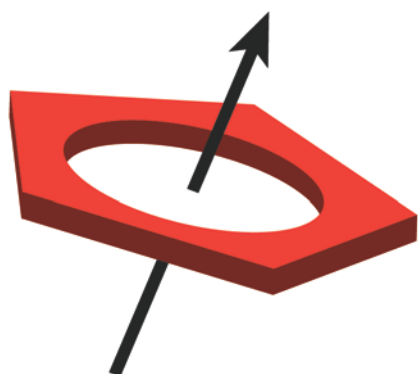

HRSMC Progress Report 2011-2016

For the SEP Evaluation of the Leiden Institute of Chemistry (LIC),
Leiden University (UL)

January 2017



**HOLLAND
RESEARCH
SCHOOL
OF MOLECULAR
CHEMISTRY**



HRSMC Progress Report 2011 – 2016

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Executive Summary

This progress report presents an overview of the research and educational activities of the Holland Research School of Molecular Chemistry (HRSMC) during the period 2011-2016. The HRSMC is a collaboration between top research groups of four Dutch Universities: the University of Amsterdam (UvA), the VU University Amsterdam (VU), Leiden University (UL) and the Radboud University (RU). The HRSMC was founded in 1994 and re-accredited three times by the Royal Netherlands Academy of Arts and Sciences (KNAW). The HRSMC harbours a powerhouse of expertise in Synthetic, Physical, and Theoretical Chemistry as well as Spectroscopy and Molecular Physics. This multidisciplinary character makes the School unique in the Netherlands and abroad; it allows it to operate in a broad field that addresses fundamental scientific problems but also challenges society currently faces in areas like sustainability, energy, and health.

Starting point for the present report is the previous re-accreditation in 2011, where the Peer Review Committee consisting of Prof. dr. Douwe Wiersma (University of Groningen, The Netherlands, chair), Prof. dr. David Milstein (The Weizmann Institute of Science, Israel) and Prof. dr. Odile Eisenstein (University of Montpellier 2, France) determined that *“the HRSMC is functioning extremely well as Graduate School and that its existence as an umbrella organization also for research is appreciated by all stake holders”*.¹ In 2015 the re-accreditation procedure for Research Schools by the KNAW has been replaced by a procedure in which the School is evaluated as part of the SEP evaluation of the institutes involved for which the present HRSMC Progress Report 2011-2016 has been prepared.

As an interuniversity research school, the HRSMC has two main targets:

- (A) to promote and facilitate research aimed at the three HRSMC research themes: (1) ‘Synthesis, Characterisation, Properties and Reactivity of Molecules’, (2) ‘Physical Chemistry and Spectroscopy’ and (3) ‘Theoretical Chemistry’. The HRSMC board strives for coherence in the research activities of its members by promoting collaboration between the research groups and safeguarding complementarities with respect to infrastructure and expertise.
- (B) to facilitate and provide a coherent, high-level educational programme to its PhD students, which offers a seamless connection to the Master degree programme. The primary aim is to teach PhD researchers to answer key questions in molecular science and to use their insights in a multidisciplinary approach.

The extensive educational programme (Schools, Courses, Symposia and other activities like career advice events) offered by the HRSMC means that for all practical purposes the school takes care of the educational program of its PhD students and safeguards their progress. Importantly, the educational activities of the HRSMC are also accessible for (advanced) MSc students and thereby seamlessly connect to the undergraduate programs of the participating universities.

In the 2011-2016 period the HRSMC has developed two novel Programmes to reinforce these research and educational objectives:

- (1) The interuniversity and multidisciplinary Excellence Master Programme *‘Sustainability, the Molecular Approach’*. This programme offers doctoral students the opportunity to develop their own research ideas for PhD research. Elected in 2012 as one of the thirteen Graduate Schools to receive substantial funding within the NWO Graduate Programme, the HRSMC has now granted three proposals for PhD research written by doctoral students in 2015-2016.
- (2) A *‘Fellowship Programme’* that finances visits by outstanding foreign researchers to HRSMC-affiliated research groups for a period up to six months.

¹ Report of the Peer Review Committee for the Holland Research School of Molecular Chemistry (HRSMC), p. 3. The full report can be found in Appendix 1.

The success of this strategy, activities and efforts can be measured by a large number of achievements of which the following deserve special mention:

- On December 31 2016, **64** staff members and **177** PhD students participated in the School. Together with postdocs, technical support, and others involved in the organisation, the HRSMC had about **340** members.
 - In the period 2011 – 2016 a total of **111** PhD theses have been published within the HRSMC (see Appendix 6). Every year, the HRSMC Board has awarded the annual Dick Stufkens Prize for the most outstanding PhD thesis within the HRSMC.
 - In the period 2011 – 2016 the following UvA/VU/UL groups joined the HRSMC:
 - the Theoretical Chemistry group of dr. J. Meyer (UL),
 - the Biocatalysis group of dr. F. Mutti (UvA),
 - the Heterogeneous Catalysis and Sustainable Chemistry of Prof. dr. G. Rothenberg, Dr. S. Grecea, Dr. N.R. Shiju, and Dr. N. Yan (UvA).
- while from the RU the following research groups became associated members:
- the Molecular Structure and Dynamics – FELIX/Molecular and Biophysics group of Prof. dr. J. Oomens, Dr. J.M. Bakker and Dr. A.M. Rijs (RU),
 - the Theoretical Chemistry group of prof. dr. ir. G.C. Groenenboom (RU).
- In the period 2011 – 2016 the HRSMC has organised:
 - **12** Schools with in total **809** participants, including **463** participants from foreign universities, **176** MSc students and **13** industrial participants,
 - **6** Courses with in total **143** participants including **23** MSc students,
 - **6** Symposia with \pm **170** attendants per symposium,
 - **3** Career Advice Events, **3** Lab visits, **1** Proposal Writing Course in combination a Peer Review Course and **1** Sustainability Workshop.
 - In the period 2011 – 2016, the HRSMC has granted
 - **3** research proposals within the NWO Graduate Programme and HRSMC Excellence Master Programme 'Sustainability: the Molecular Approach', as a result of which three PhD students have been appointed,
 - **15** Fellowship applications within the HRSMC Fellowship Programme.

For the future, the HRSMC Board strives to continue and further develop its broad educational activities as well as its Excellence Master and Fellowship programmes in order to stay an excellent platform for interuniversity and multidisciplinary cooperation and to provide an incentive for world-class education and research in molecular chemistry and physics.

1. General Information

1.1 Introduction

This supplement presents an overview of the research and educational activities of the graduate research school 'Holland Research School of Molecular Chemistry' (HRSMC) during the period 2011 - 2016. Formally, the HRSMC comprises research groups of the following institutes and universities:

- the van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam (UvA),
- the Institute for Electrons and Molecular Structure (EMS) of the VU University (VU),
- the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Leiden University (UL).

Within HRSMC there is a formal agreement between the school and the institutes in which rules are described for the supervision and the evaluation of the education of the PhD researchers (see Appendix 2).

The University of Amsterdam legally represents the HRSMC. The research school was founded in 1994 as an UvA, VU and UL collaboration. PhD students, postdocs and staff members of UvA, VU and UL can become an official member, or a *guest* member in case they are actively involved in the HRSMC but formally an official member of another Research School (e.g. NIOK or Casimir). Besides the official and guest membership, there is the *associated* membership for PhD students, postdocs and staff members outside the UL, VU and UvA. This membership has been established in 2016 when staff members from the Radboud University Nijmegen (RU) expressed their wish to the HRSMC board to become member of the HRSMC as well. An overview of all UvA, VU, UL, and RU members as of now can be found in Chapter 1.3.

The HRSMC mission is '*...to stimulate, facilitate, initiate, focus and support (collaboration in) high-level research and education in the area of chemistry concerning the connection between the three-dimensional and electronic structure of molecules, their purposeful thermal and photochemical synthesis and reactivity, as well as their physical and biological properties.*' Advances and real breakthroughs in chemistry require a thorough understanding at the molecular level. To obtain the latter a concerted effort is paramount, both in research and education, combining synthesis, spectroscopic characterization and theoretical and computational description of molecular systems. The research topics of the HRSMC are therefore organized around three different research themes in molecular chemistry which complement and mutually reinforce each other: (1) '*Synthesis, Characterisation, Properties and Reactivity of Molecules*', (2) '*Physical Chemistry and Spectroscopy*' and (3) '*Theoretical Chemistry*'. The mission and the organisational aspects of the HRSMC are further explained in Chapter 1.2 while the research themes are expanded on in Chapter 1.3.

In addition to the research training, the HRSMC offers a selection of courses to the PhD students. The HRSMC Board strives for a consistent Educational programme reflecting all research themes within the HRSMC. A certificate is presented to those PhD students that have fulfilled their Education Programme (see Chapter 2.1). Key educational activities since 1994 are:

- *HRSMC Schools* (29 Summer, Tulip or Autumn Schools)
 - * Photochemistry (1998, 2003, 2008, 2012, 2016)
 - * Modern Developments in Spectroscopy (2001, 2003, 2006, 2009, 2012, 2015)
 - * Synthetic Bio-organic Chemistry (2001, 2005, 2009, 2013)
 - * Advanced Metal-Organic Chemistry and Catalysis (1998, 2002, 2006, 2010, 2014 – with NIOK)
 - * Molecular Simulations (2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016)
- *HRSMC Courses* (29 Interuniversity Courses)
 - * Molecular Modelling (1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2008, 2013, 2016)

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- * Physical Methods in Inorganic Chemistry (1994, 1999, 2001, 2003, 2005, 2007, 2009, 2011, 2013, 2015)
 - * Photophysics, Photochemistry & Photobiology (1996, 1999, 2001, 2004, 2007, 2010, 2014)
 - Other key activities
 - * The annual HRSMC Symposium for all its members with ca. 180 scientists attending the last symposium in 2016. In 2014 a special Lustrum Symposium with ca. 225 visitors was organized to celebrate the school's 20th anniversary with lectures by the Nobel laureates Prof. Moerner (2014), Prof. Warshel (2013) and Prof. Hoffmann (1981).
 - * Since 2010, a Career Advice Activity in collaboration with Royal Dutch Chemistry Association (2010, 2012, 2013, 2015).
 - * Proposal Writing Course in combination with a Peer Review Course (2015).

The Education Programme and the related HRSMC Schools, Courses and other educational activities are further explained in Chapter 2.2 and 2.3.

Within the period 2011 – 2016, two Programmes have been developed to further reinforce the research and educational objectives of the HRSMC.

(1) HRSMC Excellence Master Programme 'Sustainability, the Molecular Approach'

Within the NWO Graduate Programme, the HRSMC was selected in 2012 as one of only thirteen Dutch Graduate Schools to receive substantial funding. This enabled HRSMC to offer young talented PhD students the opportunity to develop their own research ideas within the framework of the Graduate Programme 'Sustainability, the Molecular Approach'. As a result of this programme, the HRSMC Excellence Programme was established in 2013. This is an interuniversity (UvA-VU-UL) and interdisciplinary programme reflecting the three HRSMC Research Themes. Within this programme a special highlight was the appointment of two PhD students in 2015 and one PhD student in 2016. More information about the Excellence Master Programme can be found in Chapter 3.1.

(2) HRSMC Fellowship Programme

Besides organizing several educational activities, the HRSMC established a new Fellowship Programme in 2015. It provides funding for outstanding foreign researchers of postdoc level and higher to visit and collaborate with HRSMC-affiliated research groups, aiming specifically to set up new and challenging research lines. As of 2015, there have been two application rounds, in April and October. More information about the Fellowship Programme can be found in Chapter 3.2.

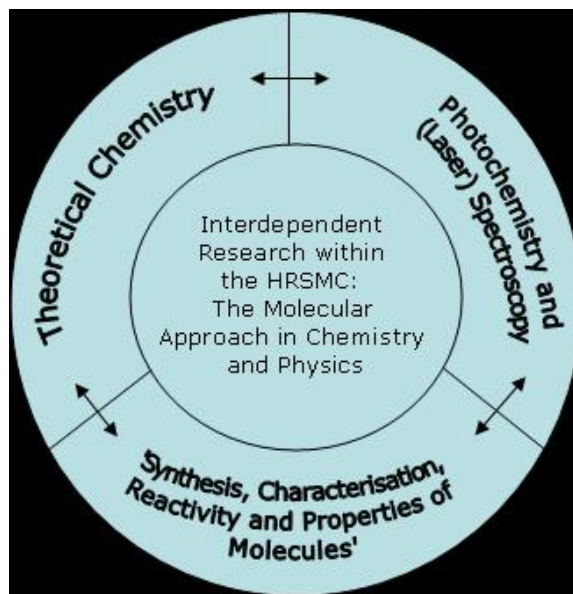
An overview of the income and expenses managed by the HRSMC over the period 2011 – 2015 (total income: € 969.017/ total expenses: € 965.085) is given in Appendix 3. The University of Amsterdam provides the core financial support to cover personnel costs and costs for key activities. Together with the contributions for the HRSMC Courses and Schools received from participants and from external sponsoring (e.g. chemical companies and foundations) the total annual budget of the HRSMC varies annually. Another financial resource managed by the HRSMC is an amount of 800 k€ granted by NWO within the NWO Graduate Programme (see Chapter 3.1).

1.2 Mission and Organisation

Mission

The official mission statement of HRSMC is: '...to stimulate, facilitate, initiate, focus and support (collaboration in) high-level research and education in the area of chemistry concerning the connection between the three-dimensional and electronic structure of molecules, their purposeful thermal and photochemical synthesis and reactivity, as well as their physical and biological properties.'

The mission emphasizes clear targets in a broad field concerning key questions in molecular sciences. The primary aim of the school is to teach PhD researchers to answer these questions and to use their insights in a multidisciplinary approach. In this respect the HRSMC is unique in the Netherlands since it does not exclusively focus on a single research area as other graduate research schools do (e.g. polymers, catalysis, materials). The approach by the HRSMC represents added value in facilitating a way of thinking based on a molecular approach where synthetic chemists, spectroscopists, and theoreticians, who are increasingly interdependent in current chemical research, are brought together in one research organisation. Such an approach is the more relevant as the molecule is nowadays no longer exclusively associated with chemistry, but is the key to a fundamental understanding in scientific disciplines that range from physics to biology and health sciences. The interdependent molecular approach of the HRSMC is therefore and crucial for effective knowledge valorisation and to meet the challenges society currently faces in areas like sustainability, energy, and health.



The main targets of the HRSMC are:

- to promote and facilitate (collaboration in) research aimed at the three HRSMC research themes: (1) 'Synthesis, Characterisation, Properties and Reactivity of Molecules', (2) 'Photochemistry and (Laser) Spectroscopy' and (3) 'Theoretical Chemistry'.
- to facilitate and provide a coherent, high-level educational programme to its PhD and MSc students, which offers a seamless connection to the Master degree programme.

The HRSMC offers excellent opportunities for achieving synergy in the research of participating groups. The board and staff have developed a coherent programme of complementary, yet interwoven, research projects. Participating groups at the four universities share expertise, readily collaborate and actively seek each other's advice. In recent years opportunities to actively direct research have been greatly expanded by the HRSMC Fellowship programme that aims to stimulate further collaborative and interdisciplinary research efforts, and allows for exploring radically new research directions.

The annual HRSMC symposia and staff meetings are very constructive in realising the continuous exchange of scientific ideas and progress and initiating new joint research projects. In addition, HRSMC takes part in discussions to achieve complementary expertise at the level of chairs in chemistry at the participating universities. Although individual research groups have their roots in HRSMC, their research activities may be in areas which also belong to or are closely related to other graduate research schools such

as NIOK (catalysis). In such cases, groups take part in two schools and PhD research students may successfully attend relevant courses at both schools.

HRSMC makes every effort to provide high-level training, such as symposia, inter-university courses and summer schools. PhD supervisors also participate in HRSMC Courses and Schools as lecturers or coordinators. The fact that they are also actively involved in Master courses confirms and further ensures that the educational needs at Master and PhD level are optimally matched. The research in the various research groups, the HRSMC PhD educational programme, and the Master programmes are therefore strongly interwoven. The Excellence Master Programme 'Sustainability, the Molecular Approach' is in this respect a success story as it has enabled the HRSMC to attract international top talent at the Master level and let them do their PhD research within the HRSMC.

International collaboration and educational exchange is encouraged and implemented by joint courses with foreign institutions. In addition, the vast majority of the lecturers who participate in the HRSMC Schools come from abroad. Announcements of HRSMC Schools are sent to international contacts of the organizing HRSMC staff members. The HRSMC Schools are internationally greatly appreciated as high-quality Schools, and thus attract PhD researchers from all over the world. On average, about 50% of the participants of the HRSMC Schools come from foreign universities.

HRSMC members are informed of HRSMC activities and scientific developments through personal contacts and via the website (www.hrsmc.nl), e-mail, newsletters, annual reports, and of course at the annual HRSMC symposia.

In short, since its foundation in 1994 HRSMC (i) has set up and maintained a simple, but highly efficient organisational structure, (ii) has developed a broad high-quality, internationally oriented educational programme, and (iii) has stimulated the collaboration and exchange of ideas between the research groups and other universities.

Organisation

The management consists of a board of three members and a scientific director (Prof. dr. W.J. Buma). In 2016, the HRSMC board consisted of Prof. dr. F.M. Bickelhaupt (VU), chairman, Prof. dr. M.T.M. Koper (UL) and Prof. dr. C.J. Elsevier (UvA).

The scientific director is assisted by an executive secretary (Mrs. Drs. H.E. Zwaan – van der Plas) and administrative officers (Mrs. R. Weijer). In addition, an external advisory committee, the PhD platform and internal committees for education and research advise the board (see Appendix 4).

The organisation of the HRSMC is schematically depicted in Fig. 1.1. On December 31 2016, 64 staff members and 177 PhD students participated in the School. Together with postdocs, technical support, and others involved in the organisation, the HRSMC had about 340 members.

