EDUCATIONAL ASSESSMENT
Theoretical Chemistry and Computational Modelling

An evaluation of the quality of the Erasmus Mundus Master of Science in Theoretical Chemistry and Computational Modelling

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vluhr

EDUCATIONAL ASSESSMENT
THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

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PREFACE BY THE VLUHR QA BOARD

The assessment panel reports its findings on the Erasmus Mundus Master of Science in Theoretical Chemistry and Computational Modelling. This programme is assessed in the spring of 2016 on behalf of the Flemish Higher Education Council (VLUHR).

First of all, this report is intended for the programme involved. This assessment report provides the reader a snapshot of the quality of the programme and is only one phase in the process of the ongoing concern for educational quality. After a short period of time the study programme may already has changed and improved significantly, whether or not as an answer to the recommendations by the assessment panel. Additionally, the report intends to provide objective information to a wide audience about the quality of the evaluated programme. For this reason, the report is published on the VLUHR website.

I would like to thank the chairman and the members of the assessment panel for the time they have invested and for the high levels of expertise and dedication they showed in performing their task. This assessment is made possible thanks to the efforts of all those involved within the institution in the preparation and implementation of the assessment site visit.

I hope the positive comments formulated by the assessment panel and the recommendations for further improvement provide justification for their efforts and encouragement for the further development of the study programme.

Nik Heerens
Chair VLUHR QA Board

SECTION 1
General Section

PART I
Educational assessment Theoretical Chemistry and Computational Modelling

1 INTRODUCTION

In this report, the assessment panel Theoretical Chemistry and Computational Modelling publishes its findings regarding the Erasmus Mundus Master of Science in Theoretical Chemistry and Computational Modelling. This programme was assessed in the spring of 2016 on behalf of the Flemish Higher Education Council (VLUHR).

This assessment procedure is part of the VLUHR activities in the domain of external quality assurance in Flemish higher education, which is designed to ensure that Flemish universities, university colleges and other statutory registered higher education institutions are in compliance with the relevant regulatory framework.

2 THE ASSESSED STUDY PROGRAMME

In accordance with its mission, the assessment panel visited the Master of Science in Theoretical Chemistry and Computational Modelling organised by KU Leuven, together with Universidad Autónoma de Madrid, Spain (coordinating institution); Rijksuniversiteit Groningen, The Netherlands; Università degli Studi di Perugia, Italy; Universidade do Porto, Portugal; Université Paul Sabatier - Toulouse III, France and Universitat de Valencia, Spain. The assessment panel visited the study programme from 19th till 20th of May 2016.

3 THE ASSESSMENT PANEL

3.1 Composition of the assessment panel

The composition of the assessment panel was ratified on October 12th, November 10th and 10 December 10th 2015 by the VLUHR Quality Assurance Board. The NVAO sanctioned the panel composition on January 18th, 2016.

The assessment panel was composed in the following way:

– Chairman of the assessment panel:
  - **Prof. dr. Gilberte Chambaud**, professor, University Paris-Est Marne la Vallée, France

– Other panel members:
  - **Prof. dr. Sir David C. Clary**, professor, Department of Chemistry, Oxford University, United Kingdom
  - **Prof. dr. Benedetta Mennucci,** professor, Department of Chemistry, University of Pisa
  - **Mr. Thijs Stuyver**, master of Science in chemistry (molecular and macromolecular design, 2014) and Ph.D. student at the Free University of Brussels (Vrije Universiteit Brussel)

Mr. Patrick Van den Bosch, staff member of the Quality Assurance Unit of the Flemish Higher Education Council is project manager of this educational assessment and acts as secretary to the assessment panel.

The brief curricula vitae of the members of the assessment panel are listed in Appendix 1.

3.2 Task description

The assessment panel is expected:
– to express substantiated and well-founded opinions on the study programme, using the assessment framework;
– to make recommendations allowing quality improvements to be made where possible;
– to inform society at large of its findings.

3.3 Assessment Process

3.3.1 Preparation

The study programme was asked to compile a self-evaluation report in preparation for the educational assessment. An assessment protocol, with a detailed description of the expectations regarding the content of the self-evaluation report, was presented by the Quality Assurance Unit of VLUHR for this purpose. The self-evaluation report reflects the accreditation framework.

The assessment panel received the self-evaluation reports some months before the on-site assessment visit, which allowed for adequate time to study the document and to prepare for the assessment visit. The members of the assessment panel were also asked to read a set of recent Master's theses for the study programme before the site visit took place.

The assessment panel held its preparatory meeting on February 22th, 2016. During this meeting, the panel members were given further information about the assessment process and they made specific preparations for the forthcoming on-site assessment visit. Special attention was given to the uniformity of the implementation of the accreditation framework and the assessment protocol. The self-evaluation reports were collectively discussed and the interviews were prepared.

