2, in a research group where (part of) the master thesis will be conducted, allowing the student to get acquainted with the actual research work in which they want to specialize for their master thesis, but also to develop skills such as accessing the scientific literature, developing research proposals, setting them in context against wider goals, and articulating courses with research. This component of module VII thereby supports and evaluates LOs such as 2a ("delineate the key problems of a research […] assignment"), 3a ("make competent use of the scientific literature") or 4d ("awareness of societal […] implications of […] scientific activities"). Performing the research in a foreign country and with involvement of supervisors from different institutions nourishes and tests the students' international orientation and ability to network with peers and international experts (LOs 7a and 7c).

The detailed aims of the Master Thesis are well described in the unit description on the KU Leuven webpage, reproduced here as Annex AdA4. This document spells out many of the elements that justify the present curriculum mapping. E.g. the aim to "Acquire attitudes to conduct scientific research in a team", by doing research "in collaboration with an entire research group", clearly maps onto LO 4c. Discussing the goals of the project with supervisors and possible collaborators, and while describing this context in the written thesis, the student will need to consider the implications of the research performed (LO 4d).

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Training in research also involves learning about scientific integrity (LO 4e) by taking part in research processes and being part of a research environment (LO 6c). This intensive period of time spent by students immersed in research groups of different institutions naturally leads to the acquisition of a broad range of technical and broader skills, and the thesis is thereby a core element of TCCM, laying the basis for the pursuit of further research or professional employment. Hence the large number of LOs associated with this Module in Annex A8: only LOs 1a and 1b (which are covered in detail by the courses comprised by Modules I, III, IVA, and VI) are not explicitly linked to the thesis, even though the in-depth use of theoretical concepts during that research period will certainly lead to reinforcement of those LOs.

3.1.3. Details of the Curriculum Mapping: Partner Institutions

Students admitted to the EMM-TCCM at KU Leuven study for the first year in Leuven. During Y2, they follow the modules VI and VII which are organized globally and have the mapping described above onto the learning outcomes. Students admitted to partner universities within the consortium instead follow modules I – V in their home institution, and these modules differ in the details of their implementation. Some details of this implementation for the Madrid partner are provided in Annex AdA5.

3.1.4. Teaching and Learning Methods used in Relation to the Targeted Learning Outcomes

The EMM-TCCM has a very carefully constructed structure, with some special teaching and learning methods chosen to optimize the in-depth understanding of the fundamentals of the field. In Y1, the main teaching techniques are lectures, as well as problem sessions and computer exercises, allowing students to gain in-depth insight. There are compulsory courses as well as optional topics tailored to the student circumstances. In Leuven, there are also two compulsory internships in which students are exposed to a research environment. This mix of teaching and learning methods is well suited to giving students a strong basic understanding of, and practical experience with, theoretical and computational chemistry.

The Y2 starts with the IC, which involves lectures, problem classes and computer exercises. By bringing the students from the whole master program together, and also teachers from within and outside the consortium, it creates an intense experience and an opportunity to learn in a more

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informal way. It is followed up by in-depth homework. This is an individual study, in which the student sends the answers directly to the lecturer for evaluation. The research project for the thesis involves additional international collaboration and experience.

Given that most universities only have staff with expertise in a few sub-areas of theoretical and computational chemistry, the present course set-up can provide a much broader and firmer education, and the IC, together with the international research project, are essential ingredients in delivering this outcome. More details on the study pathway (guidance), RIs and theses are given in Chapter 4 (4.2, 4.3 and 4.4).

Overall, the design of the modules and the choice of teaching and learning methods ensures cohesion of the curriculum, since it is built around teaching students about theoretical and computational modelling in a unified way. The practicability of the curriculum is monitored continuously through feedback from students. For example, as discussed in section 3.4 and Chapter 4, some concerns about the heavy teaching load (in the IC), have arisen and actions have been taken to remedy this.

3.2. Student Intake and Progression Policies

The program is promoted and advertised in various ways, e.g. through webpages of KU Leuven and UA Madrid… and in part by alumni. The consortium has been promoting association of our students, and an Alumni Association of TCCM Masters is set up. This association is playing an important role in promoting the program, in spreading information about it, and on helping new students in different fronts, in particular in what concerns employability. Considering the many languages, countries and institutions involved, it is a challenge to ensure that all the information about the program needed by students wishing to apply is available on the various webpages. To face this challenge, efforts shall further be invested to improve the webpages (in English) with easier access and clearer information.

The admission policy of the TCCM consortium was mentioned in Chapter 1, and is given in detail in Annex AdA2. The progression policies follow the general rules of KU Leuven. For KU Leuven, intake is typically of 5 students per year, with roughly 30 in total per year for the whole EMM-TCCM. Although bachelors in chemistry represent the largest contingent, candidates having degrees in physics, biology and (bio)-engineering have also been selected. There is a

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diversity of recruited students coming from all continents including Eastern Europe, North and South America, Africa and Asia.

For KU Leuven, recruitment of chemistry bachelor students to the EMM-TCCM was not successful. While this may be just an accident linked with the low total number of bachelor students, it could also indicate that during the bachelor years, students do not have sufficient space (only 6 ECTS on theory) to explore their interest in theoretical chemistry.

3.3. Staff Linked to the Study Program

The academic staff and assistants associated with teaching and project supervision for EMM-TCCM in KU Leuven are primarily those of the Division of Quantum Chemistry and Physical Chemistry (QCPC), and especially the six academic members active in the area of theoretical chemistry, who have a wide variety of high-level research interests. The “Computer Module” (Module II) is led by the computer manager within the division, who holds a Ph. D. in quantum chemistry. Research activity in theory and computation, and their applications, is not confined to QCPC, and indeed some of the core compulsory courses are given by other members of the Chemistry Department at KU Leuven, and one course on density functional theory given at VU Brussel. Some optional courses are taken from the curricula of other departments, and are taught by staff from these departments.

The list of staff / lecturers is given in Annex A7. As far as the QCPC staff is concerned, all lecturers are giving courses within their expertise and active research domains. The program has started the publication of the Springer series of Lecture Notes in TCCM’ in which Leuven lecturers have contributed/will contribute some textbooks. According to KU Leuven regulations, academic staff are regularly evaluated on their quality and performance in teaching, research and services.

The teaching assistants are doctoral candidates of the division (whose names are not given in Annex A7). They should follow the teaching training for Ph. D. students organized by the faculty within its professionalization program (http://wet.kuleuven.be/OO/assistenten/EN). In this course, experiences are exchanged based on, among others, the observation and questionnaire to improve the teaching skills of all PhD students.

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As under many other headings, the international nature of the EMM-TCCM is primordial here. Students interact with project supervisors from other universities, gaining exposure to research leaders from well beyond KU Leuven. This is one of the key strengths of an international program such as this one, in that it allows interaction of students with acknowledged experts in all subfields of the subject. While there are enough staff in each of the institutions for the required teaching, the absolute number in each is relatively low. At KU Leuven, this requires attention for the future as following retirements or other staff changes can have an impact on the program. The capacity of staff needs to be closely monitored in order to be able to quickly respond to changes.

The IC also plays an important role, since this important part of module VI involves teachers from staff in other departments of the consortium, as well as from invited lecturers from other parts of the world. For example, Professors Peter Gill (Australian National University), Arvi Rauk (University of Calgary, Canada), Bert De Groot (University of Göttingen, Germany), David Tew (University of Bristol, UK)… were among the lecturers in recent ICs.

3.4. Internal and External Quality Assurance

The EMM-TCCM program is subject to continuous quality assurance within each of the partner institutions, and within the consortium. The program at KU Leuven is the responsibility of the Faculty of Science POC, which delegates to the chemistry POC the responsibility to monitor the EMM-TCCM, to define solutions for problems with the program as a whole or with specific courses in particular, to prepare changes to the educational programs, to implement approved changes and to monitor and improve the quality of the program.

In the chemistry POC, elected representatives of students, lecturers, teaching assistants of all chemistry educational programs, as well as a member of the professional field of activities are represented. Input from TCCM students is specifically sought out (though as many of the courses are shared with other master programs, changes may also arise following the experiences of the other students). A summary of the actions taken and the changes made to educational program in the period of 2012-2015 is given in Annex A8. The quality of the program is a point of attention during the monthly meetings of the POC Chemistry and is also monitored in the university wide online evaluations of the individual courses. Moreover, the POC and individual POC members have the possibility to ask for e.g. hearings. The university is currently deploying COBRA, the new quality assurance system (cf. http://www.kuleuven.be/onderwijs/cobra/).

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The ISC meets regularly, among other reasons, to assess the delivery of the courses, and especially IC. Experiences and insights are shared, and decisions taken about the place in which the following IC will be organized, and the way in which the IC will run. For example, in the 2014 IC in Toulouse, student feedback indicated that small progress tests organized during the course had required too much attention, thereby distracting the students from being able to focus strongly enough on the courses. Accordingly, it was decided that from the 2015 edition, the progress tests would be lower-key.

3.5. Program-specific Facilities

The key facilities for EMM-TCCM students are classrooms, and appropriate e-learning support environments. These are provided within each home institution. One specific and necessary facility is naturally computing resources. Each of the universities in the consortium has high-performance computing (HPC) resources available for teaching and research. For example, in KU Leuven, there is a local computer within the Quantum Chemistry group (currently 83 nodes with 150 CPUs and 852 cores, attaining a power of 11 TFlop). Students also have access to KU Leuven central HPC (VSC, 2656 cores and over 130 TFlop). Computers are the key working tool for the program-specific study, and the way of learning and using computers of students also constitutes a guide for their study pathways.

3.6. Critical Reflection and Future Prospects

When preparing this SER, the panel reflected on the way the LOs map onto the courses, especially in KU Leuven. As described above, this mapping is very well suited to the overall aims. The over-arching module structure and local nature of Y1 curriculum, combined with the more internationally oriented Y2 content, mean that there is a high degree of subsidiarity in planning the courses: staff in each institution know what is needed by the begin of Y2, but can map the modules I – V onto local courses in accordance with local needs and regulations.

One reflection concerns the matching between the KU Leuven curriculum and the intake. Students come from quite different national and disciplinary backgrounds, and there is some evidence that the content of Y1 would benefit from having more flexibility for some of them, e.g. more leveling courses. Also, ensuring that up to date information about the master program is available through the webpages in various institutions remains a constant challenge. Both of these issues will be pursued both within the chemistry POC and the ISC.

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Chapter 4 Generic Quality Standard 3: Outcome Level Achieved

Following all the learning and training activities, evaluation of the knowledge and skills of students constitutes a key activity which assesses the outcomes of not only the study of an individual student, but also of the efficiency of a course or the whole program. Assessment outcomes are mainly reflected by the marks obtained. The latter measure the extent to which the LOs have been achieved by the student. Viewed more broadly, the marks also provide insight concerning the extent to which the intended LOs are being achieved. In this chapter we present the evaluation processes of EMM-TCCM involving both components of the outcomes.

Evaluation of students is classically achieved through written or oral exams. In line with the general subsidiarity principle in TCCM consortium, assessment of EMM-TCCM students is fully carried out based on the examination rules of their home institution. We are mainly concerned with KU Leuven whose examinations are organized in compliance with local regulations for all courses, internships in Y1 and Y2, and master theses. When a KU Leuven student follows a course elsewhere, the evaluation follows regulations at that place. When she/he carries out a master thesis elsewhere, the defense should however be organized at KU Leuven. We refer to the detailed document entitled 'Education and Examination Regulations 2015-2016' issued by KU Leuven (Annex A9). Assessment of RIs, IC and theses will be described in some detail in following sections.

