Holland Research School of Molecular Chemistry



Annual Report 2016

LEIDEN UNIVERSITY
UNIVERSITY OF AMSTERDAM
VU UNIVERSITY AMSTERDAM

Holland Research School of Molecular Chemistry

Address:
HRSMC - University of Amsterdam
Science Park 904
1098 XH Amsterdam
P.O. Box 94157
1090 GD Amsterdam, The Netherlands

Phone: +31 20 525 6956/ 6454
Fax: +31 20 525 6456
E-mail: hrsmc-science@uva.nl
Homepage: http://www.hrsmc.nl

Institutes participating in the HRSMC:

Van 't Hoff Institute of Molecular Sciences (HIMS)
University of Amsterdam
Science Park 904
1098 XH Amsterdam, The Netherlands
http://www.science.uva.nl/hims

Institute for Electrons and Molecular Structure (EMS)
VU University Amsterdam / FEW
De Boelelaan 1083
1081 HV Amsterdam, The Netherlands
http://www.chem.vu.nl

Institute for Lasers, Life and Biophotonics Amsterdam (LaserLaB Amsterdam)
VU University Amsterdam
De Boelelaan 1081
1081 HV Amsterdam, The Netherlands
http://www.laserlab.vu.nl/en/index.asp

Leiden Institute of Chemistry (LIC)
Leiden University - Gorlaeus Laboratoria
P.O. Box 9502
2300 RA Leiden, The Netherlands
http://lic.leidenuniv.nl/

Leiden Institute of Physics (LION)
Leiden University - J.H. Oort building
PO box 9504
2300 RA Leiden, The Netherlands
http://www.physics.leidenuniv.nl

Leiden Observatory (LO)
Leiden University - Huygens Laboratorium
Niels Bohrweg 2
NL 2333 RA Leiden, The Netherlands
http://www.strw.leidenuniv.nl

Colophon
Lay-out: H.E. Zwaan-Van der Plas / M.C.H. Smits-Weijers / R. Weijer

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1. General

1.1 Preface

This annual report presents an overview of the research and educational activities of the graduate research school 'Holland Research School of Molecular Chemistry' (HRSMC) during 2016. The University of Amsterdam legally represents the HRSMC. The research school was founded in 1994 and has been re-accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW) in 1999, 2005 and 2012. The HRSMC is now in its fourth period 2012-2018. 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 latter jointed the HRSMC in 2016, as some staff members from the RU expressed their wish to the HRSMC board to become member of the HRSMC as well.
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.

This annual report presents a survey of the activities and achievements of the HRSMC, both educational and scientific, as well as the scientific achievements of the participating research groups.
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.

Besides organizing several educational activities, the HRSMC organized two application rounds within the Fellowship Programme, which has been established in 2015. This Programme 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.

Furthermore, in 2016 eleven students participated in the HRSMC-NWO Excellence Master Graduate programme *'Sustainability: the Molecular Approach'.* Within this programme, a special highlight was the appointment of one PhD students. In the summer of 2016, the HRSMC has granted one proposal for PhD research written by MSc chemistry student Tessel Bouwens. She was appointed at the University of Amsterdam.

The success of this strategy, activities and efforts lead to the following results in 2016:

- 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.
- A total of **14** PhD theses have been published within the HRSMC (see chapter 3.3).
- The annual Dick Stufkens Prize was awarded to Dr. Lando Wolters (VU) for the most outstanding PhD thesis within the HRSMC.
- In 2016 the following UvA/VU/UL groups or staff members joined the HRSMC:
    - Dr. Irene Groot (UL), Dr. Agur Sevink (UL), Prof. dr. Tom Grossmann (VU), Dr. Tiddo Mooibroek (UvA), Dr. ir. Annemieke Petrignani-Taube (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 2016 the HRSMC has organised:
    - two Schools with in total **139** participants, including **89** participants from foreign universities, **26** MSc students and **1** industrial participants,
    - one Course with **20** participants,
    - the annual HRSMC Symposium with $\pm$ **190** attendants,
    - a Lab visit at the VU and a HRSMC-HIMS Sustainability Workshop.
- In 2016, the HRSMC has granted
    - one research proposal within the NWO Graduate Programme and HRSMC Excellence Master Programme 'Sustainability: the Molecular Approach', as a result of which Tessel Bouwens has been appointed at the UvA (two other PhD students were already appointed in 2015),
    - **9** Fellowship applications within the HRSMC Fellowship Programme (€ 67.125), of which one is the special John van Geuns Fellowship (10 kEuro) under auspices of the HRSMC.

The HRSMC is grateful to the John van Geuns foundation for its financial support for the Photochemistry School, the Sustainability Workshop and the John van Geuns Fellowship.

With its broad educational activities and graduate and fellowship programmes, the HRSMC offers an excellent platform for interuniversity and multidisciplinary cooperation, as well as an incentive for worldclass education and research in molecular chemistry and physics.

1.2 Mission and Organisation

Mission

The HRSMC is a graduate research school in which research groups from the two Universities in Amsterdam, Leiden University and the Radboud University participate. In accordance with the resolutions of the Government concerning the Graduate Research Schools, the HRSMC aims to set up and maintain a high-level training programme for its PhD students. In addition to the research training, the HRSMC offers a selection of courses to the students, which are collected in chapter 3.1 and on the HRSMC website (www.hrsmc.nl). Some of these courses are given by staff members from all three universities, others by guest lecturers from abroad. Furthermore, summer schools are regularly organised on the main research themes of the HRSMC. A certificate is presented to those PhD students, who have fulfilled their education programme (see Annex 4.5).
In order to promote the co-operation and exchanges of expertise and ideas, the members are informed about the activities and facilities of the research groups via reports, symposia, the news page of the HRSMC website and the HRSMC newsletter.

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 HRSMC is the only research school in the Netherlands with a mission in a broad field that addresses challenges society currently faces in areas like sustainability, energy, and health from a molecular perspective. Both in research and education the HRSMC efforts are internationally recognized. The highly challenging and exciting research- and educational environment attracts young and ambitious molecular scientists from all over the world. The status of HRSMC as a top leading research school is further underpinned by its track record in acquiring grants and awards and by the very good to excellent scores in QANU and other research reviews.

Organisation

The University of Amsterdam legally represents the HRSMC and provides the core financial support to cover personnel costs and costs for key activities. The research school was founded in 1994 as an UvA, VU and UL collaboration. 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.

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 can be found in Chapter 2.

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 officer (Mrs. R. Weijer). In addition, an external advisory committee, the PhD platform and internal committees for education and research advise the board (see Annex 4.1).

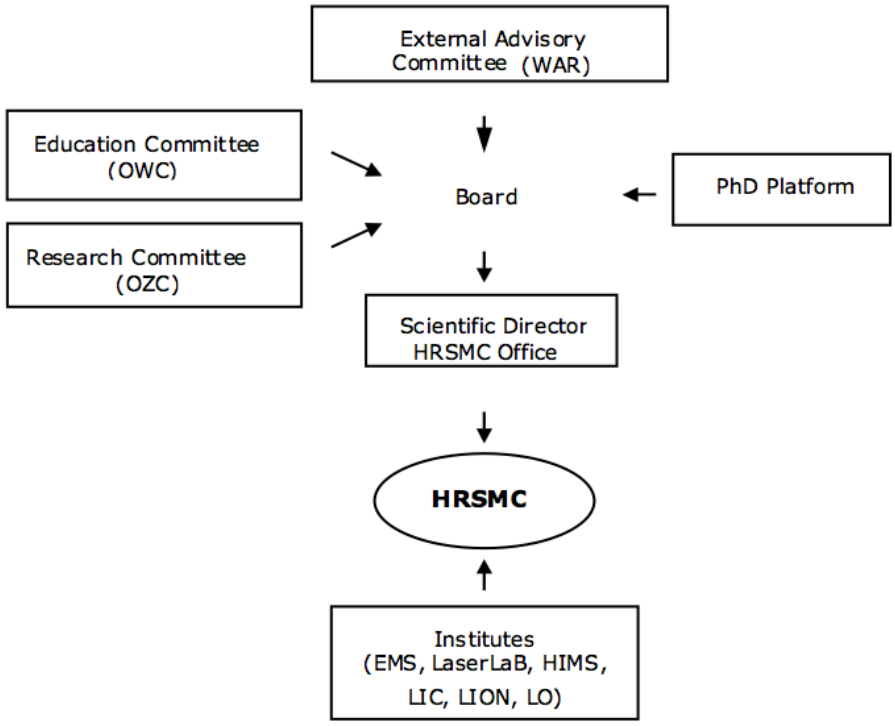


Figure 1.1 Schematic organisation of the HRSMC

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.

1.3 General Activities and Highlights of 2016

In 2016, the HRSMC has put much effort in providing the PhD students with outstanding courses and maintaining the co-operations with other research groups and institutions.

Educational Activities

The annual HRMSC Symposium was held at the Leiden University on 17 November, 2016. Besides the guest lecture of Prof. dr. Wilhelm T.S. Huck (RU), there were lectures of five PhD students and three lectures by senior scientists. In addition, the Dick Stufkens prize was awarded to Dr. Lando Wolters (former VU PhD student), who also gave a lecture. In 2008 this annual prize has been established by the board of the HRSMC for the most outstanding PhD thesis within the HRSMC. The prize, consisting of (i) a certificate and (ii) 1,000 Euro in cash, is named after the scientific director of the HRSMC from 1997 to 2001.

The symposium, which was attended by ca. 190 scientists, included poster sessions with 39 posters, mainly presented by PhD students. Further details regarding this symposium can be found in Chapter 3.2.

The HRSMC activities of 2016 consisted of:

- The two weeks HRSMC Course *'Molecular Simulation'*, organized under the auspices of CECAM (4-15 January 2016, UvA)
- HRSMC Lab visit at the LaserLaB VU for the UvA/UL groups (22 April 2016)
- HRSMC Course *'Molecular Modeling'* (6-17 June, 2016, VU)
- HRSMC introduction meeting for new PhD members of the HRSMC (10 June 2016, VU)
- HRSMC social activity for all PhD members and postdocs of the HRSMC, as well as the students of the HRSMC Excellence Master programme; this activity was organized by some members of the PhD platform (10 June 2016)
- HRSMC Summer School *'Photochemistry, Fundamentals and Applications'* (27 – 31 August, 2016, Kasteel Vaeshartel, Maastricht)
- HRSMC – HIMS Sustainability workshop (23 September 2016, Amsterdam, WCW Congreszalen)

An overview of all HRSMC inter-university Courses and Summer Schools can be found in Chapter 3.1. In this chapter, more information can be found as well on the educational activities of 2016 described above.

HRSMC Excellence Master/Graduate 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. On December 31, 2016 seven MSc students participated in this Excellence Program and three students graduated in the period of August-November 2016.

In 2016, the HRSMC has granted the proposal for PhD research written by chemistry student of Tessel Bouwens. Within the NOW Graduate Programme, Tessel Bouwens was appointed at the University of Amsterdam.
More information about this programme can be found in Chapter 3.4.

Fellowship Programme

Since 2015 the HRSMC has a Fellowship Programme. It provides funds for foreign researchers of postdoc level and higher to visit HRSMC-affiliated research groups. In 2016, there have been two rounds, in April and October. Nine Fellowship applications were awarded (€ 67.125), of which one was the special John van Geuns Fellowship (10 kEuro) under auspices of the HRSMC. More information about this programme can be found in Chapter 2.6.

Research collaborations

Besides its broad educational activities, graduate and fellowship programmes, the HRSMC aims to be an excellent platform for interuniversity and multidisciplinary cooperation between groups of the HRSMC. There are many collaborations on a formal basis (see chapter 2.4) and on an informal basis, i.e., to advice, brainstorm, and share expertise and equipment (see annex 4.5). These collaborations resulted in several joint publications in 2016, while several joint applications at CW-NWO were awarded.

(Personnel) mutations

In 2016 the following UvA/VU/UL groups or staff members joined the HRSMC:

- Dr. Irene Groot (UL), Dr. Agur Sevink (UL), Prof. dr. Tom Grossmann (VU), Dr. Tiddo Mooibroek (UvA), Dr. ir. Annemieke Petrignani-Taube (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 November 2016 Dr. Chris Slootweg and eight co-workers moved from Vrije Universiteit Amsterdam to the HIMS premises at Amsterdam Science Park.

2. Research

The research topics of the HRSMC are collected in the three research themes 'Synthesis, Characterisation, Reactivity and Properties of Molecules' (Theme 1), 'Physical Chemistry and Spectroscopy' (Theme 2), and 'Theoretical Chemistry' (Theme 3). Table 2.1 gives an overview of the research groups involved in the HRSMC in 2016. The names of all staff members, graduate students, postdocs and technical staff are listed in Annex 4.3.

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. Of course the collaborations are not restricted to research groups of a single theme. In addition, 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. Chapter 2.4 gives an overview of the collaborations in 2016, which is constantly evolving and which fluctuates annually.

Table 2.1 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], Prof. dr. C.J. Elsevier[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
	Organic and Organometallic Chemistry (VU, EMS) Dr. J.C. Slootweg, Dr. A.W. Ehlers
	Organic and Peptide Chemistry (VU, EMS) Prof. dr. T.Grossmann
	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	**Biomolecular Spectroscopy (VU, EMS)** Dr. F. Ariese
	Biophysical Organic Chemistry (UL, LIC) Prof. dr. H.J.M. de Groot, Dr. Alia, Dr. F. Buda, Dr. G.J.A. Sevink
	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. Juurlink
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

[1]also NIOK

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

Aims, activities and achievements

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 four universities eight different groups are active in this area.

The **Biocatalysis** group at the UvA is focused on cutting-edge research at the interphase between the chemical and the biological sciences. It requires therefore a high level of multidisciplinary expertise, encompassing organic synthesis, bioorganic chemistry, biochemistry, enzyme engineering and molecular biology.
Collaborations with other groups at HIMS and at other Universities complement and support our research, in particular regarding X-ray crystallisation of new enzymes and computational studied.

The mission of the **Heterogeneous Catalysis and Sustainable Chemistry group** at the UvA is to discover new catalysts and materials for sustainable chemistry applications. We start from fundamental concepts and develop practical applications. These include gas-to-liquids, biomass-to-liquids, biomass to chemicals and finding new catalytic routes to a variety of industrial materials. Our strengths are in catalyst design, catalyst synthesis and testing, and characterisation under real-life conditions. HCSC is a highly interdisciplinary group (inorganic and organic chemists, physicists, chemical engineers, electronics experts, materials scientists, chemometricians and computational chemists) and all our projects benefit from this.