3.3.2 On-site visit

During the on-site visit the panel interviewed all stakeholders directly involved with the study programme. The panel spoke with those responsible for the study programme, students, teaching staff, educational support staff, alumni, and representatives from the professional field. The conversations and interviews with all these stakeholders took place in an open atmosphere and provided the panel with helpful information to and clarifications of the self-evaluation report.

The panel visited the programme-specific facilities, including the library, classrooms, and computer facilities. There was also a consultation hour during which the assessment panel could invite people or during which people could come and be heard in confidence.

Furthermore, the programme was asked to prepare a wide variety of documents to be available during the on-site visit for the assessment

panel to consult as a tertiary source of information. These documents included minutes of discussions in relevant governing bodies, a selection of study materials (courses, handbooks and syllabuses), indications of staff competences, testing and assessment assignments, etc. Sufficient time was scheduled throughout the assessment visit for the panel to study these documents thoroughly. Additional information could be requested during the on-site visit if the assessment panel deemed that information necessary to support its findings.

Following internal panel discussions, provisional findings were presented by the chairman of the assessment panel in conclusion of the on-site assessment visit.

3.3.3 Reporting

The last stage of the assessment process was the compilation of the panel's findings, conclusions, and recommendations into the present report. The panel's recommendations are separately summarised at the end of the report.

The study programme had the opportunity to reply to the draft version of this report. The assessment panel considered this response and when deemed appropriate included elements of it into the final version.

PART II
Table with scores

The following table represents the assessment scores of the assessment panel on the two standards as formulated in the assessment framework.

For each standard the panel expresses a considered and substantiated opinion, according to a two-point scale: satisfactory or unsatisfactory. The panel also expresses a final opinion on the quality of the programme as a whole, also according to a two-point scale: satisfactory, unsatisfactory or satisfactory for a limited period.

In the report of the study programme the assessment panel makes clear how it reached its opinion. The table and the scores assigned ought to be read and interpreted in connection to the text in the report. Any interpretation based solely on the scores in the table, is unjust towards the study programme and passes over the assignment of this external assessment exercise.

Explanation of the scores of the **standard**:

Satisfactory (S)	The study programme meets the standards.
Unsatisfactory (U)	The standard is unsatisfactory.

Rules applicable to the final **opinion**:

Satisfactory (S)	The final opinion on a programme is 'satisfactory' if the programme meets all standards.
Unsatisfactory (U)	The final opinion on a programme – or a mode of study – is 'unsatisfactory' if all standards are assessed as 'unsatisfactory'.
Satisfactory for a limited period (S')	The final opinion on a programme – or a mode of study – is 'satisfactory for a limited period' , i.e. shorter than the accreditation period, if, on a first assessment, one or two standards are assessed as 'unsatisfactory'.

	Standard 1 Targeted Outcome Level	Standard 2 Educational Learning Environment	Standard 3 Outcome Level Achieved	Final Opinion
Master of Science in Theoretical Chemistry and Computational Modelling	S	S	S	S

SECTION 2
Assessment report

KU LEUVEN*
Master of Science in Theoretical Chemistry and Computational Modelling

*** TOGETHER WITH UNIVERSIDAD AUTÓNOMA DE MADRID, SPAIN (COORDINATING INSTITUTION); RIJKSUNIVERSITEIT GRONINGEN, THE NETHERLANDS; UNIVERSITÀ DEGLI STUDI DI PERUGIA, ITALY; UNIVERSIDADE DO PORTO, PORTUGAL; UNIVERSITÉ PAUL SABATIER - TOULOUSE III, FRANCE AND UNIVERSITAT DE VALENCIA, SPAIN**

SUMMARY OF THE ASSESSMENT REPORT
Master of Science in Theoretical Chemistry and Computational Modelling

From 19th till 20th of May 2016, the Master of Science in Theoretical Chemistry and Computational Modelling has been evaluated in the framework of an educational assessment by a peer review panel of independent experts. In this summary which describes a snapshot, the main findings of the panel are listed.

Profile of the programme

The TCCM programme at KU Leuven follows both European and local regulations and duties. The organization is monitored by an ISC (International steering Committee), with one representative from each consortium university. The ISC meets annually. It has full responsibility regarding the admission policy and selection of students. Every year the programme has approximately 120 applicants. The 50 best students will be selected. Most students receive a scholarship to participate in the programme.

The tasks of ISC also include analysis of student feedback, organization of IC, and quality review reports to the Education, Audiovisual and Culture Executive Agency, European Commission (EACEA). The grants are managed by the international coordinator. The programme at KU Leuven is the responsibility of the Faculty of Science POC (Permanente

Onderwijscommissie), which delegates to the chemistry POC the responsibility to monitor the TCCM, to define solutions for problems with the programme as a whole or with specific courses in particular, to prepare changes to the educational programmes, to implement approved changes and to monitor and improve the quality of the programme.

It is the aim of the TCCM master that at the end of the two years study programme the students will have acquired the following skills: a deep knowledge and understanding of theoretical chemistry and simulation techniques and their applications; the ability to use these techniques and applications 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 programme specific learning outcome targets match the current programme content requirements as they are established internationally by discipline specialists and professionals. Bringing together the best staff and students in a specific domain from different universities across Europe is the main asset of TCCM.