4.1. System of Assessment, Testing and Examination

4.1.1. Types of Assessment used in Relation to the Targeted Learning Outcomes

In general, research-based courses taught at KU Leuven encourage students to adopt an analytical and critical attitude toward a scientific issue, and this is also reflected in the way that courses are assessed. The curriculum map (Annex A5) shows that all learning outcomes are assessed in one or more modules. The evaluation format is adjusted to the learning outcomes. The following evaluation forms are commonly used:

a. *Written* and/or *oral exams*. This is the typical exam form for courses in Y1 in order to evaluate LOs described in the ECTS fiches. An exam which consists of several questions

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allows the lecturer to check whether students possess technical and scientific knowledge, and whether they understand and can analyse theory and computational methods. Examination with open book is also favoured by some lecturers (such as the courses 'Group Theory' and 'Molecular Spectroscopy').

b. Tests. In IC, short tests with *multiple-choice questions* provide continuous feedback during the course itself.

c. Individual *report* or *essay* or oral presentation. This form allows the lecturer(s) to check whether students understand and are able to formulate a problem, to analyse a new problem in searching for information in the current literature, or to critically comment on a research article. The presentation of projects after the two RIs fits well in this format, and the corresponding evaluation is described in a following section (4.2). Short essays are also the favoured type of some lecturers (such as the course 'Molecular Spectroscopy'). The main assessment of the IC is through pieces of *written homework* on different parts of the IC.

d. Evaluation of master thesis and research aptitudes. Assessing of the master thesis includes the evaluation of a written text and the defence of the thesis research in front of a jury. The whole process of preparing the thesis, which also brings in a critical attitude and an ability to set up research activities is assessed in particular. This allows the lecturer(s) to appreciate not only the research results, but also whether students can function in an interdisciplinary team, interact with other domains and can integrate information to come up with feasible solutions. As stated above (cf. 3.1.1), not all LOs are *explicitly* evaluated. These refer to general attitudes rather than specific knowledge and skills. The (collaborative and ethical) attitudes of a student are appreciated during the evaluation of his/her master thesis.

4.1.2. Method of Ensuring the Quality of Testing (Validity and Reliability)

The Faculty organizes exam sessions but it is the responsibility of the lecturers to ensure that they are correctly organized, representative, reliable and transparent. The individual lecturers prepare exam questions according to the descriptions given in the corresponding ECTS fiches and the guidelines described in the POC Evaluation Policy, they collect and correct the answers, and finally give the marks (grades). The quality of examinations is regularly monitored based on university-wide surveys of students (Course-Lecturer Evaluation). These surveys are also used by the POC to evaluate the quality of the exams and to remedy when necessary. Recently, the

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POC is revising its evaluation policies, a process that started in 2014-2015 and resulted in the renewed POC Evaluation Policy. The full implementation of the revised policy is planned and will be in place in 2016-2017.

Currently, the lecturers already make use of several important guidelines and tools found in the Evaluation Policy: In particular the validity of exams depends on whether the questions i) are effective for testing knowledge on the subject, ii) accurately reflect the learning objectives, and iii) are appropriate in volume and level of difficulty. To this purpose, some lecturers make use of peer review and check if the questions map to the learning outcomes of the course.

Regarding the reliability, the result of an exam (the mark given) should in principle be similar, irrespective of the evaluator, the moment of corrections and the determining questions to measure the student skills. When giving the marks, each lecturer makes use of a set of evaluation criteria based on learning objectives and specific or generic answer models.

4.1.3. Transparency and Feedback

Information on the courses for students is available from the webpages of the programme (cf. Chapter 1). Students can get all possible information about life and activities from the central webpage (http://www.kuleuven.be/English). When new TCCM students arrive in Leuven at the beginning of the academic year, an orientation session is organized by the Local Coordinator to provide them with a study guidance by introducing, among others, the courses and practices, the general academic requirements, the tests and exam regulations and the role of the exams ombudsperson... Each student can contact the relevant academic staff to have additional explanation on the content of the courses and practices. Each student will then select an Y1 study program. The examination schedule established by the Faculty is available online (KU Loket of students and lecturers) at the start of each semester. Information on the mode of exam (closed or open book, written or oral, reports or essay, etc.) is provided online in the ECTS fiches, and explained by the lecturer at the first and last lectures.

The feedback procedure, after an exam session, is described in the faculty regulations, and the POC evaluation policy. In view of the small number of EMM-TCCM students, varying yearly from 1 to 5, students can receive detailed feedback from lecturers concerning examination results, and from supervisors and coordinators concerning RIs and theses.

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Student representatives provide feedback on exam structure and organisation through the chemistry POC. Students can register complaints through the ombudsmen who are always present in the deliberation of examination committees. Since the existence of the TCCM up to now, during the meetings of the examination committee, no complaints have been expressed or recorded.

According to the alumni hearings, TCCM students greatly appreciated the cordial contact, and the way in which information was given (cf. Annex ElA4).

4.2. Internships (RI)

RIs are introduced in Chapter 3 (section 3.1.4). Here we describe them in more details. At KU Leuven, there are two different RIs.

A) *Research Internship 1* (Y1, RI-1, 9 ECTS). In the second semester of Y1, in consultation with the supervisor, each student selects a research group at KU Leuven for a six-week internship (RI-1). A short proposal is submitted by the student, in agreement with the supervisor. During RI-1, daily supervision is provided by a mentor, and the student is also assigned to an external promoter, who is a member of the didactic team. The student sends weekly written reports to the supervisor and external promoter. At the midpoint of internship, following discussion with the student, an evaluation form is generated to register progresses achieved as well as points of attention for the remaining period. At the end of RI-1, the supervisor and promoter individually fill in the final evaluation form (given in Annex AdA6). The student also gives an oral presentation of 15-20 minutes, followed by discussion, of the work conducted during the internship in front of the didactic team, who judges the quality of the presentation.

B) *Research Internship 2* (Y2, RI-2, 6 ECTS). During the first semester of Y2, each student perform RI-2 in a KU Leuven research group where part of the master thesis will be conducted. Daily supervision is provided by a member of this research group. RI-2 starts immediately after the student returns from IC (during this time the student is still working on written reports for IC homework). At the end of the semester, the student gives an oral presentation in front of TCCM didactic team and QCPC division members, containing both an overview of the introductory work performed during the RI-2, and a description of further research to be performed for the thesis (The RI-2 is in fact the starting part of master thesis). Evaluation of the internship is based

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on i) daily work; ii) the final presentation + discussion, and iii) style, structure, and comprehensiveness of the answers to the IC assignments (cf. Annex AdA6).

4.3. Intensive Course (IC)

The IC is also described in Chapter 3. The evaluation process and methods are common for all Y2 students irrespective of their home institution. Each partner should ensure a period of 8-12 weeks for carrying out the IC homework. At KU Leuven, this period overlaps with the RI-2.

The evaluation of IC is implemented as follows:

1. At the end of each week: multiple-choice tests are given to evaluate short-term impact of the lectures. Weight factor for the tests: 20 %
2. Up to three months after the IC: the written homework, involving exercises, calculations and literature surveys on specific study problems, is assessed by the lecturers. The resulting marks are weighted equally over the four topics of the IC: Advanced Computational Techniques, Advanced Electronic Structure Theory, Applications, Dynamic Simulations and Modelling. Weight factor for the homework: 80 %.

4.4. Master Thesis

For KU Leuven students, the assessment of theses is done following the regulations for KU Leuven – Faculty of Science master projects (cf. Annex AdA4). Each master thesis is evaluated by a KU Leuven jury, but with a mandatory participation of a member from a partner university. Also Leuven staff members evaluate theses of students of partner universities who conducted research in Leuven.

The selection of research subjects is described in Annex AdA7. At the end of Y2 second semester, students submit their theses to jury members. There are no formal guidelines on length or format, though a thesis is typically 50-60 pages long (without annexes), and contains an introduction and background, essential research results, and a discussion. During the subsequent oral defence, each student presents the conducted research (15 minutes), and the jury discusses with the students and asks questions (10 minutes). If the foreign jury member cannot attend this presentation, a filled out evaluation document should be sent on time to the coordinator of the master theses. This report is communicated to the jury during the deliberation. Written questions

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are also sent to the coordinator, and then to the student during the defence session, which are all chaired by the same chairperson to assure a uniform assessment.

The evaluation by promotors and assessors is done by means of an assessment roster (Annexes AdA8 and AdA9), which covers all aspects of research, and is filled out in conjunction with an appreciation scale (Annex AdA10). Such an evaluation follows the criteria set up by current regulations of KU Leuven Faculty of Science. The score on a thesis amalgamates the weights of three components, for a total of 30 ECTS. The mark of the promotor contributes 50% to the final mark, whereas those of two assessors contribute 15% each. The remaining 20% relates to the oral presentation and defence, and is obtained as an average of marks over all jury members. Again the assessment roster serves as a guidance.

In order to succeed, a student must obtain a sufficient mark (> 50%) for each of three components that make up the final mark respectively (from the supervisor, the average of two assessors marks, and the defense). If this is not the case for one or more of these components, the final score therefore being 9/20 or less, the student will then not be able to obtain his/her master degree. In the assessment roster, a clear distinction is made between process and product of research work. A reader only evaluates the product whereas the supervisor evaluates both. The assessment roster facilitates the discussion of the jury, and is used to give a structured feedback to the student. The items of evaluation roster are in accordance with LOs of master theses (see Curriculum Mapping, Chapter 3, Annexes A5 and A6).

Not all Y1 students could attend Y2 program. But all Leuven Y2 students were able to defend their theses in the July exam session, and successfully obtained their diploma. The average mark was 17/20, within a range from 15.6 to 19.0/20.

The surveys among the students and alumni indicated that they considered very positively the mobility for master theses, as well as the supervision and evaluation at Leuven.

4.5. Achievement of the Learning Outcomes: Suitability of Graduates for Employment in the Labour Market

Through surveys and hearings, alumni and current students are generally of the opinion that the learning outcomes of the IC and master thesis are well achieved. They have greatly appreciated and enjoyed the mobility experience. Knowledge and experience gained in training

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and research have broadly contributed to their abilities for competition in the job market, in particular for academic positions.

According to the survey of the alumni (Annex ElA4), a very high percentage ~90% of TTCM master graduates have opted for academic research. Only a few % took jobs in private sectors (banking, ICT…). Their TCCM training, strong background and high quality theses allowed them to successfully find positions and to follow doctoral studies in chemistry, physics, life and materials sciences… in different European and non-European institutions.

The framework of the master also contributes to a cultural integration through the mandatory mobility (a TCCM student spends time in three countries, namely, home, IC and thesis). We pay a particular attention to this integration by favoring interaction of students with numerous cultural activities offered by KU Leuven, and of the city. The students also are eager to collaborate in achieving this goal when other colleagues, coming from other institutions of the consortium, joint their home university. As a result, TCCM graduates could get an edge in competitive recruitment as they can easily integrate in a new cultural and social environment.

As we consistently proposed the subjects that correspond to timely topics and even hot topics (our partners have shared with much enthusiasm), the novelty of TCCM master theses led to a high percentage of publication of papers in peer-reviewed high impact factors journals in the field. Our TCCM students frequently graduated with high grades. Only master students who graduated with, at least, distinction (cum lauda, grade ≥ 14/20) could be admitted to the Arenberg doctoral school (ADS). In our division, four TCCM graduates stay further as doctoral candidates of ADS. One receives a prestigious FWO doctoral mandate. Other candidates receive scholarships from KU Leuven research projects. The list of KU Leuven TCCM master theses (students, titles, marks) is given in Annex A10, along with a list of representative theses of the whole consortium.