The **Homogeneous, Supramolecular and Bio-Inspired Catalysis** group at the UvA develops new tools for transition metal catalysis, based on rational ligand design, supramolecular concepts and bio-inspired approaches. With these new tools new and existing reactions are developed with a focus on high atom-efficiency, control of chemo-, regio-, and stereo-selectivity, and optimized activity and stability of the catalyst. The development novel reactions relevant for bio-renewable conversion as well as conventional reactions relevant for synthesis and industry revceive attention, and we also study reaction for green energy applications (water oxidation, proton reduction, formic acid decomposition, alcohol dehydrogenation, carboxylic acid hydrogenation). In addition, new solutions to homogeneous catalyst separation and recycling are investigated, as well as ways to catalytically convert unprotected carbohydrates to higher value products.

The **Metals in Catalysis, Biomimetics & Inorganic Materials (MCBIM)** group at the UL is involved in the synthesis and study of the properties of transition-metal coordination compounds and their applications as homogeneous catalysts, medicinal compounds, models for the active sites in metalloproteins, and molecular materials.

The **Organic and Organometallic Chemistry group** synthesizes novel organophosphorus compounds in the context of sustainability and catalysis by focusing on Al/P- and B/P-based frustrated Lewis pairs (FLPs), white phosphorus (P4), phosphinidenes akin to the Fischer and Schrock carbene complexes, P,N-ligands for homogeneous catalysis, and organosilicates as entry to enantioselective catalysis. They are also involved in the design of novel light-absorbing chromophores. All their molecular designs are supported by ab initio and DFT calculations.
In November 2016 Dr. Chris Slootweg, Dr. Andreas Ehlers and their co-workers moved from the VU to the HIMS premises at the Amsterdam Science Park.

The **Organic and Peptide Chemistry** group of Prof. dr. T. Grossmann (VU) joined the HRSMC in 2016. The group focuses on the design of peptide-inspired ligands for applications in proximity-induced chemical reactions and as inhibitors of protein-protein interactions. The main expertise involves peptide and amino acid synthesis as well as a number of biophysical methods (e.g. isothermal titration calorimetry and protein crystallography).

The central theme in the **Synthetic and Bio-organic Chemistry** group at the VU is the development of new synthetic methodology for the efficient and selective generation of (libraries of) biologically relevant molecules. Key topics are improvement of atom and process efficiency in organic synthesis, the development of novel tandem and multicomponent reactions for diversity and/or biology oriented synthesis, and application of advanced (bio)catalysis in the synthesis of complex and diverse molecules.

The **Synthetic Organic Chemistry (SOC)** group at the UVA develops efficient and selective, diversity-oriented synthetic methodology, in particular organocatalytic procedures, and target-oriented preparation of molecules of relevance in chemistry, biology and medicine. The main target molecules are novel enantiopure organocatalysts, indole and tetrahydroisoquinoline alkaloids, small cyclic peptides and model systems for lasso peptides and 4-membered ring-containing terpenes, like aquatolide and solanoeclepin A, the hatching agent of potato cyst nematodes. A new research line is directed at the discovery and development of robust methods for the synthesis of high value chemicals and materials using the C-H functionalization strategy.

Biocatalysis

Dr. F. Mutti (UvA)

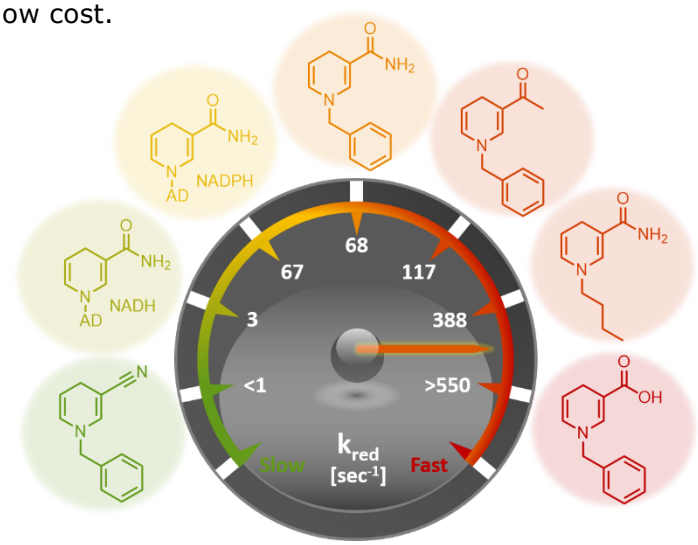
Research topics

The Biocatalysis group carries out cutting-edge research at the interphase between the chemical and the biological sciences. The research focuses on:

- The development of novel biocatalytic systems for the sustainable manufacture of chemical products.
- Identification and characterisation of novel enzymes.
- Engineering of enzymes to improve existing activities or introduce new activities.
- Kinetic and thermodynamic measurements of enzymatic reactions.
- Elucidation of enzymatic reaction mechanisms.
- Creation of artificial enzymes.

Group highlights 2016

The Biocatalysis group has published a study on a range of synthetic biomimetic compounds that can replace the relatively expensive natural nicotinamide coenzymes (NADH and NADPH) in asymmetric enzymatic redox processes. The method is applicable with diverse oxidoreductase enzymes. In particular, the team investigated the performance of the biomimetic compounds with "ene"-reductase enzymes, which catalyse the asymmetric reduction of activated alkenes. The group elucidated the performance of the biomimetics through steady-state and rapid-reaction kinetics as well as the analysis of the X-ray crystal structures of the biomimetics in complex with the ene-reductase XenA. Notably, in selected cases, these biomimetics surpasses the catalytic efficiency of the natural coenzymes. The biomimetic coenzymes are inexpensive to manufacture and more stable than their biological counterparts, that are required as hydride source in enzymatic redox reactions. The implementation of these synthetic biomimetics – as well as the design of more sophisticated analogues capable of operating with a variety of other oxidoreductases – will facilitate the use of redox biocatalysts in chemicals production. It is expected that the "Better-than-Nature" biomimetics can find widespread application in fine and specialty chemicals production by harnessing the power of high stereo-, regio-, and chemoselective redox biocatalysts and enabling reactions under mild conditions and at low cost.



Key publications 2015-2016

- Knaus, T.; Paul, C.E.; Levy, C.W.; de Vries, S.; Mutti, F.G.; Hollmann, F.; Scrutton, N.S.; Better than nature: Nicotinamide biomimetics that outperform natural coenzymes, *Journal of the American Chemical Society* **2016**, *138*, 1033-1039.
- Both, P.; Busch, H.; Kelly, P.P.; Mutti, F.G.; Turner, N.J.; Flitsch, S.L.; Whole-cell biocatalysts for stereoselective C-H amination reactions, *Angewandte Chemie International Edition* **2016**, *55*, 1511-1513.

Important Grants and Prizes in 2016

Ron Wever (em.) received the Vanadis Award 2016 at the 10th International Vanadium Symposium in Taipei, Taiwan for his seminal research on vanadium haloperoxidases.

Heterogeneous Catalysis and Sustainable Chemistry

Prof. dr. G. Rothenberg, Dr. S. Grecea, Dr. N.R. Shiju, Dr. N. Yan (UvA)

Research Topics

- Oxygen activation
- Biomass conversion
- CO_2 conversion
- Molecular Sensing
- Molecular Separations
- Asymmetric catalysis
- Fuel cells

Group highlights 2016

A collaboration between several group members together with researchers from University of Bucharest, EPFL, and Lawrence Berkeley Laboratories in California has led to the successful development of tunable multi-shell carbon materials with a host of applications in catalysis and sustainable energy. By simple tuning of the reaction pH, a series of new materials were made based on the self-assembly of two joined metal-organic frameworks. These can be easily carbonised, giving "carbon onions" with excellent accessibility. Their structure resembles a modern highway system, with interconnected wide and narrow roads. These new materials are now being applied as supercapacitors, oxidation catalysts and fuel cell electrodes.

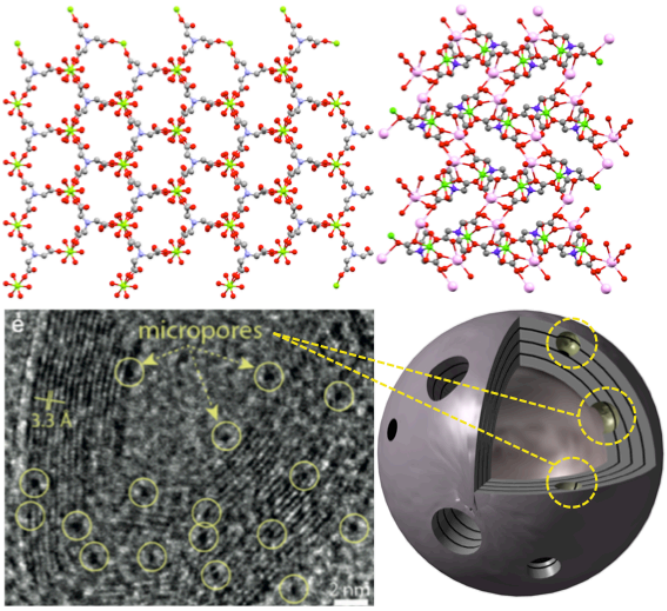


Figure 1. The self-assembly of two MOFs (above) and pyrolysis gives nested graphitic shells with interconnecting micropores (below).

A rational synthesis of hierarchically porous, N-doped carbon from Mg-based MOFs: Understanding the link between nitrogen content and oxygen reduction electrocatalysis. D. Eisenberg, W. Stroek, N.J. Geels, S. Tanase, M. Ferbinteanu, S.J. Teat, P. Mettraux, N. Yan, G. Rothenberg *Phys. Chem. Chem. Phys.,* **2016**, 18, 20778-20783.

Key publications 2015-2016

- Eisenberg, D.; Stroek, W.; Geels, N.J.; Sandu, C.S.; Heller, A.; Yan, N.; Rothenberg, G.; A Simple Synthesis of an N-Doped Carbon ORR Catalyst: Hierarchical Micro/Meso/Macro Porosity and Graphitic Shells, *Chemistry - A European Journal* **2016**, 22, 501-505.
- Slot, T.K.; Eisenberg, D.; van Noordenne, D.; Jungbacker, P.; Rothenberg, G.; Cooperative catalysis for selective alcohol oxidation with molecular oxygen *Chemistry - A European Journal* **2016**, 22, 12307–12311.
- Hernandez-Mejia, E.; Gnanakumar, E.S.; Olivos-Suarez, A.; Gascon, J.; Greer, H.F.; Zhou, W.; Rothenberg, G.; Shiju, N.R.; Ru/TiO_2-catalysed hydrogenation of xylose: the role of crystal structure of the support, *Catalysis Science & Technology* **2016**, 6, 577-582.
- Maggi, R.; Shiju, N.R.; Santacroce, V.; Maestri, G.; Bigi, F.; Rothenberg, G.; Silica-supported sulfonic acids as recyclable catalyst for esterification of levulinic acid with stoichiometric amounts of alcohols. *Beilstein Journal of Organic Chemistry* **2016**, 12, 2173-2180.
- Pagis, C.; Ferbinteanu, M.; Rothenberg, G.; Tanase, S.; Lanthanide-based metal organic frameworks: synthetic strategies and catalytic applications, *ACS Catalysis* **2016**, 6, 6063-6072.
- Eisenberg, D.; Stroek, W.; Geels, N.J.; Tanase, S.; Ferbinteanu, M.; Teat, S.J.; Mettraux, P.; Yan, N.; Rothenberg, G.; A rational synthesis of hierarchically porous, N-doped carbon from Mg-based MOFs: Understanding the link between nitrogen content and oxygen reduction electrocatalysis. *Physical Chemistry Chemical Physics* **2016**, 18, 20778-20783.
- Hua, B.; Yan, N.; Li, M.; Zhang, Y.-Q.; Sun, Y.F.; Li, J.; Etsell, T.; Sarkar, P.; Chuang, K.T.; Luo, J.L.; Novel layered solid oxide fuel cells with multiple-twinned $Ni_{0.8}Co_{0.2}$nanoparticles: the key to thermally independent CO_2 utilization and power-chemical cogeneration, *Energy & Environmental Science* **2016**, 9, 207-215.
- Hua, B.; Yan, N.; Li, M.; Sun, Y.F.; Zhang, Y.-Q.; Li, J.; Etsell, T.; Sarkar, P.; Luo, J.L.; Anode-Engineered Protonic Ceramic Fuel Cell with Excellent Performance and Fuel Compatibility, *Advanced Materials* **2016**, 28, 8922-8926.

Important Grants and Prizes in 2016

Title	Design of heterogeneous catalysts for chemo-selective synthesis of cyclohexylamines
Applicant	Dr. N.R. Shiju
Partner	DSM
Grant from	TKI Chemie, TKI Toeslag

Title	Conversion of levulinic acid from biomass in to valuable base chemicals
Applicant	Dr. N.R. Shiju
Partner	Green Future Biochemicals
Grant from	EFRO Kansen voor West

Homogeneous, Supramolecular Catalysis and Spectro-electrochemistry

Prof. dr. J.N.H. Reek, Prof. dr. B. de Bruin, Prof. dr. C.J. Elsevier, Dr. T.J. Mooibroek, Dr. M. Tromp, Dr. Ir. J.I. van der Vlugt (UvA)

Research topics

- Development of new approaches in transition metal catalysis and catalyst recovery, including supramolecular approach, ligand design, bioinspired approaches, controlled radical-type reactions, noninnocent ligands and metal complexes in unusual oxidation states.
- Combinatorial catalysis and kinetic analysis using robotics and HTE.
- Development of new reactions using rational approaches based on spectroscopic analysis, kinetics and DFT calculations.
- Application of a diverse set of analytical techniques and their application in homogeneous and heterogeneous catalysis, photocatalysis, redox catalysis and biocatalysis.
- Energy and electron transfer in (supra)molecular dyad and triad systems driven and controlled by light absorption and/or a redox reaction, relevant for photodriven reactions.
- Kinetics, in situ spectroscopy and DFT calculations on reaction mechanisms
- Bio-inspired approached, including catalyst encapsulation, bifunctional catalysis, catalyst selection
- Hydroformylation, hydrogenation, C-H activation, small molecule activation
- Metalloradicals and catalysis
- Application of reactive ligands (redox-active, chemoresponsive) for bond functionalization and catalysis
- C1-carbene chemistry
- Development of advanced spectroscopic techniques as tools in catalysis.
- Targeting unprotected carbohydrates with tailored supramolecular organo(metallic) catalysts.