Programme

TCCM is a two years master programme organized by KU Leuven and six partner universities, coordinated by Universidad Autónoma de Madrid, Spain. The general structure of the programme is organized around seven modules. In the first year (Y1) the programme management wants to bring bachelor graduates from a variety of related disciplines to a good basic knowledge of theoretical and computational chemistry and its applications. In the second year (Y2), students take part in the common Intensive Course (IC). Finally the programme provides to deepen the students' knowledge through research training. During the first year (Y1), each student follows courses in his or her home institution, whereas in year two (Y2), the whole cohort assembles for a joint international Intensive Course. Later, each student carries out a research stay in a laboratory, which must be based outside their home institution and country.

The content of the programme is very broad ranging from theoretical and computational chemistry applications in physics, biology and materials science. It starts off with fairly elementary material as the students have a very varied background and are from many countries. The levelling courses

help students to catch up. Students have to learn a foreign language. It is a common complaint of students that the workload is very high during the IC. The students are in favour to extend the IC from 4 to 6 weeks.

During the two years, the students have the opportunity to develop international relations. In the first year, even though it is essentially conducted in their home university, they participate in a winter school where they can meet the TCCM students and teaching staff from the other institutions. At the beginning of the second year, the one month intensive course of the whole TCCM group offers the students the opportunity to work with discipline specialists and informs them about the specific research topics in the other institutions. Besides this, the international mobility required during the master thesis allows the students to work on a research topic involving the collaboration between two groups of different countries. They can learn from these two different environments. Doing research for their master thesis with discipline specialists in different countries is an enormous asset of TCCM.

Applications to this master are arranged on the level of the ISC. Based on some application criteria, the coordinating University in Madrid makes a shortlist of potential students. On a meeting with a representative of each of the seven partner universities, the students are ranked and assigned to a university. In their application, students can mention their preferred university. Subsequently the selected students have an interview with the local coordinator of the university.

Evaluation and testing

The evaluation of students is classically achieved through written or oral exams in the first year of the master in all TCCM partner institutions. Assessments of students are carried out based on the examination rules of the particular institution. When a KU Leuven student follows a course elsewhere, the evaluation follows regulations at that place. When a KU Leuven student carries out a master thesis elsewhere, the defense should however be organized at KU Leuven. The level acquired at the end of Y1 is measured by a test common to all TCCM students from the partner institutions at the beginning of Y2. This is an important tool to measure that all intended Y1 learning outcomes are achieved, at least on threshold level.

Local regulations and traditions sometimes prevail in the implementation of common evaluation criteria and processes. At this moment the ISC does

not have the ownership on the final achievement of learning outcomes. The programme management ensured that in the near future, comparable processes 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.

Services and student guidance

When new TCCM students arrive in Leuven, an introduction session is organized by the local TCCM coordinator. Students receive information about study guidance, the courses and working methods, the general academic requirements, the tests and exam regulations and the role of the ombudsperson. At KU Leuven there are currently several PhD students and postdocs who have been through the TCCM Masters course. They clearly act as very good advisors for the students.

The contact with the teaching staff is intensive during the intensive courses. Afterwards, when students are back from the IC, some students are asking for more feedback on how to complete their homework. This point needs some attention, to make sure that the support offered is sufficiently active at all time.

Study success and professional opportunities

Students in theoretical chemistry who want to pursue a career in the sector, whether it is in academia or in industry, need a PhD. Thus nearly all the students start a PhD either in one of the institutions they have been linked with or elsewhere. This process seems to work very well.

ASSESSMENT REPORT
Erasmus Mundus Master of Science in Theoretical Chemistry and Computational Modelling

Preface

This report concerns the Master of Science in Theoretical Chemistry and Computational Modelling organised by KU Leuven, together with Universidad Autónoma de Madrid, Spain (coordinating institution); Rijksuniversiteit Groningen, The Netherlands; Università degli Studi di Perugia, Italy; Universidade do Porto, Portugal; Université Paul Sabatier - Toulouse III, France and Universitat de Valencia, Spain. The assessment panel (further referred to as the panel) visited the study programme from 19th till 20th of May 2016.

The panel assesses the study programme based on the three standards of the VLUHR programme assessment framework. This framework is designed to fulfil the accreditation requirements, applied by the NVAO. For each standard the panel gives a weighted and motivated judgement on a two-point scale: unsatisfactory or satisfactory. In assessing the generic quality assurance, the concept of 'generic quality' means that the standard is in place and the programme - or a mode of study of the programme - meets the quality standards that can reasonably be expected, from an international perspective, of a Bachelor's or Master's programme in higher education. The score satisfactory points out that the programme meets the generic quality because it demonstrates an acceptable level for the particular standard. The score unsatisfactory indicates that the programme does not attain the generic quality for that particular standard.