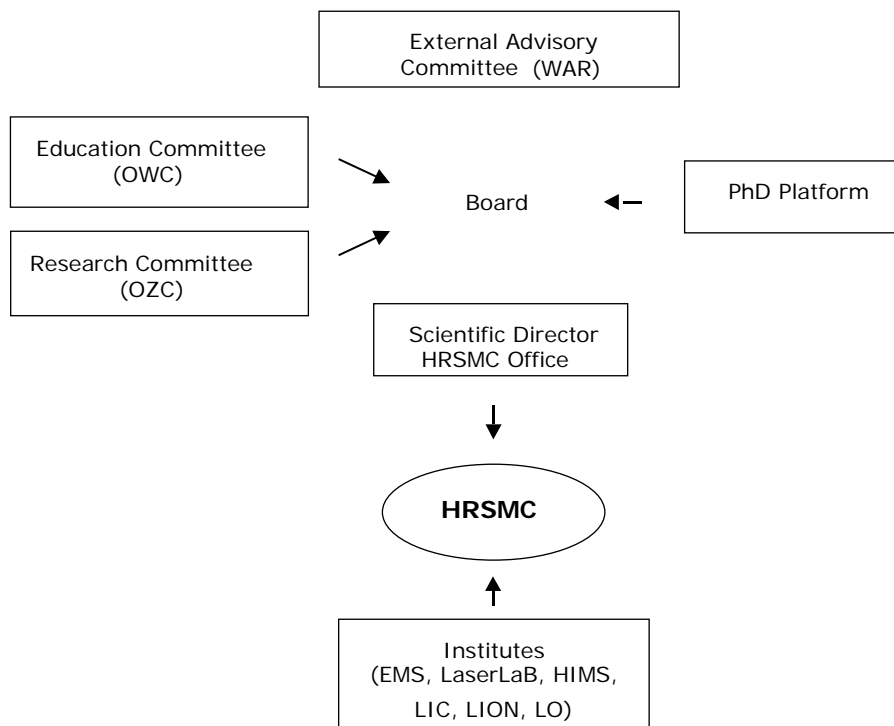


Figure 1.1 Schematic organisation of the HRSMC

1.3 Research

Advances and real breakthroughs in chemistry require a thorough understanding at the molecular level. To obtain the latter a concerted effort is paramount, both in research and education, combining synthesis, spectroscopic characterization and theoretical and computational description of molecular systems. The research topics of the HRSMC are organized around three different research themes in molecular chemistry which complement and mutually reinforce each other:

- Theme 1: 'Synthesis, Characterisation, Reactivity and Properties of Molecules'
- Theme 2: 'Physical Chemistry and Spectroscopy'
- Theme 3: 'Theoretical Chemistry'

Theme 1 - Synthesis, Characterisation, Reactivity and Properties of Molecules

The design and synthesis of compounds with novel structures are among the most essential activities in molecular chemistry research. The incentives to prepare such new molecules are, apart from curiosity, their anticipated physical, chemical or biological properties. Strategic aspects of the HRSMC synthetic research are the development of new (bio)catalytic reactions and the investigation of their mechanisms, the synthesis of magnetic and conducting materials, and the development of methodologies for the synthesis of bioactive compounds. A great variety of techniques is used for the synthesis of the compounds as well as for the elucidation of their molecular structure and physical-chemical and biological properties. From the three universities eight different groups are active in this area.

Theme 2 - Physical Chemistry and Spectroscopy

The interaction between light and molecular matter is central in a large number of fundamental and applied research areas in molecular chemistry and physics. In HRSMC it is employed to probe and utilize fundamental processes such as reaction mechanisms and dynamics, catalytic events, energy and electron transfer, conformational dynamics, and dynamic life processes. Concurrently, advanced spectroscopic techniques are used to elucidate inter- and circumstellar chemistry, and for analytical applications. Many of the groups working in this area are renowned for their development and application of new spectroscopic techniques. Various groups in the Netherlands conduct scientific research in spectroscopy, but photo-chemical and photo-physical research of inorganic and organic compounds in gas and condensed phases is increasingly confined to groups within HRSMC.

Theme 3 - Theoretical Chemistry

Understanding the structure of molecules and their chemistry from first principles represents the holy grail of theoretical chemistry. Many molecular properties can be understood directly from the electronic structure. When considering reactivity, it is usually necessary to consider the dynamics of the nuclei taking part in the reaction as well.

The research program of the HRSMC is embedded in top research groups of the VU University Amsterdam (VU), the University of Amsterdam (UvA) and Leiden University (UL). Table 1.1 gives an overview of the research groups involved in the HRSMC in 2016.

The HRSMC board strives for coherence in the research activities of its members, which are spread over the four Universities, by promoting the collaboration between the research groups and safeguarding complementarities with respect to infrastructure and expertise. Importantly, these collaborations do not only take place at the level of senior staff members, but also at the level of junior researchers. In a number of cases HRSMC collaborations have led to the appointment of a temporary researcher as (assistant) professor at another institution. Appendix 5 gives an overview of the collaborations in 2016, which is constantly evolving and which fluctuates annually.

Table 1.1 HRSMC research themes, corresponding research groups and their staff members in 2016.

Theme	Group (University, institute) staff members
1	Biocatalysis (UvA, HIMS) Dr. F. Mutti
	Heterogeneous Catalysis and Sustainable Chemistry (UvA, HIMS) Prof. dr.G. Rothenberg ¹ , Dr. S. Grecea, Dr. N.R. Shiju, Dr. N. Yan
	Homogeneous, Supramolecular and Bio-Inspired Catalysis (UvA, HIMS) Prof. dr. B. de Bruin ¹ , Prof. dr. J.N.H. Reek ¹ , Dr. M. Tromp, Dr. Ir. J.I. van der Vlugt
	Metals in Catalysis, Biomimetics & Inorganic Materials (UL, LIC) Prof. dr. E. Bouwman ¹ , Dr. S. Bonnet, Dr. D. Hetterscheid
	Molecular Inorganic Chemistry (UvA, HIMS) Prof. dr. C.J. Elsevier ¹
	Organic and Organometallic Chemistry (VU, EMS) Prof. dr. K. Lammertsma, Dr. A.W. Ehlers, Dr. J.C. Sloopweg
	Synthetic and Bio-organic Chemistry (VU, EMS) Prof. dr. ir. R.V.A. Orru, Dr. E. Ruijter
	Synthetic Organic Chemistry (UvA, HIMS) Prof. dr. H. Hiemstra ¹ , Prof. dr. J.H. van Maarseveen, Prof. dr. P. Timmerman, Dr. M.Á. Fernández-Ibáñez, Dr. S. Ingemann
	2
Biophysical Organic Chemistry (UL, LIC) Prof. dr. H.J.M. de Groot, Dr. Alia, Dr. F. Buda	
Raymond and Beverly Sackler Laboratory Astrophysics and Astrochemistry (UL, LION) Prof. dr. H. Linnartz	
Molecular Structure and Dynamics – FELIX/Molecular and Biophysics (RU) Prof. dr. J. Oomens, Dr. J.M. Bakker, Dr. A.M. Rijs	
Molecular Nano-Optics and Spins (UL, LION) Prof. dr. E.J.J. Groenen, Prof. dr. M. Orrit, Dr. P. Gast, Dr. M. I. Huber	
Molecular Photonics (UvA, HIMS) Prof. dr. A.M. Brouwer, Prof. dr. W.J. Buma, Prof. dr. S. Woutersen, Dr. R. M. Williams, Dr. H. Zhang, Prof. dr. J. Oomens	
Surface Chemistry and Catalysis (UL, LIC) Prof. dr. M. Koper ¹ , Dr. W.T. Fu, Dr. I.M.N. Groot, Dr. D. Hetterscheid, Dr. L.B.F. Jurlink	
3	Computational Chemistry (UvA, HIMS) Prof. dr. P.G. Bolhuis, Prof. dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede
	Theoretical Chemistry (VU, EMS) Prof. dr. F.M. Bickelhaupt ¹ , Prof. dr. L. Visscher, Dr. C. Fonseca Guerra, Prof. dr. P. Gori Giorgi, Dr. O. Gritsenko
	Theoretical Chemistry (UL, LIC) Dr. J. Meyer
	Theoretical Chemistry (RU) Prof. dr. ir. G.C. Groenenboom

¹also NIOK

2. Education and Research Training

2.1 HRSMC Education Programme and Dick Stufkens Prize

The objective of the HRSMC Educational programme is to supply highly qualified scientific practitioners who are equipped to quickly build successful careers in several professional fields, varying from a researcher at a University/a (chemical) company/industry/a governmental research organisation (TNO), to a job as secondary or postsecondary educator, or to a job as government regulator or policy maker. The advantage of a multidisciplinary organization such as the HRSMC is that the PhD students are broadly trained and educated scientists, which increases their career prospects.

Within the HRSMC each Course and Summer School is evaluated. This evaluation is extensively discussed in meetings of the Education Committee and the HRSMC board, and in the annual staff meeting. The lecturers concerned are informed about the outcome as well. Furthermore, the contact with our PhD researchers via these surveys is used as an opportunity to receive feedback on the variety and quality of HRSMC activities in general. Since 2009, a PhD platform has been established to get feedback on existing activities and proposed changes.

HRSMC Education Programme

The main mission of the HRSMC is to provide its PhD students with high-level education training. Apart from completing a research project, the PhD students of the HRSMC follow an individual education and training programme. For this purpose the education committee supplies them with a selection of courses, which are announced in newsletters/ashes and on the HRSMC website. The board of the school presents HRSMC certificates to those students who have fulfilled their education programme with a minimum of 15 ECTS:

ECTS system	1 ECTS = 28 h
Literature research, Paper (see remarks for explanation) and Colloquium (see remarks for explanation)	6, all three together
HRSMC school	2-3
HRSMC course	2-3
External course of + 1 week	1-3, the validation of the responsible organization will be used.
Course on didactics	1-2
Presenting a poster at an (inter)national conference	1
Giving a lecture at an (inter)national conference	2
2x attendance of a guest lecture and a scientific discussion	10 attendances=1 EC
Research in another laboratory (preferring outside Holland)	max. 6
Minimum	15

Remarks:

- Every PhD needs to follow at least one HRSMC course and one HRSMC school for the HRSMC certificate. If there is no HRSMC school or course available supporting the aspects of the PhD research, an external course can be chosen instead (but for 95% of the PhD student this is not necessary). The other items are optional: for the certificate it is not 'a must' to do a course on didactics or a research in another laboratory, but when this is done a maximum of 6 ECTS can be given for this activity.
- The Han-sur-Lesse Winter school 'Theoretical Chemistry & Spectroscopy' is not organized by the HRSMC, but many HRSMC staff members are involved. Therefore, this course is considered as a HRSMC school for the HRSMC certificate.

-
- A colloquium is a presentation, which a PhD gives at the beginning (normally after 3-6 months). A PhD researcher presents his/her research plans and gives a general background of the project. This colloquium can be based on the paper.
 - A paper should not be confused with a scientific article. A paper is a document, which a PhD researcher normally makes at the beginning of his/her research. This paper includes items like:
 - The general background of the research project
 - The plans a PhD researcher has for the first years of his/her research project

Dick Stufkens prize

In recognition of the high quality of research performed by PhD researchers participating in the HRSMC, the board of the HRSMC has established in 2008 the annual Dick Stufkens Prize for the most outstanding PhD thesis within HRSMC. The prize consists of a certificate and a cash prize of 1,000 Euros. The prize is named after the late scientific director of the HRSMC from 1997 to 2001, Prof. dr. Dick Stufkens, who forged new bonds between the participating groups and was always actively seeking to enhance the possibilities the School could offer to its Ph.D. students. An overview of the Dick Stufkens prize 2011 – 2016 can be found in Appendix 7.

2.2 HRSMC Interuniversity Courses and Schools

HRSMC Courses

The HRSMC has developed three specialised, multidisciplinary courses, or so-called HRSMC interuniversity courses, which are given by a team of HRSMC staff members. Lecturers outside the HRSMC (even from abroad) will occasionally be invited. The interuniversity courses are in general organised according to a two/three year cycle. HRSMC members/PhD students, advanced MSc students and participants from other universities can attend the following courses:

- **Molecular Modelling**

- HRSMC theme 1 and 2; 3 ECs for PhD and MSc students.
- The course is intended for PhD students who (consider to) use computational chemistry methods in their experimental research. The aim is to provide participants with enough background and hands-on experience to get started in modelling chemical structures and reactions.
- Organized in 1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2008, 2013, 2016.

- **Physical Methods in Inorganic Chemistry**

- HRSMC theme 1; 2 ECs for PhD students, 3 ECs for MSc students after the fulfilment of an exam.
- The course is intended to provide participants with important applications of various spectroscopic techniques and methods in research in inorganic and organometallic chemistry.
- Organized in 1994, 1999, 2001, 2003, 2005, 2007, 2009, 2011, 2013, 2015.

- **Photophysics, Photochemistry, and Photobiology**

- HRSMC theme 2; 3 ECs for PhD and MSc students.
- This course provides an overview of experimental aspects of optical spectroscopy, and the application to a variety of systems, with examples ranging from inorganic/molecular to biological/medical fields.
- Organized in 1996, 1999, 2001, 2004, 2007, 2010, 2014.

During the 2011 – 2016 period six Courses were organized (see Appendix 8A).

HRSMC Schools

The HRSMC has developed several HRSMC Schools. Most of them differ with the interuniversity Courses in a way that it is more organized like a conference with lectures, discussion sessions and poster sessions. In addition, the vast majority of the lecturers who participate in the HRSMC Schools come from abroad. Announcements of HRSMC Schools are sent to international contacts of the organizing HRSMC staff members. The HRSMC Schools are internationally greatly appreciated as high-quality Schools, and thus attract PhD researchers from all over the world. On average, about 50% of the participants of the HRSMC Schools come from foreign universities.

The following Schools are organized:

- **Molecular Simulations**

- HRSMC theme 3; 3 ECs for PhD and MSc students.
- The MolSim School provides training in the field of simulation techniques for the study of many-particle (molecular) systems. It targets doctoral and post-doctoral researchers, as well as advanced master students, who want to learn these techniques to study topics in physics, chemistry or biology.
- Organized in 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016.

- **EPA Summer School on Photochemistry**

- HRSMC theme 2; 2 ECs for PhD students, 3 ECs for MSc students after the fulfilment of an exam.
- The lecturers in this school represent a few of the many branches of modern photochemistry. They are leading experts in areas such as single molecule spectroscopy, molecular photochemical reactivity, nanoparticle spectroscopy,

photobiology, time-resolved spectroscopy, organic light emitting materials, and medical photonics.

- Organized in 1998, 2003, 2008, 2012, 2016.

- **Modern Developments in Spectroscopy**

- HRSMC theme 2; 2 ECs for PhD students, 3 ECs for MSc students after the fulfilment of an exam.
- Highly qualified scientists present introductory and specialized lectures on various topics in the field of spectroscopic and dynamical studies of molecular systems. The topics range from frequency resolved spectroscopic studies of gaseous biomolecules, time-resolved studies in chemical and biological systems, dynamics in proteins and membranes, photodissociation dynamics, dynamics and control in femtochemistry, and molecular nanophotonics.
- Organized in 2001, 2003, 2006, 2009, 2012, 2015.

- **Synthetic Bio-organic Chemistry**

- HRSMC theme 1; 2 ECs for PhD students, 3 ECs for MSc students after the fulfilment of an exam.
- During this meeting participants receive high-level education in contemporary synthetic organic chemistry, including biocatalysis and supramolecular chemistry, and with a focus on biological applications.
- Organized in 2001, 2005, 2009, 2013.

- **Advanced Metal-Organic Chemistry and Catalysis**

- HRSMC theme 1; 2 ECs for PhD students, 3 ECs for MSc students after the fulfilment of an exam.
- The main purpose of the school is to inform PhD and master students of the latest developments in homogeneous catalysis, organometallic and coordination chemistry.
- Organized in 1998, 2002, 2006, 2010, 2014 – with NIOK.

During the 2011 – 2016 period twelve Schools were organized (see Appendix 8B).

2.3 The annual HRSMC Symposium and other HRSMC Activities

The annual HRSMC Symposium

The annual HRSMC symposium is organized for its HRSMC members (PhD students, Postdocs and staff members), MSc students from the HRSMC Excellence Programme and other scientists (from other universities or from the industry). With various poster sessions and guest, PhD, postdoc and staff lectures, it is a unique opportunity to network and to discuss novel trends in chemical research. The symposium usually attracts 150-180 scientists and closes with the lecture of the annual Dick Stufkens prize winner for the most outstanding PhD thesis (1,000 Euro). A special highlight was the HRSMC Symposium of 2014, where three Nobel laureates spoke at the school's 20th anniversary: Prof. Moerner (2014), Prof. Warshel (2013) and Prof. Hoffmann (1981). The symposium took place at 'the place of birth', the Royal Netherlands Academy of Arts and Sciences (KNAW). The symposium, which was attended by ca. 200 scientists, also included poster sessions with 42 posters, mainly presented by PhD students.

KNCV/HRSMC Career Advice Activity

For PhD students and postdocs, an afternoon is organized with various lectures regarding career possibilities and job-application. In addition, each participant gets 30 min. quality time with a career consultant.

(2010, 2012, 2013, 2015)

Lab visit Theme 2

Within HRSMC Research Theme 2, Photochemistry and (Laser) Spectroscopy, a lot of specialised equipment is used. Therefore, lab visits are organized to share expertise and knowledge, and to stimulate collaboration.

(2011, 2014, 2016)

Proposal Writing/Peer Review Workshop (2 EC)

The Proposal Writing workshop (4 days) is aimed at graduate research students and post-docs who have some experience in scientific writing and might have taken an introductory workshop on scientific writing. This workshop is most useful to researchers who plan to submit grant proposals. The Peer Review workshop (1 day) is aimed at graduate research students and post-docs who are planning or have submitted a manuscript to a peer-reviewed journal. This workshop is most useful to researchers who are beginning to publish peer-reviewed research. This new Workshop was organized for the first time in 2015 and the HRSMC Board intends to organize this workshop biannually.

(2015)

Sustainability Workshop (HRSMC-HIMS)

The workshop, organized in the context of the HRSMC Excellence Master 'Sustainability: the Molecular Approach' and the UvA's Research Priority Area Sustainable Chemistry, is intended for HIMS and HRSMC PhD students, postdocs and staff members, as well as for MSc students.

(2016)

Introduction activity for first years and Social activity for all PhD/PD

On a regular basis (annually or biannually) an information meeting with drinks are organized for new PhD students. Furthermore a (biannual) Social activity for all PhD and postdocs within the HRSMC is organized by the PhD platform.

More information about the annual HRSMC Symposia and other activities between 2011 – 2016 can be found in Appendix 8C en D.