Group highlights 2016

The nanoconcentrator, a new catalytic nanosphere concept has been developed in the context of the ERC Advanced Grant research program 'Nature Inspired Transition Metal Catalysis'. The new nanocontainers are formed by self-assembly: mixing 12 palladium metals and 24 so-called ditopic nitrogen ligands leads to formation of nano-sized spheres. The ditopic nitrogen ligands are modified with guanidinium binding motifs such that the resulting nanocontainers are able to bind sulfonates and carboxylates in their interior. Sulfonate guests are bound much more strongly than carboxylates because of so-called cooperative binding. This has been used to firmly fix sulfonated gold-based catalyst, while the remaining binding sites are available for the pre-organisation of the carboxylate moieties that are to be converted (the substrates). The working principles of this 'nanoconcentrator' system was established using a gold-catalysed cyclization reaction. The local high concentration of the metal catalyst combined with the pre-organization of the substrate resulted in dramatically enhanced reaction rates in

comparison to common systems where the catalyst and the reactants are not pre-organised but just both dissolved in a solvent. Reactions usually increase with catalyst and substrate concentration; but this is generally limited solubility issues or unfavorable catalyst/reactant ratios. This has now been solved by taking advantage of local concentrations in the self-assembled nanoconcentrator (*Nature Chemistry ,*2016).

Key publications 2015-2016

- Wang, Q.; Gonell Gomez, S.; Leenders, S.H.A.M.; Dürr, M.; Ivanović-Burmazović, I.; Reek, J.N.H.; Self-assembled nanospheres with multiple endohedral binding sites pre-organize catalysts and substrates for highly efficient reactions, *Nature Chemistry*, **2016**, 8, 225-230.
- Becker, R.; Amirjalayer, S.; Li, P.; Woutersen, S.; Reek, J.N.H.; An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media, *Science Advances* **2016**, 2, e1501014 DOI: 10.1126/sciadv.1501014.
- Das, B.G.; Chirila, A.; Tromp, M.; Reek, J.N.H; de Bruin, B.; Co^{III}-Carbene Radical Approach to Substituted 1H-Indenes, *Journal of the American Chemical Society* **2016**, 138, 8968−8975.
- Kuijpers, P.F.; Otte, M.; Dürr, M.; Ivanović-Burmazović, I.; Reek, J.N.H.; de Bruin, B.; A Self-Assembled Molecular Cage for Size-Selective Epoxidation Reactions in Aqueous Media, *ACS Catalysis* **2016**, 6, 3106–3112.
- Vreeken, V.; Broere, D.L.J.; Jans, A.C.H.; Lankelma, M.; Reek, J.N.H.; Siegler, M.A.; van der Vlugt, J.I.; Well-defined dinuclear gold complexes for preorganization-induced selective dual-gold catalysis, *Angewandte Chemie International Edition* **2016**, 55, 10042-10046.
- Bagh, B.; Broere, D.L.J.; Siegler, M.A.; van der Vlugt, J.I.; Redox-active ligand mediated formation of an acyclic trinuclear ruthenium complex with bridging nitrido ligands, *Angewandte Chemie International Edition* **2016**, 55, 8381-8385.
- Korstanje, T.J.; van der Vlugt, J.I.; Elsevier, C.J.; de Bruin, B.; Hydrogenation of Carboxylic Acids with a Homogeneous Cobalt Catalyst, *Science*, **2015**, 350 (6258), 298-302. DOI: 10.1126/science.aaa8938.
- Siebel, A.; Gorlin, Y.; Durst, J.; Proux, O.; Hasché, F.; Tromp, M.; Gasteiger, H.A.; Determination of HOR catalyst structure using operando EXAFS', *ACS Catalysis* **2016**, 6, 7326-7334.
- Wandt, J.; Freiber, A.; Thomas, R.; Gorlin, Y.; Siebel, A.; Jung, R.; Gasteiger, H.A.; Tromp, M.; Transition metal dissolution and deposition in Li-ion batteries investigated by operando x-ray absorption spectroscopy, *Journal of Materials Chemistry A* **2016**, 4, 18300-18305.
- Bauzá, A. Frontera, A.; Mooibroek, T.J.; π-Hole Interactions Involving Nitro Compounds: Directionality of Nitrate Esters, *Crystal Growth & Design* **2016**, 16, 5520-5524.

Important Grants and Prizes in 2016

Title	Chemical industry made natural!
Applicant	dr. T.J. Korstanje
Grant from	NWO Veni
Amount	k€ 250

Title	Operando XAS measurements of a novel Iron electrode for low-cost energy storage
Applicant	M. Tromp, with T. van Dijk, E-Stone Batteries B.V. (Netherlands)
Grant from	NWO KIEM, 2016
Amount	k€18,75

Title	Preparation of Complex Systems – Influence of Precipitation and Treatment Conditions on Metal Oxide Properties
Applicant	M. Tromp with Clariant (Germany)
Grant from	NWO LIFT grant, 2016-2020
Amount	k€300

Title	In-situ Ageing and Conservation Studies on Metal-containing Works of Art
Applicant	M. Tromp with Dr. K. Keune and the Rijksmuseum
Grant from	NICAS NOW Seed money, 2016-2017
Amount	k€25

Title	Supramolecular catalysts for the one-pot selective synthesis of carbohydrate derivatives
Applicant	dr. T.J. Mooibroek
Grant from	NWO Vidi
Amount	k€ 800

Title	Making amines out of thin air
Applicant	dr. D.L.J. Broere
Grant from	NWO Rubicon
Amount	24 month postdoc at Yale University

Title	Redox Mediators in Dye-sensitized Photoelectrochemical Cells for CO_2-reduction
Applicants	Prof. dr. Joost Reek, dr. Remko Detz, prof.dr. Fred Brouwer, prof.dr. Wim Sinke (IoP, ECN), dr. Erik Garnett (AMOLF)
Partners	AMOLF, ECN, Merck
Grant from	NWO Solar to Products (CW/FOM)
Amount	k€ 557 (2 PhD students for HIMS)

Title	Against the Odds: Regioselective Hydroaddition via Single-Electron Catalysis with Noble Metals
Applicant	Dr. J.I. van der Vlugt
Grant from	NWO CW ECHO
Amount	k€ 260 (1 PhD student for HIMS)

Metals in Catalysis, Biomimetics & Inorganic Materials

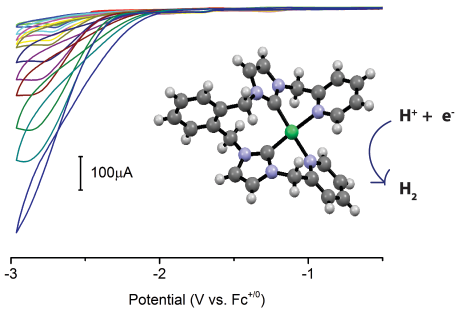
Prof. dr. E. Bouwman, Dr. S. Bonnet, Dr. D.G.H. Hetterscheid (UL)

Research topics

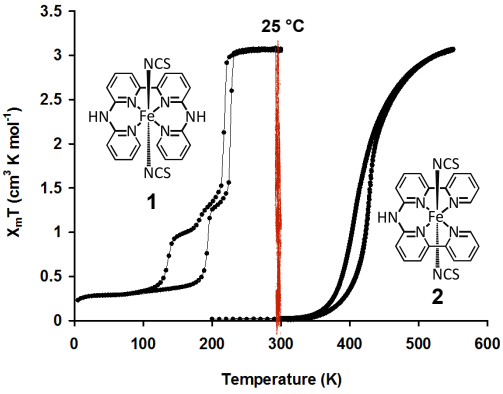
- Inorganic chemistry
- Homogeneous- and photo-catalysis (reported within NIOK)
- Biomimetic and bioinorganic chemistry
- Molecular materials

Group highlights 2016

Two bis-(benz)imidazolium salts alkylated with pyridyl side arms, H_2**L1**Br_2 and H_2**L2**Br_2 were used in the synthesis of nickel compounds containing N-heterocyclic carbenes (Ni-NHCs). The four Ni-NHC complexes [Ni(**L1**)Br]Br (**1a**), [Ni(**L1**)]$(PF_6)_2$ (**1b**), [Ni(**L2**)]Br_2 (**2a**) and [Ni(**L2**)]$(PF_6)_2$ (**2b**) were isolated and characterized by various methods, and the X-ray crystal structures of **1a**, **2a** and **2b** were determined. The compounds with an imidazole-based carbene revealed much higher activity in electrocatalytic proton reduction and better acid tolerance, although their overpotentials are higher than those of the benzimidazole-based compounds. The presence of bromide ions has an adverse effect on the redox potentials as well as the overpotentials for proton reduction. Complex **2b**, having the most planar coordination geometry, appeared to have the highest catalytic efficiency for proton reduction in DMF (i_c/i_p = 50, k_{obs} = 490 s^{-1} at 0.1 V/s) when using acetic acid as the proton source. (S. Luo, M.A. Siegler, E. Bouwman, *Eur. J. Inorg. Chem.*, 2016, 4693-4700.)

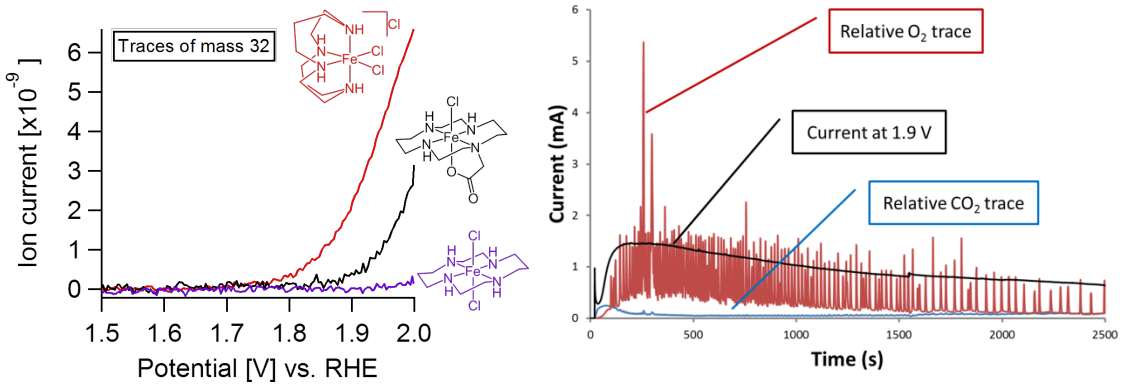


Last year, we published the preparation of the new tetrapyridyl ligand bbpya (bbpya = N,N- bis(2,2'-bipyrid-6-yl)amine) and of its mononuclear iron(II) compound [Fe(bbpya)(NCS)2] (**1**). According to different techniques this ligand strongly stabilizes the low-spin state of the iron complex. As a consequence, **1** exhibits spin crossover at an exceptionally high transition temperature 418 K characterized by a wide (21 K) and dissymmetric hysteresis cycle. DFT and CASPT2 calculations under vacuum demonstrate that the bbpya ligand generates a stronger ligand field around the iron(II) core than its analogue bapbpy (N,N'-di(pyrid-2-yl)-2,2'-bipyridine-6,6'-diamine), which stabilizes the LS state compared with [Fe(bapbpy)$(NCS)_2$] (**2**). (S. Zheng, N. Reintjens, M. A. Siegler, O. Roubeau, E. Bouwman, A. Rudavskyi, R. W. A. Havenith, S. Bonnet, *Chem. Eur. J.* 2016, 22, 331-339). The two ligands bapbpy and bbpya, originally developed for



spin crossover research, are now being used in combination with ruthenium(II) ions, to make light-activatable anticancer compounds.

Finally, innovative techniques are necessary to prove the behavior of molecular compounds. For example in the past year several molecular catalysts for the oxygen evolution reaction were monitored by on-line electrochemical mass spectrometry in order to detangle the oxygen evolution reaction with other oxidative processes such as electrode or catalyst degradation at very early stages in the catalytic reaction (i.e. within seconds). This approach allowed us to pinpoint catalytic activity to the iron cyclam acetate and the *cis* cyclam complex (see Figure), whereas the *trans* complex is inactive (*ChemCommun* 2016, 52, 2643). In case of the iridium complex $[Ir^{III}Cl_3(pic)(MeOH)]^-$ on the other hand evolution of CO_2 from the complex must occur first (see Figure) prior to any catalytic activity is obtained (*ACS Catalysis* 2016, 6, 7872).



The O_2 trace of recorded by OLEMS as a function of applied potential for three different iron cyclam complexes (left) and the O_2 trace (red), CO_2 trace (blue) and current (black) depicted versus time in case of $[Ir^{III}Cl_3(pic)(MeOH)]^-$ at an applied potential of 1.9 V.

Key publications 2015-2016

- Liu, X.; Akerboom, S.; de Jong, M.; Mutikainen, I.; Tanase, S.; Meijerink, A.; Bouwman, E.; Mixed-Lanthanoid Metal–Organic Framework for Ratiometric Cryogenic Temperature Sensing, *Inorganic Chemistry* **2015**, 54, 11323-11329.
- Limburg, B.; Wermink, J.; van Nielen, S.S.; Kortlever, R.; Koper, M.T.M.; Bouwman, E.; Bonnet, S.; Kinetics of photocatalytic water oxidation at liposomes: membrane anchoring stabilizes the photosensitizer, *ACS Catalysis* **2016**, 6, 5968-5977.
- van Rixel, V.H.S.; Siewert, B.; Hopkins, S.; Askes, S.H.C.; Busemann, A.; Siegler, M.A.; Bonnet, S.; Green light-induced apoptosis in cancer cells by a tetrapyridyl ruthenium prodrug offering two trans coordination sites, *Chemical Science* **2016**, 7, 4922-4929.
- Lameijer, L.N.; Hopkins, S.L.; Brevé, T.G.; Askes, S.H.C.; Bonnet, S.; L- versus D-glucose conjugation: Mitochondrial targeting of a light-activated dual-mode of action ruthenium-based anticancer prodrug, *Chemistry – A European Journal* **2016**, 22, 18484-18491.
- Abril, P.; del Rio, M.P.; Tejel, C.; Verhoeven, M.W.G.M.; Niemantsverdriet, J.W.; van der Ham, C.J.M.; Kottrup, K.G.; Hetterscheid, D.G.H.; Detangling Catalyst Modification Reactions from the Oxygen Evolution Reaction by Online Mass Spectrometry, *ACS Catalysis* **2016**, 6, 7872.