The panel's opinions are supported by facts and analyses. The panel makes clear how it has reached its opinion. The panel also expresses a final opinion on the quality of the programme as a whole, also according to the same two-point scale.

The panel assesses the quality of the programme as it has been established at the time of the site visit. The panel has based its judgement on the self-evaluation report and the information that arose from the interviews with the programme management, with lecturers, students, representatives of the professional field, alumni and personnel responsible at programme level for internal quality assurance, internationalization, study guidance and student tutoring. The panel has examined the course materials, master theses, test and evaluation assignments and standard answering formats,

and relevant reports available. The panel has also visited the educational facilities such as classrooms, the research facilities and library during the site visit at the KU Leuven.

In addition to the judgement, the panel also formulates recommendations with respect to quality improvement. In this manner, the panel wants to contribute to improving the quality of the programme. The recommendations are included in the relevant sections of the respective standard. At the end of the report there is an overview of improvement suggestions.

Context of the study programme

In November 2003 representatives of European Universities met to establish a European Master programme in Theoretical and Computational Chemistry (TCCM). 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.

In 2009 TCCM 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 programme was approved in May 2010 and installed as a separate master programme in the Faculty of Science. In 2015, the TCCM recognition was renewed by the European Commission for three more years.

This two-year master programme is cross-European, and involves finally a consortium of seven European partner institutions.
- Universidad Autónoma de Madrid, Spain (coordinating institution)
- Rijksuniversiteit Groningen, The Netherlands
- Università degli Studi di Perugia, Italy
- Universidade do Porto, Portugal
- Université Paul Sabatier - Toulouse III, France
- Universitat de Valencia, Spain
- KU Leuven, Belgium.

During the first year (Y1), each student follows courses in his or her home institution, whereas in year two (Y2), the whole cohort assembles for a joint international Intensive Course (IC). Later, each student carries out a research stay in a laboratory, which must be based outside their home institution and country.

The TCCM programme at KU Leuven follows both European and local regulations and duties. The organization is monitored by an ISC (International Steering Committee), with one representative from each consortium university. The ISC meets annually. It has full responsibility regarding the admission policy and selection of students. Every year the programme has approximately 120 applicants. The 50 best students will be selected. Most students receive a scholarship to participate the programme.

The tasks of ISC also include analysis of student feedback, organization of IC, and quality review reports to the Education, Audiovisual and culture Executive Agency, European Commission (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 Erasmus Mundus Scholars, feedback on the past and organization of the next IC, and verification of mobility criteria for master theses.

The programme at KU Leuven is the responsibility of the Faculty of Science POC (Permanente Onderwijscommissie), which delegates to the chemistry POC the responsibility to monitor the TCCM, to define solutions for problems with the programme 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 programme.

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 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).

Standard 1 – Targeted Outcome Level

The panel evaluates the targeted outcome level as satisfactory.

The **objectives** of the Master of Science in Theoretical Chemistry and Computational Modelling are:

- 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.

It is the **aim** of the TCCM master that at the end of the two years study programme the students will have acquired the following skills: a deep knowledge and understanding of theoretical chemistry and simulation techniques and their applications; the ability to use these techniques and applications 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.

It is the panels' opinion that the targeted **programme-specific learning outcomes** are appropriate to the required master level and orientation as defined in the Flemish qualification framework and to the validated discipline-specific learning outcomes. The master is almost exclusively meant to be a preparatory master to a PhD. The intended professional field for graduates of this master is the academic (research) area, which is a legitimate choice according to the panel.

The panel is convinced that the TCCM master is well designed to achieve a very good master level, with a specific international environment. The **international collaboration** between experts in the domain of TCCM from seven universities assures a match with the current requirements from an international perspective by discipline specialists. 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 TCCM. The TCCM master bundles the qualitative and quantitative benefits of working together with seven institutions. The panel indicates that bringing together the best staff and students in a specific domain from different universities across Europe is the main asset of TCCM.

All in all, it is the panels' opinion that the targeted programme specific learning outcomes fit the domain specific outcomes and the Flemish qualification framework. The programme specific learning outcomes targets also match the current programme content requirements as they are established internationally by discipline specialists and professionals.

Standard 2: Educational Learning Environment

The panel evaluates the Educational Learning Environment as satisfactory.

TCCM is a two year master programme organized by KU Leuven and **six partner universities**, coordinated by Universidad Autónoma de Madrid, Spain. The general structure of the programme is organized around seven modules (I to VII). In the first year (Y1) the programme management wants to bring bachelor graduates from a variety of related disciplines to a good basic knowledge of theoretical and computational chemistry and its applications. In the second year (Y2), students take part in the common IC of module VI. Finally the programme provides to deepen the students' 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:

- 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.

It is the panel's opinion that the **content and structure** of the curriculum are very good. The programme structure with a locally-organized Y1 and an international Y2 including an intensive course aiming at presenting advanced methods and techniques is quite effective. The panel noticed a good progression of the learning process during the two master years.