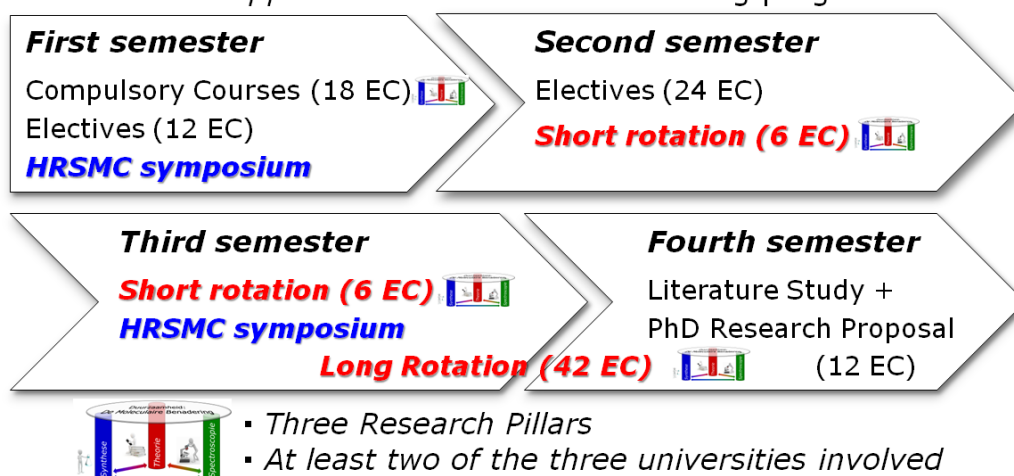
3. HRSMC Excellence Master and Fellowship Programme

3.1 HRSMC Excellence Master Programme 'Sustainability: the Molecular Approach'

Apart from providing and organizing an outstanding educational programme for PhD students which is also accessible to (advanced) MSc students, the HRSMC has been elected in 2012 as one of the thirteen Graduate Schools to receive substantial funding from NWO. With this funding the HRSMC can offer young PhD students the opportunity to develop their own research ideas within the framework of the programme "*Sustainability, the Molecular Approach*". The funding is part of NWO's Graduate Programme and aims to develop Dutch PhD Educational Programmes. As a result of this programme, the HRSMC Excellence Programme was established in 2013, which is an interuniversity (UvA-VU-UL) and interdisciplinary programme, reflecting the three HRSMC Research Themes.

The HRSMC Board aims for the top 10 percent of students - not only at the HRSMC universities but also from other institutions and abroad. Selected students are talented in various disciplines and have a broad vision. Admission is granted based on a strict selection procedure which comprises a written application and an interview with the HRSMC Board and the Director of the Education Committee. In the period of 2013 – 2016, 16 students participated in the HRSMC Excellence Master Programme, of which 3 students were appointed as PhD students within the NWO Graduate Programme based on their research proposal.

The two-year HRSMC Honours Master Programme "*Sustainability: The Molecular Approach*" consists of the following programme:



General outline of the programme:

The interuniversity HRSMC Excellence Master 'Sustainability: the Molecular Approach' prepares talented chemistry students for a scientific career. Researchers of the University of Amsterdam (UvA), the VU University Amsterdam (VU) and Leiden University (the HRSMC partners) composed a unique, demanding and interdisciplinary programme characterised by strong integration of theory, spectroscopy and synthesis. Only the best 10 percent of the chemistry students are eligible for the programme. A crucial part is the preparation of a proposal for PhD research to be performed by the students themselves. Four proposals are rewarded with an actual PhD position, financed through the Graduate Programme of the Netherlands Organisation for Scientific Research (NWO).

The students are getting more guidance from a special committee mentoring the selected students during the different stages of this Excellence Master (e.g. progress and choice of

internships). In December 2016, this special 'Advisory Committee' consisted of Dr. S. Bonnet (UL, director of education), Dr. C. Fonseca Guerra (VU) and Dr. E. Ruijter (VU).

Three PhD proposals selected in HRSMC/NWO excellence programme

During the second year, typically during their graduation internship, the students choose one or more staff members of the HRSMC for discussions and consultations regarding the research subject for their proposed PhD research project. Students have complete freedom in choosing a topic as long as it fits within the research programme of the HRSMC. Students are encouraged to involve more than one HRSMC research groups in their proposal, and they write their proposal following a template that is downloadable from the HRSMC website. Students present and defend their proposal in a meeting with an Assessment Panel consisting of Prof. dr. G. van Koten (UU), Prof. dr. R. van Santen (TUE) and Prof. dr. D. Wiersma (RUG) as external members, as well as HRSMC Board members and the chairs of the Education and Research Committee. The best proposals are selected on the basis of scientific quality, novelty, feasibility and level of interdisciplinarity.

In 2015, the HRSMC has granted two proposals for PhD research. The laureates were Hans de Bruijn (UL) (*An experimental and theoretical study of the hydroaminomethylation of internal olefins to linear amines with a Co-based catalytic system*; supervisors Prof. dr. E. Bouwman (Leiden) and Prof. dr. F.M. Bickelhaupt (VU Amsterdam) and Kaj van Vliet (VU) (*Creative Advances in visible light photoredox catalysis*; supervisors Prof. dr. B. de Bruin (UvA) and Prof. A.M. Brouwer (UvA)). Both students received their Master's degree with honours (cum laude). In 2016, the HRSMC has granted the proposal of Tessel Bouwens (UvA): *Photoredox shuttles for efficient solar fuel devices*; supervisors Prof. dr. J.N.H. Reek (UvA), Prof. dr. S. Woutersen (UvA) en Prof. dr. L. Visscher (VU). According to the panel the selected proposals excelled not only in academic quality but also in their interdisciplinary and interuniversity approach, illustrative of both the Excellence Master and the HRSMC research school.

3.2 The HRSMC Fellowship Programme

In 2015 the HRSMC established a new Fellowship Programme. It provides funding for foreign researchers of postdoc level and higher to visit and collaborate with HRSMC-affiliated research groups, aiming specifically to set up new and challenging research lines. Annually, there are two application rounds: in April and October.

General outline of the Fellowship Programme:

The HRSMC Fellowship programme aims to support and reinforce high-quality research within the HRSMC. Within the programme, visits by outstanding foreign researchers (postdoc level and higher) to HRSMC-affiliated research groups are financed.

The HRSMC strongly welcomes applications, which

- stimulate cross-fertilization between differently-affiliated HRSMC research groups, involving 2 or more applicants from different groups, and
- support fundamental, not directly application-driven research.

Staff and associated members of the HRSMC with a permanent position can apply. Applications in which staff members of 2 or more different research groups are involved have a higher priority for funding (if other aspects are comparable).

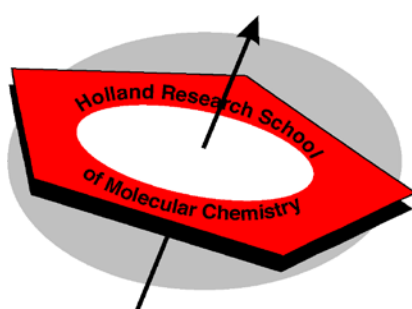
Visits by outstanding, foreign researchers with a minimum of 2 weeks and a maximum of 6 months are supported. Grants can be requested to help to meet the costs of subsistence and travel. The following rates apply:

- *Subsistence costs*: €1750 per month for an experienced researcher or €2000 per month for a full professor.
- *Travel costs*: The maximum amount of grant depends on the country in which the researcher is appointed. For researchers based in Europe the maximum is €500, for researchers based outside Europe €1500. There is no compensation for consumables or other research costs.

An overview of the awarded Fellowships in 2015 and 2016 can be found in Appendix 9.



REPORT OF THE PEER REVIEW COMMITTEE
FOR THE
HOLLAND RESEARCH SCHOOL OF MOLECULAR
CHEMISTRY (HRSMC)



Site visit Amsterdam, May 16-18 2011

Prof. dr. Odile Eisenstein (CNRS, IGG University Montpellier 2, France)

Prof. dr. David Milstein (Weizmann Institute, Israel)

Prof. dr. Douwe Wiersma (chair, University of Groningen, the Netherlands)

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Preface

Graduate research in the Netherlands is done at Research Institutes or in Graduate Research schools ('Onderzoekscholen'). While most Research Institutes are local, Graduate Research Schools can be either local or, more often, comprise several universities in a particular field, as, for instance, polymer chemistry. While the emphasis in Research Institutes is on research, the emphasis in Graduate Research Schools is on teaching of the PhD students. Interestingly enough, the interaction between the different research groups in a Graduate School through Courses and Symposia aimed at graduate students, will also affect the groups in their research direction. While the Dutch universities have introduced the bachelor/master system, they are still struggling with some of the implications of the new educational model. The evolution of the Dutch PhD trajectory towards the American Graduate School model is also in progress. This process also affects the Holland Research School for Molecular Chemistry, which emphasizes its educational role for graduate students, while at the same time trying to stimulate collaborative research in the themes the School covers.

The Committee reviewing the Holland Research School of Molecular Chemistry (HRSMC) was pleased to determine, by discussions with staff members and PhD students, that the HRSMC is functioning extremely well as Graduate School and that its existence as an umbrella organization also for research is appreciated by all stake holders.

The Committee enjoyed very much the presentations by staff members on the ongoing research projects and also appreciated the meetings with the HRSMC Board, the dean of the UvA-faculty and the Institute's Director, as well as the scientific staff and the PhD students.

Prior to its site visit, the Committee received the following information on the HRSMC:

- The Annual Reports of the years 2005 – 2010 including the lists of publications.
- The 'PRC Supplement', which presented a survey of the activities and achievements of the HRSMC, both educational and scientific, over the past six years.¹

This information has helped considerably the Committee in preparing a report covering the functioning of the HRSMC during the period 2005-2010 and in making recommendations for the future.

We are grateful to all those involved in the discussions on the HRSMC and to the Director's staff for providing the necessary data for the present report. We hope and entrust that our recommendations will enable the HRSMC to maintain its high quality and added value to PhD students and staff members of the participating research groups.

Prof. dr. O. Eisenstein
Prof. dr. D. Milstein
Prof. dr. D.A. Wiersma

¹ *This Supplement was based on the ECOS re-accreditation form and additional information was given in several appendices. As the Application for Re-Accreditation should not exceed 10 pages, this Supplement is not included in the Application for Re-Accreditation but is available upon request.*

1. Mission, Structure and Management

INTRODUCTION

The Holland Research School for Molecular Chemistry (HRSMC) was founded in 1994 and comprises 18 research groups of the following institutes and universities:

- The Van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam (UvA, also the legal representative of the HRSMC)
- The Institute for Electrons and Molecular Structure (EMS) of the Free University (VU)
- The Leiden Institute of Chemistry (LIC), the Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Leiden University (UL)

As a Research School, the mission of the HRSMC is

'...to stimulate, facilitate, initiate, focus and support (collaboration in) high-level research and education in the area of chemistry concerning the connection between the three dimensional and electronic structure of molecules, their purposeful thermal and photochemical synthesis and reactivity, as well as their physical and biological properties.'

With this broad mission, the primary aim of the school is to teach PhD students to use their insights in a multidisciplinary approach to answer key questions in molecular sciences. In this respect the HRSMC is unique in the Netherlands as it does not focus on a single research area as most other graduate research schools do (e.g. polymers, catalysis, materials).

The HRSMC Board consists of three representatives from the universities representing the various scientific domains covered and the Scientific Director. The Scientific Director is assisted by a part-time executive secretary and a part-time administration officer. An External Advisory Committee and several internal committees (the Education Committee, the PhD Platform and the Research Committee) advise the Board.

FINDINGS AND CONCLUSIONS

Mission

The Committee is satisfied with the way the Research School's mission is implemented. The interactions between the different research groups have shown to be fruitful and the PhD students testify that the activities of the HRSMC greatly contribute to their scientific training and to their network. Both staff members and PhD students very much appreciate the Symposia, Courses and Schools organized by the HRSMC. The Research School also offers a variety of activities for PhD students in order to gain more specialized expertise, as well as a broader comprehension of the field they are working in.

Management and Structure

The quality and effectiveness of the management of the HRSMC is excellent. The Board constantly looks for opportunities to diversify the organization with new research groups.

To implement one of the recommendations of the Accreditation Committee for Research Schools (ECOS) made at the previous re-accreditation in 2005, a PhD Platform has been established in 2009. The Committee believes that with this Platform the HRSMCs organizational structure is optimal.

Overall impact

Despite limited financial means the HRSMC has managed to establish a remarkably successful research and educational program. This is impressive, because this success is

only due to the desire of the participating staff to work together for the benefit of their graduate students and to stimulate interdisciplinary research. To intensify this collaborative research effort the Committee strongly encourages the participating universities to increase the budget of the HRSMC.

2. Research

INTRODUCTION

The research of the HRSMC takes place at the heart of chemistry and physics and focuses on the chemical, physical and biological properties of small to moderately sized molecules in relation to their electronic and spatial structures. Research topics are grouped in three themes: (1) Synthesis, Characterisation, Reactivity and Properties of Molecules; (2) Photochemistry and (Laser) Spectroscopy; and (3) Theoretical Chemistry.

The HRSMC aims to stimulate collaboration between the research groups and supports activities that aim to improve the research infrastructure. One of the key activities to accomplish this goal is the annual HRSMC symposium. Traditionally, several staff members and PhD students present their latest scientific accomplishments to a broad audience of inorganic and organic chemists, physical and theoretical chemists, etc. On the advice of the Education Committee and the PhD Platform, the format of the symposium in 2010 has been changed to further stimulate the interaction between all different research groups of the School. To achieve that aim, more and shorter presentations by PhD students were scheduled and visits to all posters by staff and students encouraged by the award of a public prize per research theme.

In the period 2005 – 2010, 18 research groups from the VU, UvA and UL participated in the HRSMC. All but one of these groups have been recently evaluated by an international peer review panel related to the assessment of the Quality Assurance Netherlands Universities (QANU). The outcome of this evaluation for the 18 groups is given in Annex 2.

Seven research groups of the HRSMC (Baerends/Bickelhaupt, Elsevier, Hiemstra, Koper, Lammertsma, Orru, Bouwman/Reedijk, Reek and Wever) also participate in the National Research School Combination Catalysis Controlled by Chemical Design (NRSC-Catalysis).

As a graduate school the HRSMC is not a granting organization and therefore does not have the financial means to contract PhD students or to direct the research of the research groups. The participating groups are usually embedded in a Research Institute at their own University and financed on the group level by the corresponding university, the Netherlands Organisation for Scientific Research (NWO), the EU, or by granting organisations such as STW.

In addition to discussions with the Board, the Committee has spoken with all group leaders (or their representatives) during three interview sessions related to the three Research Themes. A major topic for discussion was the added value of the School with regard to the education of PhD students and collaborative research efforts.

FINDINGS AND DISCUSSION

Quality of Research

The universities and the individual research groups are well represented within the three Research Themes. Considering the SEP evaluations given in the QANU reports (see Annex 2) and the presentations of the research groups given during the committee's visit (May 17th), the Committee is impressed with the quality of the research within the HRSMC, which is very good to outstanding.

Collaboration

The HRSMC plays an important role by promoting interaction and collaboration between the various research groups. This results in a significant number of joint ventures between the different groups of the participating universities. Although not all contacts lead to joint papers, the network has clearly demonstrated its added value through regular discussions between the various groups, joint meetings and the equipment shared among the members of the HRSMC. Because of its 15 year existence, staff members are well aware of the scientific expertise available in the HRSMC and appreciate what the School offers for PhD students in terms of Symposia and special courses.

In addition to the local interdisciplinary research projects, several staff members participate in projects with other Dutch universities and in projects outside the Netherlands, in particular with groups from the University of Münster (see Chapter 4).

Research Strategy

The Committee has noted that the HRSMC has no jurisdiction to impose a research strategy on the research groups, which in the committee's opinion is just fine. The only and important mission of the HRSMC is to facilitate the interaction between the different research groups and to stimulate interdisciplinary research.

Financial situation for Research in the Netherlands

The Committee was informed by the dean of the faculty, Prof. dr. Bart Noordam, about the new financial model of the Dutch Ministry for scientific research. The Department of Economic Affairs, Agriculture and Innovation apparently has chosen 10 priority areas judged as being vital to the Dutch economy. On advice of a national committee it has been decided that 50% of NWO budget should be allocated to applied research in these 10 areas, of which chemistry is one. However, the committee notes that progress in Science is dependent on the advancement in all branches of Science. The Committee was therefore very surprised and concerned by the fact that physics and mathematics are not among the designated priority areas.

3. Education and Training of PhD students

INTRODUCTION

To provide PhD students with a broad knowledge of multidisciplinary research in a university or industrial setting, the HRSMC organizes an annual Symposium, four different so called Schools (once every three to four years) and six different interuniversity courses (organized every year or every two or three years) covering all research themes. In addition to these educational activities, the HRSMC offers seminars, lab visits, a Career Advice event for PhD students and social events for staff and PhD students.

The School awards a certificate to PhD students that have fulfilled their educational requirements (18 ECT credit points). This certificate is also a prerequisite to apply for the Dick Stufkens prize for the best thesis within the HRSMC.

Each course or school is evaluated by the participants. In addition to a questionnaire focusing on the level and quality of the course and its relevance to the research of the PhD students, there is a survey about the functioning of the HRSMC in general. Furthermore the educational activities and planning for the coming years is reviewed annually by the Education Committee and PhD platform. The outcome of these surveys and the input of the PhD Platform and Education Committee has led to several new activities in the period 2005 – 2010: (1) the course 'Molecular Simulation', (2) Synthetic Chemistry Problem Solving sessions, (3) the course Medicinal Chemistry, (4) lab visits within Research Theme 2, (5) a career advice event, and (6) an Introduction for first-year PhD students and (7) a social event for all HRSMC members.

During the visit, the Committee received detailed information about the educational activities organized by the HRSMC. The Committee had discussions with students of the PhD Platform, staff members and members of the Education Committee about the impact of these educational activities on their PhD program.

FINDINGS AND DISCUSSION

Education Programme

The HRSMC has managed to establish an effective and greatly appreciated educational programme despite limited financial means. The general programme of the HRSMC reflects a broad range of interdisciplinary activities. However, to more effectively bridge the different research topics in the programme, the Committee advises courses to be offered at both an introductory and advanced level.

The Committee also recommends a new course, named 'Intellectual Property' to be given to provide the PhD students with a basic understanding of the wide range of issues concerning the legal regulation of intellectual property.