• Kottrup, K.G.; Hetterscheid, D.G.H.; Evaluation of iron-based electrocatalysts for water oxidation – an on-line mass spectrometry approach, *Chemical Communications*, **2016**, 52, 2643.

Organic and Organometallic Chemistry

Dr. A.W. Ehlers, Dr. J.C. Slootweg (VU, EMS)

Research topics

- The design of and catalysis with frustrated Lewis pairs
- Syntheses and applications of organophosphorus reagents and compounds
- Catalytic reactions that eliminate organophosphorus waste
- Transition metal complexes with phosphorus ligands
- Sustainable building blocks, polydentate ligands, and catalysts
- Synthesis of chiral silicates

Group highlights 2016

On 9-10 March, 2016 our group organized the 2nd international conference on sustainable phosphorus chemistry in Berlin, Germany (www.susphos.eu/icspc). The program consisted of a set of 10 distinguished speakers from industry and academia, who illustrated the many and wide-ranging aspects of phosphorus chemistry, focusing on the sustainable use of phosphorus, as well as the application of phosphorus chemistry for sustainability, covering topics such as P4 synthesis and application, P-based catalysis, and P-based polymers and flame retardants. With its emphasis on industrial applications and the sustainable use of phosphorus, this conference was an outstanding opportunity to build new academic-industrial relations and a unique possibility to discuss the latest developments in sustainable phosphorus chemistry.

In 2016 Chris Slootweg became Associate editor of RSC Advances.
Andreas Ehlers was appinted as Associate Professor at the Univeristy of Johannesburg, South-Africa.

In November 2016 Slootweg, Ehlers and seven co-workers moved from Vrije Universiteit Amsterdam to the HIMS premises at Amsterdam Science Park.

Key publications 2015-2016

- Borger, J.E.; Ehlers, A.W.; Lutz, M.; Slootweg, J.C.; Lammertsma, K.; Stabilization and Transfer of the Transient $[Mes^*P_4]^-$ Butterfly Anion Using BPh_3, *Angewandte Chemie International Edition* **2016**, *55*, 613–617.
- Borger, J.E.; Bakker, M.S.; Ehlers, A.W.; Lutz, M.; Slootweg, J.C.; Lammertsma, K.; Functionalization of P_4 in the coordination sphere of coinage metal cations, *Chemical Communications* **2016**, *52*, 3284–3287. (Inside front cover picture)
- Devillard, M.; Declercq, R.; Nicolas, E.; Ehlers, A.W.; Backs, J.; Merceron-Saffon, N.; Bouhadir, G.; Slootweg, J.C.; Uhl, W.; Bourissou, D.; A Significant but Geometrically-Frustrated Pt-Al interaction: Fixation of CO_2 and CS_2, Activation of H_2 and $PhCONH_2$, *Journal of the American Chemical Society* **2016**, *138*, 4917−4926.
- Wit, J.B.M.; de Jong, G.B.; Schakel, M.; Lutz, M.; Ehlers, A.W.; Slootweg, J.C.; Lammertsma, K.; $iPr_2N{-}P{=}Fe(CO)_4$ in Olefinic Solvents: A Reservoir of a Transient

Phosphinidene Complex Capable of Substrate Hopping, *Organometallics* **2016**, *35*, 1170−1176.

Organic and Peptide Chemistry

Prof. dr. T.N. Grossman (VU, EMS)

Research topics

- Peptidomimetics
- Proximity-induced reations
- Inhibition of protein-protein interactions
- Molecular materials

Group highlights 2016

Together with the groups of Herbert Waldmann (MPI Dortmund) and Alois Fürstner (MPI für Kohlenforschung) we developed orthogonal ring-closing alkyne and olefin metatheses for the solid-phase synthesis of bicyclic peptides. This method was used to generate inhibitors of protein-protein interactions involving a small GTPase and the protein 14-3-3, respectively.

Key publications 2015-2016

- Cromm, P.M.; Wallraven, K.; Glas, A.; Bier, D.; Fürstner, A.; Ottmann, C.; Grossmann, T.N.; Constraining an irregular peptide secondary structure through ring-closing alkyne metathesis, *ChemBioChem* **2016**, 17, 1915–1919.
- Cromm, P.M.; Schaubach, S.; Spiegel, J.; Fürstner, A.; Grossmann, T.N.; Waldmann, H.; Orthogonal ring-closing alkyne and olefin metathesis for the synthesis of small GTPase-targeting bicyclic peptides, *Nature Communications* **2016**, 7, 11300.

Important Grants and Prizes in 2016

ERC starting grant (European Research Council)

Synthetic & Bio-Organic Chemistry

Prof. dr. ir. R.V.A. Orru, Dr. E. Ruijter (VU)

Research topics

- Natural product synthesis
- Diversity-oriented synthesis
- Multicomponent reactions
- Biocatalysis
- Palladium catalysis

Group highlights 2016

Isocyanide based multicomponent reactions (IMCRs) are widely used for the synthesis of valuable compound libraries.[1,2] These reactions provide rapid access to skeletally diverse scaffolds from simple starting materials.[3] However, most IMCRs are limited in their application since the products have a similar backbone. This limitation can be overcome by the introduction of smart functional groups that allow post-modifications of the IMCR scaffold.[1]

Another important drawback of IMCR chemistry is the availability of the isocyanide input. Unlike the other components, only few isocyanides are commercial available, especially with relevant functionalized side chains. In addition, the isocyanide input produces a very stable secondary amide in many IMCRs (such as the Ugi[4] and Passerini[5] reaction) . To address this limitation the concept of a 'convertible' or 'universal' isocyanide was introduced.[6] Ideally, this is a practical isocyanide which has the ability to be converted into any other functional group under mild conditions. Furthermore, the reagent should be versatile, easily synthesized and preferably recyclable since the majority of the isocyanide (everything but the carbon atom) does not end up in the final product.

In the past two decades several promising convertible isocyanides have appeared in the literature and they can be divided in two different groups: (i) isocyanides that can directly be converted after the IMCR[6-9] and (ii) isocyanides that require activation upon cleavage.[8,10-13]

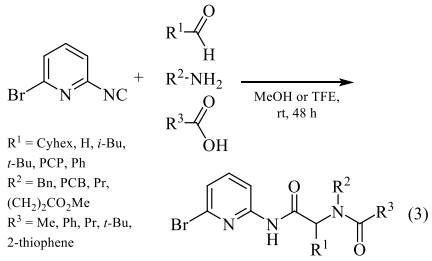
The first group can be subdivided into (a) isocyanides that are converted under acidic conditions[6-8] and (b) isocyanides that are converted under basic conditions.[9] The scope of the conversion to different functional groups is in most cases limited for these isocyanides. However, since these isocyanides do not need to be activated, they have the advantage that the conversion of the secondary amide can generally be performed in the same pot as the IMCR.

The second group of isocyanides is based on activation of the secondary amide to a much better leaving group (like an acyl indole[11] or pyrrole[13]). This requires an additional (sometimes difficult) reaction step and/or a relatively complex isocyanide, but afterwards the convertibility potential is much greater (milder reaction conditions and conversion to a broader range of functional groups).

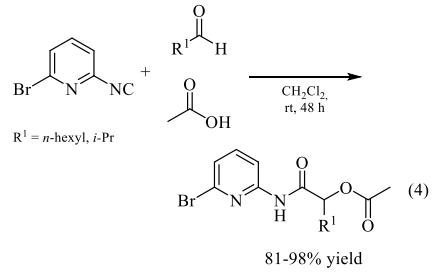
2-Bromo-6-isocyanopyridine was recently reported as an attractive alternative, since it combines the advantages of both groups of isocyanides.[14] The isocyanide is readily

cleaved without additional activation, under both basic and acidic conditions to a broad range of different functional

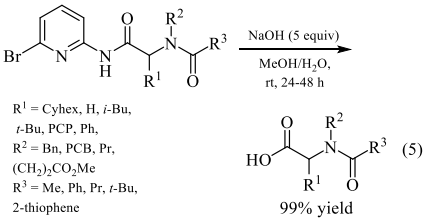
Ugi reactions. 2-Bromo-6-isocyanopyridine provides the corresponding Ugi-product when reacted with several different amines, aldehydes and carboxylic acids in protic solvents (eq 3).[14] Especially 2,2,2-trifluoroethanol (TFE) is a good solvent for these transformations and greatly improves the yields for less activated substrates such as aromatic aldehydes.



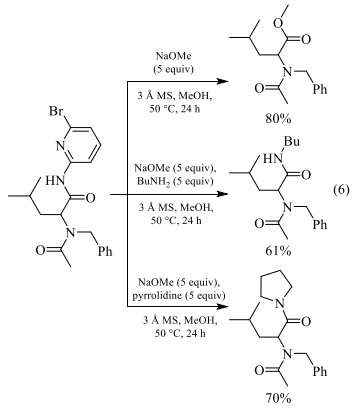
Passerini reactions. In combination with aliphatic aldehydes and acetic acid, 2-bromo-6-isocyanopyridine provides the corresponding α-acyloxyamides in excellent yields under standard Passerini conditions (81%-92%, eq 4).[14] The choice of the carboxylic acid component in this reaction is irrelevant, since this functional group is also removed during the post IMCR modifications. Therefore, on basis of cost and availability, acetic acid was used as the carboxylic acid input for this reaction.



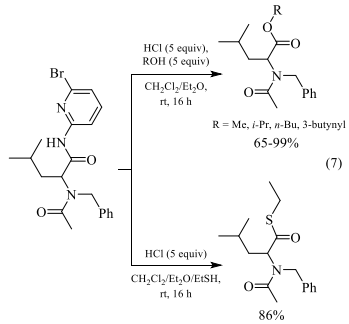
Transacylation of Ugi products under basic conditions. Post-modification of the Ugi products at the secondary amide side provides many new possibilities for library diversification. The conversion to the corresponding carboxylic acid can be considered the most valuable transformation. The coupling chemistry of carboxylic acids is well established and provides access to a broad range of carboxylic acid derivatives. The pyridyl amides (Ugi products from eq 3) are converted to the corresponding carboxylic acids by treatment with aqueous NaOH in MeOH in excellent yields (typically 99%, eq 5).[14] Since MeOH is generally the solvent of choice for the Ugi reaction, both the Ugi reaction and the hydrolysis step can be combined in a one-pot procedure to provide the amido acids directly in comparable yields. The reaction is somewhat sensitive to steric bulk at the stereogenic center (resulting from bulky aldehydes), and consequently some Ugi products require higher temperatures or longer reaction times to reach full conversion. The purification of the amido acids is in most cases readily accomplished by a simple acid base extraction.



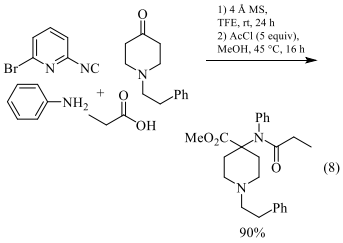
A slight modification of the reaction conditions (from NaOH to NaOMe) provided access to the corresponding methyl ester (eq 6).[14] Molecular sieves are an essential additive to ensure anhydrous conditions, since traces of water lead to the irreversible saponification of the generated ester. Interestingly, addition of an amine nucleophile (like butylamine or pyrrolidine) to the reaction mixture directly provided the corresponding secondary or tertiary amide (eq 6).



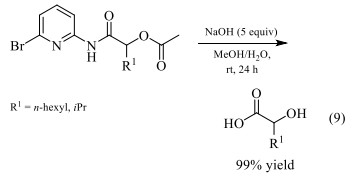
Transacylation of Ugi products under acidic conditions. The basic pyridyl nitrogen embedded in the isocyanide also allows acid–mediated transacylation reactions. The required acid is generally hydrochloric acid and can either be added to the reaction mixture as a commercial solution (*e.g.* in Et_2O) or generated *in situ* by the addition of acetyl chloride to a protic solvent. With these conditions several different esters and thioesters were obtained in good to excellent yield (65%-99%, eq 7).[14]



2-Bromo-6-isoycanopyridine was also used in the short and efficient synthesis of the extremely potent opioid carfentanil (eq 8).[14,15]



Basic hydrolysis of Passerini products. The Passerini products (α-acyloxy amides) were hydrolyzed under similar conditions as the Ugi products to the α-hydroxy acids (eq 9).[14] The products were purified by extraction, which should be done carefully, because the products are typically water-soluble.



Key publications 2015-2016

- Van der Heijden, G.; Jong, J.A.W.; Ruijter, E.; Orru R.V.A.; 2-Bromo-6-isocyanopyridine as a Universal Convertible Isocyanide for Multicomponent Chemistry, *Organic Letters* **2016**, 18, 984-987.
- Saya, J.M.; Oppelaar, B.; Cioc, R.C., van der Heijden, G.; Vandevelde, C.M.L.; Orru, R.V.A.; Ruijter, E.; Synthesis of polycyclic spiroindolines by highly diastereoselective interrupted Ugi cascade reactions of 3-(2-isocyanoethyl)indoles, *Chemical Communications* **2016**, 52, 12482-12485.
- Cioc, R.C.; Preschel, H.D.; van der Heijden, G.; Ruijter, E.; Orru, R.V.A.; Trityl Isocyanide as a Mechanistic Probe in Multicomponent Chemistry: Walking the Line between Ugi- and Strecker-type Reactions, *Chemistry - A European Journal* **2016**, 22, 7837-7842.
- De Graaff, C.; Bensch, L.; Boersma, S.J.; Cioc, R.C.; van Lint, M.J.; Janssen, E.; Turner, N.J.; Orru, R.V.A.; Ruijter, E.; Asymmetric Synthesis of Tetracyclic Pyrroloindolines and Constrained Tryptamines by a Switchable Cascade Reaction, *Angewandte Chemie International Edition* **2015**, 54, 14133-14136.