As for the content of the programme, the panel learned that there may be **differences in the courses** depending on the university at which the student attends his or her first year. At KU Leuven, the Y1 courses are selected among the courses given in different masters of KU Leuven that focus on theoretical concepts, computational methodologies and physico-chemical techniques for molecules, molecular materials and solid state. This assures a level homogenous with that of the other KU Leuven master programmes. Even so, this allows an integration of the TCCM students with the students from the other master programmes. The TCCM programme contains two modules that were specifically designed for the programme, namely: 'Module II: computational techniques' (Y1) and the intensive course (Y2). Between the universities, the indicated number of ECTS credits is subject to small deviations, and the denomination of the courses can also vary. By the start of the second year, all students have to pass a test to examine whether they have reached a common threshold level to start their second year.

The **content of the programme** is very broad ranging from theoretical and computational chemistry applications in physics, biology and materials science. It starts off with fairly elementary material as the students have a very varied background and are from many countries. The panel is positive about the levelling courses that help some students to catch up. The panel supports the fact that students have to learn a foreign language. At KU Leuven most of the foreign students take a Dutch course. It stimulates their ability to interact with local students. At KU Leuven students start a research internship in their first year which allows them to have a direct experience with research activities in computational chemistry before starting their Master thesis.

The second year starts with the **intensive course** (IC) period, including advanced learning in many different fields, allowing a more specific orientation of the research work. Even if the work load seems rather heavy during the IC, the students appreciate to have access to all the most important theoretical methods and computational approaches used in the computational chemistry research. By bringing the students from the whole master programme together, and also teachers from within and outside the consortium, it creates an intense experience and an opportunity to learn in a more informal way. It is followed up by in-depth homework. During this period the students can have active contacts with the IC professors.

It is a common complaint of students that the **workload is very high during the IC**. The students are in favour to extend the IC from 4 to 6 weeks. The panel realizes that this will bring additional costs for students and the host university, but recommends searching a solution to this problem, together with the students.

An impressive and possible unexpected outcome of the IC is **a series of books** written by the professors describing some of the lectures given. These are not only very useful for the students on the TCCM course but will also have much wider use by theoretical chemistry students at the research level worldwide and will bring distinction to the quality of the TCCM course.

The panel noted that the presence of some **learning outcomes** was rather implicitly present in the programme. At KU Leuven, the scientific integrity is now taught for starting PhD's, though scientific integrity is one of the intended learning outcomes of this programme. The panel recommends to touch this learning outcome more explicit in the current compulsory courses. The panel is confident that the programme management will adjust this item. Other learning outcomes that where lacking in the course programme such as the learning outcomes on ethical issues have been discussed within the ISC. Those learning outcomes are now incorporated in a special session in the IC. Also a communication workshop was added to the programme of the IC after hearings with the students.

The panel learned from the self-evaluation report that one of the main objectives of the TCCM programme is "to work with innovative pharmaceutical, petrochemical and new-materials industries". The panel found few evidence that this objective is present in the programme's

educational learning environment. The panel understands the current focus on academic research, but reminds the programme management that there could be more attention to this objective. After all, in the near future European funding of this programme will possibly stop. From this perspective, cooperation with various industries is advisable.

The panel is satisfied with the **working and learning methods** that are used in the different courses. TCCM has a very carefully constructed structure, with teaching and learning methods chosen to optimize the in-depth understanding of the fundamentals of the field. In the first year, 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. At KU 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 give students a strong basic understanding of, and practical experience with, theoretical and computational chemistry.

The panel is laudatory about the **international aspect** of the programme. During the two years, the students have the opportunity to develop international relations. In the first year, even though it is essentially conducted in their home university, they participate in a winter school where they can meet the TCCM students and teaching staff from the other institutions. At the beginning of the second year, the one month intensive course of the whole TCCM group offers the students the opportunity to work with discipline specialists and informs them about the specific research topics in the other institutions. Besides this, the international mobility required during the master thesis allows the students to work on a research topic involving the collaboration between two groups of different countries. They can learn from these two different environments. Doing research for their master thesis with discipline specialists in different countries is an enormous asset of TCCM.

The programme is promoted and advertised in various ways such as the webpages of KU Leuven and UA Madrid and also by alumni. Recently an Alumni Association of TCCM Masters is set up. This association is playing an important role in promoting the programme, in **spreading information** about it, and in helping new students on different fronts, in particular on employability. The programme management is aware that ensuring up to date information about the master programme on the webpages in various institutions remains a constant challenge.

Applications to this master are arranged on the level of the ISC. Based on some **application criteria**, the coordinating University in Madrid makes a shortlist of potential students. On a meeting with a representative of each of the seven partner universities, the students are ranked and assigned to a university. In their application, students can mention their preferred university. Subsequently the selected students have an interview with the local coordinator of the university. The panel finds this a good practice.