Networking activities

To increase the interaction between the groups, the Committee recommends that group meetings and lectures are announced on the website. Furthermore, PhD students should be encouraged to go to other group meetings. This idea is in line with the view of the PhD Platform. According to this Platform, PhD students strongly value opportunities to network and thereby intensify scientific relations. The committee also advises to put the PhD research projects on the group's website. This suggestion is about to be implemented by the HRSMC staff.

HRSMC Schools

The Committee noticed that the Schools organized by the HRSMC are strongly appreciated by staff members and PhD students. The Committee endorses this School concept and has some recommendations to further increase the effectiveness of these Schools for students. Besides high-quality invited talks, the Committee recommends that PhD students get an opportunity to present their work in short, 12-15 min., talks. Participation by foreign PhD students should be further encouraged through the staff's network.

4. Internationalisation

INTRODUCTION

Besides the international collaborations of the individual research groups, the HRSMC plays a prominent role in a number of important European Research Centers as LaserLab Amsterdam (part of LaserLab Europe) and CECAM (Centre Européen de Calcul Atomique et Moléculaire) to which the Amsterdam Center for Multiscale Modeling (ACMM) also belongs.

At the HRSMC Schools most lecturers come from universities outside the Netherlands. Internationally renowned scientists also contribute to the courses given and often present invited papers at the HRSMC's annual Symposium.

Since 2001 the HRSMC collaborates with the WWU Münster. The current program, the *International Research Training Group (IRTG) 'Generation of Supramolecular Functional Cavities - Container Molecules, Macrocycles and Related Compounds'*, started in February 2007 and was funded for 4.5 years by the DFG and by the NWO. The IRTG promotes and supports the exchange of PhD students and guest lecturers, as well as the organisation of joint courses and summer schools.

During the visit, the Committee discussed the international collaborations with the Board and staff members. Concerning the collaboration with WWU Münster, the Committee had a meeting with two HRSMC staff members, including the coordinator of the Dutch section, and with two staff members of the WWU Münster, including the spokesperson and coordinator of the German section.

FINDINGS AND DISCUSSION

International Status of the HRSMC

The list of the most important international collaborations is given in the PRC Supplement. The most important collaboration is that with the WWU Münster. HRSMC staff members are enthusiastic about this collaboration and about the resulting joint educational activities. Despite the fact that there is currently no prospect for a continuation of funding after September 2011, there is a strong wish from both sides to continue the joint activities.

In the current program the DFG provides funds for the appointment of PhD students. In fact the German groups in Münster received 1.885 M€ (including funding for 10 PhD students) for collaboration with the HRSMC. In contrast the HRSMC received only 199 k€ from NWO relating to this program.

International character of HRSMC Schools

The Committee greatly appreciates the international character of the HRSMC Schools with attendance of foreign students sometimes exceeding 50% of the total number of participants. In cases where attendance of foreign students is lower, staff members should use their network to advertise these Schools to their colleagues. This would be beneficial to all and further enhance the international visibility of the HRSMC.

5. Addressing the ECOS Recommendations of 2005

INTRODUCTION

After the previous re-accreditation of the HRSMC by the Royal Netherlands Academy of Arts and Sciences (KNAW) in 2005, the Accreditation Committee for Research Schools (ECOS) gave the following recommendations:

1. The Committee strongly urges the School to keep a close eye on whether the procedures concerning the monitoring of the progress of PhD students are carried out in a strict fashion and complied with.
2. The Committee recommends to establish a PhD Platform
3. The Committee strongly urges the School in the coming period of accreditation to give a high priority to the implementation of an effective strategy that will reduce the average graduation period - as seems to have occurred since 1998 - even more and bring it back to a maximum of 4.5 years.
4. The Committee recommends the School to anticipate in supporting the PhD students in their preparations for a career after their PhD. The Committee thinks here in particular of a course in the area of management skills for all PhD students.
5. The Committee argues in favour of increasing the role of the School in the development of a strategic research programme by becoming more facilitating between the HRSMC research groups.

In the PRC Supplement, the response given to the ECOS recommendations is as follows:

1] Monitoring progress of PhD students. This is primarily a responsibility of the participating institutes (see Appendix B of the PRC Supplement²). To facilitate this process, the following measures have been taken: (1) these findings were communicated to all directors of the involved institutes and they were asked to address this in their staff meetings and to take adequate measures (e.g. to keep track of the official annual assessment of their PhD students), (2) during staff meetings the subject has been discussed regularly and (3) the HRSMC has prepared a checklist for the annual assessment discussing the Education and Supervision Plan.

2] PhD Platform. In 2009 a PhD Platform has been established. This has led to several changes, such as several new activities, a new format of the annual symposium and the renewal of the website and newsletter (see Section 3-1a and 3-2d of the PRC Supplement³).

3] Graduation period. To shorten the graduation period to 4.5 years the measures described under 1] have been taken. As result the percentage of students that graduated in less than 4.5 years increased from 17% (Cohort 2003) to 67% (Cohort 2006). The percentage of students graduating within 5 years rose from 66% to 77% for these cohorts.

4] Career and Management courses. To implement appropriate measures, extensive discussions have taken place in the Educational Committee and PhD Platform. Furthermore, surveys have been organized amongst HRSMC PhD students. On this basis, the HRSMC Board has concluded that various Management Courses are already offered by the three universities (UvA, VU and UL) and other organizations. There is thus no need for the HRSMC to organize such a course. Instead, an overview of the different courses and the

² Or Appendix 3 of the Application for Re-Accreditation

³ Or Section 3-1a and 3-2d of the Application for Re-Accreditation

corresponding organizations is now given on the HRSMC website. The Board also concluded that more information about career opportunities is needed. In 2010 the first biannual career advice event was organized together with the Royal Dutch Chemical Society (KNCV).

5] Influence on strategic research programme. Apart from the strong involvement of the HRSMC Board on the research programme of the institutes as an ‘umbrella organisation’ (see Section 2a⁴), the Board has taken a number of specific measures to be more facilitating between the HRSMC research groups and thereby obtain more influence on the strategic research programme:

1] The annual symposium is a unique and important activity for the HRSMC since it engages the entire scope of molecular chemistry and physics (see Section 1 of the PRC Supplement). The following changes were implemented:

(a) With better communication and more involvement of the staff members, the Board has succeeded to almost double the attendance from 2005 to 2010.

(b) The set-up of the annual HRSMC symposium has been changed to get more cross-fertilization. Besides more and shorter PhD lectures, there are less posters per session. Visits of participants to posters from other Themes than their own is encouraged by the introduction of a public prize per Theme.

(c) To celebrate the 15-year anniversary of the HRSMC, a two-day symposium has been organized in 2009 that was attended by 225 participants. Besides poster sessions and lectures from HRSMC PhD students and staff members, several prominent (inter)national lecturers were invited to further enhance the reputation of the annual symposium.

2] New activities are organized like the Problem Solving Sessions within Theme 1. Furthermore, as within Research Theme 2 (Photochemistry and (Laser) Spectroscopy) a lot of specialized equipment is used, lab visits are organized to share expertise and knowledge, and to stimulate collaboration.

3] As of 2011, an Introduction Activity for all first-year PhD students and a Social Activity for all HRSMC members (PhD students and staff members) are organized.

4] More staff members are involved in HRSMC activities as coordinators and lecturers

5] Since 2006, three times a year an e-mail newsletter is sent. Besides information on HRSMC activities, it contains information of the groups (new PhD students/staff, research highlights, grants, etc.).

FINDINGS AND DISCUSSION

The Committee concludes with respect to the recommendations made by the ECOS that the HRSMC has fully complied with these recommendations and that the measures taken have been successful. In particular the Committee is impressed with the remarkable reduction in average graduation time that was achieved by the implementation of stricter procedures regarding the monitoring of the progress of graduate students in their PhD projects.

⁴ Or Section 2a of the Application for Re-Accreditation

6. Conclusions and Recommendations

In summary, the overall conclusion of the Committee is that the HRSMC *has managed to establish itself as a very successful Research School.*

To further increase the School's impact, the Committee recommends the following:

1. To intensify research collaborations within the School, the Committee emphasizes the importance of an increase of the School's budget.
2. To increase the interaction between the staff and students of the different research topics the Committee advises courses at both an introductory and advanced level.
3. To provide PhD students with a basic understanding of the wide range of issues concerning the legal regulation of intellectual property, a Seminar on 'Intellectual Property' is recommended. As many PhD students will end up in Industry, a Seminar on "Industrial Chemistry", preferably given by an industrial chemist, is also advised.
4. To stimulate interaction between the research groups, the Committee recommends that group meetings and lectures are announced on the website and that PhD students are encouraged by their supervisors to attend these meetings. PhD projects should also be put on the website.
5. The Committee is in favour of continuing the collaboration with the University of Münster after the official end of the current program. Even without external funding the groups should maintain their scientific contacts.
6. To further increase the international visibility of the Schools the staff should be encouraged to use its network to attract PhD students from all over Europe to attend the HRSMC-Courses.
7. PhD students should present their work in short talks at HRSMC Schools.

Annex 1. The Peer Review Committee and programme of the site visits.

The Peer Review Committee

Prof. dr. Douwe Wiersma, Professor of Physical Chemistry
University of Groningen, The Netherlands (Chairman)

Prof. dr. David Milstein, Professor of Organic Chemistry
The Weizmann Institute of Science, Israel

Prof. dr. Odile Eisenstein, Professor of Theoretical Chemistry
Institut Charles Gerhardt Montpellier, University of Montpellier 2, France

Drs H.E. Zwaan – van der Plas, HRSMC executive secretary,
University of Amsterdam, The Netherlands (Secretary)

The programme

Date	Start	End	Event
May 16	18:30		Welcome Dinner with the HRSMC Board and Executive Secretary HRSMC
May 17	9:00	9:30	Official welcome and introduction by the Scientific Director of the HRSMC, the Dean of the Faculty of Science and the Director of HIMS
	9:30	10:20	Interview with the Director, Board of the HRSMC and Administration Officer
	10:30	11:20	Interview with the HRSMC group leaders and staff members Research Theme 2: Photochemistry and (Laser) Spectroscopy.
	11:30	12:15	Interview with the HRSMC group leaders and staff members Research Theme 3: Theoretical Chemistry.
	12:15	13:15	Lunch
	13:15	13:55	Interview with members HRSMC/WWU Münster IRTG (research & education)
	14:00	15:00	Interview with Education Committee and Executive Secretary
	15:00	16:00	Internal Committee meeting
	16:00	16:50	Interview with the HRSMC group leaders and staff members Research Theme 1: Synthesis, characterisation, Reactivity and properties of molecules.
	17:00	18:00	Interview with PhD students of the PhD Platform
	18:15		Departure for hotel by taxi
	19:30		Diner with the External Advisory Committee of the HRSMC
May 18	9:15	11:15	Internal Committee meeting preparing final interview with the Board of the School
	11:15	12:30	Preliminary report Peers to Director and Board of the HRSMC
	12:30	14:00	Lunch and departure

Annex 2. VSNU Quality Assessment.

An overview of the research groups with corresponding SEP evaluation

	QANU page	Quality	Productivity	Relevance	Viability
Theme 1 groups: 'Synthesis, Characterisation, Reactivity and Properties of Molecules'					
<u>Bouwman (UL)</u> , Metals in Catalysis, Biomimetics & Inorganic Materials	P130	5	5	5	3
<u>Elsevier (UvA)</u> , Coordination and Organometallic Chemistry ¹	P73	4	5	5	5
<u>Orru (VU)</u> , (Bio) Organic Chemistry ²	P117	4	5	4	5
<u>Hiemstra/Timmerman (UvA)</u> , Biomolecular Synthesis ³	P71	4	4	4	4
<u>Lammertsma (VU)</u> , Organophosphorus, Organometallic and Computational Chemistry ²	P117	4	5	4	5
<u>Overkleef/ vdMarel (UL)</u> , Bio-organic Synthesis	P125	5	4	5	5
<u>Reek/Hartl (UvA)</u> , Supramolecular Catalysis ¹	P73	4	5	5	5
<u>Wever (UvA)</u> , Bio-organic Chemistry & Bio-catalysts ³	P71	4	4	4	4
Theme 2 groups: 'Photochemistry and (Laser) Spectroscopy'					
<u>Buma/ Brouwer (UvA)</u> , Molecular Photonics	P79	4	5	4	5
<u>Linnartz (UL)</u> , Laboratory Astrophysics and Astrochemistry	P18/ 19 ⁴	5	5	4.5	5
<u>Gooijer (VU)</u> , Analytical Chemistry Applied Spectroscopy	P111	3	4	5	4
<u>Groenen/Orrit/Völker (UL)</u> , Molecular Nano-Optics and Spins	The Physics evaluation is presently in progress				
<u>de Groot/Buda (UL)</u> , Biophysical Organic Chemistry	P140	4	4	4	4
<u>Koper (UL)</u> , Surface Chemistry and Catalysis	P129	4	3	4	4
<u>Janssen (VU)</u> , Physical Chemistry	P119	4	4	4	3
Theme 3 groups: 'Theoretical Chemistry'					
<u>Baerends/Bickelhaupt/Visscher (VU)</u> , Theoretical Chemistry	P121	5	5	5	5
<u>Neugebauer (UL)</u> , Theoretical Chemistry	P141	4	3	4	5
<u>Bolhuis/Meijer (UvA)</u> , Computational Chemistry & Physics	P75	5	5	5	3

QANU Research Review Chemistry 2010 Report

5=Excellent, 4=Very Good, 3=Good, 2=Satisfactory, 1=Unsatisfactory

On www.hrsmc.nl, an overview of the groups with a direct link to their website is given.

¹In the QANU report, the group of Prof. dr. C.J. Elsevier and Prof. dr. J.N.H. Reek are evaluated together with the group of Prof. dr. G. Rothenberg who is not a member of the HRSMC

²In the QANU report, the group of Prof. dr. R.V.A. Orru and the group of Prof. dr. K. Lammertsma are evaluated together

³In the QANU report, the group of Prof. dr. R. Wever and the group of Prof. dr. H. Hiemstra are evaluated together

⁴A different QANU report.

Annex 3. Abbreviations

ACMM	Amsterdam Center for Multiscale Modeling
DFG	Deutsche Forschungs Gemeinschaft (German Research Council)
ECOS	Erkenningscommissie Onderzoekscholen Accreditation Committee (for Research Schools)
EMS	the Institute for Electrons and Molecular Structure of the VU University
HIMS	the van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam
HRSMC	Holland Research School of Molecular Chemistry
IRTG	International Research Training Group
KNCV	Koninklijke Nederlandse Chemische Vereniging/ Royal Netherlands Chemical Society
KNAW	Koninklijke Nederlandse Academie voor Wetenschappen/ Royal Netherlands Academy of Arts and Sciences
LIC	Leiden Institute of Chemistry
LION	Leiden Institute of Physics
LO	Leiden Observatory
NWO	Nederlandse Organisatie voor Wetenschappelijk Onderzoek The Netherlands Organisation for Scientific Research
NRSC-C	National Research School Combination-Catalysis
QANU	Quality Assurance Netherlands Universities
STW	Stichting Technisch Wetenschappelijk onderzoek
UvA	Universiteit of Amsterdam University of Amsterdam
UL	Universiteit Leiden Leiden University
VU	Vrije Universiteit Amsterdam VU University Amsterdam
WWU Münster	Westfälische Wilhelms-Universität Münster

Appendix 2. Agreement between the participating institutes of all three universities

RELATIONSHIP BETWEEN THE HRSMC AND THE PARTICIPATING RESEARCH INSTITUTES IMC (UVA), LIC (UL) AND EMS (VU)

1. Research projects of the HRSMC PhD researchers/postdocs are approved by the director of the research institute, who judges the projects in the light of the work programme of the institute.
2. Group leader and director of the institute are responsible for the selection of candidates for the PhD project or postdoc position.
3. Group leader and PhD researcher draw an education plan that has to be approved by the director. The management of the school receives a copy of the plan and checks it with the educational requirements of the school.
4. On behalf of the HRSMC, the director of the institute judges and reports once a year the progress of the research/education of a PhD researcher. The HRSMC receives a copy of this report.
5. The director draws the annual report and work programme of his institute. All matters that concern the HRSMC are put to the board of the school for approval. The board checks these matters with the scientific mission of the school, the adjustment between the participating institutes, and the guaranteed staffing of the school.
6. The director of the institute informs the board of the school about all (intended) changes in personnel that take part in the school. This holds for the PhD researchers and postdocs as well as for the scientific, technical and administrative staff.
7. Within the framework of its scientific mission, the board of the school advises the director of the institute and the dean of the faculty concerning the policy with respect to chairs and adjustment of research with the other institutes. The board nominates an expert who sits on the Appointment Commission for the occupation of an HRSMC chair.
8. At least once a year the directors of the institutes and the school evaluate the collaboration and the course of affairs in relation to this agreement.

Appendix 3. A financial overview of the HRSMC over the period 2011 – 2015

Income 2011 - 2015	Total	Expenses 2011 - 2015	Total
Contribution UvA - Faculty	420.000	Personnel Costs	342.749
Contribution UvA - HIMS	205.000	Donation HIMS Institute ^{1]}	200.000
		Fellowship Programme	43.357
Contribution UL	27.224	Board	5.767
Contribution VU	27.224	Bureau Costs	5.401
JvGeuns foundation	30.000	Annual Reports (printing)	5.226
Schools	246.429	Schools	243.043
Symposium	8.160	Symposium	87.979
Other	1.007	Dick Stufkens PhD prize	5.000
Interest	3.611	Courses/Lab visits	9.073
KNCV/HRSMC Career Advice Event	362	KNCV/HRSMC Career Advice Event	362
		Excellence MSc Programme ^{2]}	1.712
		HRSMC website	897
		Re-accreditation 2011/2012	9.045
		Social Activity	4.075
		Other	1.399
	<hr/> € 969.017		<hr/> € 965.085

1] As of 2014, a new agreement between the VSNU (Association of universities in the Netherlands) and SODOLA (the Dutch network of accredited research schools in all fields of academic research) became applicable for the funding of Research Schools. Based on this agreement, as of 2015, the HRSMC should get funding of 300 kEuro. Instead of 50 kEuro from the faculty and 5 kEuro from the HIMS Institute, the contribution of the faculty was raised to 150 kEuro and 150 kEuro for the HIMS Institute. As this increase for the HIMS Institute would strongly affect HRSMC affiliated research groups from the UvA/HIMS Institute, the HRSMC Board decided to donate 150 kEuro to the HIMS Institute.