Important Grants and Prizes in 2016

- Dr. E. Ruijter, NWO/CW ECHO grant
- Dr. E. Ruijter, Thieme Journal Award
- We chaired the 16th European Colloquiem on Heterocyclic Chemistry (Beurs van Berlage, Amsterdam, approx. 350 participants)

Synthetic Organic Chemistry

Prof. dr. H. Hiemstra, Prof. dr. P. Timmerman, Prof. dr. J.H. van Maarseveen, Dr. S. Ingemann, Dr. M.A. Fernández Ibáñez (UvA)

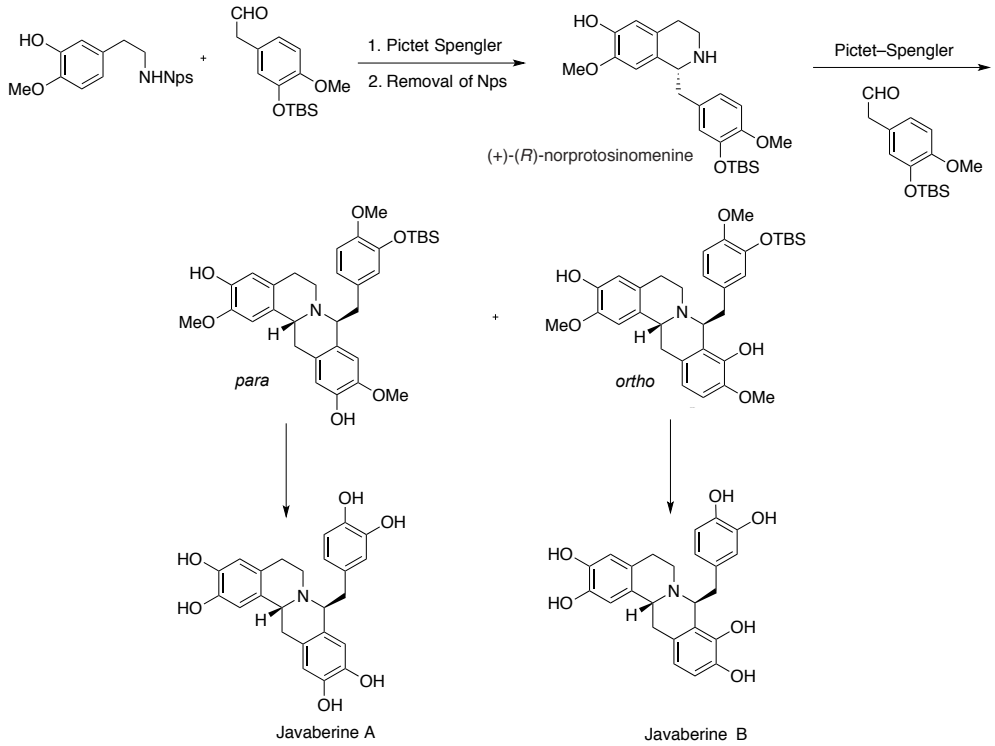
Research topics

- Synthetic methodology development
- Target-oriented synthesis
- Organocatalysis
- Chemical biology

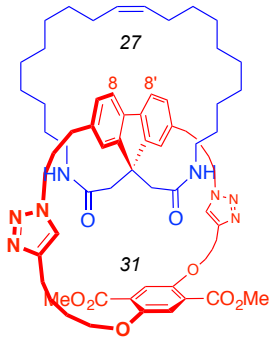
Group highlights 2016

Total synthesis of javaberine (Ingemann)

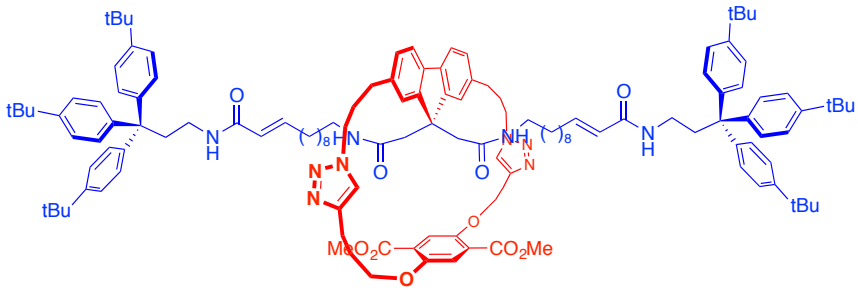
An enantioselective organocatalytic synthesis of the natural 8-benzylprotoberberines (+)-javaberine A and (+)-javaberine B was developed based on two consecutive Pictet–Spengler (PS) condensations with protected 3,4-dihydroxyphenylacetaldehydes. The first PS reaction between a dopamine derivative carrying a *N*-*o*-nitrophenylsulfenyl (Nps) group and an appropriately protected 3,4-dihydroacetaldehyde was catalyzed with 5 mol% of (*R*)-TRIP to afford (+)-(*R*)-norprotosinomenine in 90 % *ee.* The second PS reaction proceeded without any catalyst to form two regioisomers in a ratio that was highly dependent on the solvent. In trifluoroethanol the ratio between the *para* and *ortho* regioisomers was 99:1, while in the apolar solvent toluene we observed preferential formation of the *ortho* isomer. Subsequently, the para isomer was deprotected to afford (+)-javaberine A in 48% overall yield and the ortho isomer converted to (+)-javaberine B in 35% yield.



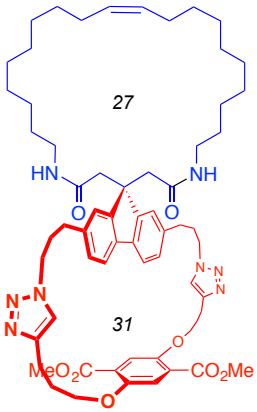
Synthesis of quasi-[1]rotaxanes and quasi-[1]catenanes (Van Maarseveen)
During our methodology development studies towards the total synthesis of the naturally occurring lasso peptides a new molecule class was revealed. Along the road we realized that our backfolding strategy to make interlocked molecules may also provide access to the unprecendented inverted spiro geometry. We have successfully disclosed this new class of molecules that we coined quasi [1]catenanes. Although the regular spiro and quasi [1]catenane geometries only differ by inversion of the configuration of the center-of-symmetry tetrahedral carbon they relate as diastereomers with inherent different physical properties. By starting from the same tetrahedral C-centered acyclic precursor and the same backfolding concept the structurally related mechanically locked quasi [1]rotaxane and its unwinded conformer were obtained.



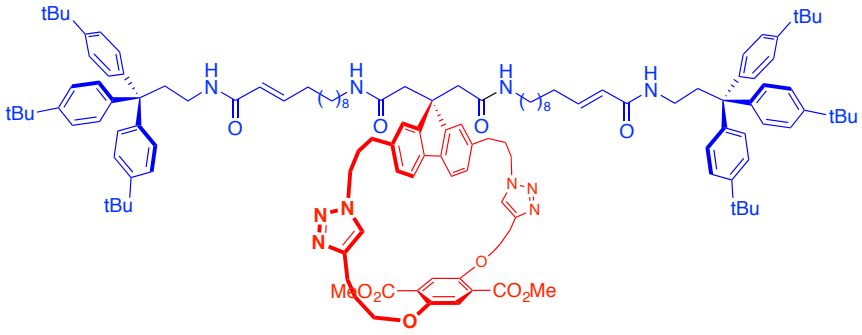
quasi [1]catenane



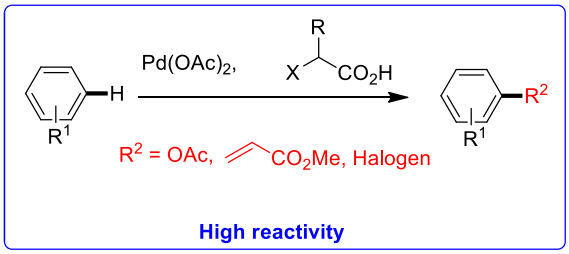
quasi [1]rotaxane



spiro bicycle



Catalytic C-H functionalization of non-activated arenes (Fernández-Ibáñez)
Direct C-H functionalization shortens classical organic synthetic routes yielding direct benefits both in energy costs and atom-economy. However, the low reactivity of C-H bonds and the poor selectivity are the main obstacles in the development of efficient C-H bond transformations. The vast majority of the existing methodologies rely on the use of directing groups within the substrate to assist the process. A challenging, but more attractive approach, is to develop new catalytic systems that can provide effective and selective C-H functionalization reactions. We have developed an inexpensive and easy accessible new type of bidentate ligand capable of promoting the palladium-catalyzed C-H olefination of simple arenes. The new catalytic system is operationally simple, scalable and can also be applied in late-stage functionalization of complex molecules. The broad applicability of this novel ligand has been showcasted in other transformations such as palladium-catalyzed C-H acetoxylation and allylation reactions.



Key publications 2015-2016

- Valderas, C.; Naksomboon, K.; Fernández-Ibáñez, M.Á.; Ligand-Promoted Palladium-Catalyzed C-H Acetoxylation of Simple Arenes, *ChemCatChem* **2016**, *8*, 3213.
- Veguillas, M.; Solà, R.; Fernández-Ibañez, M.Á.; Maciá, B.; Catalytic enantioselective addition of methyltriisopropoxititanium to aldehydes, *Tetrahedron: Asymmetry* **2016**, *27*, 643.
- Bosschert, V.; Frisch, C.; Back, J.W.; van Pee, K.; Weidauer, S.E.; Muth, E.M.; Schmieder, P.; Beerbaum, M.; Knappik, A.; Timmerman, P.; Mueller, T.D.; The sclerostin-neutralizing antibody AbD09097 recognizes an epitope adjacent to sclerostin's binding site for the Wnt co-receptor LRP6, *Open Biology* **2016**, 6(8), 160120.
- Wentink, M.Q.; Hackeng, T.M.; Tabruyn, S.P.; Puijk, W.C.; Schwamborn, K.; Altschuh, D.; Meloen, R.H.; Schuurman, T.; Griffioen, A.W.; Timmerman, P.; Targeted vaccination against the bevacizumab binding site on VEGF using 3D-structured peptides elicits efficient antitumor activity, *Proceedings of the National Academy of Sciences* **2016**, 113(44), pp. 12532-12537.
- Kayhan, J.; Wanner, M.J.; Ingemann, S.; van Maarseveen, J.H.; Hiemstra, H.; Consecutive Pictet-Spengler Condensations toward Bioactive 8-Benzylprotoberberines: Highly Selective Total Syntheses of (+)-Javaberine A, (+)-Javaberine B, and (-)-Latifolian A, *European Journal of Organic Chemistry* **2016** (22), 3705-3708. This paper was highlighted in *SYNFACTS*, Highlights in Current Synthetic Organic Chemistry **2016**, 12(10) 1011.
- Breman, A.C.; van der Heijden, G.; van Maarseveen, J.H.; Ingemann, S.; Hiemstra, H.; Synthetic and Organocatalytic Studies of Quinidine Analogues with Ring-Size Modifications in the Quinuclidine Moiety, *Chemistry: A European Journal* **2016**, *22*(40), 14247-14256.
- Saya, J.M.; Vos, K.; Kleinnijenhuis, R.A.; van Maarseveen, J.H.; Ingemann, S.; Hiemstra, H.; Total synthesis of aquatolide, *Organic Letters* **2015**, 17, 3892–3894. This paper was highlighted on the website http://www.organic-chemistry.org/Highlights/ 2016/29August.shtm.
- Kleinnijenhuis, R.A.; Timmer, B.J.J.; Lutteke, G.; Smits, J.M.M.; de Gelder, R.; van Maarseveen, J.H.; Hiemstra, H.; Formal synthesis of solanoeclepin A: enantioselective allene diboration and intramolecular [2+2] photocycloaddition for the construction of the tricyclic core, *Chemistry: A European Journal* **2016**, *22*(4), 1266-1269.
- Popovic, S.; Wijsman, L.; Landman, I.R.; Sangster, M.F.; Pastoors, D.; Veldhorst, B.B.; Hiemstra, H.; van Maarseveen, J.H.; Fine-tuning the balance between peptide thioester cyclization and racemization, *European Journal of Organic Chemistry* **2016** (3), 443-446.

- Streefkerk, D.E.; Richelle, G.J.J.; van Maarseveen, J.H.; Timmerman, P.; Multicyclic CLIPS Peptides: Next Generation Therapeutic Peptide Drugs, Patent Application: EP16202466.

Important Grants and Prizes in 2016

Prof. dr. Jan H. van Maarseveen received the 2016 KNCV Van Marumpenning in recognition of his contributions to the societal relevance and the public image of chemistry.

Grants:

Title	Synthese van volledig L-geconfigureerde gespannen kleine cyclische peptiden gebaseerd op asymmetrische hydrogenering van dehydro aminozuren
Applicant	Prof.dr. Jan van Maarseveen
Partner	InCatT
Grant from	NWO NCI-Kiem
Amount	k€ 35

Title	Artificial Metalloenzyme for the Selective C-H Alkenylation of Arenes
Applicant	Dr. M. A. (Tati) Fernandez
Partner	Dr. Francesco Mutti
Grant from	HRSMC

2.2 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.

In the **Biomolecular Spectroscopy group** of VU-LaserLaB Amsterdam, laser spectroscopic methods, in particular Raman Spectroscopy in a variety of modes are developed for biophotonics, biomedical and other purposes. Emphasis is currently on the development of special Raman modes for future Mars missions, surface enhancement and resonance enhancement of Raman signals. non-linear Raman spectroscopy (SRS) for fast imaging and for the in-flow detection of micro/nanoparticles, spectroscopy at the nanoscale based on scanning near-field optical microscopy (SNOM), and depth analysis through nontransparent samples using time-resolved Raman spectroscopy.

The **Biophysical Organic Chemistry group** at the UL is highly recognized for its studies in high-resolution Magic Angle Spinning Solid State NMR studies. The research takes place in the European center for ultra-high field solid state NMR in Leiden and is carried out also in combination with quantum chemical modeling (Buda) and mesoscale simulations (Sevink). The main focus is on the relation between electronic/spatial structure and function of membrane proteins involved in visual signal transduction and photosynthetic energy conversion. In addition, ultrahigh field micro-MRI (Alia) allows imaging and visualizing the metabolic processes in vivo. The aim is to translate the understanding of general principles used in natural systems into concepts for novel artificial photosynthesis devices.

In the **Raymond and Beverly Sackler Laboratory for Astrophysics** (UL) experimental studies are performed that focus on simulating the chemical processes in the interstellar medium. Part of the experiments is performed with the aim to provide spectroscopic data, both of molecular gas phase transients and ices, to interpret and guide astronomical observations. Other experiments study the cryogenic formation of new molecules on interstellar dust grains upon vacuum UV irradiation or bombardment with atoms for fully controlled conditions. Besides bottom-up research – generating more complex species from smaller precursors – recently also top-down astrochemical processes have been studied experimentally, by investigating the photo-induced dissociation of astronomically relevant PAHs.