4.6. Critical Reflection and Future Prospects

We can state that the *LOs described above are realized*. The evaluation policy in the educational programs of the chemistry department complies with the view of the KU Leuven and Faculty of Science on education and evaluation. Currently, the evaluation activities in use are to a great extend in agreement with the new POC evaluation policy. The full implementation of the

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POC evaluation policy is currently being prepared in cooperation with educational supporting staff of the faculty and of the university educational office. Details of this implementation will be discussed during the bi-annual *Chem-E-Days*, organized for the chemistry department, and planned near the 2016 Easter recess. Thus, in the coming academic year (2016-2017) this new policy will be implemented in all its details.

The *international character of the program*, in both learning process and participants, is an attractiveness but also induces intrinsic challenges. On the one hand, foreign students need to adapt to novel methods of teaching, learning and evaluation. On the other hand, a high level of coordination between partner institutions is required. Surveys of current students and alumni consistently pointed out the demanding study load, in particular in the IC, which is very challenging to some students. Efforts to manage the load and hence enhance practicability of the curriculum have been already been undertaken (see Annex A8).

In view of the fact that strong *local traditions* often prevail in the implementation, the consortium requests all partners to consider specific regulations for IC and master theses in order to have harmony not only in preparation but also in evaluation criteria and process. In a near future, comparable process for selection of subjects and assessment method shall be applied for master theses in all partner institutions in order to ensure that a similar quality can be expected. This constitutes a challenge in the coming years for the EMM-TCCM program.

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Chapter 5 Conclusions

5.1. An SWOT Analysis

The 15-month-long extensive discussion allowed us to look back, to carefully consider again the desired *learning outcomes* which lay behind the design of this master program, to explore exactly how the teaching is structured in order to deliver these outcomes, and to honestly assess how well these outcomes are met by students, and how good are the approaches for assessing the students' learning.

Overall, we believe that this Erasmus Mundus master program is a valuable presence in the European education landscape opened up by the Bologna reforms. Theory and computational modelling are of increasing importance in chemistry, yet by their nature, only small numbers of students in each higher education institution are motivated to specialize in this area. Also, only small numbers of staff have expertise in this area. Yet cumulatively across Europe, the numbers become significant, and specific training, similar but distinct from general chemistry master programs, is essential for training the experts in this field that academia and industry need. The current master program plays a key role in filling this niche. This represents a major strength of the program, and indeed an on-going opportunity. At the same time, our analyses in previous chapters acknowledge the challenges in the way the program runs at present.

We therefore start by reviewing the strengths (S), weaknesses (W), opportunities (O) and threats (T) of the current EMM-TCCM program.

Strengths

- The study program is focused on theoretical and computational modelling in chemistry, a unique focus in Flanders;
- The program is recognized internationally, not least through having twice been awarded Erasmus Mundus and Erasmus+ funding. All selected students received scholarships;
- The program has an intrinsically international character through the teaching staff, and the mandatory stays in more than one country;

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- The program exploits synergies between multiple institutions to deliver an original program;
- The students carry out their master thesis research projects in leading theoretical groups from across Europe;
- The students meet in joint intensive courses, workshops, research stays,… and that creates a spirit of belonging to a community, and
- Alumni find employment, at present mostly in competitive Ph. D. programs.

Weaknesses

- The study load is heavy, and can be very challenging to some students, given the very diverse background of the intake, and
- Gaining information about the program is rather complex given the many institutions, countries and languages involved. Some of the learning outcome deserve more attention. For example, ethical aspects that have in part been remedied through the IC 2015, but also communication skills.

Opportunities

- The program can build on its trail-blazing record to establish standards for education on TCCM within Europe;
- The program stimulates close cooperation between the participating groups in education and research;
- The program can exploit its growing reputation to recruit excellent master students within Flanders, Belgium, Europe and globally;
- Through synergies with the new TCCM doctoral ITN, the masters can demonstrate its qualities as an ideal route into high-quality doctoral research, and
- The EMM-TCCM can forge further links with end-users in academia and industry to ensure that it continues to deliver a valued skill-set.

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Threats

- The program has relatively small numbers of students in each participating institution, and is therefore vulnerable to being considered uneconomical to teach;
- The program has some travel and communication overhead costs, especially for the intensive course, that need to continue to be covered;
- The program is dependent on European funding, whose future is unclear;
- The course is carried out by the expertise and goodwill of a relatively small number of staff in each institution. A few career changes and retirements can have significant impact, and
- The program relies for its intake mostly on chemistry bachelor graduates. The teaching content of Bachelors at KU Leuven, as far as theoretical chemistry is concerned, is insufficient. The current curriculum does not succeed in attracting the interest of bachelor students in theory, and
- The delivery of the program is dependent on synergy with other masters programs. If the content of other programs changes, it will become a challenge to deliver the required teaching.

5.2. Perspectives and Options for the Future.

In the next years, our effort will be devoted to improving the aspects suggested by the present SER, in conjunction with the partner institutions. This can already be started from the following ISC meeting.

Concerning the longer term, it is to be mentioned that the current funding from Erasmus+ will elapse by the middle of 2019. Compared to the previous period, the number of scholarships is already reduced from two/three per institution per year to just one.

At the same time, the opportunities for experts in the TCCM field will certainly remain high, or indeed increase in coming years. This combination of developments will certainly play a big role in the medium term. Although it is likely that from 2019, the TCCM master program shall be self-supporting, we trust that inventive solutions will be found to sustain a fruitful master in TCCM program in KU Leuven by open scholarships of the Flemish Ministry for Education,

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VLIR, of KU Leuven (IRO, Faculty of Science…), and of industrial partners of the ITN doctoral program.

More importantly the program needs to attract (a. o. by more extensive advertisement) self-supporting students including bachelor students graduated not only from KU Leuven but also from other Flemish, and Walloon and European universities. As the TCCM program is suitable for bachelors not only in chemistry, but also in physics, biology, life science and engineering, there is a realistic perspective for recruitment.

Staff turnover in this area will be substantial in coming years, but a commitment of the university to the future is already starting to be put in place through recruitment of the next generation. Continued investment in the area will certainly lead to the enthusiasm and inventiveness needed to prolong this important but niche educational activity, and we believe that the Master in TCCM has a bright future.

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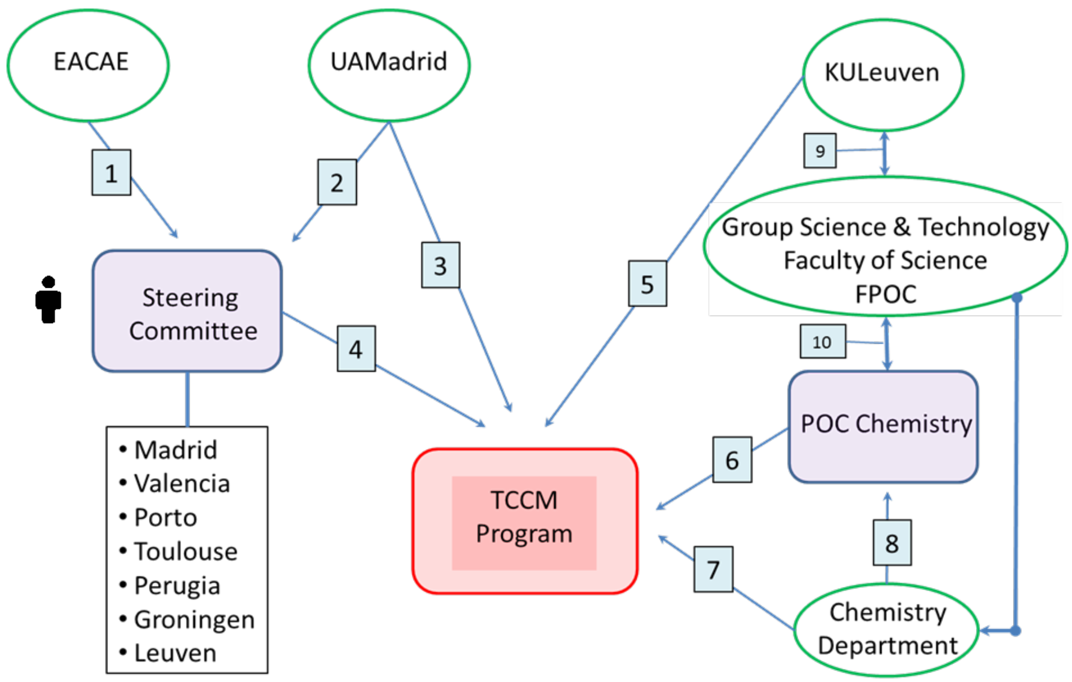
Compulsory Annexes

Annex A1: Organizational Chart



The chairman of the steering committee is the international coordinator. At each partner institute a member of the steering committee acts as local coordinator.

1 Award of Erasmus Mundus label

Finance: grants, scholarships, participation costs

Quality reviews, annual reporting

2 Administrative support and control

3 Joint Diploma

4 Selection of candidates

International program aspects: intensive course, mobility, collaboration

5 KULeuven Diploma

6 Local program aspects: M1, thesis requirements

Quality review, student representatives

7 Staff and infrastructure

8 Elected representatives of the teaching staff

9 KUL is structured in three groups: Science & Technology, Biomedical Sciences, Humanities

10 The Faculty of Science is responsible for education.

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Annex A2. EMM TCCM: Programme-Specific Learning Outcomes (Chapter 2)

The student:

1. Knowledge and Understanding

a) has acquired a sound knowledge of the fundamentals and methodology of theoretical chemistry and simulation techniques;
b) has a clear idea of the potential of these techniques in chemistry, and related fields such as molecular physics, material science, and biological chemistry;
c) has an advanced and precise knowledge of and can make original contributions to the particular field and application in which he/she has developed his/her research project.

2. Professional Abilities

a) can delineate the key problems of a research or project assignment and link it to theoretical insight and computational techniques. He/she can define the underlying hypotheses and postulates, and design problem solving steps;
b) can work autonomously in an organized and efficient way, within the framework of theoretical and computational objectives;
c) can apply existing scientific computational codes, and has the ability to select among existing codes and methods which one is suitable to address the requirements associated with research or productive activities.

3. Acquisition and Use of Information

a) can make competent use of the scientific literature;
b) can process and integrate new information from data files, codes, and informatics tools;
c) can critically evaluate complex information in the field of chemical sciences and distinguish scientifically sound protocols.

4. Communication and Social Skills

a) is able to communicate in English to peers and experts in oral or written form on his/her results and achievements in a structured way;
b) can communicate to a broader audience on topics of scientific interest;

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c) has the skills to function and collaborate in an interdisciplinary team;
d) has awareness of societal, and possible ethical and environmental implications of his/her scientific activities;
e) has developed a positive attitude towards scientific integrity.

5. Learning Skills

- is able to master autonomously additional knowledge or methodologies that are relevant for the project or assignment at hand

6. Motivation and Attitudes

a) can take responsibilities and initiatives with respect to computational and theoretical challenges to improve and advance research projects.;
b) is open to complementary input from other scientific disciplines;
c) has a stimulating effect on his/her research environment through active interest and collaborative attitude.