2] For the HRSMC-NWO Graduate Programme 'Sustainability: The Molecular Approach', the HRSMC received separately **800 kEuro** for the appointment of 4 PhD students in 2012. Within this programme, two PhD students were appointed in 2015 and one in PhD student in 2016. These finances are not included in this overview.

Appendix 4. HRSMC Organisation on 31 December 2016

Organisation Structure

The interuniversity research school HRSMC is a cooperation between the University of Amsterdam (UvA), the Vrije Universiteit Amsterdam (VU), Leiden University (UL) and the Radboud University (RU), UvA being the university in charge of the HRSMC ('penvoerder'). The HRSMC organisation structure consists of:

Scientific Director and Managing Staff

- Prof. dr. W.J. Buma (UvA), Scientific Director
- Drs. H.E. Zwaan-Van der Plas, Executive Secretary
- Mrs R. Weijer, Administration Officer

Board

- Prof. dr. F.M. Bickelhaupt (VU, chairman)
- Prof. dr. C.J. Elsevier (UvA)
- Prof. dr. M. Koper (UL)

The scientific director and executive secretary of the HRSMC prepare and attend the meetings of the Board.

Research Committee (OZC)

- Dr. F. Buda (UL, research theme 2/3)
- Prof. dr. H. Hiemstra (chairman, UvA, research theme 1)
- Dr. F. Ariese (VU, research theme 2)

Education Committee (OWC)

- Dr. L. Juurlink (UL, research theme 2)
- Dr. M. Tromp (UvA, research theme 1)
- Prof. dr. L. Visscher (VU, chairman, research theme 3)
- E. Schippers, MSc (UvA, research theme 1, PhD student)

External Advisory Committee (WAR)

- Prof. dr. E.J. Baerends (emeritus VU)
- Dr. R. Hage (Catexel)
- Prof. dr. J. Reedijk (emeritus UL)
- Prof. dr. J.W. Verhoeven (emeritus UvA)
- Prof. dr. E. Vogt (Albemarle)

PhD Platform

- S. Askes, MSc; Nicole Smits, MSc and Hans de Bruijn, MSc; PhD students in the Metals in Catalysis, Biomimetics & Inorganic Materials group at the UL
- S. Auras, MSc; PhD student in the Catalysis & Surface Chemistry group at the UL
- D. Petrova, MSc; PhD student in the Molecular Photonics group at the UvA
- E. Schippers, MSc and C. te Grotenhuis, MSc; PhD students in the Homogeneous, Supramolecular and Bio-inspired catalysis group at the UvA
- F. Zaccaria, MSc; PhD student in the Theoretical Chemistry group at the VU
- D. Boom, MSc and J. Borger, MSc; PhD students in the Organophosphorus, Organometallic and Computational Chemistry group at VU

Appendix 5. HRSMC Co-operations on 31 December 2016

Research topic	Co-operating groups	Theme	University
2-D IR of Protein folding	Woutersen/Bolhuis	2.3	UvA
Adaptive QMMM methods	Ensing/Bulo	3	UvA, VU
Applications of chiroptical spectroscopies	Buma/Ariese	2	UvA/VU
Aromaticity in inter/circumstellar ice analogues a combined experimental and theoretical approach	Linnartz/Fonseca Guerra/Bickelhaupt	2.3	UL, VU
Calculations on homogeneous catalytic mechanisms	Ehlers/Bouwman	1	UvA, UL
Circular dichroism in plants	Buma/Ariese	2	UvA, VU
Calculations on Multicomponent Syntheses	Bickelhaupt/Orru/Fonseca Guerra	1.3	VU
Chemistry Behind CuI- μ -thiolate and CuI-disulfide complexes	Bouwman/Fonseca Guerra/Bickelhaupt	1.3	VU
Chiral anion-mediated catalysis	Orru/Lammertsma	1	VU
Developing broad spectrum light-harvesting antennas for organic solar cells	Bickelhaupt/Fonseca Guerra/Lammertsma	1.3	VU
Development of device compatible charge separators	Orru/Lammertsma	1	VU VU, UL, UvA
Dutch Compound Library	Orru/v.Maarseveen	1	UvA
Early stage dynamics of protein folding	Woutersen/Bolhuis	2.3	UvA
Electrocatalysis of immobilized molecular catalysts for water oxidation	Koper/Reek/Hetterscheid	2.3	UL, UvA
Electronic structure calculations on organometallic complexes	Baerends/Lammertsma	1.3	VU
Electronic structure of phosphinidene complexes	Baerends/Lammertsma	1.3	VU
Ester hydrogenolysis and (de)hydrogenations using firstrow transition metals	Elsevier/de Bruin/vd Vlugt/Van Maarseveen	1	UvA
Experimental and theoretical studies of molecules of astrochemical interest	Bickelhaupt/Fonseca Guerra/ Linnartz/Ubachs	1.2	VU, UL
Fluorescent organocatalysts	Brouwer/Hiemstra	1.2	UvA
Fragment-oriented rational design of catalysis	Bickelhaupt/Reek	1.3	VU, UvA
Homogenous Catalysis in transition metal complexes	Meijer/Reek/De Bruin	1.3	UvA
Homogeneous vs. heterogeneous electrocatalysis	Koper/Bouwman	1.3	UL
Hydrogenation of Carboxylic Acids with a Homogeneous Cobalt Catalyst	Elsevier/de Bruin	1	UvA
Infrared studies of (di)manganese carbonyl ions	Buma/Ingemann	1.2	UvA
Isotope-labeled peptides	Woutersen/Van Maarseveen	1.2	UvA
IR spectroscopy of metal clusters	Bakker/Buma/Oomens/Visscher	2.3	RU, UvA, VU

Light harvesting dyes	Brouwer/Orru/Lammertsma	1.2	UvA, VU
Light Harvesting Molecules	Lammertsma/ Bickelhaupt/ Buma	1.2.3	VU, UvA
Luminescence enhancement of lanthanoid complexes; Orrit/Bouwman	Orrit/Bouwman	1.2	UL
Measuring and simulating chemistry in cometary processes	Bickelhaupt/Linnartz	3.2	VU, UL
Modeling of conformation of peptidomimetics	Orru/Ehlers	1	VU
Molecular separations	Grecea/Dubbeldam	1.3	UvA
Molecular sensing	Grecea/Bouwman/Zhang	1.2	UvA,UL
Non radiative energy transfer in three-component lipid membranes: upconversion followed by FRET	Bonnet/Kennis	1.2	UL, VU UVA, VU, UL
PAHs in the laboratory and in space	Buma/Ubachs/Linnartz	2	UL
Palladium catalysis, click chemistry involving NHC-triazole compounds	Elsevier/Hiemstra/Van Maarseveen	1	UvA
Pd-Catalyzed Z-Selective Semihydrogenation of Alkynes: Determining the Type of Active Species	Elsevier/de Bruin	1	UvA
Photocatalysis	Brouwer/Reek/Hartl/vdVlugt	1.2	UvA
Photocatalysis	Reek/vd Vlugt/De Groot	1.2	UvA, UL
Photosynthesis	De Groot/Koper	2.3	UL
Proton conductivity	Grecea/Ensing/Woutersen	1.2.3	UvA
Protons in aqueous environment	Meijer/Ensing/Woutersen	2.3	UvA
Radical copper-phenolate compounds	Bouwman/De Bruin	1.3	UL, UvA
Renewable fuels	Buma/Visscher	1.3	UvA,VU
Solar energy conversion	Lammertsma/ Bickelhaupt/Buma	1.2.3	VU, UvA
Spectroscopy (2D-IR)	Reek/vd Vlugt/Woutersen	1.2	UvA
Stimulated Raman in cells	Bonnet/Ariese	1.2	UL, VU
Time-dependent spectroscopy of photocatalytic liposomes	Bonnet/Brouwer	1.2	UL, UvA
TR spectroscopy applied to supramolecular catalysis	Reek/Brouwer	1.2	UvA
Ester hydrogenolysis and (de)hydrogenations using firstrow transition metals	Elsevier/de Bruin/vd Vlugt	1	UvA
Various Synthetic products	Hiemstra/Orru/ v.Maarseveen	1	UvA, UL
Vibrational circular dichroism	Woutersen/Buma/De Bruin	1.2	UvA
Vibrational circular dichroism: applications and theory	Buma/Visscher	1.3	UvA, VU
Water oxidation catalysis	Buda/de Groot/Koper/Hetterscheid	2.3	UL

Appendix 6. HRSMC PhD Graduations 2011 – 2016

2011

Dzik, W.I.

Group 9 open-shell organometallics: reactivity at the ligand

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Prof. dr. B. de Bruin

January 11, 2011

Postdoctoral Researcher at TU Kaiserslautern

Warsink, S.

Palladium complexes bearing nitrogen donor functionalized N-heterocyclic carbene ligands: application in transfer semihydrogenation

Promotor: Prof. dr. C.J. Elsevier

January 19, 2011

Wawrzyniak, P.K.

Ab initio modeling of primary processes in photosynthesis: Protein induced activation of bacteriochlorophylls for efficient light harvesting and charge separation

Promotor: Prof. dr. H.J.M. de Groot

January 26, 2011

IT Consultant for Electronic Payments at Collis

Smolarek, S.

UV and IR laser spectroscopy of isolated molecular structural dynamics

Promotor: Prof. dr. W.J. Buma; co-promotors: Dr. M. Drabbels, Dr. A.M. Rijs

January 26, 2011

Postdoc in field of optics at Radboud University Nijmegen

Znabet, A.

Biocatalysis & Multicomponent Reactions: The Ideal Synergy. Asymmetric Synthesis of Substituted Proline Derivatives

Promotors: Prof. dr. R.V.A. Orru, Prof. dr. M.B. Groen

January 26, 2012

PostDoc at NKI, Amsterdam, The Netherlands

Hauwert, P.

Zerovalent palladium (N-heterocyclic carbene) complexes for transfer hydrogenation of alkynes

Promotor: Prof. dr. C.J. Elsevier

February 17, 2011

R&D Engineer at Frames

Ernsting, J.E.

DNA as a scaffold for phosphine-based metal catalysts

Promotors: Dr. P.C.J. Kamer, Prof. dr. J.N.H. Reek; co-promotor: Prof. dr. P.W.N.M. van Leeuwen

April 17, 2011

Highschool Teacher Chemistry at Zaanlands Lyceum

Colonna, F.

On the stability of old and novel carbon phases: a computer simulation study

Promotor: Prof. dr. A. Fasolino; co-promotor: Prof. dr. E.J. Meijer

June 8, 2011

Scientist at Fraunhofer Institute for Mechanics of Materials IWM

Raja, T.N.

Fluorescence spectroscopy and imaging of dynamics and microstructure of acrylic polymer emulsions

Promotor: Prof. dr. A.M. Brouwer

June 14, 2011

Zeist, W.J. van

Activating Bonds. Theoretical studies of chemical bonds and their catalytic activation by palladium

Promotor: Prof. dr. F.M. Bickelhaupt

June 15, 2011

Consultant/researcher at Blonk Milieu Advies

Schor, M.

From peptide chains to chains of peptides: multiscale modelling of self-assembling fibril-forming polypeptides

Promotor: Prof. dr. P.G. Bolhuis

September 20, 2011

Post Doctoral Research Associate at National Physical Laboratory, University of Edinburgh

Nguyễn, V.A.

Photoinduces processes in Functionalized and Organized Dye Systems

Promotor: Prof. dr. A.M. Brouwer; co-promotors: Dr. R.M. Williams, Prof. dr. Lê Công Hòa

September 21, 2011

Scientist, Hanoi University of Technology

Knijnenburg, A.D.

Synthetic modifications of the antibiotic peptide gramicidin S

Promotor: Prof. dr. H.S. Overkleeft

September 29, 2011

Associate Scientist at DSM Research

Lutteke, G.

Studies towards the total synthesis of solanoeclepin A: enantioselective synthesis of the right-hand substructure

Promotor: Prof. dr. H. Hiemstra; co-promotor: Dr. J.H. van Maarseveen

September 29, 2011

Postdoc Leiden University

Lammers, I.

Chiral discrimination by phosphorescence

Promotor: Prof. dr. C. Gooijer

November 14, 2011

Study director Analytical and Physical Chemistry at WIL Research

Tardioli, S.

Optical Methods For Structure Elucidation Of Protein-Ligand Interactions: Fluorescence and Ultraviolet Resonance Raman Spectroscopy

Promotor: Prof. dr. C. Gooijer

November 15, 2011

Duivenvoorden, B.A.

Synthesis & Biological Applications of Glycosylated Iminosugars

Promotors: Prof. dr. H.S. Overkleeft, Prof. dr. J.M.F.G. Aerts

December 15, 2011

Joya, K.S.

Molecular Catalytic System for Efficient Water Splitting

Promotor: Prof. dr. H.J.M. de Groot

December 21, 2011

Linden, W.A. van der

Towards subunit specific proteasome inhibitors

Promotor: Prof. dr. H.S. Overkleeft

December 22, 2011

Mooibroek, T.J.

The palladium diphosphane catalyzed reduction of nitrobenzene

Promotors: Prof. dr. E. Drent, Prof. dr. E. Bouwman

December 22, 2011

Sai Sankar Gupta, K.B.

Spin torch experiments observed in reaction centers of Rhodobacter sphaeroides

Promotor: Prof. dr. H.J.M. de Groot

December 22, 2011

Interim-Head of NMR Facility at Leiden University

2012

Plugge, M.

On the fluorescence properties of chromophores near metallic nanostructures.

Promotor: Prof. dr. A.M. Brouwer

February 16, 2012

Alvaro Galué, H.

Infrared spectroscopy of mass-selected aromatic and diamondoid molecular ions: a laboratory quest for the organic inventory in space

Promotor: Prof. dr. J. Oomens

May 16, 2012

PostDoc at VU University Amsterdam, The Netherlands

Bellini, R.

Chiral supramolecular ligands in transition metal catalysis

Promotor: Prof. dr. J.N.H. Reek

September 18, 2012

PostDoc at KTH, School of Chemical Science and Engineering, Stockholm, Sweden

Tecmer, P.

Towards reliable modeling of excited states of uranium compounds

Promotor: Prof. dr. L. Visscher

October 2, 2012

PostDoc at ETH Zurich, Switzerland

Weymiens, W.

Phosphorus Molecular Frameworks based on the Phosphole and Phosphine-Acetylene Building Block

Promotor: Prof. dr. K. Lammertsma

December 3, 2012

Trainee Patent Attorney, Nederlandsch Octrooibureau, Den Haag, The Netherlands

Hahn, C.

Step away from flat land; employing a cylindrical crystal in gas-surface dynamics studies

Promotor Prof. dr. A.W. Kleyn, co-promotor L.B.F. Juurlink

December 11, 2012

PostDoc at University of Wisconsin – Madison, Department of Chemistry, US

Franssen, N.M.G.

Functional (co)polymers from carbenes: scope, mechanism & polymer properties.

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Dr. B. de Bruin

December 11, 2012

Researcher Biodomain Shell Global Solutions

Vallés Pardo, J.L.

In silico study of reaction mechanisms and design principles for water oxidation catalysts

Promotor: Prof. dr. H.J.M. de Groot

December 19, 2012

PostDoc at EMPA (ETH) Zurich, Switzerland

M. Mooijman

C2-functionalized 2-imidazolidines and 2-imidazolines. Multicomponent Synthesis and Synthetic Potential

Promotor: Prof. dr.ir. R.V.A. Orru, Prof. dr. M.B. Groen

December 20, 2012

Area Product Manager, Anton Paar Benelux BVBA, Oosterhout, The Netherlands

2013

Beyhan, M.

Subsystem Density Functional Theory Studies

Promotor: Prof. dr. L. Visscher

January 16, 2013

Junior Fiduciair Manager at Kempen & Co, Amsterdam, The Netherlands

Babich, L.

Enzymatic cascade reactions involving phosphorylated intermediates: immobilization and process optimization. UvA Universiteit van Amsterdam (150 pag.)

Promotor: Prof. dr. R. Wever.

January 25, 2013

Researcher at Crucell, Leiden, The Netherlands

Smeenk, L.E.J.

Double-CLIPS Technology for the Mimicry of Structurally Complex Antibody Binding Sites on Proteins

Promotor: Prof. dr. P. Timmerman; co-promotor: Dr. J.H. van Maarseveen

March 22, 2013

PostDoc at the ETH, Zürich, Switzerland (group of Prof. dr. H. Wennemers)

Isokoski, Karoliina

Physics and Chemistry of Interstellar Ice

Promotors: Prof. dr. H.V.J. Linnartz, Prof. dr. E.F. van Dishoeck

March 26, 2013

Research professional, Sydney, Australia

Lehmann, C.S.

Novel applications of femtosecond electron-ion coincidence imaging: from coherent control to mass-selective discrimination of chiral molecules

Promotor: Prof. dr. M.H.M. Janssen

May 16, 2013

Postdoc at Advanced Photon Source, Argonne National Laboratories, Illinois, USA

Iping Petterson, I.E.

Time-resolved Raman spectroscopy for depth analysis of scattering samples

Promotor: Prof. dr. C. Gooijer; co-promotor: Dr. F. Ariese
May 27, 2013
PostDoc at University of Exeter, UK

Olivos Suárez, A.I.

Hypovalent substrates in transition metal catalysis: C–H bond functionalisation, ring-closing reactions & polymer synthesis.

Promotors: Prof. dr. J.N.H. Reek, Prof. dr. B. de Bruin
June 4, 2013

Lapoutre, V.J.F.

Infrared spectra of strongly bound clusters: Extending the limits of action spectroscopy.

Promotor: Prof. dr. J. Oomens; co-promotor: Dr. J.M. Bakker
June 21, 2013

Software developer Optiver

Yorulmaz, M.

Absorption, luminescence and scattering of single nano-objects

Promotor: Prof. dr M. Orrit

June 26, 2013

Postdoc at Rice University (Houston, USA)

Kwon, Y.

Biomass Electrochemistry: from cellulose to sorbitol

Promotor: Prof. dr. M.T.M. Koper

September 5, 2013

Postdoc at Lawrence Berkeley National Laboratory, USA

Carpentier, C.E.