In the **Molecular Nano-Optics and Spins** (UL), the subgroup of **Orrit** is interested in the optical detection and study of single fluorescent molecules and of single gold nanoparticles. The projects have contacts with biophysics, physical chemistry, soft matter physics and solid state physics. Important new developments are applications of gold nanorods to sensing, fluorescence enhancement, and the detection of single weak emitters. The subgroup of **Groenen** concentrates on the development and application of electron-paramagnetic-resonance (EPR) spectroscopy. Resolution, sensitivity and stability of EPR at high microwave frequencies are being enhanced continuously, which brings new applications within reach. Presently the focus is on the study of the (electronic) structure and dynamics of biomolecules and transient intermediates of enzymatic reactions using spin labels and transition metal ions.

The **Molecular Photonics** group at the UvA aims to extend the fundamental knowledge of excited states. The spectroscopic tools and the scientific competences that are required to do this enable the team to enter into numerous projects in which light-matter interaction is essential. This leads to the application of a photonic approach to the broader scientific and technological fields of molecular biology, polymer science, nanoscience, catalysis, solar energy conversion and medical imaging and phototherapies.

The Molecular Structure and Dynamics and Molecular and Biophysics-groups at the FELIX Laboratory (RU) aim at employing free-electron laser based action spectroscopy methods to obtain insight into molecular structure, conformational structure and dynamics, (photo-)chemistry and biological function of isolated, gas-phase molecules mostly of biological interest. We have developed novel methodologies and instrumentation based on the coupling between (far-)IR laser spectroscopy and mass spectrometry. Our studies focus on fundamental physical chemistry questions of molecular structure of interest in ion chemistry, mass spectrometry, gas-phase biomolecular chemistry, cluster physics and fundamentals of catalysis and astrochemistry. We also address applied problems of molecular structure identification, particularly the identification of low-abundance compounds hidden in complex mixtures, for instance in metabolomics, drug development and biomarker discovery.

The **Surface Chemistry and Catalysis group** at the UL studies chemical reactions of interest for sustianable energy conversion on well-defined, mostly single crystalline, surfaces at the molecular level, and on surfaces modified with well-defined molecular catalysts. The group combines state-of-the-art experimental setups to study surface catalytic reactions using a variety of spectroscopic techniques, both at the metal-uhv and metal-liquid interface, with computational techniques. Their aim is to unravel mechanistic and kinetic aspects of important catalytic reactions that feature in industrial processes, fuel reforming, fuel cells, the hydrogen economy, and environmental catalysis. The group is also part of NRSC-Catalysis and NIOK.

Biomolecular Analysis and Spectroscopy

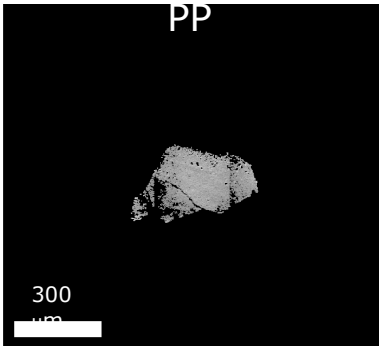
Dr. F. Ariese (VU)

Research topics

- Pico-second time-gated Raman spectroscopy for analyzing nontransparent samples
- Optimization of Raman methods for (fossilized) bacteria for future Mars missions.
- Surface-enhanced, resonance and UV-resonance Raman spectroscopy
- Stimulated Raman scattering, for microscopy and for identifying microplastics
- Spectroscopy at the nanoscale

Group highlights 2016

In a collaborative project within the TA-COAST program, stimulated Raman spectroscopy (SRS) is developed for the detection and identification of microplastics in environmental samples. Following density separation these microplastic particles can be detected on a flat filter using conventional Raman and/or SRS microscopy. The latter is significantly faster, with a scanning speed of 10-100 microsecond per pixel. A set of SRS wavelength pairs is used for multiplex detection of the most prevalent polymer types. This approach is currently being tested on samples from a laboratory-controlled marine mesocosm study and on marine sediment samples from the Loswal NW dumping site off the port of Rotterdam.



SRS microscopy detection of a polypropylene (PP) particle from a marine mesocosm sample.

The parttime visiting professorship of F. Ariese at the Raman Spectroscopy group of Prof. S. Umapathy, Indian institute of Science, Bangalore, was continued. This collaboration is highly inspiring and fruitful, and provides excellent opportunities for exploring new Raman modes and new applications, including femtosecond stimulated Raman of excited state dynamics, triplet excited state spectroscopy, Raman microscopy of diseased tissues, and terahertz Raman.

Key publications 2015-2016

- Besemer, M.; Ariese, F.; Bloemenkamp, R.; van Manen, H.J.; Identification of multiple water-iodide species in concentrated NaI solutions based on the Raman bending vibration of water *Journal of Physical Chemistry* **2016**, 120, 709-714.
- Kumar, V.R.; Ariese, F.; Umapathy, S.; Triplet excited electronic state switching induced by hydrogen bonding: a transient absorption spectroscopy and time dependent-DFT study, *Journal of Chemical Physics* **2016,** 144**,** 114301.

Biophysical Organic Chemistry

Prof. dr. H.J.M. de Groot, Dr. A. Alia, Dr. F. Buda, Dr. G.J.A. Sevink (UL)

Research topics

- Membrane Proteins and Solid State NMR, Natural and Artificial Photosynthesis

Group highlights 2016

Water oxidation catalysts

The controlled surface deposition of a robust and high-performance nanostructured copper-oxide (CuO_x-NLs) electrocatalyst for water oxidation is presented. The material exhibits a characteristic leaf-type morphology and self-assembles on a copper substrate by straightforward constant-current anodization. The oxygen onset occurs at about 1.55 V versus RHE (η = 320 mV), which is 400−500 mV less than for amorphous Cu-oxide films. A Tafel slope of 44 mV dec^{-1} is obtained, which is the lowest observed relative to other copper-based materials. Long-term catalytic performance and stability tests of the electrocatalytic CuO_x-NLs sample show a stable current density of >17 mA cm^{-2} for oxygen evolution, which was sustained for many hours.

Quantum chemical modeling

A series of mononuclear ruthenium water oxidation catalysts of the form $[Ru(cy)(L)(H_2O)]^{2+}$ (cy = p-cymene, L = 2,2'-bipyridine and derivatives) is considered. The proposed catalytic cycle and intermediates are examined using density functional theory (DFT), radiation chemistry, spectroscopic techniques and electrochemistry to establish the water oxidation mechanism. The stability of the catalyst is investigated using Online Electrochemical Mass Spectrometry. The comparison between the calculated absorption spectra of the proposed intermediates with experimental ones, as well as free-energy calculations with electrochemical data, provides strong evidence for a water oxidation catalytic cycle involving four proton-coupled electron transfer (PCET) steps. The thermodynamic bottleneck is identified in the third PCET step involving the O-O bond formation. The good agreement between the optical and thermodynamic data with DFT predictions further confirms the general applicability of this methodology as a powerful tool in the characterisation of water oxidation catalysts and for the interpretation of experimental observables.

Computer simulations of membrane fusion

Two peptides, Coil-K and Coil-E, form a parallel heterodimeric coiled coil, CC-K/E, and have been shown to promote membrane fusion. We examine the effects of reversing the sequence of Coil-E (to yield Coil-Er), on coiled-coil formation and membrane fusion. Coiled-coil assembly was studied using circular dichroism spectroscopy, paramagnetic proton NMR, fluorescence spectroscopy, analytical ultracentrifugation and computational simulations. Combined, the data show that Coil-K and Coil-Er combine in a 1:1 ratio to form an antiparallel tetramer, reinforcing previous studies that show small changes to peptide sequences strongly affect the stoichiometry and orientation of the resulting assemblies. Cholesterol-modified Coil-K and Coil-Er variants were subsequently tested for their ability to promote membrane fusion and the results were compared to the CC-K/E

model system. Surprisingly, no significant differences were found between the two systems, despite the Coil-K/Er complex being 'nonzipper-like'.

Metabolic profiling of intact *Arabidopsis thaliana* leaves using MAS NMR

Arabidopsis thaliana is the most widely used model organism for research in plant biology. In this work we use high resolution-magic angle spinning nuclear magnetic resonance (HR-MAS NMR) to establish the *in vivo* metabolic profile directly from the intact *Arabidopsis thaliana* leaves without metabolite extraction. Combining one- and two-dimensional ^{1}H HR-MAS NMR allowed the identification of several metabolites including sugars and amino acids in intact leaves. Multivariate analysis on HR-MAS NMR spectra of leaves throughout the circadian cycle revealed modules of primary metabolites with significant and consistent variations of their molecular components at different time points of the circadian cycle. Since robust photosynthetic performance in plants relies on the functional periodicity of the circadian rhythm, our results show that HR-MAS NMR promises to be an important non-invasive method that can be used for metabolomics of the *Arabidopsis thaliana* mutants with altered physiology and photosynthetic efficiency.

Key publications 2015-2016

- Monti, A.; Negre, C.F.A.; Batista, V.S.; Rego, L.G.C.; de Groot, H.J.M.; Buda, F.; Crucial Role of Nuclear Dynamics for Electron Injection in a Dye-Semiconductor Complex, *Journal of Physical Chemistry Letters*, **2015**, 6, 12.
- Najdanova, M.; Janssen, G.J.; de Groot, H.J.; Matysik, J.; Alia, A.; Analysis of electron donors in photosystems in oxygenic photosynthesis by photo-CIDNP MAS NMR, *Journal of Photochemistry and Photobiology B: Biology* **2015**.
- Bulacu, M.; Sevink, G.J.A.; Computational insight in the role of fusogenic lipopeptides at the onset of liposome fusion, *Biochimica et Biophysica Acta (BBA)* **2015**, 1848.
- Augustijn, D.; Roy, U.; van Schadewijk, R.; de Groot, H.J.M.; Alia, A.; Metabolic Profiling of Intact Arabidopsis thaliana Leaves during Circadian Cycle Using H-1 High Resolution Magic Angle Spinning NMR, *Plos One* **2016**, 11, 9.
- Joya, K.S.; de Groot, H.J.M.; Controlled Surface-Assembly of Nanoscale Leaf-Type Cu-Oxide Electrocatalyst for High Activity Water Oxidation, *ACS Catalysis* **2016**, 6, 3.
- de Ruiter, J.M.; Purchase, R.L.; Monti, A.; van der Ham, C.J.M.; Gullo, M.P.; D'Angelantonio, M.; Barbieri, A.; de Groot, H.J.M.; Buda, F.; Electrochemical and Spectroscopic Study of Mononuclear Ruthenium Water Oxidation Catalysts: A Combined Experimental and Theoretical Investigation, *ACS Catalysis* **2016**, 6.
- Zheng, T.; Bulacu, M.; Daudey, G.; Versluis, F.; Voskuhl, J.; Martelli, G.; Raap, J.; Sevink, G.J.A.; Kros, A.; Boyle, A.L.; A non-zipper-like tetrameric coiled coil promotes membrane fusion, *RSC Advances* **2016**, 6, 10.
- Joya, K.S.; Ahmad, Z.; Joya, Y.F.; Garcia-Esparza, A.T.; de Groot, H.J.M.; Efficient electrochemical water oxidation in neutral and near-neutral systems with a nanoscale silver-oxide catalyst, *Nanoscale* **2016**, 8, 32.

Important Grants and Prizes in 2016

- NWO Solar to Products Design and optimization of a photoanode for solar fuel production, F. Buda, H.J.M. de Groot, L. Visscher, S. van Gisbergen, NWO, 733.000.007, date of granting: 01-09-2016 (€560.000), position still open.

- CSC- studentship Design of dye-based responsive matrices for quantum coherent photochemical conversion, Yang Shao
- NWO, Netherlands Magnetic Resonance Research School (Joint research school, €200.000,-) A.P.M. Kentgens, M. Baldus, R. Boelens, A. Bonvin, M. Ubbink, H.J.M. de Groot, H. van As, J. van Duynhoven, A. Velders, K. Nicolay, P.C.M.M. Magusin, O.F. van den Brink, NWO, 022.005.029, start date PhD: 19-09-2016
- Nog niet officieel toegekend: Verlengingsaanvraag FOM/ALW programma 'Towards biosolar cells' H.J.M. de Groot, FOM-16.1864, technician position

Raymond and Beverly Sackler Laboratory for Astrophysics

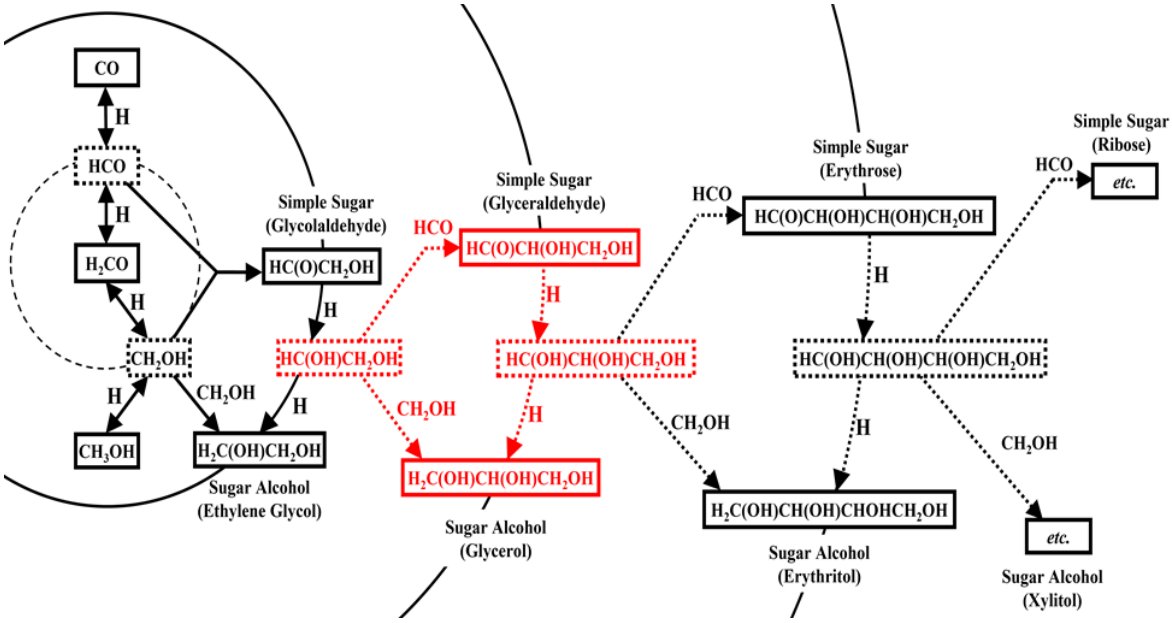
Prof. dr. H. Linnartz (UL)

Research topics

- Laboratory astrophysics and astrochemistry
- High resolution IR (2500-4000 cm^{-1}) and UV/VIS (200-1000 nm) molecular spectroscopy
- Molecular transients of astrophysical interest
- Interstellar ice: spectroscopy and molecular dynamics

Group highlights 2016

In 2016 we demonstrated that molecules as complex as glycolaldehyde and ethylene glycol are efficiently formed on icy dust grains via non-energetic atom addition reactions between accreting H atoms and CO-molecules [Chuang et al. 2016], a process that dominates surface chemistry during the 'CO-freeze out stage' in dense cores of dark interstellar clouds, when icy dust grains are covered by a CO-coating. Based on this work, facilitating backbone growth through radical recombinations, we also showed that a similar mechanism results in the formation of the biologically relevant molecule glycerol, a three-carbon bearing sugar alcohol necessary for the formation of membranes of modern living cells and organelles [Fedoseev et al., 2017]. The physical chemical processes at work enrich the molecular complexity of interstellar ices without the need of thermal activation. This shows that astronomically complex species are already formed during the first stages of star and planet formation, fully in line with the recent identification of such species on comet P67/C-G, a piece of highly pristine material reflecting the chemical composition of our Solar System some 4.5 billions yrs ago.