7. International Orientation

a) has a broad international orientation, and experience of working on different locations with international teams;
b) has a basic knowledge of European culture and of a second European language besides English;
c) can make use of networking with peers and international experts for exchange of scientific ideas.

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Annex A3. TCCM: Theoretical Chemistry and Applications Discipline-Specific Learning Outcomes (Chapter 2)

1. Having a general knowledge and understanding of theoretical chemistry and its applications in chemistry and chemistry related disciplines such as biochemistry, material science and physical chemistry.
2. Having advanced knowledge of a specialized branch of theoretical chemistry and insight into its applications.
3. Having a general scientific attitude to critically assess, analyze and develop problem solving steps for well-defined problems in relation to theoretical chemistry and its applications.
4. Having experience in data acquisition and literature surveys.
5. Having knowledge of and experience with the computational and mathematical techniques of theoretical chemistry.
6. Being prepared to work as an expert in the use and development of computational techniques in molecular sciences, to work with innovative pharmaceutical, petrochemical and new-materials industries.
7. Being prepared for doctoral research studies using theoretical and computational chemistry methods within the fields of chemistry, physics, life science or materials science.

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Annex A4: A mapping showing the interconnections between PLO's and DLO's (Ch. 3)

	Discipline specific learning outcomes (DLOs)						
PLO Module	General knowledge	Specialized knowledge	Scientific attitude	Data and literature	Technical experience	Professional training	Research training
1a,b	✓						
1c		✓					
2a,b						✓	✓
2c					✓		
3a,b				✓			
3c			✓				
4a							✓
4b,c						✓	
4d,e			✓			✓	✓
5						✓	✓
6			✓				✓
7							✓

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Annex A5: Curriculum Mapping (Chapter 3)

Curriculum Mapping between Learning Objectives 1a–7c / Teaching Modules I-VII

	Year 1 Modules							**Year 2 Modules**	
LO	I	II	III	IVa	IVb**	IVc	V	VI	VII
1a	E		E	E				E	
1b	E		E	E				E	
1c			S					E	E
2a						E			E
2b		E				E			E
2c		E		E*				E	E
3a					S	E			E
3b		S						E	E
3c					S	E			E
4a				E*		E		E	E
4b					E				E
4c						E		S	E
4d									E
4e						S			E
5		S			E	S			S
6a						S			E
6b					E	S			S
6c						E			E
7a								S	E
7b							E		S
7c								S	E

S = this LO is supported by the teaching and supervision provided as part of this module.

E = this LO is evaluated through exams and/or marking of projects. Any LO that is evaluated in a module is also supported by this module.

*Only in the course "Computational Chemistry"

**Excluding the course "Advanced Computational Chemistry", which is elective, but should in this matrix be placed under module I.

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Annex A6: Schematic Overview of the Curriculum (Chapter 3)

Schematic overview of the curriculum, indicating the number of credits awarded for each part of the study program.

[In the preamble to this chapter, the content of the Masters is described in terms of a number of high-level learning modules. Each partner university provides the training associated with a given module in terms of one or several local courses. In order to facilitate the following discussion, it is useful to list the specific courses associated with each module for KU Leuven students]:

- **Module I: General Background (16 ECTS)**
  - Quantum Chemistry (3 ECTS)
  - Density Functional Theory (4 ECTS)
  - Electronic structure of molecular materials (3 ECTS)
  - Reactive systems (6 ECTS)
- **Module II: Computational Techniques (5 ECTS)**
  - Computer module (5 ECTS)
- **Module III: Basic Applications (12 ECTS)**
  - Chemical Applications of Group Theory (6 ECTS)
  - Dynamics of Chemical and Biochemical Systems (6 ECTS)
- **Module IV: Elective and Leveling courses (24 ECTS)**
  - Leveling courses (IVa) (Quantum Physics, Computational Chemistry) (0-6 ECTS)
  - Elective courses (IVb) (9–15 ECTS)
  - Research internship I (IVc) (9 ECTS)
- **Module V: Foreign language (3 ECTS)**
- **Module VI: International Intensive Course (24 ECTS)**
- **Module VII: Research Activity - Master Thesis (36 ECTS)**
  - Research Internship II (6 ECTS)
  - Master Thesis (30 ECTS).

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Annex A7. Staff employed in EMM-TCCM, classified by function (1 October 2014) (Chapter 3)

Function	Name staff member	Department/Division	FTE in institution	Number of credits to the training
Full professor				
	1 Nguyen Minh Tho	Chemistry/ Quantum Chemistry and Physical Chemistry	1	6
	2 Nies Erik	Chemistry/ Polymer chemistry and -materials	1	4.49
	3 Ceulemans Arnout	Chemistry/ Quantum Chemistry and Physical Chemistry	1	37.73
	4 Clays Koen	Chemistry/ Molecular Imaging and Photonics	1	6
	5 De Feyter Steven	Chemistry/ Molecular Imaging and Photonics	1	2.4
	6 De Maeyer Marc	Chemistry/ Biochemistry, Molecular and Structural Biology	1	2.11
	7 Harvey Jeremy	Chemistry/ Quantum Chemistry and Physical Chemistry	1	3
	8 Hofkens Johan	Chemistry/ Molecular Imaging and Photonics	1	1.4
	9 Lievens Peter	Physics/Solid State Physics and Magnetism	1	3
	10 Verbiest Thierry	Chemistry/ Molecular Imaging and Photonics	1	3
Professor				
	1 Pierloot Kristine	Chemistry/ Quantum Chemistry and Physical Chemistry	1	9.01
	2 Robben Johan	Chemistry/ Biochemistry, Molecular and Structural Biology	1	1.7
Associate professor				
	1 Hendrickx Marc	Chemistry/ Quantum Chemistry and Physical Chemistry	1	3
	2.Mizumo Hideaki	Chemistry/ Biochemistry, Molecular and Structural Biology	1	11.51
	3. Carl Shaun	Chemistry/ Quantum Chemistry and Physical Chemistry	1	3
	4 Cibotaru Liviu	Chemistry/ Quantum Chemistry and Physical Chemistry	1	7.26
Other				
	1 Matthijs Edward	TC Chemische Procestechn. Gent-Aalst	1	3
	2 Ivasenko Oleksandr	Chemistry/ Molecular Imaging and Photonics	1	1.2
	3 Vansweevelt Hans	Chemistry/ Quantum Chemistry and Physical Chemistry	1	5

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ALL STAFF CLASSIFIED BY GENDER AND AGE

NUMBERS		Gender		Age category					Total
		M	F	20-29	30-39	40-49	50-59	60 plus	
Senior academic staff		20	1	0	1	10	7	3	**21**
Junior academic staff	Research assistant	0	0	0	0	0	0	0	**0**
	Teaching assistant	0	0	0	0	0	0	0	**0**
	Postdoctoral assistant	0	0	0	0	0	0	0	**0**
Associate academic staff outside operating funds		9	4	7	5	1	0	0	**13**
Other (support and guidance)		0	0	0	0	0	0	0	**0**
TOTAL		**29**	**5**	**14**	**14**	**6**	**8**	**3**	**34**

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Annex A8: Changes made to TCCM educational program in the period 2012-2015 (Ch. 3)

Changes made by the ISC

The ISC supervises the organization of the ICs. During its annual meeting in Madrid, a report is presented on the previous IC. It includes feedback by the participants. Since the start of the TCCM program, the following changes have been made:

1) In view of the intensive character of the courses and the lack of study time during the lecture weeks, it was decided to schedule a free afternoon on Wednesdays, and to shift the weekly tests on Saturday to the next Monday morning (except for the final week where the test is rescheduled on Friday).

2) The quotation scheme for the Multiple Choice questions (which accounts for 20 % of the marks) was fine tuned to focus more on attention during the lectures rather than on acquired knowledge.

3) Also the homework study load and relevance was reconsidered.

The homework must reflect the four important subjects of IC: *i)* Advanced Electronic Structure and Condensed Matter, *ii)* Advanced Computational Techniques, *iii)* Chemistry and Molecular Dynamics and Simulation and Modelling, and *iv)* Applications.

Homework assignments were allocated to the lecturers accordingly. In previous editions all lecturers were invited to present homework, which often led to unequal distribution of work load and extensions beyond the deadline on December 1.

4) In the last two editions, a level test was organized in the beginning of the course. Students could fill it in anonymously. The purpose was to evaluate how well the objectives for the first master year were met.

In addition the ISC examines proposals for organization of workshops and winter schools that are of potential interest to TCCM students. When appropriate it issues recommendations to the partners to send students to these events. Since several years now the Université Paul Sabatier at Toulouse organizes a winter school on various aspects of theoretical chemistry and computational chemistry in the Pyrenées, France. This school is also sponsored by CECAM and attended by a majority of TCCM students.

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Changes made by the POC Chemie KU Leuven

Changes to the educational programs of chemistry at the KU Leuven are the responsibility of the Faculty of Science. The changes to the programs are prepared by the POC Chemie which are then proposed, evaluated and approved by the FPOC. A list of changes and actions relevant to the Educational program EM TCCM are presented below.

	Topic	Description	Who	Timing
1	***Quality Assurance*** Changes to education in response to comments of visitation of bachelor and Master of chemistry	Preparation and remediation of visitation comments on bachelor and master of chemie/chemistry programs	POC Chemistry, regular POC meetings	2011-2014 2015-
2	***Chem-E-Day*** biannual Educational day of the educational programs of chemistry	Organisation, planning, reporting of the results and actions of the Chem-E-Days, follow-up results and actions by POC	All lecturers , teaching assistants, large delegation of students (typically 5 per study year)	2012 2014 2016
3	***Professionalization*** Staff	"Hapje Onderwijs "	Educational staff of faculty, lecturers	2012, recurrent
4	***Quality Assurance*** Online evaluation	Online evaluations of the education (courses-lecturers evaluations)	POC Chemistry, Students	2012 2015 2016
5	***Quality assurance*** Online evaluation	Communication results online evaluation and follow-up on the results	Program director	2013 2016 ----
6	***Educational program*** Research Internship	Reorganise, make internship more research oriented (critical reflection)	POC Chemistry	2011-2012
7	***Professionalization*** New Staff	Information session for new ZAP staff	Faculty, onderwijsondersteuners, ZAP	2012 recurrent
8	***Professionalization*** Training	Training for teaching assistants	Faculty	2012 recurrent
9	***Quality Assurance/Improvement*** Evaluation policy	Evaluation criteria MSc thesis fully implemented in master programs	POC/Faculty	Active since 2012-2013
10	***Quality Improvement*** Bachelor research	Internal application for funding educational project Experimental skills attitudes and bachelor research	**POC-ad hoc subcommittee educational project**	2011-2012 2012-2013
12	***Quality Assurance*** Evaluation policy	Inventory evaluation forms	POC/FPOC	2012-203