Three-dimensional visualization of contact networks in granular material

Promotors: Prof. dr. D. Bonn, Prof. dr. A.M. Brouwer; co-promotor: Dr. P. Schall

September 26, 2013

No position yet

Fayolle, Edith

From ice to gas; constraining desorption mechanisms in interstellar ice.

Promotors: Prof. dr. H.V.J. Linnartz, Prof. dr. J.-H. Fillion; co-promotor: Dr. K.I. Oberg

October 1, 2013

Postdoc Harvard University, USA (Rubicon laureate)

Schouten, K.J.P.

Electrocatalytic carbon dioxide reduction

Promotor: Prof. dr. M.T.M. Koper; co-promotor: Dr. L.B.F. Juurlink

October 8, 2013

Jr. Project Leader at Avantium, Amsterdam, the Netherlands

Yang Jian

Promotion of the Electrocatalytic Reduction of Nitrate

Promotor: Prof. dr. M.T.M. Koper

October 24, 2013

Postdoc at Faculty of Science & Technology, University of Twente, the Netherlands

Akerboom, S.

Ln(III) Complexes as Potential Phosphors for White LEDs

Promotor: Prof. dr. E. Bouwman; co-promotor: Dr. W.T. Fu

October 29, 2013

Researcher at Nalco, Leiden, The Netherlands

Yuan, H.

Single molecules in soft matter: a study of biomolecular conformation, heterogeneity and plasmon enhanced fluorescence

Promotor: Prof. dr. M. Orrit

October 29, 2013

Postdoc at KU Leuven (Belgium)

Pavlov, A.

Understanding the Role of Aqueous Solution in Chemical Reactions A Computational Study

Promotors: Prof. dr. E.J. Meijer

October 30, 2013

PostDoc at Georgia University of Technology, Atlanta, Georgia, USA

Kleijn, S.E.F.

Electrocatalysis at Single Nanoparticles

Promotor: Prof. dr. M.T.M. Koper

November 13, 2013

Research Associate at SMARTPhotonics, Eindhoven, the Netherlands

Diaz-Leines, G.

Path-Metadynamics. A computational study of conformational transitions in proteins

Promotors: Prof. dr. P.G. Bolhuis; co-promotor: Dr. B. Ensing

November 15, 2013

PostDoc at Ruhr University Bochum, Bochum, Germany

Dydio, P.F.

Supramolecular control of selectivity in transition metal catalysis: Substrate preorganization & cofactor-steered catalysis

Promotor: Prof. dr. J.N.H. Reek

November 22, 2013

Kara, F.

Monitoring Alzheimer's disease in transgenic mice with ultra high field magnetic resonance imaging

Promotor: Prof. dr. H.J.M. de Groot; co-promotor: Dr. A. Alia

December 3, 2013

PostDoc at Universiteit of Antwerp

Janssen, G.

The heart of oxygenic photosynthesis illuminated

Promotor: Prof. dr. H.J.M. de Groot; co-promotor: Dr. A. Alia

December 4, 2013

April 2012 to January 2013: Consultant at People in Science

February 2013: Director Business Development at Crystallics

Panman, M.R.

Observing invisible machines with invisible light: The mechanics of molecular machines

Promotor: Prof. dr. W.J. Buma; co-promotor: Dr. S. Woutersen

December 5, 2013

Postdoc at University of Amsterdam, The Netherlands

Rosa Domingos, S.M.

Amplified vibrational circular dichroism

Promotor: Prof. dr. W.J. Buma; co-promotor: Dr. S. Woutersen

December 11, 2013

Bahreman, A.

Lipid Bilayers Decorated with Photosensitive Ruthenium Complexes

Promotor: Prof. dr. E. Bouwman; co-promotor: Dr. S. Bonnet

December 17, 2013

PostDoc at Leiden University, with dr. A. Kros

Raoufmoghaddam, S.

Development of Homogeneous Catalysts for the Selective Conversion of Levulinic Acid to Caprolactam

Promotors: Prof. dr. E. Bouwman, Prof. dr. E. Drent

December 17, 2013

PostDoc at University of Amsterdam, with Prof. dr. J.N.H. Reek

Walters, A.J.C.

Mechanistic insight in rhodium-mediated carbene polymerization

Promotors: Prof. dr. B. de Bruin, Prof. dr. J.N.H. Reek

December 18, 2013

2014

Ras, E.J.

Descriptors for solid catalysts: 21st century discovery tools

Promotor: Prof. dr. G. Rothenberg

January 14, 2014

Surendran, S.T.

Towards photo-CIDNP MAS NMR as a generally applicable enhancement method

Promotors: Prof. dr. H.J.M. de Groot en Dr. J. Matysik

February 20, 2014

No employment direct after ending contract (pregnancy)

Jansen, E.

Transition Metal Catalysts for the Conversion of Biomass Inspired Substrates

Promotors: Prof. dr. C.J. Elsevier, Prof. dr. B. de Bruin

April 10, 2014

Science Laboratory Specialist, VSO Volunteer (Cambodia)

Terrade, F.G.

Nature inspired catalytic systems using sulfoninamido-phosphorus based complexes

Promotor: Prof. dr. J.H.N. Reek

April 29, 2014

Huerta Viga, A.

Coupled Vibrations in Peptides and Proteins

Promotor: Prof. dr. Sander Woutersen

May 9, 2014

Postdoctoral researcher

Vlaar, T.

Isocyanides' Latest Trick: Palladium-Catalyzed Imidoylative Cross-Coupling Reactions

Promotor: Prof. dr. ir. Romano V.A. Orru; co-promotor: Dr. Eelco Ruijter

Date of defense: May 15, 2014

Albemarle Amsterdam

Weina Du

Advanced path sampling of the kinetic network of small proteins

Promotor: Prof. dr. Peter Bolhuis

Date of defense: June 13, 2014

Postdoctoral researcher

Zheng, S.

Mononuclear spin-transition materials based on the bapbpy scaffold

Promotor: Prof. dr. E. Bouwman; co-promotor: Dr. S. Bonnet

June 25, 2014

Postdoc at TU Delft, team Dr. Marcel de Puit (forensic science)

Lizhe Zhu

Molecular simulations of receptor proteins

Promotor: Prof. dr. Peter Bolhuis; co-promotor: Dr. Jocelyne Vreede

September 5, 2014

Postdoctoral researcher

Strassberger, Z.

Converting Lignin to Aromatics - step by step

Promotor: Prof. dr. G. Rothenberg; co-promotor: Dr. S. Grecea

September 18, 2014

Breman, A.C.

Novel Cinchona Derived Organocatalysts: New Asymmetric Transformations and Catalysis

Promotor: Prof. dr. H. Hiemstra, co-promotor: Dr. S. Ingemann

September 30, 2014

Postdoc in the Institute of Chemistry, University of Leiden (Overkleeft group)

Kiliç, M.

Molecular Simulations in Electrochemistry: Electron and Proton Transfer Reactions Mediated by Flavins in Different Molecular Environments

Promotor: Prof. dr. Evert Jan Meijer; co-promotor: Dr. Bernd Ensing

October 1, 2014

Postdoctoral researcher

Bashlakov, D.

Interaction of Oxygen and Carbon Monoxide with Pt(111) at Intermediate Pressure and Temperature. Revisiting the Fruit Fly of Surface Science

Promotor: Prof. dr. M.T.M. Koper

October 14, 2014

Drost, R.

The Pd-Catalyzed Semihydrogenation of Alkynes to Z-alkenes: Catalyst Systems and the Type of Active Species

Promotors: Prof. dr. C.J. Elsevier, Prof. dr. B. de Bruin

October 21, 2014

PostDoc in South Africa

Gumrukcu, Y.

Direct Activation of Allylic Alcohols in Palladium Catalyzed Coupling Reactions

Promotors: Prof. dr. J.H.N. Reek, Prof. dr. B. de Bruin

October 21, 2014

Heshmat, M.

Theoretical Study on Conformational Flexibility and Weak Interactions of Asymmetric Organocatalysts in Solution: The Case of Cinchona Derivatives and Binaphthyl Ligands

Promotor: Prof. dr. E.J. Baerends

November 6, 2014

Postdoc (Theoretical Chemistry, VU University Amsterdam)

Navarro Pérez, P.

Stable single molecules for quantum optics and all-optical switches

Promotor: Prof. dr.M.A.G.J. Orrit

November 13, 2014

Tan, E.

Structural dynamics of isolated biological and synthetic photoswitches

Promotor: Prof. dr. Wybren Jan Buma, Prof. dr. Jos Oomens

November 25, 2014

NXP Semiconductors

Fedoseev, G.S.

Atom Addition Reactions in Interstellar Ice: new pathways towards molecular complexity in space

Promotor: Prof. dr. H.V.J. Linnartz

December 10, 2014

Postdoc Sackler Laboratory for Astrophysics (UL)

van Son, M.

Spin-label EPR approaches to protein interactions

Promotor: Prof. dr. E.J.J. Groenen, co-promotor: Dr. M.I. Huber

December 4, 2014

Eisenmayer, T.

Coherent Dynamics in Solar Energy Transduction

Promotor: Prof. dr. H.J.M. de Groot; co-promotor: Dr. F. Buda

December 15, 2014

Research position Computational Chemistry; company Albemarle, Amsterdam

Kai Liu

Functionalized Upconversion Nanoparticles for Cancer Imaging and Therapy

Promotor: Prof. dr. Wybren Jan Buma, Prof. dr. X.G. Kong

December 16, 2014

Postdoctoral Researcher

Boulens, P.A.

Sulphonamido-Phosphorus Nickel Complexes for the Selective Oligomerisation of Olefins

Promotor: Prof. dr. J.H.N. Reek

December 17, 2014

2015

Rutters, J.P.A.,

Auxiliary mediated synthesis of ring-strained lactams

Promotor: Prof. dr. H. Hiemstra; co-promotor: Prof. dr. J.H. van Maarseveen

January 13, 2015

Assessor physical and chemical properties at Dutch Board for the Authorisation of Plant Protection Products and Biocides

Bosch, B. van den

Complexes for electro- and photocatalytic proton reduction

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Prof. dr. S. Woutersen

January 27, 2015

Chief Material Officer, MgAubel/Guest Resarcher TU Delft Experimental MicroMechanics

Mirtschink, A.,

Energy Density Functionals from the Strong-Interaction Limit of Density Functional Theory

January 29, 2015

Promotor: Prof. dr. E. J. Baerends

Co-Promotor: Dr. P. Gori-Giorgi

Post-doctoral Researcher, VU

Ording-Wenker, E.C.M.

Biomimetic redox reactions of the Cu(II) μ -thiolate complex

Promotor: Prof. dr. E. Bouwman

March 11, 2015

Programme Manager, NWO

Janssen, G.V.

Enantioselective synthesis of diverse compounds using asymmetric catalysis and chiral auxiliaries.

Promotor: Prof. dr. ir. R.V.A. Orru; co-promotor: Prof. dr. K. Lammertsma

April 28, 2015

Postdoctoral Researcher, Antoni van Leeuwenhoek

Loop, van der, T.F.

Hydrogen-bond dynamics and proton transfer in nanoconfinement

Promotor: Prof. dr. S. Woutersen; co-promotor: Prof. dr. H.J. Bakker

June 15, 2015

Management Consultant, Financial Risk Capgemini Consulting

Kumpulainen, T.

Proton-transfer reactions in "super" photoacids and supramolecular assemblies

Promotor: Prof. dr. A.M. Brouwer; co-promotor: Prof. dr. S. Woutersen

May 21, 2015

Postdoctoral Researcher, Université de Genève

Meuzelaar, H.

New light on protein folding: Unraveling folding and unfolding mechanisms using time-resolved and two-dimensional vibrational spectroscopy

Promotor: Prof. dr. S. Woutersen; co-promotor: Dr. J. Vreede

June 30, 2015

Lecturer in Chemistry, Hogeschool Inholland

Sluiter, S.N.

Multidentate Di-N-heterocyclic carbene ligands for transition metal catalyzed hydrogenation reactions

Promotor: Prof. dr. C.J. Elsevier; co-promotor: Dr.ir. J.I. van der Vlugt

September 18, 2015

Project Manager Chemical Innovation at MatrixIC & Port of Amsterdam

Hooijschuur, J.H.

Raman Spectroscopy as a Potential Method for the Detection of Life Signatures

Promotor: Prof. dr. G.R. Davies; co-promotors: Prof. dr. C. Gooijer, Dr. F. Ariese

September 24, 2015

R&D Specialist Raman Spectroscopy and Service Specialist Analysis, ASaP BV

Luiken, J.A.

Self-Assembly of Functionalized Colloids and Short Amyloidogenic Peptides. Modelling, Theory and Simulations

Promotor: Prof. dr. P.G. Bolhuis; co-promotor: Prof. dr. E.J. Meijer

November 11, 2015

Diaz Morales, O.A.

Catalysis of the electrochemical water oxidation to oxygen

Promotor: Prof. dr. M.T.M. Koper,

Co-Promotor: Dr. F. Calle-Vallejo

November 19, 2015

Postdoctoral researcher, Stockholm University

Shen, J.

Electrocatalytic reduction of CO₂ and nitrate on immobilized metal porphyrins

Promotor: Prof. dr. M.T.M. Koper

Co-promotor: Dr. D.G.H. Hetterscheid

December 9, 2015

Den Dunnen, A.

Surface-structure dependencies in catalytic reactions

Promotor: Prof. dr. M.T.M. Koper

Co-Promotor: Dr. L.B.F. Juurlink

December 9, 2015

Postdoctoral Researcher, Guest, Leiden University

Monti, A.

Taking control of charge transfer : strategic design for solar cells

Promotor: Prof. dr. Huub J. M. de Groot

Copromotor: Dr. Francesco Buda

December 21, 2015

Kortlever, R.G.H.

Selective and efficient electrochemical CO₂ reduction on nanostructured catalysts

Promotor Prof. dr. M.T.M. Koper

Co-promotor: Dr. L.B.F. Juurlink

December 22, 2015

Postdoctoral Researcher, Caltech

2016

Chen, H.C.

Solar Fuels via Artificial Photosynthesis – From Homogeneous Photocatalysis in Solution to a Photoelectrochemical Cell

Promotors: Prof. dr. A.M. Brouwer, Prof. dr. J.N.H. Reek; co-promotor: Dr. R.M. Williams

January 14, 2016

Leenders, S.H.A.M.

Transition Metal Catalysis in Confined Spaces

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Prof. dr. B. de Bruin

March 11, 2016

Wolters, L.P.

Chemical Bonding and Catalysis

Promotor: Prof. dr. F.M. Bickelhaupt

March 22, 2016

Torres Knoop, A.

Entropy-driven separations in nanoporous materials

Promotor: Prof. dr. E.J. Meijer; co-promotor: Dr. D. Dubbeldam

April 28, 2016

Singhal, K.

From flexibility to function. Molecular dynamics simulations of conformational changes in chaperones and photoreceptors

Promotor: Prof. dr. P.G. Bolhuis; co-promotor: Dr. J. Vreede

De Graaff, C.

Cascade Reactions with a Twist. Chemoenzymatic Synthesis of Biologically Relevant Heterocycles

Promotors: Prof. dr. ir. R.V.A. Orru, Dr. E. Ruijter

May 2, 2016

Broere, D.L.J.

New Avenues for Redox-Active Ligands

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Dr.ir. J.I. van der Vlugt

June 7, 2016

Ledezma, Yanez I.D.

The role of water in hydrogen electrocatalysis

Promotor: Prof. dr. M.T.M. Koper

June 16, 2016

de Boer, S.Y.

Proton-Responsive Pyridine-Based Ligands. Synthesis, Coordination Chemistry and Catalysis

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Dr. ir. J.I. van der Vlugt

June 28, 2016

Becker, R.

Hydrogenase Mimics for Proton Reduction Catalysis

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Dr.ir. J.I. van der Vlugt

September 14, 2016

Jongbloed, L.S.

Fundamental Reactivity of the Metal-Carbon Bond in Cyclometalated PCN-Complexes

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Dr.ir. J.I. van der Vlugt

September 28, 2016

Badan, C.

Surface-structure dependence of water-related adsorbates on platinum

Promotor: Prof. dr. M.T.M. Koper

November 22, 2016

Askes, S.

Upconverting nanovesicles for the activation of ruthenium anticancer prodrugs with red light

Promotor: Prof. dr. E. Bouwman; co-promotor: Dr. S. Bonnet

November 24, 2016

Vreeken, V.