Key publications 2015-2016

- Chuang, K.-J.; Fedoseev, G.; Ioppolo, S.; van Dishoeck, E.F.; Linnartz, H.; H-atom addition and abstraction reactions in mixed CO, H2CO and CH3OH ices; An extended view on complex organic molecule formation, *Monthly Notices of the Royal Astronomical Society* **2016**, 455, 1702.
- Linnartz, H.; Fedoseev, G.; Ioppolo, S.; Atom addition reactions in interstellar ices, *International Reviews in Physical Chemistry* **2015**, 34, 205

Important Grants and Prizes in 2016

- Three NWO grants within Dutch Astrochemistry II call on 'Circumstellar ice and snow lines - Photochemistry at the edge' (Hogerheijde/Linnartz), 'Molecular complexity in interstellar ices – a combined experimental /theoretical study' (Linnartz/Cuppen) and 'Photo-absorption and dissociation of CH and carbon-based radicals' (Ubachs/Linnartz).
- Two ITN H2020 grants within EUROPAH (www.europah.eu), a large European research and training consortium to investigate the role of PAHs in the interstellar medium.

Molecular Structure and Dynamics – FELIX/Molecular and Biophysics

Prof. dr. J. Oomens, Dr. J.M. Bakker, Dr. A.M. Rijs (RU)

Research topics

- Structure of peptides
- Far-Infrared Spectroscopy to probe Hydrogen Bond Signatures
- Biomarker discovery via IR ion spectroscopy (IRIS)
- Ion Chemistry
- Astrochemistry

Group highlights 2016

New infrared action spectroscopy tool for neutral gas-phase molecules

Infrared spectroscopy is an efficient tool for the structural analysis of (bio)molecules, especially when experiments are performed in a cooled gas phase environment and combined with theoretical quantum-chemical calculations. This article demonstrates a new infrared spectroscopy technique, which significantly extends the scope of the molecules that can be studied in the gas phase. It is particularly suitable for neutral peptide molecules lacking an ultra-violet (UV) chromophore. The demonstrated technique also enables infrared spectroscopy of molecular complexes: several molecules bound together by means of weak interactions such as hydrogen bonding. This creates unique opportunities to selectively study the interactions that are responsible for the structure of the (bio)molecules, either originating from intrinsic molecular properties, or from the surrounding environment. The authors believe that the demonstrated technique will significantly advance the field of structural studies of molecules and molecular complexes.

Infrared ion spectroscopy, another dimension in mass spectrometry

FELIX researchers have demonstrated the first use of infrared ion spectroscopy (IRIS) to characterize the structures of peptide fragments generated by electron transfer dissociation (ETD). They related previously predicted product ion structures of an often studied model tryptic peptide ([AlaAlaHisAlaArg+2H]2) to experimental IR spectra of mass-selected ETD product ions to establish their molecular structure. These results are published in Nature Communications (June 9, 2016). Comparing theory and experiment reveals that structural assignments based on computed thermodynamic considerations alone often do not correspond to the experimentally formed species. This highlights the potential for infrared ion spectroscopy using a tunable free electron laser (FELIX) to diagnostically identify product ion structures in tandem MS and, more specifically, the mechanisms associated with peptide fragmentation in electron attachment methods.

Key publications 2015-2016

- Yatsyna, V.; Bakker, D.J.; Salén, P.; Feifel, R.; Rijs, A.M.; Zhaunerchyk, V.; Infrared Action Spectroscopy of Low-Temperature Neutral Gas-Phase Molecules of Arbitrary Structure, *Physical Review Letters* **2016**, *117*, 118101.

- Bakker, D.J.; Peters, A.; Yatsyna, V.; Zhaunerchyk, V.; Rijs, A.M.; Far-Infrared Signatures of Hydrogen Bonding in Phenol Derivatives, *Journal of the Physical Chemistry Letters* **2016,** *7*, 1238.
- Martens, J.; Grzetic, J.; Berden, G.; Oomens, J.; Structural identification of electron transfer dissociation products in mass spectrometry using infrared ion spectroscopy, *Nature Communications* **2016** *7*, 11754.
- Alvaro Galue, H.; Oomens, J.; Buma, W.J.; Redlich, B.; Electron Flux Infrared Response to Varying p-Bond Topology in Charged Aromatic Monomers, Nature Communications **2016**, *7*, 12633.
- Lang, S.M.; Bernhardt, T.M.; Kiawi, D.M.; Bakker, J.M.; Barnett, R.N.; Landman, U.; The Interaction of Water with Free $Mn_4O_4^+$ Clusters: Deprotonation and Adsorption-Induced Structural Transformations, Angewandte Chemie International Edition **2015**, *54*, 15113.

Important Grants and Prizes in 2016

- NWO Dutch Astrochemistry Network II grant (2 PhD positions)
- EUROPAH MCSA-ITN Network 722346 (Coord U Aarhus, Denmark), 1 ESR at FELIX

Molecular Nano-Optics and Spins

Prof. dr. E.J.J. Groenen, Prof. dr. M. Orrit, Dr. P. Gast, Dr. M. I. Huber (UL)

Research topics

- Electronic and geometric structure determination and dynamics by multifrequency, cw and pulsed Electron Paramagnetic Resonance (EPR) and Electron Nuclear Double Resonance (ENDOR).
- Single-molecule fluorescence and absorption spectroscopy, microscopy of single metal nanoparticles, optical trapping and diffusion of single nanoparticles.
- Photophysics, conformational dynamics and relaxation processes of (bio)molecular systems probed by high-resolution, site-selective laser spectroscopy and optical hole-burning.

Group highlights 2016

The Groenen group has developed a multi-frequency EPR approach to determine the spin-spin coupling parameters of DNP agents (Gast et al.)

The Orrit group has demonstrated optical detection of the electrochemical switching of a single molecule under an externally controlled potential (Zang et al.)

Key publications 2015-2016

- Shabestari, M.H.; Meeuwenoord, N.J.; Filippov, D.; Huber, M.; Interaction of the amyloid beta peptide with sodium dodecyl sulphate as a membrane-mimicking detergent, *Journal of Biological Physics* **2016**, 42.
- Schilder, J.; Liu, W.M.; Kumar, P.; Overhand, M.; Huber, M.; Ubbink, M.; Protein docking using an ensemble of spin labels optimized by intra-molecular paramagnetic relaxation enhancement, *Physical Chemistry Chemical Physics* **2016**, 18.
- Zhang, W.; Caldarola, M.; Pradhan, B.; Orrit, M.; Gold Nanorod Enhanced Fluorescence Enables Single-Molecule Electrochemistry of Methylene Blue, Angewandte Chemie Int. Ed. **2017**, 56, DOI: 10.1002/ange.201612389.
- Hou, L.; Adhikari, S.; Tian, Y.X.; Scheblykin, I.G.; Orrit, M.; Absorption and Quantum Yield of Single Conjugated Polymer Poly [2-methoxy-5-(2-ethylhexyloxy)-1,4-phynylenevinylene] (MEH-PPV) Molecules, *Nano Letters* **2017**, 17, DOI: 10.1021/acs.nanolet.6b04726.

Important Grants and Prizes in 2016

- E.J.J. Groeinen appointed fellow of the International EPR Society.
- M. Orrit received the Physica Prize 2016 of the NNV and the Edison-Volta Prize 2016 of the EPS.

Molecular Photonics

Prof. dr. W.J. Buma, Prof. dr. A.M. Brouwer, Prof. dr. S. Woutersen, Dr. ir. A. Petrignani-Taube, Dr. R.M. Williams, Dr. H. Zhang (UvA), Dr. S. Castellanos Ortega (ARCNL)

Research topics

- Dynamics of supramolecular and biomolecular systems
- Photoprocesses in nanostructures
- Photochemical processes

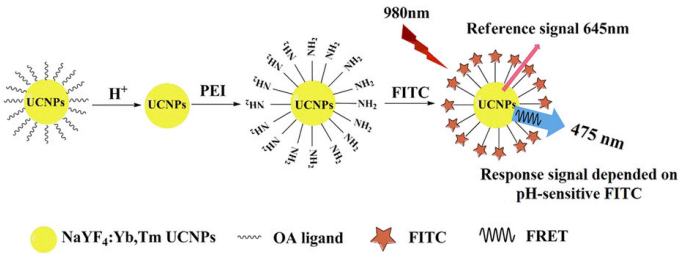
Group highlights 2016

Molecular grapheme

The interaction of delocalized π-electrons with molecular vibrations is key to charge transport processes in π-conjugated organic materials based on aromatic monomers. The application of advanced infrared multiple-photon dissociation action spectroscopic techniques and quantum-chemical calculations has allowed us to show how the molecular edge topology is ultimately responsible for determining how the electron distribution is linked to the vibrational dynamics of the carbon skeleton. These results rationalize the differences of electronic properties of armchair- versus zigzag-type families of technologically relevant organic molecules, and allow for a rational design of new materials (*Nature Communications* 2016, 7, 1263).

Nanoprobes for self-ratiometric pH sensing

The accurate quantification of the intracellular pH (pH_i) is of great importance in revealing the cellular activities and early warning of diseases. A series of fluorescence-based nano-bioprobes composed of different nanoparticles or/and dye pairs have already been developed for pH_i sensing. Till now, biological auto-fluorescence background upon UV-Vis excitation and severe photo-bleaching of dyes are the two main factors impeding an accurate quantitative detection of pH_i. We have developed a self-ratiometric luminescence nanoprobe based on Förster resonant energy transfer (FRET) in which upconversion nanoparticles (UCNPs) (as energy donor) were covalently conjugated with pH-sensitive Fluorescein isothiocyanate (FITC) (as energy acceptor) for an accurate and quantitative probing of pH_i. Under 980 nm excitation upconversion emission bands at 475 nm and 645 nm of $NaYF_4:Yb^{3+},Tm^{3+}$ UCNPs were used as pH_i response and self-ratiometric reference signal, respectively. This direct sensing approach has circumvented the traditional software-based subsequent processing of images which may lead to relatively large uncertainty of the results. Due to efficient FRET and the absence of fluorescence background, a highly sensitive and accurate sensing has been achieved, featured by 3.56 per unit change in pH_i value 3.0-7.0 with deviations less than 0.43. This approach will facilitate the intracellular researches and development of the intracellular drug delivery systems (*Scientific Reports* 2016, 6:38617).

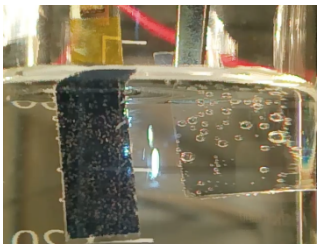


Vibrational Circular Dichroism

Vibrational Circular SDichroism (VCD) is one of the most powerful tools to determine and study the stereochemistry of chiral molecular systems but its routine application suffers from the extensive theoretical efforts that need to be made to come to an unambiguous assignment of experimental spectra. In collaboration with Scientific Computing & Modelling N.V. and BioTools Inc. we have developed new theoretical methods that enable a faster and more reliable analysis. With these methodologies we have shown that the currently employed analysis methods that consider the molecule as conformationally static in general lead to an incorrect interpretation of the spectrum. Indeed, only when the conformational dynamics are explicitly taken into account full agreement between experiment and theory can be obtained (*Chemistry – A European Journal* 2016, *22*, 704; *Physical Chemistry Chemical Physics* 2016, *18*, 21202; *ibid* 21213).

Solar Fuels

In 2016 the Molecular Photonics group contributed to the development of light driven water oxidation for solar fuels. We made new robust photoactive chromophores that absorb light and drive photo-catalysis. We anchored highly electron-deficient benzo[ghi]-perylene-tris-imide (BPTI) chromophores to a metal oxide electrode surface and showed that reversible formation of their radical anions can occur in air-saturated aqueous buffer solution. BPTI is a robust molecular chromophore that can function as the electron acceptor in water splitting artificial photosynthetic devices in aqueous phase. Next to these perylene tris-imides, we also used new beta substituted porphyrins. Very photo-stable tetra-chloro-metallo-porphyrins (Cu(II) and Ni(II)) were used as sensitizers for visible-light-driven water oxidation coupled to cobalt based water-oxidation catalysts in concentrated phosphate buffer solution. We successfully demonstrated long-term (>3 h) visible-light-driven water oxidation using a molecular system (*Chemistry - A European Journal* 2016, *22*(16), 5489-5493; *Physical Chemistry Chemical Physics* 2016, *18*(22), 15191-15198).



Surprising finding under the hood of molecular motors

Time-resolved vibrational-spectroscopy experiments on the molecular motor of Nobel laureate Ben Feringa show that its operation cycle involves an electronic 'dark state', that results in a short (picosecond) stutter at the onset of its rotational movement, and strongly influences the quantum efficiency of the molecular motor. This knowledge is essential for the design of the next generation of these motors: to improve the efficiency of the photon-to-rotation conversion one should focus on the 'dark state', and not on the optically accessible excited electronic state that was the focus of attention so far (*Journal of Physical Chemistry A* 2016, *120*, 8606-8612).

Key publications 2015-2016

- Becker, R.; Amirjalayer, A.; Li, P.; Woutersen, S.; Reek, J.N.H.; An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media, *Science Advances* **2016**, *2*, e1501014.