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14	***Educational programs*** 3-6-9 initiatiative	Adapt the courses contents to match 3, 6 or 9 ECTS credits in the programs of bachelor 1, bachelor 2, bachelor 3, master 1, master 2	POC Chemistry preparation of program changes FPOC approve and activate in the programs	2012-2013 2013-2014
15	***Quality Assurance*** Study guide	Check of ECTS-fiches information	POC-subcommittee ECTS	2013-2014 2014-2015 2015-2016
16	***Evaluation policy*** Updating Evaluation policy	Develop and updated evaluation policy of educational programs	POC	2013-2014 2014-2015
19	***Quality Improvement*** Student hearings	Hearing concerning the learning track : experimental skills, attitude and bachelor research	POC-ad hoc subcommittee educational project	2014-2015
23	***Quality assurance*** Working procedures POC	Involve MSc of Chemistry and TCCM in a systematic and frequent manner in POC	Program director	2014-2015
24	***Quality improvement*** Learning tracks	Mapping OPO's on Learning tracks (response to the research visitation and the request of the division of quantum chemistry and physical chemistry)	POC-ad hoc subcommittee per bachelor learning track: Learning tracks Theoretical chemistry	2014-2015
25	***Educational program*** TCCM, MSc in chemie, Msc chemistry	Change in content Advanced computational chemistry	POC prepared changes, FPOC approved	2014-2015 Active since 2015-2016
26	***Educational program*** Bachelor program	Changes in tolerances in bachelor program for basic sciences (mathematics) in preparation for the course *Computationele chemie*	POC	2014-2015 Active since 2015-2016
27	***Educational program*** Bachelor program	Pre-knowledge changed for the course *Computationele chemie* to make the students better prepared for this course.	POC	2014-2015 Active since 2015-2016

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Annex A9. Regulations on Education and Examinations 2015-2016 (Chapter 4)

See the following KU Leuven webpage:

https://www.kuleuven.be/education/regulations/2015/

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Annex A10: List of TCCM master theses at KU Leuven and at partner institutions

(Chapter 4)

A) Theses at KU Leuven

2010-2012

1. NGUYEN Huyen Thi

Title: Computational study of conjugated polyelectrolytes and silole-based polymers

Promotor: Minh Nguyen, Copromotor: Ria Broer (Groningen)

Mark: 17.2

http://limo.libis.be/KULeuven:ALL_CONTENT:32LIBIS_ALMA_DS71169813560001471

2. PHUNG Manh Quan

Title: First-principles Study of Ruthenium Complexes Involved in Atomic Layer Deposition

Promotor: Kristine Pierloot, Co-promotor: Luis Seijo (Madrid)

Mark: 19.0

http://limo.libis.be/KULeuven:ALL_CONTENT:32LIBIS_ALMA_DS71169813470001471

3. HRSAK Dalibor

Title: Electronic Topology and Magnetic Interactions of Möbius Annulenes and Polyphyrins.

Promotor: Arnout Ceulemans, Co-promotor: M. Alcamí Pertejo (Madrid).

Mark: 17.2

http://limo.libis.be/KULeuven:ALL_CONTENT:32LIBIS_ALMA_DS71169813490001471

2011-2013

1. SMYRNOVA Daryna

Title: Molecular Dynamics and Hybrid Quantum Mechanics/Molecular Mechanics of Cis-Trans Isomerisation in Dronpa and mAG.

Promotor: Arnout Ceulemans, Co-promotor: Iñaki Tuñón (Valencia).

Mark: 16.2

http://limo.libis.be/KULeuven:ALL_CONTENT:32LIBIS_ALMA_DS71174076590001471

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2012-2014

1. YANG Hui

Title: Application of the Reactive Force Field Model, ReaxFF, to B_n Boron Clusters (n=2-6):

Parameterization and Structural Modeling

Promotor: Arnout Ceulemans and Minh Tho Nguyen; Copromotor: Ria Broer and Remco Havenith (Groningen)

Mark: 15.6

http://limo.libis.be/KULeuven:ALL_CONTENT:32LIBIS_ALMA_DS71177583920001471

2. SANZ Ana

Title: Is C_{50} a Superaromat? Evidence from Ring Currents and Electronic Structure.

Promotor: Arnout Ceulemans, Copromotor: Manuel Alcami (Madrid)

Mark: 17.0

http://limo.libis.be/KULeuven:ALL_CONTENT:32LIBIS_ALMA_DS71177581160001471

2013-2015

1. FURTADO Jonathan

Title: Broken-symmetry Two-component DFT Methodology for the Calculation of the Parameters of Ising Exchange Interaction in Strongly Anisotropic Magnetic Complexes

Promotor: Liviu Chibotaru, Co-promotor: Remco Havenith (Groningen)

Mark: 16.2

2. ENGELMANN Yannick

Title: Plasma-Enhanced Growth Mechanism of Titanium Dioxide Nanolayers

Promotor: A. Ceulemans, Copromotor: Patrice Raynaud (Toulouse)

Mark: 17.2

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B) A Selection of Theses at Partner Institutions (electronic versions available):

2010-2012

First Name	Family Name	Home University	Mobility	Thesis
Rodrigo	Perez Garcia	Groningen Prof. Ria Broer Dr. Remco Havenith	Perugia Prof. Antonio Laganà	PCBM Derivatives and Copolymer for Organic Photovoltaic Devices: Computational Modelling and Analysis
Daniel	Sethio	Groningen Dr. Remco Havenith Prof. Ria Broer	Leuven Dr. Steven Vancoillie Prof. Kristine Pierloot	Spin Crossover In $Fe^{II}(L)N(NCS)_2$ Complexes: A CASPT2 Study
Humberto	Silva	Madrid Dr. Sergio Díaz-Tendero Victoria	Toulouse Dr. Mathias Rapaciolli	1^{st}-Order Time-Dependent Perturbation Theory for Description of Charged Fullrene Fragmentation
Riccardo	Verzeni	Madrid Prof. Inés Corral Pérez	Porto Prof. Álvaro Cimas	MS-CASPT2 Study of the Low-Lying Electronic Excited States of Sulfur Dithiosubstituted Formic Acid Dimers
Alberto	Muzas	Madrid Dr. Cristina Díaz	Leiden Prof. Geert-Jan Kroes	Vibrational Deexcitation and Rotational Excitation of H_2 and D_2 Scattered from Cu(111): Adiabatic versus Non-adiabatic Dynamics
Dilara	Öksüz	Perugia Prof. Antonio Laganà Dr. Noelia Faginas Lago	Madrid Prof. Fernando Martin	Adsorption of Hydrogen Molecules on Carbon Nanotubes Using Quantum Chemistry and Molecular

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2011-2013

First Name	Family Name	Home University	Mobility	Thesis
Shehryar	Khan	Groningen Prof. Ria Broer Dr. Remco Havenith	Toulouse Dr. Isabelle Dixon	Theoretical Investigation of Novel Materials for Solar Cell Application
Rodrigo Hernan	Recabarren Hurtado	Groningen Dr. Alex de Vries	Valencia Prof. Iñaki Tuñón	Spectral Properties and Orientational Analysis of the Voltage-Sensitive Dye Annine-6 in Popc Bilayers
Dumitru-Claudiu	Sergentu	Groningen Prof. Ria Broer Dr. Remco Havenith	Valencia Dr. Daniel Roca-Sanjuan	Revisiting the Intersystem Crossing in Benzophenone
Habibur-rahman	Zulfikri	Groningen Prof. Ria Broer Dr. Remco Havenith	Toulouse Dr. Helene Bolvin Prof. Nathalie Guihery	Crystal-Field Parameters of Mononuclear Lanthanoid Sandwich Complexes
Kathy	Chen	Madrid Prof. Inés Corral Pérez	Toulouse Prof. Martial Boggio-Pasqua	Stereoisomeric Discrimination between Homo-/Heterochiral Metal-Chalcogen Complexes & Deactivation Pathways of 4-Thiouracil and 2,4-Dithiouracil
Dariusz	Pierkarski	Madrid Dr. Sergio Díaz-Tendero	Porto Prof. Maria João Ramos	Theoretical Study of the Stability and Fragmentation Dynamics of Neutral and Ionized Glycine, β-Alanine

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				and Clusters of β-Alanine in Gas Phase
Patricia	Vindel Zandbergen	Madrid Dr. Ignacio Sola Reija	Toulouse Dr. Christoph Meier	Applying Local Control Techniques to Single Electron Processes with Ultrafast Pulses
Md Musleh Uddin	Munshi	Perugia Dr. Filippo De Angelis Prof. Paola Belanzoni	Groningen Dr. Remco Havenith	Simulation of Structural, Electronic and Optical Properties of Cyclometalated Ru(Ii)-Complexes for Solar Cells Applications
Lucy	Cusinato	Toulouse	Groningen Prof. Ria Broer Dr. Remco W. A. Havenith	Magnetic Interactions in Organic-Inorganic Hybrid Copper Materials

2012-2014

First Name	Family Name	Home University	Mobility	Thesis
Riccardo	Alessandri	Groningen Dr. Remco W. A. Havenith Prof. Ria Broer	Toulouse Dr. Helene Bolvin Prof. Nathalie Guihery	What Determines the Ground State of Lanthanoid Sandwich Complexes: the Physics Behind the Crystal Field Parameters
Salma- haminati	Salma-haminati	Groningen Dr. Remco Havenith Prof. Ria Broer	Valencia Dr. Daniel Roca-Sanjuán	Photophysics and Photochemistry of Sunlight-Absorbing Amino Acids: a CASSCF/CASPT2 Study

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Azat	Gubay-dullin	Madrid Dr. Paula Riviere	Toulouse Prof. Christoph Meier	High Harmonic Generation From the H_2^+ Molecular Ion
Katerina	Leminsko	Madrid Prof. Merced Montero-Campillo Prof. Manuel Yáñez	Perugia Prof. Francesco Tarantelli	The Behavior of Carboxylic Acids upon Complexation with Beryllium Compounds
Sebastian	Brickel	Perugia Prof. Francesco Tarantelli	Toulouse Prof. Nathalie Guihéry	Excited State Description-Dressing the Con Guration Interaction Matrix Between Singly Excited Determinants under the Effect of Doubly and Triply Excited Determinants
Rami	Shafei	Perugia Dr. Andrea Lombardi Dr. Noelia Faginas Lago	Madrid Prof. Manuel Alcami Dr. Sergio Diaz Tendero	Solvation Structure of Na^+ and K^+ in Liquid Water and Ion-Water Clusters: Ab Initio and Molecular Dynamics Study
Juan	Sanz Garcia	Toulouse	Groningen Prof. Ria Broer Dr. Remco Havenith	Theoretical Analysis of the Environment Influence on the Photochromic Response of the Trans-$[RuCl(NO)Py_4](PF_6)_2 \cdot 1/2H_2O$ Crystalline Structure

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First Name	Family Name	University	Mobility	Thesis
Elena	Kusevska	Madrid Prof. Merced Campillo Prof. Manuel Yáñez	Leuven Prof. Minh Tho Nguyen	Global Optimization on the Potential Energy Surfaces of Small Boron Clusters, Doped by One or Two Vanadium Atoms. A Look at the Chemical Bonding
Andrés Felipe	Ordoñez	Madrid Prof. José Luis Sanz Vicario	Toulouse Prof. Christoph Meier	Plasma Screening Effects on the Electronic Structure of H_2^+ and H_2
Marcos	Cordones	Madrid Prof. Cristina Díaz Blanco	Leiden Prof. Geert-Jan Kroes	Theoretical Study of Noble Gases Diffraction from Ru(0001) Using Van Der Waals DFT-Based Potentials
Fedaa	Attana	Valencia Prof. Iñaki Tuñón Dr. Juan Aranda	Leuven Prof. Arnout Ceulemans Prof. Mathy Froeyen	Investigating the Molecular Mechanisms of Some DNA Methylation Inhibitors using Computational Tools
Meilani Kurniawati	Wibowo	Valencia Dr. Mercedes Rubio Dr. Daniel Roca-Sanjuán	Groningen Prof. Ria Broer Dr. Remco Havenith	The Photosensitizers Porphycene and Benzophenone: A RASPT2 Study

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Additional Annexes

Annex AdA1. List of KU Leuven EMM-TCCM SER Committee (Chapter 1)

Name	Function in KU Leuven	Function in TCCM SER Committee
Arnout CEULEMANS	Gewoon Hoogleraar Head Division of Quantum Chemistry and Physical Chemistry; Local Coordinator	Member
Jonathan FUTARDO	Student 2d Year EMM TCCM 2013-2015	Member (until July 2015)
Inge GROENINCKX	Educational Policy Department Staff	Member (until 1/5/2015; back from 1/10/2015)
Jeremy HARVEY	Gewoon Hoogleraar	Member
Marc HENDRICKX	Hoofddocent	Member
Minh Tho NGUYEN	Gewoon Hoogleraar	Faculty Coordinator Chair
Erik NIES	Gewoon Hoogleraar, Department Program Director Chair POC Chemie	Member
Iris PEETERS	Faculty of Science, Staff	Member (until 1/5/2015)
Kristine PIERLOOT	Hoogleraar	Member
Eszter Sarolta POS	Student, 1st Year EMM TCCM 2014-2016	Member
Phung QUAN	Ph D Candidate, Former TCCM student 2010-2012	Member
Inge SERDONS	Faculty of Science, Staff	Member (from 1/5/2015)
Daryna SMYRNOVA	Ph D Candidate, Former TCCM student 2011-2013	Member
Hans VANSWEEVELT	ATP, Computer Manager	Member
Alexandra VERHAGEN	Educational Policy Department, Staff	Member (from 1/5 to 1/10/2015)

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Annex AdA2: Criteria of the TCCM Consortium for Selection of Students (Chapter 1).