PNP Pincer Ligands in Late Transition Metal Nitrido Chemistry and Gold Catalysis

Promotor: Prof. dr. J.N.H. Reek; co-promotor: Dr.ir. J.I. van der Vlugt

December 1, 2016

Appendix 7. Dick Stufkens Prize 2011 – 2016

- 2011: Dr. Sergio Ioppolo (UL)
Surface formation routes of interstellar molecules
- 2012: Dr. Héctor Alvaro Galué (UvA, FOM)
Studying the Molecular Organic Inventory in Space with FELIX
- 2013: Dr. Linde Smeenk (UvA)
Natura in Minima Maxima - Functional Mimicry of Discontinuous Protein Binding Sites using Bio-Orthogonal Chemistry
- 2014: Dr. Tjøstil Vlaar (VU)
Efficient Access to Diverse Privileged Scaffolds by Palladium-Catalyzed Imidoylative Cross-Coupling Reactions
- 2015: Dr. Tatu Kumpulainen (UvA)
Proton-Transfer Reactions in 'Super' Photoacids and Supramolecular Assemblies
- 2016: Dr. Lando Wolters (VU)
Chemical Bonding and Catalysis

Appendix 8A. HRSMC Courses 2011 – 2016

Details of the courses that were organised in the past five years are:

HRSMC Course Physical Methods in Inorganic Chemistry (January 24, 28, 31 and February 1, 2011, UvA/UL)

Coordinators: Dr. S. Bonnet, Prof. dr. E. Bouwman, Dr. B. de Bruin, Prof. dr. C.J. Elsevier, I. Weijer (HRSMC), drs H.E. Zwaan-van der Plas (HRSMC)
Lecturers: Dr. S. Bonnet, Prof. dr. E. Bouwman, Dr. B. de Bruin, Prof. dr. C.J. Elsevier, Dr. W. Fu, Prof. dr. F. Hartl, Dr. S. Ingemann Jørgensen and Dr. R. Williams
Guest Lecturers: Dr. H. Kooijman and a Reaxys demonstration by Dr. B. Furter
Participants: 19 (4 Master students, 14 PhD en 1 postdoc, 9 UvA en 10 UL)

HRSMC Course Physical Methods in Inorganic Chemistry (Jan. 30 – Feb. 7, 2013, UvA/UL)

Coordinators: Dr. S. Bonnet (UL), Prof. dr. E. Bouwman (UL), Dr. B. de Bruin (UvA), Prof. dr. C.J. Elsevier (UvA), I. Weijer (HRSMC), drs H.E. Zwaan-van der Plas (HRSMC)
Lecturers: Dr. S. Bonnet (UL), Prof. dr. E. Bouwman (UL), Prof. dr. B. de Bruin (UvA), Prof. dr. C.J. Elsevier (UvA), Dr. W. Fu (UL), Dr. S. Ingemann Jørgensen (UvA), Dr. L. Juurlink (UL), Prof. dr. M. Koper (UL) and Dr. R. Williams (UvA)
Guest Lecturers: Prof. dr. S. DeBeer (Max-Planck-Institut fuer Chemische Energiekonversion) and Dr. H. Kooijman (Shell)
Participants 33 (26 HRSMC members (PhD students) and 7 MSc students from the UvA and UL)

HRSMC Course Molecular Modeling (May 13 - 24, 2013, VU)

Coordinators: Dr. C. Fonseca Guerra (VU), and I. Weijer (HRSMC), drs H.E. Zwaan-van der Plas (HRSMC)
Lecturers: Prof. dr. F.M. Bickelhaupt, Dr. C. Fonseca Guerra and Prof. dr. L. Visscher (allemaal van de VU)
Hands-on Sessions: Dr. G. Paragi, M. Franchini M. Sc., Dr. V.P. Nicu, H. Schoot M. Sc., Dr. A. de Cozar, Dr. F. Goumans, L.P. Wolters M. Sc., R.J. Mulder M. Sc., Dr. M. Heshmat and Dr. E. van Lenthe (all VU employees)
Mini projects: Prof. dr. F.M. Bickelhaupt, Dr. C. Fonseca Guerra and Prof. dr. L. Visscher (allemaal van de VU)
Participants: 24 (23 HRSMC members (PhD students) and 1 Belgian PhD student from Leuven)

HRSMC Course Photophysics, Photochemistry & Photobiology (March 31 - April 11 2014, UvA/VU)

Coordinators: Dr. René Williams (UvA), Ineke Weijer (HRSMC) and drs Hilde Zwaan (HRSMC)
Lecturers: Dr. Freek Ariese (VU), Prof. dr. Fred Brouwer (UvA), Dr. Francesco Buda (UL), MSc. Joris Snellenburg (VU), Dr. René Williams (UvA) and Dr. Gert van der Zwan (VU)
Guest Lecturers: Prof. dr. Maurice Aalders and Dr. Ivo van Stokkum
Participants 14 participants (13 PhD students and 1 MSc student)

HRSMC Course Physical Methods in Inorganic Chemistry – PhMIC2015 29 January - 6 February 2015, UvA/UL

Organisation: Prof. dr. E. Bouwman (UL), Dr. S. Bonnet (UL), Prof. dr. B. de Bruin (UvA), Prof. dr. C.J. Elsevier (UvA) Dr. M. Tromp (UvA), I. Weijer (HRSMC) and drs. H.E. Zwaan (HRSMC)

HRSMC Lecturers: Dr. S. Bonnet (UL), Prof. dr. E. Bouwman (UL), Prof. dr. B. de Bruin (UvA), Prof. dr. C.J. Elsevier (UvA), Dr. D.G.H. Hetterscheid (UL), Dr. S. Ingemann Jørgensen (UvA), Dr. L. Juurlink and Dr. Moniek Tromp (UvA)

Guest Lecturers: Dr. H. Kooijman (Shell)

Participants: 33 participants, of which:

- 10 MSc students (9 UvA-VU, 1 UL; 9 students passed the MSc exam)
- 22 PhD students (12 UvA, 7 UL, 3 VU)
- 1 Postdoc (UvA).

HRSMC Course Molecular Modeling (6-17 June, 2016, VU)

Coordinators: Dr. C. Fonseca Guerra (VU), en I. Weijer (HRSMC), drs H.E. Zwaan-van der Plas (HRSMC)

Lecturers: Prof. dr. F.M. Bickelhaupt, Dr. C. Fonseca Guerra and Prof. dr. L. Visscher (all VU staff members)

Hands-on Sessions: Dr. G. Paragi (VU) and Dr. J. Poater (HRSMC Fellow at the VU, University of Barcelona, Spain)

Mini projects: Dr. C. Fonseca Guerra, Dr. G. Paragi and Dr. J. Poater

Participants: 20 (14x PhD student, 5x Postdoc and 1x MSc student)

Appendix 8B. HRSMC Schools 2011 – 2016

Details of the Schools that were organised in the past five years are:

HRSMC School 'Understanding Molecular Simulation', Molsim 2011 (January 3-14 2011, UvA)

Coordinators: Dr. B. Ensing (UvA), Dr. E.J. Meijer (UvA) en I. Weijer (HRSMC)
Lecturers: Prof. dr. P. Bolhuis (UvA), Dr. E.J. Meijer (UvA)
Guest Lecturers: Dr. S. Abeln (VU), Prof. dr. D. Frenkel (AMOLF), Dr. C.P. Lowe (UvA), Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)
Participants: 89 (about 25% Master students and about 80 foreign participants)

HRSMC School 'Understanding Molecular Simulation', Molsim 2012 (UvA, January 9-20, 2012)

Coordinators: Dr. B. Ensing (UvA), Prof. dr. E.J. Meijer (UvA) and I. Weijer (HRSMC)
Lecturers: Prof. dr. P. Bolhuis (UvA), Dr. E.J. Meijer (UvA)
Guest Lecturers: Dr. S. Abeln (VU), Prof. dr. D. Frenkel (AMOLF), Dr. C.P. Lowe (UvA), Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)
Participants: 75 of which 56 were foreign participants (4 HRSMC PhD students and 11 Dutch MSc students; in total 64 MSc students, 11 PhD students)

Tulip School 2012 'Modern Developments in Spectroscopy' (Noordwijk, April 10-13, 2012)

Coordinators: Prof. dr. W.J. Buma, Prof. dr. M.H.M. Janssen, I. Weijer (HRSMC), Drs. H.E. Zwaan-van der Plas (HRSMC)
Lecturers: Prof. dr. S. Hell, Prof. dr. A. L`Huillier, Prof. dr. K. Kuipers, Prof. dr. F. Merkt, Prof. dr. H. Stapelfeldt, Prof. dr. M. de Vries
Participants: 59 (22 HRSMC members, 8 from other Dutch universities and 29 from foreign universities)

Photochemistry Summer School 2012 'Fundamentals and Applications' (Wijk aan Zee, September 15-19, 2012)

Coordinators: Prof. dr. F. Brouwer, Dr. F. Buda, Dr. G. van der Zwan, R. Janssen, I. Weijer (HRSMC), Drs. H.E. Zwaan-van der Plas (HRSMC)
Lecturers: Prof. dr. R. van Grondelle, Prof. dr. A.P. de Silva, Dr. S. Woutersen, Dr. C. Frochot, Prof. dr. M. Orrit, Dr. A. Sinicropi
Participants: 39 (15 HRSMC members, 4 from other Dutch universities and 20 from foreign universities)

HRSMC School 'Understanding Molecular Simulation', Molsim 2013 (UvA; January 7-18, 2013)

Coordinators: Dr. B. Ensing (UvA), Prof. dr. E.J. Meijer (UvA) and I. Weijer (HRSMC)
Lecturers: Prof. dr. P. Bolhuis (UvA), Dr. E.J. Meijer (UvA)
Guest Lecturers: Dr. S. Abeln (VU), Prof. dr. D. Frenkel (AMOLF), Dr. C.P. Lowe (UvA), Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)
Participants: 82 of which 57 were foreign participants (13 MSc from UvA/VU)

Summer School 2013 'New Vistas For Organic Synthesis' (July 1-4, 2013, Maastricht)

Coordinators: Prof. dr. H. Hiemstra (UvA, voorzitter), Dr J.H. van Maarseveen (UvA), Prof. dr ir R.V.A. Orru (VU), Dr E. Ruijter (VU), M. Smits-

Lecturers: Weijers (VU), I. Weijer (HRSMC), drs H.E. Zwaan-van der Plas (HRSMC)
Prof. dr. V.K. Aggarwal (University of Bristol), Prof. dr. C. Bolm (RWTH Aachen University), Prof. dr. D. Crich (Wayne State University, Detroit), Prof. dr. K. Gademann (University of Basel), Prof. dr. A.K. Yudin (University of Toronto)
Prof. dr. I. Marek (Israel Institute of Technology, Haifa) was op het laatste moment verhinderd. In zijn plaats hebben Prof. dr. B. Maes (Universiteit Antwerpen) en Prof. dr. Magnus Rueping (RWTH Aachen University) een bijdrage gegeven.

Guest Lecturers: Dr. H. Gijssen (Janssen, Pharmaceutical Companies of Johnson and Johnson) en Prof. dr. R. van Benthem (DSM/TUE)

Participants: 71 (38 HRSMC PhD students, 15 PhD students from other Dutch universities, 7 PhD students from foreign universities and 11 participants from the industry).

HRSMC School 'Understanding Molecular Simulation', Molsim 2014 (January 6– 17, 2014, UvA)

Coordinators: Dr. B. Ensing (UvA), Prof. dr. E.J. Meijer (UvA) en I. Weijer (HRSMC)

Lecturers: Prof. dr. P. Bolhuis (UvA), Prof. dr. E.J. Meijer (UvA)

Guest Lecturers: Dr. S. Abeln (VU), Prof. dr. R. Everaers, ENS Lyon, France, Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)

Participants: 80 participants, (61 PhD students, 19 MSc students)

HRSMC/NIOK Summer School 'Advanced Metal-Organic Chemistry and Catalysis' (June 30 – July 4 2014 - Willibrordhaeghe, Deurne)

Coordinators: Dr. Sylvestre Bonnet (UL), Prof. dr. Bas de Bruin (UvA), Dr. Andreas Ehlers (VU), Sjouke Goeree (NIOK), Dr. Irene Hamelers (NIOK), Prof. dr. Bert Klein Gebbink (UU), Dr. Edwin Otten (RUG), Miep Smits-Weijers (HRSMC), Dr. ir. Jarl Ivar van der Vlugt (UvA), Ineke Weijer (HRSMC), drs. Hilde Zwaan (HRSMC)

Lecturers:

Introduction Course: Dr. Sylvestre Bonnet (UL), Dr. Edwin Otten (RUG), Dr. Jarl Ivar van der Vlugt

General Course: Prof. Enzo Alessio (University of Trieste), Prof. Frank Neese (MPI, Mülheim an der Ruhr), Prof. Pher Andersson (University of Stockholm), Prof. Paul Chirik (Princeton University) and Prof. Dieter Vogt (Edinburgh)

Participants:

Introduction Course: 16 participants, 11 PhD students (of which 9 participants were HRSMC/NIOK members), 4 MSc students (2 VU and 2 RU) and 1 industrial participant

General Course: 46 participants, 40 PhD students (of which 37 participants were HRSMC/NIOK members), 5 MSc students (2 VU, 1 UL and 2 RU) and 1 industrial participant

HRSMC School 'Understanding Molecular Simulation', MOLSIM2015 5-16 January 2015, UvA

Organisation: Dr. B. Ensing (UvA), Prof. dr. E.J. Meijer (UvA) and I. Weijer (HRSMC)

HRSMC Lecturers: Prof. dr. P. Bolhuis (UvA), Dr. E.J. Meijer (UvA)

Guest Lecturers: Dr. S. Abeln (VU), Prof. dr. D. Frenkel (AMOLF), Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)

Participants: 81 participants; 23 MSc students and 58 PhD students (of which 51 participants came from foreign universities and 7 from Dutch universities including 2 HRSMC members)

**HRSMC TULIP School 'Modern Developments in Spectroscopy'
14-17 April 2015, De Witte Raaf Noordwijk**

Organisation: Prof. dr. W.J. Buma (UvA), Prof. dr. J. Herek (University of Twente), Prof. dr. M.H.M. Janssen (VU), M.C.H. Smits (HRSMC), I. Weijer (HRSMC) and drs. H.E. Zwaan (HRSMC)

Guest Lecturers: Prof. dr. P. Corkum (National Research Council-Canada, University of Ottawa, Canada), Prof. dr. J. Doyle (Harvard University, USA), Prof. dr. K. Eikema (VU), Prof. dr. J. Enderlein (Universität Göttingen, Germany), Prof. dr. M. Havenith (Ruhr-Universität Bochum, Germany), Prof. dr. D. Nesbitt (University of Colorado, Boulder, USA)

Participants: 48 participants, of which:

- 6 MSc students (5 UvA-VU, 1 UL)
- 42 PhD students (21 Dutch Universities: 4 UvA, 5 UL, 8 VU, 4 Radboud University)

**HRSMC School 'Understanding Molecular Simulation', Molsim 2016
(January 4-15, 2016, UvA)**

Coordinators: Dr. B. Ensing (UvA), Prof. dr. E.J. Meijer (UvA) en I. Weijer (HRSMC)

Lecturers: Prof. dr. P. Bolhuis (UvA), Prof. dr. E.J. Meijer (UvA)

Guest Lecturers: Dr. S. Abeln (VU), Prof. A. Alavi (University of Cambridge), Dr. S. Bonella (University of Rome), Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)

Participants: 91 participants (69 PhD students and 22 MSc student, of which 1 MSc student from the HRSMC Excellence Master, 1 HRSMC PhD member, and 67 participants came from foreign universities)

**HRSMC Summer School 'Photochemistry, Fundamentals and Applications'
27 – 31 August, 2016, Kasteel Vaeshartel, Maastricht**

Coordinators: Prof. dr. Fred Brouwer (University of Amsterdam), Dr. Gert van der Zwan (VU University Amsterdam), Dr. Sylvestre Bonnet (Leiden University), Mw. Ineke Weijer, drs. Hilde Zwaan.

Lecturers: Prof. Gary Brudvig (Solar fuels), Yale University, USA,
Prof. Paola Ceroni (Supramolecular photochemistry and luminescence), University of Bologna, Italy
Prof. Edith Glazer (Inorganic photochemistry for therapy), University of Kentucky, USA
Prof. Stefan Hecht (Efficient photochemical transformations) Humboldt-Universität zu Berlin, Germany
Prof. Massimo Olivucci (Computational photochemistry), University of Siena, Italy; Bowling Green State University, USA
Prof. Claus Seidel (Fluorescence spectroscopy and imaging), Heinrich Heine University, Düsseldorf, Germany
Axel Wiegand (Andor Technology)
Roel Gronheid (IMEC Leuven)

Participants: 48 (4 MSc students; 43 PhD students (11 UvA, 2 VU, 5 UL, 3 other Dutch universities and 22 foreign universities); 1 participant from the industry.

Appendix 8C. The Annual HRSMC Symposium 2011 – 2016

The annual HRSMC symposia are an excellent breeding ground for starting new and fostering existing research co-operations. The symposia are one-day events, and include lecture sessions as well as poster sessions. The lectures are presented by staff members, PhD students and guest lecturers.

Symposium 2011 (November 4, VU University)

The symposium, which was attended by ca. 140 scientists, also included poster sessions with 45 posters, mainly presented by PhD students. The following lectures were given:

Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Dr. Eelco Ruijter (VU)
"New tricks for (smelly) old dogs: exploiting atypical reactivity of isocyanides"
- PhD lecture of Sipeng Zheng (UL, group of Prof. dr. Lies Bouwman)
"From molecules to materials: tuning the transition temperature and cooperativity of bapbpy-based mononuclear spin-crossover compounds"
- PhD lecture Pawel Dydio (UvA, group of Prof. dr. Joost Reek)
"Supramolecular control of selectivity in transition metal catalysis using ligand functionalized with Anion Binding Pockets"

Theme 2 'Physical Chemistry and Spectroscopy'

- Prof. dr. Fred Brouwer (UvA)
"Looking into materials with fluorescence microscopy"
- Postdoc lecture of Dr. Bhargava Ram Niraghatam (VU, group of Prof. dr. Maurice Janssen)
"A femtosecond mass-resolved microscope for chiral molecules"
- Postdoc lecture of Peter Zijlstra (UL, group of Prof. dr. Edgar Groenen, Prof. dr. Michel Orrit and Prof. dr. Silvia Völker)
"Detection of single non-absorbing proteins using a gold nanorod"

Theme 3 'Theoretical Chemistry'

- Dr. Francesco Buda (UL)
"Modeling key processes in photosynthesis"
- PhD lecture of Kush Singhal (group of Prof. dr. Peter Bolhuis and Dr. Evert Jan Meijer)
"A molecular dynamics study of chaperone-protein binding"

Guest lectures

- Prof. dr. P. Gros, (UU)
"Insights Into the Molecular Mechanisms of the Complement System"
- IRTG and PhD lecture of Steffi Roters (WWU Münster)
"Al-P heterocycles and their reactivity towards small molecules"
- Dr. Sergio Ioppolo, *winner Dick Stufkens Prize 2011 (UL)*
"Surface formation routes of interstellar molecules"

Symposium 2012 (November 22, UvA)

The symposium, which was attended by ca. 130 scientists, also included poster sessions with 44 posters, mainly presented by PhD students. The following lectures were given:

Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Prof. dr. E Bouwman (UL)
"Organometallic chemistry of palladium in the catalytic reduction of nitrobenzene with CO"
- PhD/Postdoc Lecture: Mark Rong (VU, group Lammertsma)
"N-Heterocyclic Carbene Conformational Change: New Method to Tune the Reactivity of Transition Metal Complexes"
- PhD/Postdoc lecture: Pawel Dydio (UvA, group Reek/Hartl)
"Supramolecular control of selectivity in transition metal catalysis using ligands functionalized with anion binding pocket"

Theme 2 'Physical Chemistry and Spectroscopy'

- Dr. G. van der Zwan (VU)
"Proton Tautomerization Kinetics"

- PhD/Postdoc Lecture: Steven Kleijn (UL, group Koper)
"Landing and Catalytic Characterization of Individual Nanoparticles on Electrode Surfaces"
- PhD/Postdoc lecture: Heleen Meuzelaar (UvA, group Buma/Brouwer)
"The Folding Dynamics of Trp-Cage: Evidence for an Intermediate State from Time-Resolved Infrared Spectroscopy"

Theme 3 'Theoretical Chemistry'