The **staff** associated with teaching and project supervision for 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 PhD in quantum chemistry. Research activity in theory and computation, and their applications, is not confined to QCPC, and some of the core compulsory courses are given by other members of the Chemistry Department at KU Leuven. One course on density functional theory is given by teaching staff of the Free University of Brussels (VUB). Some optional courses are taken from the curricula of other departments, and are taught by staff from these departments.

The teaching assistants at KU Leuven are doctoral candidates of the QCPC division. Based on the meetings with the teaching assistants the panel noted that they all followed a teaching training for PhD students organized by the faculty. At KU Leuven, a large part of the supporting staff also followed this TCCM programme. They have a direct experience of the possible difficulties that the TCCM students can encounter. Most of the teaching staff have international reputations and the supporting staff are highly motivated. According to the panel, this is an important factor in enabling the students to achieve high quality learning outcome targets. The teaching quality is further improved through the teaching trainings organised by the education services of the faculty of Science within its professionalization programme.

Overall, there are many staff members as there are 7 different departments collaborating. The **student to staff ratio** is excellent, making it possible to give personal support to every student. While there is enough teaching staff in each of the institutions, the quantitative number of staff members is relatively low at each institution. At KU Leuven, this requires attention for the future as upcoming retirements or other staff changes can have

an impact on the programme. The capacity of staff needs to be closely monitored in order to be able to quickly respond to changes.

A question mark can be raised whether the **English proficiency of all staff members** is adequate for teaching in an English language programme. KU Leuven professors have to provide some proof that they meet a certain level of the English language, but no similar requirement seems to be in place in some other members of the consortium. The lack of such a requirement might cause some issues with the intelligibility of particular lectures in the intensive course. Students have also mentioned this problem in the hearings that were performed during the preparation of the self-evaluation report and during their meeting with the panel. Expanding the requirement on English language proficiency to all universities that take part in the master programme could easily solve this issue.

The key **facilities for TCCM students** are classrooms and appropriate e-learning support environments. These are provided within each home institution. Each of the universities in the TCCM consortium has high-performance computing (HPC) resources available for teaching and research, which was confirmed to the panel by the students. According to the panel, the infrastructure in Leuven is brand new and top-notch both in terms of computational facilities and more general student-oriented facilities such as the library and study rooms.

When new TCCM students arrive in Leuven, an introduction session is organized by the local TCCM coordinator. Students receive **information** about study guidance, the courses and working methods, the general academic requirements, the tests and exam regulations and the role of the ombudsperson. Students at KU Leuven can find more information and a lot of documents concerning their courses on Toledo, the electronic learning environment of KU Leuven.

The teaching staff and the supporting staff are available for the students whenever students ask for further information. As mentioned above, at KU Leuven there are currently several PhD students and postdocs who have been through the TCCM Masters course. They clearly act as very good advisors for the students. The supporting staff and the supervisors are available for students during the preparation of their master thesis. The contact with the teaching staff is intensive during the intensive courses. Afterwards, when students are back from the IC, some students are asking for more feedback on how to complete their homework. This point needs

some attention, to make sure that the support offered is sufficiently active at all time.

All in all, the curriculum, staff and facilities link very well together to make up a coherent and effective learning environment. The international nature of the course is a special feature and allows for variety in course material and teaching approaches and enables the students to become independent and responsible. During the panel's visit, they could verify the strong support of the consortium members.

Standard 3 - Outcome Level Achieved

The panel evaluates the outcome level achieved as satisfactory.

The evaluation of students is classically achieved through written or oral exams in the first year of the master in all TCCM partner institutions. The panel learned that assessments of students are carried out based on the **examination rules** of the particular institution. When a KU Leuven student follows a course elsewhere, the evaluation follows regulations at that place. When a KU Leuven student carries out a master thesis elsewhere, the defense should however be organized at KU Leuven.

The level acquired at the end of Y1 is measured by **a test common to all TCCM students** from the partner institutions at the beginning of Y2. The panel finds this an important tool to measure that all intended Y1 learning outcomes are achieved, at least on threshold level.

At KU Leuven, the exams are organised by the Faculty of Sciences but it remains the responsibility of the lecturers to ensure that the exams are correctly organized, **representative, reliable and transparent**. The individual lecturers prepare exam questions according to the descriptions given in the corresponding ECTS files and the guidelines described in the POC Evaluation Policy, they correct the answers, and finally give the marks. At KU Leuven, the panel has examined the course materials, master theses, test- and evaluation assignments and standard answering formats. Based on this information and the discussions with all stakeholders, the panel concludes that the exam materials allow students to achieve the intended learning outcomes.

In the second semester of Y1, in consultation with the supervisor, each student at KU Leuven selects a research group at KU Leuven for **a six**

week internship. A short proposal for this is submitted by the student in agreement with the supervisor. During this internship daily supervision is provided by a mentor, and the student is also assigned an external promoter, who is a member of the didactic team. The student sends weekly written reports to the supervisor and the external promoter. At the midpoint of the internship an evaluation form is generated to register progress as well as points of attention for the remaining period. At the end of the internship, the supervisor and promoter individually fill in the final evaluation form. 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, which judges the quality of the presentation. The panel finds the way the research internship is shaped and evaluated an example of good practice to assure that the learning outcomes are achieved on a high level.