Erasmus Mundus Master Course in

THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

(EMMC TCCM)

Under the Framework Partnership agreement: 2010 - 0147

SELECTION CRITERIA

The selection process is made taking into account only excellence criteria.

The maximum qualification per student is 15 points, being each of the five following areas qualified up to 3 points (according to the standards detailed below).

Every area is evaluated according to the personal information filled in the online application form (corrected when needed based on the documents received) and the supporting documentation sent to us (motivation letter, curriculum vitae, academic records, academic degree, languages and other certificates and proof of nationality).

- *Applications lacking for more than 2 of the requested documents have been directly excluded.*
- *Applicants not complying with the 12-month rule have been relocated into Category B selection process.*
- *Applicants who manifested their intention to apply to more than 3 EM Master Courses or Joint Doctorates for an Erasmus Mundus grant, where warned of the upper limit of 3 applications per students and requested to explain if EMTCCM Master was among their choice.*

Area 1. The relationship of the degrees studied with the TCCM Master studies. (up to 3 points)

The following ranking is followed although the recommended mark may be corrected in case that the subjects listed in the academic record sent {contain more / does not contain all} the usual required subjects in a common Eurobachelor.

a. Chemistry, Physics, Material Science — 3 points

b. Chemical Engineering, Pharmacy, Biotechnology, Informatics, Mathematics, Materials Engineering, Electronics Engineering, and other related bachelors. — 2 points

c. Other (e.g., BEd, Cosmeceutics, Food Technology, ...) — 1 point

Area 2. The academic excellence, as shown in the academic record sent and/or by other awards received (up to 3 points)

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Area 3. The worldwide reputation of the institution of origin. (up to 3 points)

According with the ranking of the best 12000 universities of the world provided by the web http://www.webometrics.info/ :

University Ranking	*Points*
1-1000	3
1001-2000	2.75
2001-3000	2.5
3001-4000	2.25
4001-5000	2
5001-6000	1.75
6001-7000	1.5
7001-8000	1.25
8001-9000	1
9001-10000	0.75
10001-11000	0.5
11001-12000	0.25

Area 4. The continuity in studies and extra degrees. (up to 3 points)

Item 1. A consecution of academic achievements in accordance with the age of the student is favoured (BSc at 22-24 years old, MSc at 24-26, PhD at 26-28). Academic breaks; degrees taking more than the expected years to be concluded; and deviations from a research oriented career, are considered as a decrease in the excellence of the students. (up to 2 point)

Item 2. Extra academic achievements apart to the ones considered above. (up to 1 point)

Area 5. Extra activities. (up to 3 points)

Item 1. English level (up to 0,5 points)

Item 2. Other languages (up to 0,5 points)

Item 3. Chemistry packages know (up to 0,5 points)

Item 4. Programming skills (up to 0,5 points)

Item 5. Publications, posters, attendance to conferences (up to 0,5 points)

Item 6. References (up to 0,5 points)

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Annex AdA3. Program of the Intensive Course in Leuven–Groningen, September 2015

(Chapter 3)

In 2005, a consortium of 47 universities from 8 European countries has launched a European Master Course on Theoretical Chemistry and Computational Modelling (TCCM), under the coordination of the Universida Autónoma de Madrid, which aims at forming scientists able to address problems in modern science by the combination of the tools of Theoretical Chemistry and Computational Science.

This Master is structured in two years, equivalent to 120 ECTS credits. The first year (M1) is arranged locally at each member University, including courses that provide the student with the background required by the university and necessary to follow the second year of the Master (M2), which has a marked international research character.

The first part of the second year is an Intensive Course, that took place in the academic years

- 9th International Intensive Course - Toulouse, France - September 2014
- 8th International Intensive Course - Madrid, Spain - September 2013
- 7th International Intensive Course - Perugia, Italy - September 2012
- 6th International Intensive Course - Valencia, Spain - September 2011
- 5th International Intensive Course - Porto, Portugal - July 2010
- 4th International Intensive Course - Groningen, The Netherlands & Leuven, Belgium - Aug/Sept 2009
- 3rd International Intensive Course - Toulouse, France - September 2008
- 2nd International Intensive Course - Madrid, Spain - September 2007
- 1st International Intensive Course - Perugia, Italy - September 2006

For 2015-2016 it was again jointly organized in the University of Groningen and KU Leuven. This 10th IC was divided into two periods. From 30th August to 12th September 2015, the lectures were given in Leuven. On Sunday 13th September, all the participants were transferred by bus to Groningen for the second two-week period of the course.

Intensive Course Leuven/Groningen: Lectures

LEUVEN

Weeks 1 and 2 in Leuven address general aspects, covering the main TCCM categories. Each topic includes practical computer sessions and/or paper and pencil exercises.

Advanced Electronic Structure Theory
Single and multi-reference methods: Kristine Pierloot
Modern efficient and accurate approaches to electron correlation: David Tew
Wavefunction and bonding analysis: Manuel Yañez

Condensed Matter Theory
Introduction to solid-state electronic structure and properties. Liviu Cibotaru

Mathematical Methods in Chemistry
Group theory and topology, applied to vibronic coupling: Arnout Ceulemans

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Advanced Comptational Techniques
Introduction to structure of modern high-performance computers, and aspects of their use: Ingrid Barcena (HPC)

Applied Computational Chemistry
Molecular structure and reaction mechanisms: Minh-Tho Nguyen
Multi-scale chemical modelling: Jeremy Harvey (Harvey1)

Molecular and Chemical Dynamics
Introduction to time-dependent description of atomic motion, including classical molecular dynamics and Monte Carlo methods: Jeremy Harvey (Harvey2)

GRONINGEN

Weeks 3 and 4 in Groningen are devoted to advanced topics and applications. Each topic includes practical computer sessions and/or paper and pencil exercises.

Valence Bond Theory: Remco Havenith

Magnetic Interactions: Coen de Graaf

Transition-Metals: open shell and relativistic calculations: Hélène Bolvin

Spectroscopic methods: Wibren Jan Bruma

Solid state theory: Gilles de Wijs

Density Functional Methods: ADF/DFT Marcel Swart

Applications of TDDFT: Stener

Molecular Dynamics: Alex de Vries

Understanding biological systems with Kohn-Sham MO theory: Celia Fonseca Guerra

Supercomputing in Chemistry: Tjerk Straatsma

Ethics in Science: Beatriz Noheda

Theoretical/computational chemistry, quo vadis? Rutger Van Santen

Notes: - The total IC represents 24 ECTS credits.

- Evaluation is on the basis of tests during the course (20 %), and on homework assignments (80%), to be completed afterwards (submission deadline: 1 December 2015)

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Annex AdA4: 'Aims' and "Activities" of Master Thesis (Chapter 3)

cf. the webpage: http://wet.kuleuven.be/studenten/mastersthesis/objectives

Objectives of the master's thesis

As is the case with every programme unit, at the end of a master's thesis a list of objectives should be reached. These objectives are closely related to the attainment targets of the study programme. Therefore, the link with the rest of the programme is very important: which skills do students have when they start their master's thesis? What can be expected?
For the master's thesis the emphasis lies on competences of students to actively contribute to scientific research. At the Faculty of Science the following specific objectives are aimed for and evaluated:

- Formulating research questions with the help of the supervisor, and elaborating the research.
- Acquiring information independently and assessing its relevance for answering the research questions.
- Acquiring attitude to work on scientific research in a team (with colleague master students, PhD students,…).
- Learning to communicate in a scientific language through collaboration with fellow students and researchers.
- Following up and analysing developments in the chosen area, through training and by making contact with the current research in one of the areas.
- Using adequate experimental or theoretical methods and techniques.
- Critically analysing the results and their interpretation.
- Reporting and presenting the original results in an orderly way and placing the open questions in the right perspective. Linking techniques and results from literature as well as actual research and future research lines with the research.

In order to reach these objectives students should receive enough guidance without restraining their autonomy.

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Other related documents:

1) Master thesis concept note of the Faculty of Science

http://wet.kuleuven.be/studenten/mastersthesis/mastersthesisconceptnote

2) Faculty regulations for the master's thesis:

http://wet.kuleuven.be/reglement/MastersThesis

http://wet.kuleuven.be/studenten/mastersthesis/guidance#guidingteam

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Annex AdA5: Curriculum TCCM Madrid (Chapter 3)

ECTS Specification for the Module/Course Unit Descriptions

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Module 1

- Course title: Mathematics
- Course code: M1M
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: First semester
- Number of credits allocated (workload based): 4.5
- Objective of the course (expected learning outcomes and competences to be acquired): To acquire a good level in Linear algebra: vectorial spaces, dual spaces, vectors, matrices, Hilbert spaces. Special functions: Hermite polynomials, Legendre polynomials, Laguerre polynomials. Numerical analysis: numerical integration, discrete variable representation, B-spline functions, matrix diagonalization. Partial differential equations
- Prerequisites: Those to access the Master
- Course contents: Calculus of one and several variables. Linear algebra, including scalar products, linear operators, adjoint, hermitian, unitary, representation in a given basis and change of it, linear systems, algebraic eigenvalue equations
- Recommended reading:
  Numerical Recipes in Fortran 90, Cambridge University Press,
  http://www.nrbook.com/a/bookf90pdf.html
  Handbook of Mathematical Functions. M. Abramovich, I. A. Stegun. National Boureau of Standard, 1968
  Linear Algebra, Jim Hefferon. Mathematics. Saint Michael's College Colchester, Vermont USA 05439
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions and final written examination
- Language of instruction. That of the home Institution

- Course title: Molecular quantum mechanics
- Course code: M1MQM
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: First semester
- Number of credits allocated (workload based): 6
- Objective of the course (expected learning outcomes and competences to be acquired)
  To provide the students a sound knowledge on the basic ideas that govern molecular quantum dynamics and that will be required to achieve a good understanding of the most commonly used methods in quantum chemistry.
- Prerequisites: Those to access the Master
- Course contents: Foundations of quantum mechanics, angular momentum, group theory, perturbation theory, variational methods, atomic spectra and atomic structure, introduction to molecular structure, MO theory, electron correlation, molecular rotations