- Dr. A. Cruz Cabeza (UvA)
"Discovering Polymorphland"
- PhD/Postdoc lecture: Jose Luis Valles Pardo (UL, group De Groot/Buda)
"Computational study of thermodynamics and reaction path of novel mono-nuclear water oxidation catalysts"

Guest Lectures:

- Prof. dr. A. Minnaard (RUG)
"Catalytic carbon-carbon bond formation applied in the synthesis of natural products"
- Dr. Jens Müller (WWU Münster)
"Silver(I)-mediated base pairs - a combined experimental and computational approach"
- Dr. Héctor Alvaro Galué, *winner Dick Stufkens prize 2012 (UvA)*
"Studying the Molecular Organic Inventory in Space with FELIX"

Symposium 2013

(21 November, National Museum of Natural History 'Naturalis' Leiden)

The symposium, which was attended by ca. 150 scientists, also included poster sessions with 42 posters, mainly presented by PhD students. The following lectures were given:

Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Prof. dr. J.N.H. Reek (UvA),
"Supramolecular strategies to control selectivity in Transition metal catalysis and application in synthesis"
- PhD/PostDoc Lecture: Sanne Bouwman (VU)
"Highly Stereoselective Synthesis of Fluorinated Aminoglycosyl Phosphonates"
- PhD/PostDoc Lecture: Erica Ording-Wenker (UL)
"The chemistry behind Cu^{II}- μ -thiolato and Cu^I-disulfide complexes"

Theme 2 'Physical Chemistry and Spectroscopy'

- Prof. dr. M. Orrit
"Spectroscopy and microscopy of single molecules and single gold nanoparticles"
- PhD/PostDoc Lecture: Eric Tan (UvA)
"Azobenzene at work... but how? "
- PhD/PostDoc Lecture: Angela Den Dunnen (UL)
"Dynamics of Oxygen Adsorption on Pt(553)"

Theme 3 'Theoretical Chemistry'

- Dr. P. Gori Giorgi
"Teaching Electrons a New Trick"
- PhD Lecture: Thomas Eisenmayer (UL)
"Charge transfer and coherent dynamics"

Guest Lectures:

- Guest Lecture Prof. A.J.R. Heck (UU)
"From the Top Down; MS and its Role in Studying Intact Proteins and Protein Complex Structure, Dynamics, and Assembly"
- Prof. dr. J. Neugebauer (WWU Münster)
"Beyond QM/MM: Multiscale Modelling Based on SubsystemDensityFunctional Theory"
- Dr. Linde Smeenk, *Winner Dick Stufkens prize 2013 (UvA)*
"Natura in Minima Maxima - Functional Mimicry of Discontinuous Protein Binding Sites using Bio-Orthogonal Chemistry"

Symposium 2014 (20 and 21 November, KNAW Amsterdam)

On 20 and 21 November 2014 the annual HRSMC symposium celebrated the 20-year HRSMC anniversary. The symposium took place at 'the place of birth', the Royal Netherlands Academy of Arts and Sciences (KNAW). Keynote lectures were held by Prof. dr. Erick W. Carreira and Nobel laureates Prof. dr. W.E. Moerner (2014), Prof. dr. Arieh Warshel (2013) and Prof. dr. Roald Hoffmann (1981).

Guest Lectures:

- Prof. dr. E. Carreira (ETH Zürich)
"Recent Advances in Asymmetric Catalysis"
- Prof. dr. R. Hoffmann (Cornell University)
"The Chemical Imagination at Work in very tight Places"
- Prof. dr. W.E. Moerner (Stanford University)
"Single Molecules as Nanoscale Light Sources for Super-Resolution Microscopy and for Sensing Dynamics of Individual Biomolecules"
- Guest Lecture Prof. dr. A. Warshel (USC)
"Multiscale Modeling of the Function of Biological Systems"
- Dr. Tjøstil Vlaar, *Winner Dick Stufkens prize 2014 (VU)*
"Efficient Access to Diverse Privileged Scaffolds by Palladium-Catalyzed Imidoylative Cross-Coupling Reactions"

Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Dr. J. van Maarseveen (UvA)
"C-Terminal peptide activation: learning lessons from Nature"
- PhD Lecture: Julien Daubignard (UvA)
"Substrate Orientation via Hydrogen Bonds to control the selectivity in the Rhodium Catalyzed Hydrogenation"
- PhD Lecture: Bart Limburg (UL)
"Enhanced photoinduced electron transfer at the surface of liposomes"
- PhD Lecture: Leon van der Boon (VU)
"Configurationally Stable Pentaorganosilicates"

Theme 2 'Physical Chemistry and Spectroscopy'

- Dr. L.B.F. Juurlink (UL)
"HxOy at Pt surfaces"
- PhD Lecture: Gleb Fedoseev (UL)
"Atom Addition Reactions in Interstellar Ices: new pathways towards molecular complexity in space"
- PhD Lecture: Miriam Moester (VU)
"Biomedical Imaging with Stimulated Raman Scattering Microscopy"
- PhD Lecture: Tatu Kumpulainen (UvA)
"Shuttling in Photoswitchable Hydrogen-Bonded Rotaxanes: The Effect of Thread and End Station"

Theme 3 'Theoretical Chemistry'

- Dr. C. Fonseca Guerra (VU)
Resonance-Assisted Hydrogen and Halogen Bonds in Guanina Quadruplexes
- PhD Lecture: Ariane Torres Knoop (UvA)
"Separating Xylenes Isomers by Commensurate Stacking of p-Xylene within Channels of MAF-X8"
- PhD Lecture: Brijith Thoms (UL)
"Expanding the NMR Palette: Insights on Artificial Charge Separators"

Symposium 2015 (5 November, VU University)

The symposium, which was attended by ca. 190 scientists, also included poster sessions with 44 posters, mainly presented by PhD students. The following lectures were given:

Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Dr. Chris Slootweg (VU)
Cooperative Lewis Acid/Base Catalysis
- Linda Jongbloed (UvA)

-
- A NiC-He in Nickel C-H activation
 - Luuk Steemers (UvA)
Research towards the scaffold assisted synthesis of a rotaxane

Theme 2 'Physical Chemistry and Spectroscopy'

- Prof. dr. Sander Woutersen (UvA)
Water at its weirdest: The strange case of PEG vs. POM
- Aquiles Carattino (UL)
In situ tuning of gold nanorod plasmon through oxidative cyanide etching
- Adriano Monti (UL)
Crucial Role of Nuclear Dynamics for Electron Injection in a Dye-Semiconductor Complex

Theme 3 'Theoretical Chemistry'

- Dr. Jörg Meyer (UL)
Hot or not? - Energy conversion dynamics of chemical processes at surfaces from 1st principles
- Abel de Cozar (VU)
Aggregation and Cooperative Effects in the Aldol Reaction of Lithium Enolates

Guest Lectures:

- Prof. dr. ir. B.M. (Bert) Weckhuysen (UU)
Catalytic Materials studied at the Level of Single Particles, Molecules and Atoms
- Dr. Tatu Kumpulainen, *Winner Dick Stufkens prize 2015 (UvA)*
Proton-Transfer Reactions in 'Super' Photoacids and Supramolecular Assemblies

Symposium 2016 (17 November, UL)

The symposium, which was attended by ca. 190 scientists, also included poster sessions with 39 posters, mainly presented by PhD students. The following lectures were given:

Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Dr. Tom Grossman (VU)
"Peptide-Inspired Ligands for the Modulation of Biological Function"
- PhD/PostDoc Lecture: Anne Jans (UvA)
"A Switchable Gold Catalyst by Encapsulation in a Self-Assembled Cage"
- PhD/PostDoc Lecture: Jordi Amat Cuello-Garibo (UL)
"Photoactivity and Phototoxicity of a series of strained Ruthenium-based complexes with N,S Coordinating Ligands"

Theme 2 'Physical Chemistry and Spectroscopy'

- Dr. Martina Huber (UL)
"Electron Paramagnetic Resonance: Radar and Tachometer on the Nano-scale"
- PhD/PostDoc Lecture: Camiel van Hoorn (VU)
"Fast Screening Method for Reactive Surfaces Using Raman and AFM"
- PhD/PostDoc Lecture: Tomislav Suhina (UvA)
"Molecular Rotors Shedding Light on Contact Mechanics and Friction"

Theme 3 'Theoretical Chemistry'

- Prof. dr. Evert Jan Meijer (UvA)
"Modeling Chemical Reactions in an Aqueous Environment"
- PhD/PostDoc Lecture: Francesco Nattino (UL)
"Methane dissociation on metalsurfaces: quantitative modeling of reaction probabilities and insight into lattice motion"

Guest Lectures:

- Prof. dr. Wilhelm T.S. Huck (RU)
"Synthesis of out-of-equilibrium chemical reaction networks: understanding complexity at the molecular level"
- Dr. Lando Wolters, *winner Dick Stufkens prize 2016 (VU)*
"Molecular Orbital Perspectives on Catalyst Design and Halogen Bonds"

Appendix 8D. Other HRSMC Activities 2011 – 2016

KNCV/HRSMC Career Advice Event for PhD students and postdocs (UvA, March 2, 2012)

With various lectures regarding career possibilities and job-application. In addition, each participant got 30 min. quality time with a career consultant.

Coordinators: MSc D. Henning (KNCV), Drs. J. van der Zwan (KNCV), R. Weijer (HRSMC) en Drs. H.E. Zwaan (HRSMC)

Participants: 30 (17 HRSMC PhD students, 13 other Dutch Universities)

KNCV/HRSMC Career Advice Activity for PhD students and postdocs, November 28 2014, UvA

With various lectures regarding career possibilities and job-application. In addition, each participant got 30 min. quality time with a career consultant.

Coordinators: MSc S. Blanken, MSc D. Henning (KNCV), R. Weijer (HRSMC) en drs. H.E. Zwaan (HRSMC)

Participants: 28 (16 HRSMC PhD students, 10 from other Dutch universities, 2 PhD students from Germany)

HRSMC 4-day Proposal Writing Course in combination with 1-day Peer Review Course (5-9 October 2015, UL)

Organisation: I. Weijer (HRSMC) and drs. H.E. Zwaan (HRSMC)

Guest Lecturer: Dr. Ulrike Muller (California State University Fresno, USA)

Participants: 1 MSc student, 8 PhD student, 2 Postdoc for the 4-day Course.
2 PhD students extra for the 1-day Course.

KNCV/HRSMC Career Advice Activity for PhD students and postdocs, 13 October 2015, UL - Gorlaeus

With various lectures regarding career possibilities and job-application. In addition, each participant got 40 min. quality time with a career consultant.

Organisation: S. Blanken (KNCV), J. Dijkzeul (UL), R. Weijer (HRSMC) and H. Zwaan (HRSMC)

Participants: 30 (19 HRSMC members)

HRSMC Lab visit at the LaserLaB VU for the UvA/UL groups (22 April 2016):

Organisation: Dr. Freek Ariese, Ineke Weijer (HRSMC) and drs Hilde Zwaan (HRSMC)

Schedule: From 13.30 – 14.45 h several presentations, from 15.00 – 16.45 u the lab visit and drinks afterwards.

Participants: outside the VU, about 20 people came from the UvA and UL (in total about 30 people)

HRSMC – HIMS Sustainability workshop, 23 September 2016, Amsterdam, WCW Congreszalen

Programme committee: drs. Marcel Bartels (UvA-HIMS); Hans de Bruijn, MSc (UL); Dr. Ludo Juurlink (UL); Prof. dr. Jan van Maarseveen (UvA); Kaj van Vliet, MSc (UvA); drs. Hilde Zwaan (UvA-HRSMC)

Organizers (HRSMC): Ineke Weijer and drs. Hilde Zwaan

Lecturers:

Prof. dr. Jacqueline Cramer (UU) Towards a circular economy: challenges and opportunities'.

Dr. René Kleijn (UL) Theme 1: Recycling and materials - 'Resource scarcity & circular economy'

Prof. dr. Gert Jan Kramer (UU) Theme 2: Energy - 'Fixing the Energy/Climate problem: calibrating the pace of change'

Prof. dr. Appy Sluijs (UU)

Theme 3: Climate - 'Climate and Carbon Cycling during the Eocene Greenhouse World'

Followed by three parallel Workshops of Dr. René Kleijn (UL) for theme 1, Prof. dr. Gert Jan Kramer (UU) for theme 2 and Prof. dr. Jan Maarseveen (UvA) for theme 3.

Participants first 4 lectures: \pm 65

Total participants Workshops: 50

Appendix 9. Awarded HRSMC Fellowships in 2015 and 2016

Awarded Fellowships – 1st Call, April 2015:

Time-resolved spectroscopic study on functional nanomaterials and/or nano-cavities

Guest: Dr. Pengtao Jing; hosted by Dr. H. Zhang (UvA) and Dr. S. Grecea (UvA).
A visit of 5 months.

Fundamental understanding on gas-surface interaction

Guest: Dr. Arban Uka; hosted by Dr. L. Juurlink (UL) and Prof. dr. W.J. Jan Buma (UvA).
A visit of 1.5 months.

Unravelling interstellar chemical recipes: solid state formation of proteins, sugars, and fats.

Guest: Dr. Sergio Ioppolo; hosted by Prof. dr. H. Linnartz (UL).
Four one-week visits over a period of one year.

Awarded Fellowships – 2nd Call, October 2015:

Unraveling the mechanism of proton transport in proton-conducting MOFs

Guest: Dr. Saeed Amirjalayer (WWU/CeNTech Münster); hosted by Dr. B. Ensing (UvA), Dr. S. Grecea (UvA) and Prof. dr. S. Woutersen (UvA).
An application for 3 months, in the period from 16-11-2015 to 30-04-2017; approximately 6 stays of 15 days.

Palladium-Catalyzed Oxidative Aerobic Isocyanide Insertion – A Mechanistic Study

Guest: Dr. Jordi Poater (University of Barcelona, Spain); hosted by Dr. E. Ruijter (VU), Prof. dr. R.V.A. Orru (VU), Prof. dr. F.M. Bickelhaupt (VU).
A visit of 6 months.

Awarded Fellowships – 1st Call, April 2016:

Modelling and spectroscopy of excitation energy migration in NaYF₄ nanosystems

Dr. Tu Langping (Changchun Institute of Optics, China); hosted by Prof. dr. E.J. Meijer, Dr. H. Zhang (UvA).
A visit of 5 months, co-sponsored by the Stichting John van Geund fonds, under auspices of the HRSMC.

Probing the fundamental link between chemo and electrocatalysis for biomass conversion

Dr. Vitaly Gitis (Ben Gurion University of the Negev) and Dr. Amanda C. Garcia (São Carlos Chemistry Institute (IQSC)/São Paulo University); hosted by Dr. Shiju Raveendran (UvA) and Prof. dr. M.T.M. Koper (UL).
Two researchers, each a visit of 3-4 months.

Artificial Metalloenzyme for the Selective C-H Alkenylation of Arenes

Dr. Alejandro Orden (National University of San Luis, Argentina); hosted by Dr. M. Á. Fernández-Ibáñez (UvA) and Dr. F. Mutti (UvA).
A visit of 6 months.

Well-Defined Transition Metal Complexes on Oxide Surfaces as Models for Heterogeneous Catalysis

Prof. dr. Klaus Köhler (Technical University of Munich, TUM, Germany); hosted by Prof. dr. M. Tromp (UvA).
A visit of 2 weeks.

Discovering reaction mechanisms with first principles molecular dynamics simulations

Dr. Gareth Tribello (Queen's University Belfast, Northern Ireland); hosted by Dr. Ir. B. Ensing (UvA), Prof. dr. J.N.H. Reek (UvA) and Prof. dr. S. Woutersen (UvA).

A visit of 2 weeks.

Awarded Fellowships – 2nd Call, October 2016:

Study of metal clusters with new theoretical methods and Infrared Multiple Photon Dissociation Spectroscopy

Guest: Dr. Zahra Jamshidi (Chemistry and Chemical engineering Research Center of Iran); hosted by Prof. dr. L. Visscher (VU) and Dr. J. Bakker (RU).

A visit of 4 months.

Upconverting nanoparticles for the activation of ruthenium-based anticancer drugs

Guest: Dr. Marta Maria Natile (National Research Council (CNR) - Institute of Condensed Matter Chemistry, and Energy Technologies (ICMATE) of Padova, Italy); hosted by Dr. S. Bonnet (UL).

A visit of 8 weeks.

Simulating the binding modes of the bacterial DNA organizing protein H-NS

Guest: Dr. Enrico Riccardi (Norwegian University of Science and Technology NTNU, Trondheim, Norway); hosted by Dr. J. Vree de (UvA).

A visit of 3 months.

The design of better nanostructures for more efficient luminescence upconversion for application in biomedicine and solar energy utilization

Guest: Dr Xiaomin Liu (State Key Laboratory of Luminescence and Applications, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences); hosted by Dr. H. Zhang (UvA) and Prof. dr. G. Rothenberg (UvA).

A visit of 5 months.

Appendix 10. Abbreviations

ACMM	Amsterdam Center for Multiscale Modeling
CECAM	Centre Européen de Calcul Atomique et Moléculaire
ECOS	Erkenningscommissie Onderzoekscholen Accreditation Committee (for Research Schools)
EMS	the Institute for Electrons and Molecular Structure of the VU University
EC	European Credits
ETCS	European Credit Transfer System
FOM	Stichting Fundamenteel Onderzoek der Materie
HIMS	the van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam
HRSMC	Holland Research School of Molecular Chemistry
IRTG	International Research Training Group
KNCV	Koninklijke Nederlandse Chemische Vereniging/ Royal Netherlands Chemical Society
KNAW	Koninklijke Nederlandse Academie voor Wetenschappen/ Royal Netherlands Academy of Arts and Sciences
LIC	Leiden Institute of Chemistry
LION	Leiden Institute of Physics
LO	Leiden Observatory
NIOK	Nederlands Instituut voor Onderzoek in de Katalyse Netherlands Institute for Catalysis Research
NWO	Nederlandse Organisatie voor Wetenschappelijk Onderzoek The Netherlands Organisation for Scientific Research
RU	Radboud University
TNO	the Netherlands Organisation for applied scientific research
UvA	Universiteit of Amsterdam University of Amsterdam
UL	Universiteit Leiden Leiden University
VU	Vrije Universiteit Amsterdam VU University Amsterdam
WWU-Münster	Westfälische Wilhelms-Universität Münster