By the start of the second master year all TCCM students come together in one of the partner universities for a set of many **intensive courses** during a four-week period that brings them up to speed on theoretical chemistry in all the different areas. The evaluation process and methods are common for all Y2 students irrespective of their home institution. Each partner university ensures a period of 8-12 weeks for carrying out the IC homework. At KU Leuven, this period overlaps with the second research internship.

At the end of each week, IC multiple-choice tests are given to evaluate short-term impact of the lectures. The weight factor for the tests is 20 %. Up to three months after the course, the IC students have to hand over the written homework, involving exercises, calculations and literature surveys on specific study problems. 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.

Several students told the panel they would like to have **feedback** on the evaluations of their written reports on the intensive course. Nowadays, students only receive their marks. The panel learned from the students that some of them felt somewhat isolated in completing their homework for the intensive course. Communication with the teaching staff who are based in different countries is only possible by email. Feedback from the teachers explaining the reasons for the students' grades would be useful for the students in order to better understand their progress and

to fix possible deficiencies. However, the students said that collective discussions on social media with the students in other countries helped a lot and delivered added value.

The panel learned from the programme management that local regulations and traditions sometimes prevail in the implementation of common evaluation criteria and processes. At this moment the ISC does not have the **ownership** on the final achievement of learning outcomes. The programme management ensured the panel that in the near future, comparable processes 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.

Before the site visit the panel had the opportunity to read several **master theses**. The assessment of the master thesis includes the evaluation of a written text and the defense of the thesis research in front of a jury. For KU Leuven students, the assessment of theses is done following the regulations for KU Leuven – Faculty of Science master projects. Each master thesis is evaluated by a KU Leuven jury, including the mandatory participation of a member from a partner university. Besides, KU Leuven staff members evaluate theses of students of partner universities who conducted research in Leuven.

The evaluation by promotors and assessors is done by an assessment schedule which covers multiple learning outcomes. The final mark of the thesis is composed of 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 from all members of the jury.

The panel is convinced that the quality of the theses is in most of the cases of a very high level. Some of the work in the theses gets published. Although this is not a requirement of the course it demonstrates the quality of the students' research work. The panel learned from its discussions with students and from the surveys among the students and alumni that they consider the evaluation of the thesis at KU Leuven as highly valuable.

Every year one or two students leave the programme without graduation. Most of these students stop at the beginning of the second semester of Y1, when they receive their marks of the first exams. According to an alumni

survey almost 90% of TCCM master **graduates** have opted for academic research. Only a few % took jobs in private sectors such as banking and 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. At least some alumni from Asia told the panel that they can easily have a permanent academic position in their native country after PhD and eventual post-doc due to the high level of recognition of the TCCM master.

Students in theoretical chemistry who want a career in the sector, whether it is in academia or in industry, need a PhD. Thus nearly all the students start a PhD either in one of the institutions they have been linked with or elsewhere. This process seems to work very well. The panel found strong evidence from reading the theses, discussions with the students and the graduates that this master, and especially the final research project, makes the students highly motivated to continue research in theoretical chemistry through a PhD.

The panel finds it important to plan **how TCCM can be continued** in some form when its finance from the Erasmus scheme finishes in 2019 because the possibility of renewal seems unclear. It may be necessary to have discussions with the university and local and international funding agencies on future possibilities and this will need to start soon. Nevertheless the panel felt a strong involvement of the Faculty of Science at KU Leuven to continue this master, which is rather optimistic for the future.

All in all, the programme has an appropriate system of assessment, testing and examination and demonstrates that the targeted learning outcomes are achieved.

Final judgement of the assessment panel

As **Standard 1** is evaluated as satisfactory, S**tandard 2** is evaluated as satisfactory and the **Standard 3** is evaluated as satisfactory, the final judgement of the assessment panel about the Master of Science in Theoretical Chemistry and Computational Modelling is satisfactory, according to the decision rules.

Summary of the recommendations for further improvement of the study programme

Standard 1 – Targeted Outcome Level

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Standard 2 – Educational Learning Environment

- Investigate how the workload during the IC can be limited or better spread.
- Touch 'scientific integrity' more explicit in the current compulsory courses.
- Pay more attention to working with innovative pharmaceutical, petrochemical and new-materials industries.
- Ensure up to date information about the programme on the webpages of all participating universities.
- Expand the requirements on English language proficiency to all universities that take part in the master programme.
- Monitor the capacity of staff closely in order to be able to quickly respond to changes.
- Give students after the IC more feedback on how to complete their homework.

Standard 3 – Outcome Level Achieved

- Give feedback on the evaluation of the IC, instead of only the marks.
- Assure the ISC's ownership on the achievement of learning outcomes.
- Plan how TCCM can be continued in some form when its finance from the Erasmus scheme finishes in 2019.