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and vibrations, molecular electronic transitions, electric and magnetic properties, scattering theory

- Recommended reading:
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions and final written examination
- Language of instruction. That of the home Institution

- Course title: Statistical Mechanics
- Course code: M1SM
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: First semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired): The goal sought by this course is to teach student how to apply to apply statistical ideas to the solution of problems involving both classical and quantum dynamics of molecular systems. The lectures will develop the methods of statistical mechanics systematically, and illustrate their application with numerous examples and applications to a number of carefully selected problems.
- Prerequisites: Those to access the Master
- Course contents: Basic concepts in statistical thermodynamics, distribution of states, internal energy and entropy, the canonical partition function, heat capacities, equations of state, equilibrium constants
- Recommended reading: Pippard, A. B., "The Elements of Classical Thermodynamics"(Cambridge University Press, London, 1957)
  Chandler, D., "Introduction to Modern Statistical Mechanics", (Oxford University Press, London, 1986)
  Toda, M., Kubo, R., Saito, N., "Statistical Physics I, (Spriger-Verlag, Heidelberg, 1992)
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions and final written examination
- Language of instruction. That of the home Institution

Module 2

- Course title: Programming and Numerical Methods
- Course code: M1PNM
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: First semester
- Number of credits allocated (workload based): 6

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- Objective of the course (expected learning outcomes and competences to be acquired) Advanced knowledge of scientific computer programming. To be able to read and modify ab initio codes in FORTRAN. To be able to develop new algorithms for codes in FORTRAN
- Prerequisites: Those to access the Master
- Course contents: Basic Fortran 90/95. Numerical integration. Rudiments of integral equations and their numerical resolution. Nonlinear equations
- Recommended reading:
  W. Press, B. P. Flannery, S. A: Teukolsky, W. T. Vetterling, "Numerical Recipes. The Art of Scientific Computing". Cambridge University Press, New York, 1986.
  J. Andrés, J. Bertrán, Eds. "Química Teórica y Computacional". Universitat Jaume I, Castellón, 2000
- Teaching methods: Lectures. Practical sessions in the computational laboratory. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Evaluation of the codes produced by the student.
- Language of instruction. That of the home Institution

Module 3

- Course title: Group Theory
- Course code: M1GT
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired) Development of the theory of finite groups and group representations. To be able to use symmetry to understand select properties: electric dipole moment, chirality, bonding through molecular orbital diagrams, spectroscopic properties. Introduction to SU(2) and the rotation group. Double groups and spin-orbit interactions. Crystal symmetry: crystallographic point groups, Bravais lattices and space groups.Prerequisites: Those to access the Master
- Course contents: Point Groups. Irreducible representations. Continuous and special groups. Tensors. Applications
- Recommended reading:
  P.R. Bunker, and P. Jensen, Fundamentals of Molecular Symmetry (Bristol: Institute of Physics, 2005).
  J. S. Ogden, Introduction to Molecular Symmetry (Oxford U.P., 2001)
  F. A. Cotton, Chemical Applications of Group Theory (Wiley, 1990)
  P.R. Bunker, and P. Jensen, Molecular Symmetry and Spectroscopy (Ottawa: NRC Research Press, 1998).
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions

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- Assessment methods: Continuous evaluation through weekly tutorial sessions. Final written examination
- Language of instruction. That of the home Institution

- Course title: Basic Spectroscopy
- Course code: M1S
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired). To provide the students with basic concepts in molecular spectroscopy, both from experimental and theoretical viewpoints. At the end of the course the student should be able to understand the differences between basic types of spectroscopy involving electronic, vibrational, and rotational degrees of freedom, to extract relevant information from experimental sources, and apply the essential quantum chemical models to the solution of the spectroscopic problems, in particular to absorption and emission spectra.
- Prerequisites: Those to access the Master
- Course contents: Radiation-matter interaction. Time-dependent Schroedinger equation. Rotational, vibrational, and ro-vibrational spectroscopies. Raman. Electronic spectroscopy. Lasers
- Recommended reading:
  J. L. McHale, *"Molecular Spectroscopy"*, Prentice Hall, Upper Saddle River, 1999.
  A. Requena, J. Zúñiga. "*Espectroscopía*", Proentice Hall, Madrid, 2004
  M. Diem, *"Introduction to Modern Vibrational Spectroscopy"*, Wiley, 1993.
  D. L. Andrews and A. A. Demidov, *"An Introduction to Laser Spectroscopy"*, Springer, 2002.
  N. J. Turro, *"Modern Molecular Photochemistry"*, University Science Books, Sausalito, 1991.
  Eds. P. Jensen and P. R. Bunker, *"Computational Molecular Spectroscopy"*, Wiley, Chichester, 2000.
  Ed. M. Olivucci, *"Computational Photochemistry",* Elsevier, Amsterdam, 2004.
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Final written examination
- Language of instruction. That of the home Institution

- Course title: Basic Reaction Dynamics
- Course code: M1RD
- Type of course: C
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 4.5
- Objective of the course (expected learning outcomes and competences to be acquired) A detailed understanding of how the nuclear motion governs the

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chemical reactions, what are the energy requirements for a chemical reaction to occur, what happens when reactant molecules meet, how the energy is redistributed among the different degrees of freedom, what factors determine the reaction rates and, finally, how to control chemical function through dynamics

- Prerequisites: Those to access the Master
- Course contents: Potential Energy Surfaces. Collision Theory. Semiclassical methods. Wavepackets. Transition State Theory. Quantum Effects. Rate constants
- Recommended reading: J.I. Steinfeld, J.S. Francisco and W.L. Hase, "Chemical kinetics and dynamics", Prentice Hall, New Jersey, USA, 1999, second ed.
  R. Levine. “Molecular Reaction Dynamics.” Cambridge University Press. Cambridge (UK). 2005
  Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Final written examination
- Language of instruction. That of the home Institution

Module 4

Levelling Course

As indicated in the application in the levelling course we have three different modules of 6 ECTS credits each and with the following contents:

Levelling module in Mathematics:

Linear Algebra. Scalars and vectors. Vector spaces and linear dependence. Matrices and determinants. Integrals. Integral theorems. Vector fields. Differential equations. Partial differential equations.

Levelling module in Physics:

Kinematics. One-particle dynamics. Energy and work. Thermodynamics. Classical oscillators. Dynamics of many-body systems and solids. Gravitation. Wave mechanics. Electric field. Gauss law. Electric potential. Maxwell equations. Optics.

Levelling module in Chemistry:

Notions of atomic and molecular structure. Chemical bonding. Transition metal complexes. Crystal field theory. Chemical equilibrium. Acids and bases. Aqueous equilibria. Elements of chemical kinetics. Organic chemistry: hydrocarbons and functional groups. Biochemistry

Semioptional disciplines

- Course title: Fundamentals of Solid State Chemistry
- Course code: M1SSC
- Type of course: E
- Level of course: Basic
- Year of study: First year

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- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired): To provide the students with basic methodology to treat periodic systems, crystals and polymers.
- Prerequisites: Those to access the Master
- Course contents: Finite models. Covalent and Ionic crystals, Metals. Periodic Models. Bloch Theorem. Bands theory. Applications
- Recommended reading: C. Kittel. "Introducción a la Física del Estado Sólido". 3º Ed., Reverté, Barcelona, 19993.
  P. Fulde, "Electron correlations in molecules and solids", Solid-State Science, Springer Verlag, Berlin, 1995
  J.L. Whitten and H. Yang, "Theory of Chemisorption and reactions on metal surfaces" Surf. Sci. rep. 24, 59 (1996)
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Elaboration of periodic reports
- Language of instruction. That of the home Institution

- Course title: Simulation Techniques and Molecular Modelling
- Course code: M1SSC
- Type of course: E
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired): To provide the students with basic ideas related to intermolecular interactions, molecular mechanics and quantitative structure-activity relationships.
- Prerequisites: Those to access the Master
- Course contents: Intermolecular Forces. Long range. Short range. Hydrogen bonding. Non-pairwise additivity. Foundamentals of molecular mechanics. Force fields (MM3, AMBER, CHARMM…), QSAR relationships. Validation of QSAR models. Solvation.
  Recommended reading: A.R. Leach, "Molecular Modelling. Principles and Applications". Logman, Essex, 1996.
  R.W. Hockney and J.W. Eastwood, "Computer simulations using particles" McGraw-Hill, New York, 1981
  D. Frenkel and B. Smit, "Understanding molecular simulation" Academic Press, San Diego, 1996
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Elaboration of periodic reports
- Language of instruction. That of the home Institution

- Course title: Ionization and dissociation by ultrashort laser pulses

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- Course code: M1IDL
- Type of course: E
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired): Methods to treat the electronic molecular continuum; the role of the vibrational motion in the ionization process; control of molecular response by using ultrashort pulses.
- Prerequisites: Those to access the Master
- Course contents: Laser-matter interaction. Perturbation methods. Discretized continuum methods. B-splines basis functions. The vibrational continuum. Resonant states.
- Recommended reading: Bachau H, Cormier E, Decleva P, Hansen J E and Martín F 2001 *Rep. Prog. Phys.* **64** 1815; Martín F 1999 *J. Phys. B (Topical Review)* **32** R197
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Elaboration of periodic reports
- Language of instruction. That of the home Institution

- Course title: Heavy elements, effective core potentials, and embedding.
- Course code: M1ECP
- Type of course: E
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired): After the course, the students should be able: to identify when and what relativistic effects are necessary in electronic structure calculations, to know the basics of the methods that include them, to know the basics and details of non-relativistic and relativistic effective core potential methods and to use them, to identify when embedding effects are necessary, and to know and use embedding methods.
- Prerequisites: Those to access the Master
- Course contents: Introduction to relativistic quantum chemistry. Effective core potentials. Relativistic effective potentials. Embedding methods and embedding potentials.
- Recommended reading: Introduction to Relativistic Quantum Chemistry, K. G. Dyall and K. Faegri, (Oxford Univ. Press, USA, 2007); Computational Chemistry: Reviews of Current Trends, Vols. 1 and 4, edited by J. Leszcynski, (World Scientific, Singapore, 1999); Introduction to Computational Chemistry, F. Jensen, (Wiley, Sussex, 1999).
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Elaboration of periodic reports

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- Language of instruction. English or that of the home Institution

- Course title: Chaos theory. Fundamentals and applications
- Course code: M1CT
- Type of course: E
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired): Basic skills to recognize chaotic behaviour in dynamical systems and mathematical ways to analyze it. Use of the Kolmogorov-Arnold-Moser theorem as the fundamental tool for the analysis of generic systems in Chemical Physics. Relation between dynamics and spectroscopy through Fourier transform between correlation function and spectra. Computation and analysis of vibrational excited states in small polyatomic molecules
- Prerequisites: Those to access the Master
- Course contents: Deterministic Chaos. Lyapunov's exponent and other chaos indexes. Logistic Maps. Stability and bifurcations. Chaos in continuous systems. Attractors. Fractals. Applications to the dynamics of vibrational excited states and infrared spectroscopy.
- Recommended reading: Lieberman and Lichtenbeg, *Regular and Stochastic Motion* (Springer, NY, 1983); Letokhov, *Laser Spectroscopy of Highly Vibrationally Excited Molecules* (Adam Hilger, Bristol, 1989).
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Elaboration of periodic reports
- Language of instruction. That of the home Institution

- Course title: Modelling processes of interest in atmospheric chemistry and astrochemistry
- Course code: M1AC
- Type of course: E
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 3
- Objective of the course (expected learning outcomes and competences to be acquired) : To learn how to simulate vibrational and rotational spectra and to obtain the thermodynamic state functions (S, G...).To know the basic techniques necessary to model processes in the atmosphere: evaluation of Potential Energy Surfaces (PES) for reactions in the atmosphere, localization of reaction intermediates, transition states and calculation of the intrinsic reaction coordinates. To become familiar with the intrinsic problems due to the existence of states either of the same or different spin multiplicities and with the evaluation of conical intersections and intersystem crossings. To learn how to calculate rate constants using the information contained in the PES.