APPENDICES

APPENDIX I
Curricula vitae of the members of the assessment panel

Gilberte Chambaud

Gilberte Chambaud is Professor Emeritus in University of Paris-Est-Marne-la-Vallée. She is an expert in Theoretical Molecular Physical Chemistry specialized in reactivity, stability and identification of intermediate molecular species, structural determination of molecular systems and accurate spectroscopic characterisation. A large part of her activity is also on the structure and spectroscopy of molecular metallic compounds (MX, MX2) and on the physisorption interaction of H2 molecules on metallic surfaces. She recently oriented her interest on multiscale models for mechanical and piezoelectric properties of nanowires of semiconductors and related multi-scale properties. She has supervised 18 PhD students and has written more than 140 publications in International Journals, 150 Conference Proceedings and was invited in more than 70 national and international conferences. She is author or co-author of 8 text-books in Physical Chemistry. She was President of the Education Division in the French Chemical Society in 2000-2004, and member of the European network "Tuning Project" for the European harmonization of the University trainings according to the Bologna Process. She created in 2006 the French Network of Theoretical Chemistry and in 2008 she launched the French-Chinese network in theoretical Chemistry. She has been administrator of the French Chemical Industry Association and of the synchrotron SOLEIL. She is Member of the Academia Europaea. She has been the Scientific Director of the Institute of Chemistry at CNRS (2006-2011) and Scientific Advisor at the AERES (2011-2014). She is presently President of the French

Chemical Society (2015). She was distinguished by the French Legion d'Honneur in 2007, and Officer of Palmes Académiques in 2012.

David Clary

David Clary has been President of Magdalen College Oxford since 1 September 2005. He also runs a research group in the Chemistry Department at Oxford University. Before coming to Magdalen he was Head of the Division of Mathematical and Physical Sciences at Oxford University and a Professorial Fellow of St John's College. He has held faculty positions at Manchester, Cambridge and UCL. He was a Fellow and Senior Tutor at Magdalene College Cambridge where he is now an Honorary Fellow. His PhD was at Cambridge where he also holds the Sc.D. He was an undergraduate at the University of Sussex where he recently was awarded the Doctor of Science, honoris causa. He was the first Chief Scientific Adviser to the Foreign Office from 2009-13 and before that was President of the Faraday Division of the Royal Society of Chemistry. Sir David has been elected to several academies including the Royal Society, the American Association for the Advancement of Science, the International Academy of Quantum Molecular Science, and the American Academy of Arts and Sciences. He was knighted in the 2016 Queen's birthday honours for services to international science. Professor Clary is Editor of Chemical Physics Letters and is on the Board of Reviewing Editors of Science. He teaches a graduate course on Quantum Chemistry and he also gives undergraduate tutorials in this subject.

Benedetta Mennucci

Benedetta Mennucci is Professor in Physical Chemistry at the University of Pisa in Italy. Since 2014 she is President of the Theoretical and Computational Chemistry Division of the Italian Chemical Society and Senior Editor for the Journal of Physical Chemistry Letter of the American Chemical Society. Her scientific activity is mainly focused on the development of hybrid quantum-mechanical/classical models to describe the effects of the environment on properties and processes of (supra)molecular systems. In the last years she has received important fundings from the European Union through the "NanoScience" ERANET network with a transnational project entitled "Molecules and Light in individual Metal Nanostructures" (MOLIMEN) and through the European Research Council (ERC) with a ERC consolidator grant on a project entitled "The interplay between quantum coherence and environment in the photosynthetic electronic energy transfer and light- harvesting: a quantum chemical picture" (EnLight).

Thijs Stuyver

Thijs Stuyver is a PhD fellow of the Research Fund – Flanders (FWO) in the Department of Chemistry of the Vrije Universiteit Brussel. He graduated summa cum laude from the same university and his master thesis was selected as the winner of the Royal Chemistry Society Flanders (KVCV) prize for the most meritorious student in chemistry. He has been a member of the student council of the Vrije Universiteit Brussel (2014-2016) and president of the student delegation in the education council of the Vrije Universiteit Brussel (2015-2016). He is currently representative for the OAP-section in the same education council (2016-…). His particular research interests are conceptual Density Functional Theory (DFT) and molecular electronics. As a visiting scholar he recently spend 2 months in the Hoffmann group (Cornell University, U.S.A).

APPENDIX II
Visit schedule

May 19, 2016	
9:00–12.30	internal consultation + lunch
12:30–13:45	programme management
13:45–14:15	Internal consultation
14:15–15:15	students
15:15– 15:30	internal consultation
15:30–16:30	teaching staff
16:30–17:15	internal consultation
17:15–18:15	graduats and professional field
18:15	diner panel

May 20, 2016	
9:00–10:00	programme-specific infrastructure
10:00–11:00	supporting staff
11:00–12:00	consultation hour
12:00–13:00	lunch
13:00–13:30	programme management
13:30–15:30	final consideration
15:30	oral reports