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- Prerequisites: Those to access the Master
- Course contents: High-level ab initio methods for the evaluation of thermodynamic properties. Potential energy surfaces evaluation. Spin-orbit coupling. Conical intersections. Evaluation of rate constants. Applications in atmospheric chemistry and astrochemistry.
- Recommended reading:
    - Computational Molecular spectroscopy. P. Jensen and P. Bunker. John Wiley and Sons. 2000
    - Atmospheric Chemistry and Physics. J.H. Seinfeld and S.N. Pandis. John Wiley and Sons. 1998
    - Unimolecular Reactions: A Concise Introduction, W. Forst, Cambridge University Press, 2003
- Teaching methods: Lectures. Problem-solving classes. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Elaboration of periodic reports
- Language of instruction. That of the home Institution

- Course title: UNIX and LINUX system managing
- Course code: M1UNIX
- Type of course: E
- Level of course: Basic
- Year of study: First year
- Semester/trimester: Second semester
- Number of credits allocated (workload based): 5
- Objective of the course (expected learning outcomes and competences to be acquired) **:** The aim is to get a knowledge about system management in complex servers based in different flavours of Unix operating systems (Including Linux, which is becoming very popular) . This management knowledge includes daily operations, security hints, and the procedures needed to assure high availability of servers.
- Prerequisites: Those to access the Master
- Course contents: Unix Language Systems. Different types of UNIX systems. Fundamental commands. Vi editor. Fundamental aspects of the UNIX management system.
- Recommended reading:
- 1) Unix system administration handbook. Evi Nemeth, Garth Snyder, Scott Seebass, Trent R. Hein. Ed. Prentice Hall, 2001.
  2) Unix Power tools. Jerry Peek, Tim. Ed. O'Reilly, Mike Loukides. O'Reilly 1997.
- Teaching methods: Lectures. Practical work in the drylab of the Centro de Computación Científica de la UAM. Tutorial sessions
- Assessment methods: Continuous evaluation through weekly tutorial sessions. Practical examination on Unix system management.
- Language of instruction. That of the home Institution

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Annex AdA6. Form for the Final Evaluation of Research Internship (Chapter 4)

Student – intern
Name: ______________________________
First name: ______________________________
Student number: ______________________________

Laboratory
Name: ______________________________
Promoter: ______________________________
Mentor: ______________________________
Supervisor: ______________________________

	excellent	very good	good	average	fair	unsatisfactory	not applicable
Quantity of work							
Quality of work							
Independance							
Efficiency							
Initiative							
Degree of knowledge							
Critical analysis							
Proper use of logbook or electronic notebook							
Safety and environmental consciousness							
Verbal communication skills							
Quality of weekly reports							
Collaboration with superiors, colleagues…							
Account of points raised in mid-term evaluations							
Final presentation							

Global impression							

*Depending on the evaluator some criteria may be not/insufficiently applicable

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Evaluation Result

…./20

Scale:

Excellent	18-20	The mean score is 14/20.
Very good	16-17	Scores above should have a
Good	14-15	justifiable higher quality!
Fair to average	10-13	Scores from 18/20
Unsatisfactory	< 10	are very exceptional.

The evaluation result is not communicated to the student until after the deliberation.

Remarks and motivation evaluation result

Completed by

Name: ______________________________

Function: ______________________________

Date: ______________________________

Signature: ______________________________

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Annex AdA7. Selection of Research Project for Master Theses (Chapter 4)

Two main selections concern each master thesis, namely, the setting up of a research project and the choice of a partner laboratory where the student will compulsorily spend three months.

At the KU Leuven, the list of proposals for theses is made available to the students during the course of the second semester of Y1. The Standing Committee also has offered research subjects, with suggestions for joint studies. A student can also propose an own research project after consulting a suitable promoter.

After selecting a research subject at the end of Y1, the student discusses with the promoter about the stay abroad. Students receive information about research projects from local professors, central and partner webpages, or mostly during the IC where they can talk to their fellow students. When staying in a partner group, a student can continue the home research project. An obvious advantage is that with a new supervisor, a new approach or a new method can possibly be applied. The same research project can then be performed under a new eye. The student can also choose a project which differs from his/her home project. An advantage is that the student can enter a new field. In practice, each Y2 student starts carrying out research work from early October, after the IC, during an internship (6 ECTS, see above). The 3-month stay in a partner laboratory spans during the period from February to May of the following year, in such a way that the student can write up the thesis, and present it at the end of June or early July. During this stay, the student is fully supervised by the partner staff, but in regular contact with the home promoter.

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Annex AdA8:
Thesis assessment roster: supervisor

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Educational programme:

Name student:

Name examiner:

Title master's thesis:

Date defence:

	Insufficient	Weak	Moderate	Good	Very good	Excellent	not applicable
PROCESS *(supervisor/cosupervisor)*							
Planning / organisation / regularity							
Effort / willingness to learn							
Scientific attitude							
Independence / self-criticism							
Insight							
Problem solving ability							
Functioning in team							
Health, Safety and Environment (HSE)							
CONTENT *(readers + supervisor/cosupervisor)*							
Introduction and problem statement							
Research method / scientific character							
Argumentation							
Results: discussion / interpretation							
General conclusion							
Coherence / logical composition							
Originality / creativity / depth							
References							
FORM *(readers + supervisor/cosupervisor)*							
Layout / structure / readibility							
Tables / figures							
Language / spelling / style							
Size (within directive programme)							
DEFENCE *(consensus defence committee)*							
Presentation: used language							
Presentation: content / accessibility							
Presentation: form / composition / timing							
Answering questions: correctness / insight							
Answering questions: self-criticism							

GLOBAL MOTIVATION

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Mark of supervisor: /50 (integer number)

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Annex AdA9:
Thesis assessment roster: assessor

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	Educational programme:
	Name student:
	Name examiner:
Date defence:	Title master's thesis:

	Insufficient	Weak	Moderate	Good	Very good	Excellent	not applicable
PROCESS *(supervisor/cosupervisor)*							
Planning / organisation / regularity							
Effort / willingness to learn							
Scientific attitude							
Independence / self-criticism							
Insight							
Problem solving ability							
Functioning in team							
Health, Safety and Environment (HSE)							
CONTENT *(readers + supervisor/cosupervisor)*							
Introduction and problem statement							
Research method / scientific character							
Argumentation							
Results: discussion / interpretation							
General conclusion							
Coherence / logical composition							
Originality / creativity / depth							
References							
FORM *(readers + supervisor/cosupervisor)*							
Layout / structure / readibility							
Tables / figures							
Language / spelling / style							
Size (within directive programme)							
DEFENCE *(consensus defence committee)*							
Presentation: used language							
Presentation: content / accessibility							
Presentation: form / composition / timing							
Answering questions: correctness / insight							
Answering questions: self-criticism							

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Mark of assessor: /15 (integer number)

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Annex AdA10: 1/2

Appreciation scale master's thesis Faculty of Science

18-20	"Excellent work" **PROCESS** The research was lead independently based on the ability to gain insight and solve problems. Only minor things had to be added and the communication with the involved team was very fertile/excellent. **CONTENT** The research question and the analysed research have the scientific quality of a publication or are of original quality. The methods and techniques were used adequately, the results are valid and reliable and are analysed very critically. The findings are perfectly related with actual research and proposed future research steps are highly relevant. The whole can be considered as "state of the art". **FORM** Fulfills the highest standards of the field. **DEFENCE** The research was presented in a highly structured and coherent way with the use of the correct terminology. The questions were answered very clearly and correctly and were approached in a very critical way.
16-17.9	"Very good work" **PROCESS** After a growing phase the research was lead independently with a very high ability to gain insight and solve problems. The communication with the involved team was very good. **CONTENT** The research question and the analysed research have a high scientific quality. The methods and techniques were used adequately, the results are valid and reliable and are analysed very critically. The findings relate well with actual research and the proposed future research steps are relevant. **FORM** Possibility for very minor revision. **DEFENCE** The research was presented in a structured and coherent way with the use of the correct terminology. The questions were answered clearly and correctly and were approached in a very critical way.
14-15.9	"Good work" **PROCESS** When enough guidance was foreseen the research was lead relatively independently, with a sufficient ability to gain insight and solve problems. The communication with the involved team was good. **CONTENT** The research question and the analysed research have an acceptable scientific quality. The methods and techniques were used adequately, the results seem valid and reliable and are analysed critically. The findings relate well with actual research and the proposed future research steps were relevant, however for (at least one of) both some issues were neglected. **FORM** Possibility for minor revision. **DEFENCE** The research was presented in a relatively structured and coherent way with a few incorrect usages of terminology. The questions were answered pretty clearly and predominantly correct and were approached in a critical way.

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ISSN: 2279-8773

VIRT&L-COMM.9.2016.1

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Appreciation scale master's thesis Faculty of Science

12-13.9	"Moderate work" **PROCESS** The research was lead with a lot of guidance, with a very moderate ability to gain insight and solve problems. Most of the time the communication with the involved team was good. **CONTENT** The research question and the analysed research have a moderate scientific quality. The methods and techniques were used adequately most of the time, most of the results seem valid and reliable and are analysed critically. The findings relate in a limited way with actual research and proposed future research steps are mostly relevant, however for (at least one of) both some crucial issues are neglected. **FORM** Possibility for moderate revision. **DEFENCE** The research was mostly presented relatively structured and in a coherent way but with incorrect usages of terminology. Most of the time most questions were answered correctly and were approached in a critical way.
10-11.9	"Weak work" **PROCESS** The research was lead with guidance given throughout, with a deficient ability to gain insight and solve problems. The communication with the involved team was not always good. **CONTENT** The research question and the analysed research have a minimal scientific quality. The methods and techniques were not always used adequately, the results don't always seem valid and reliable and are not analysed very critically. The findings relate in a limited way with actual research and proposed future research steps are not always relevant, however for both some crucial issues are neglected. **FORM** Major revision is necessary. **DEFENCE** The research was not always presented in a structured and coherent way and with many incorrect usages of terminology. The questions were not always answered correctly and were not approached in a critical fashion.
6-9.9	"Insufficient work" **PROCESS** The needed guidance was out of proportion, with no ability to gain insight and solve problems. The communication with the involved team was not good. **CONTENT** The research question and the analysed research have a a lack of scientific quality. The methods and techniques were insufficiently adequately used, the results are not very valid and reliable and are analysed insufficiently critically. The findings relate insufficiently with actual research and proposed future research steps are not relevant. **FORM** Major revision is necessary. **DEFENCE** The research was not presented in a structured and coherent way and had many incorrect usages of terminology. Most questions were answered incorrectly and were not approached in a sufficiently critical fashion.

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ISSN: 2279-8773