- Bruijn, J.R.; Van der Loop, T.H.; Woutersen, S.; Changing Hydrogen-Bond Structure during an Aqueous Liquid–Liquid Transition Investigated with Time-Resolved and Two-Dimensional Vibrational Spectroscopy, *Journal of Physical Chemistry Letters* **2016**, *7*, 795–799.
- Chen, H.-C.; Williams, R.M.; Reek, J.N.H.; Brouwer, A.M.; Robust Benzo[Ghi]Perylenetriimide Dye-Sensitized Electrodes in Air-Saturated Aqueous Buffer Solution, *Chemistry - A European Journal* **2016**, *22*, 5489-5493.
- Cong, T.; Ding, Y.; Xin, S.; Zhang; Liu Y.; Solvent-Induced Luminescence Variation of Upconversion Nanoparticles, *Langmuir* **2016**, *32*, 13200-13206.
- Galué, H.A.; Oomens, J.; Buma, W.J.; Redlich, B.; Electron-flux infrared response of varying π-bond topology in charged aromatic monomers *Nature Communications* **2016**, *7*, 12633.
- Maltseva, E.; Petrignani, A.; Candian, A.; Mackie, C.J.; Huang, X.; Lee, T.J.; Tielens, A.G.G.M.; J. Oomens, J.; Buma, W.J.; High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons in the 3-mm region: Role of periphery, *Astrophysical Journal* **2016**, *831*, 58.
- Nicu, V.P.; Domingos, S.R.; Strudwick, B.H.; Brouwer, A.M.; Buma, W.J.; Interplay of exciton coupling and large-amplitude motions in the vibrational circular dichroism spectrum of dehydroquinidine, *Chemistry – A European Journal* **2016**, *22*, 704-715.
- Suhina, T.; Amirjalayer, S.; Mennucci, B.; Woutersen, S.; Hilbers, M.; Bonn, D.; Brouwer, A.M.; Excited-State Decay Pathways of Molecular Rotors: Twisted Intermediate or Conical Intersection?, *Journal of Physical Chemistry Letters* **2016**, *7*, 4285–4290.
- Meuzelaar, H.; Panman, M.R.; Woutersen, S.; Guanidinium-induced denaturation by breaking of salt bridges, *Angewandte Chemie International Edition* **2015**, *54*, 15255-15259.
- Suhina, T.; Weber, B.; Carpentier, C.E.; Lorincz, K.; Schall, P.; Bonn, D.; Brouwer, A.M.; Fluorescence microscopy visualization of contacts between objects, *Angewandte Chemie International Edition* **2015**, *54*, 3688-3691.
- Tan, E.M.M.; Amirjalayer, S.; Smolarek, S.; Vdovin, A.; Zerbetto, F.; Buma, W.J.; Fast photodynamics of azobenzene probed by scanning excited state potential energy surfaces using slow spectroscopy, *Nature Communications* **2015**, *6*, 5860.
- Tu, L.; Liu, X.; Wu, F.; Zhang, H.; Excitation energy migration dynamics in upconversion nanomaterials, *Chemical Society Reviews* **2015**, *44*, 1331-1345.

Important Grants and Prizes in 2016

Grants:

Title	High-resolution vibrational and electronic spectroscopy of the isolated aromatic universe
Applicants	Prof. dr. Wybren Jan Buma and Dr. Anouk Rijs (RU)
Grant from	NWO Astrochemistry DAN-II
Amount	k€ 214 (1 PhD student)

Title	The reaction dynamics of ionic and neutral PAHs
Applicants	Dr. Annemieke Petrignani
Grant from	NWO Astrochemistry DAN-II

Amount	k€ 214 (1 PhD student)
Title	Redox Mediators in Dye-sensitized Photoelectrochemical Cells for CO_2-reduction
Applicants	Reek, Koch, Detz, Brouwer, Sinke, Garnett
Grant from	NWO Solar to Products
Amount	k€ 557
Title	ELENA Low energy electron driven chemistry for the advantage of emerging nano-fabrication methods
Applicants	ELENA Consortium. A.M. Brouwer member
Grant from	European Commission, HORIZON 2020 program,
Amount	k€ 1067 (k€ 255, 1 PhD student at ARCNL; defence at UvA)

Prizes:
H. Zhang, award of *The 4th International Symposium on Rare Earth Resource Utilization and the 7th International Symposium on Functional Materials*.

Surface Chemistry and Catalysis

Prof. dr. M.T.M. Koper, Dr. D.G.H. Hetterscheid, Dr. L.B.F. Juurlink, Dr. I.M.N. Groot (UL)

Research topics

- Electrocatalysis for sustainable energy conversion, water splitting, carbon dioxide reduction
- Surfaces, both in UHV and electrochemical environments
- Theoretical electrochemistry
- Model catalysts
- In situ spectroscopy and in situ scanning probe imaging under realistic conditions

Group highlights 2016

Three papers in Nature Communications

In August 2016, papers by Oscar Diaz-Morales, Yi-Fan Huang and Thom Hersbach were published in Nature Communications.

The three papers are:

- Diaz-Morales, O.; Raaijman, S.; Kortlever, R.; Kooyman, P.J.; Wezendonk, T.; Gascon, J.; Fu, W.T.; Koper, M.T.M.; Iridium-based double perovskites for efficient water oxidation in acid media, *Nature Communications*, vol. 7.
- Huang, Y.; Kooyman, P.J.; Koper, M.T.M.; Intermediate stages of electrochemical oxidation of single-crystalline platinum revealed by in situ Raman spectroscopy, *Nature Communications*, vol. 7.
- Hersbach, T.J.P.; Yanson, A.I.; Koper, M.T.M.; Anisotropic etching of platinum electrodes at the onset of cathodic corrosion, *Nature Communications*, vol. 7.

Double-stranded water on platinum on the cover of PRL

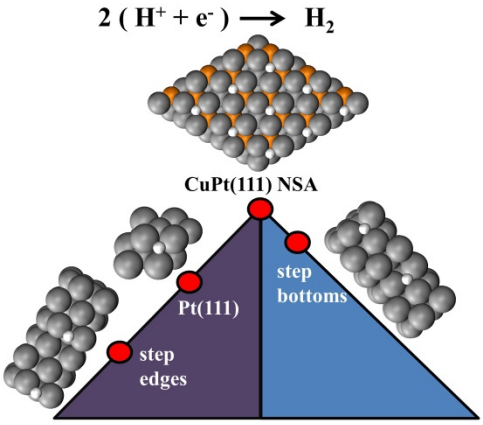
A paper by Manuel Kolb on water adsorption on stepped platinum surfaces, in collaboration with the group of Dan Killelea at Layola University in Chicago, features on the cover of *Physical Review Letters*.



Boost of Water Electrolysis - Article In Nature Communications

Researchers from Leiden University, Ruhr-Universität Bochum and the Technical University of Munich have boosted the efficiency of water electrolysis. They located a layer of copper atoms near the surface of conventional platinum electrodes. Because of that, reaction intermediates could desorb a bit more easily from the surface, making the

catalyst more efficient. The modified system generated twice the amount of hydrogen than a platinum electrode without a copper layer. The research team published these results in the journal "Nature Communications".
Tymoczko, J.; Calle-Vallejo, F.; Schuhmann, W.; Bandarenka, A.S.; Making the hydrogen evolution reaction in polymer electrolyte membrane electrolysers even faster, *Nature Communications*, vol. 7:10990, pp. 1-6.

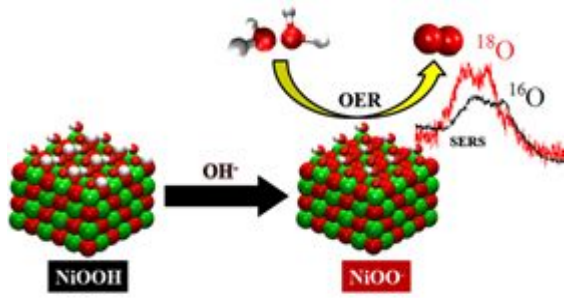


Water at stepped platinum surface on the cover of PCCP

A paper by Manuel Kolb on the adsorption of water on the stepped Pt(533) surface features on the cover of PCCP.



Mechanism of oxygen evolution on nickel oxyhydroxide electrodes in JACS and Chemical Science



Two papers from the spectro-electrochemical work of Oscar Diaz-Morales on the mechanism of the oxygen evolution reaction on nickel oxyhydroxide electrodes, one in collaboration with the group of Wilson Smith at the TU Delft, have been published in JACS and Chemical Science. The papers highlight, and provide an explanation for, the pH dependence of the catalytic activity.

Key publications 2015-2016

- Diaz-Morales, O.; Raaijman, S.; Kortlever, R.; Kooyman, P.J.; Wezendonk, T.; Gascon, J.; Fu, W.T.; Koper, M.T.M.; Iridium-based double perovskites for efficient water oxidation in acid media, *Nature Communications* **2016**, 7, 12363.

- Hersbach, T.J.P.; Yanson, A.I.; Koper, M.T.M.; Anisotropic etching of platinum electrodes at the onset of cathodic corrosion, *Nature Communications* **2016**, 7, 12653.
- Huang, Y.; Kooyman, P.J.; Koper, M.T.M.; Intermediate stages of electrochemical oxidation of single-crystalline platinum revealed by in situ Raman spectroscopy, *Nature Communications* **2016**, 7, 12440.
- Kolb, M.J.; Farber, R.G.; Derouin, J.; Badan, C.; Calle-Vallejo, F.; Juurlink, L.B.F.; Killelea, D.R.; Koper, M.T.M.;Double-Stranded Water on Stepped Platinum Surfaces, *Physical Review Letters* **2016**, 116, 13.
- Van Spronsen, M.A.; Weststrate, K.J.; Juurlink, L.B.F.; A Comparison of CO Oxidation by Hydroxyl and Atomic Oxygen from Water on Low-Coordinated Au Atoms, *ACS Catalysis* **2016**, 6, 10, 7051-7058.
- Kottrup, K.G.; Hetterscheid, D.G.H.; Evaluation of iron-based electrocatalysts for water oxidation - an on-line mass spectrometry approach, *Chemical Communications* **2016**, 52, 12, 2643-2646.
- Mom, R.V.; Rost, M.J.; Frenken, J.W.M.; Groot, I.M.N.; Tuning the Properties of Molybdenum Oxide on Al2O3/NiAl(110): Metal versus Oxide Deposition, *Journal of the Physical Chemistry C* **2016**, 120, 35, 19737-19743.
- Badan, C.; Heyrich, Y.; Koper, M.T.M.; Juurlink, L.B.F.; Surface Structure Dependence in Desorption and Crystallization of Thin Interfacial Water Films on Pt, *Journal of Physical Chemistry Letters* **2016**, 9, 1682–1685, DOI: 10.1021/acs.jpclett.6b00320.

Important Grants and Prizes in 2016

- Dr. I.M.N. Groot receives an Horizon 2020 grant for the project 'Development of continuous two-dimensional defect-free materials by liquid-metal catalytic routes'
- The International Society of Electrochemistry (ISE) has awarded Marc Koper with the biennial Brian Conway Prize for Physical Electrochemistry. The prize will be presented at the 2017 Annual Meeting of the ISE in Providence, RI, USA.

2.3 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 three theoretical chemistry groups of HRSMC work in both areas of research.

The research in the **Computational Physics and Chemistry** groups of Bolhuis and Meijer (UvA) focuses on the study of materials, biological systems, and solution chemistry. Development and application of novel computational techniques and connection with experimental techniques are essential components of the research program. International collaboration with experimental and computational groups plays an important role.

The **Theoretical Chemistry** groups of VUA concentrate their efforts on developing chemical theories and methods for rationally designing and spectroscopically characterizing molecules, nano-structures and materials as well as chemical processes toward these compounds, based on quantum mechanics and computer simulations. This ties in very well with the development of both density (matrix) functional and wave function based methods. The group is active in structure and reactivity, molecular recognition and nanostructures, (bio)catalysis, accurate calculation of properties (NMR, electric field gradients, excitations and many other response properties) where relativistic effects are important, and biochemistry. The group also participates in the ARC-CBBC and NIOK.

This year the **Theoretical Group of Dr. J. Meyer** (UL) joined the HRSMC. His research aims at a better fundamental understanding of energy concersion at interfaces by combining existing as well as developing new computational techniques.

This year the **Theoretical Group of Prof. dr. ir. Gerrit C. Groenenboom** at the RU also joined the HRSMC. The group includes tenured members Dr. Herma M. Cuppen and Dr. ir. Gilles A. de Wijs and emeritus Prof. Ad van der Avoird. Groenenboom and Van der Avoird work on electronic structure and dynamics of molecules, Cuppen focuses on dynamics of molecular clusters and solids, and De Wijs' research interest is electronic structure of materials.

Computational Chemistry

Prof. dr. P.G. Bolhuis, Prof. dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede, Dr. R. Ni (UvA)

Research topics

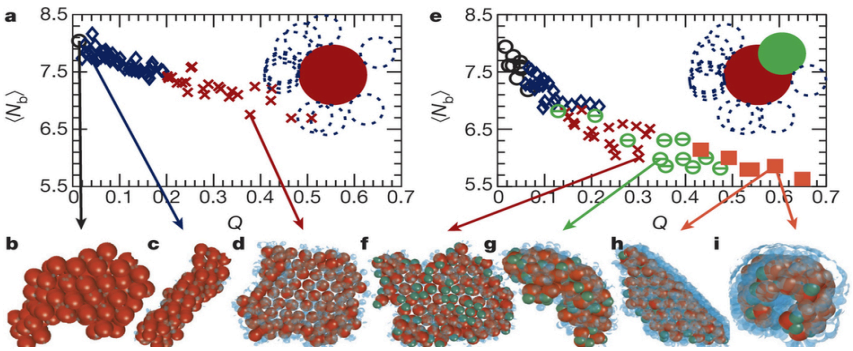
- Development of computational techniques to model properties of many-particle systems
- Nanoporous materials
- Micellar structures
- Reactivity in complex environment
- Polymers in flow
- Stability and structure of carbon materials
- Biological membranes
- Protein folding
- Photoactive proteins
- Signalling proteins
- Protein fiber formation
- Crystal stability and polymorphism
- Carbon materials

Group highlights 2016

Soft (Bio)Matter (Researcher: Peter Bolhuis)

The role of colloidal bond hybridization and anisotropy in self-assembly of microcapsules, published in Nature.

Particles with directional interactions are important building blocks for novel functional materials and may serve as models for biological structures. For example, mutually attractive deformable nanoparticles may spontaneously order themselves in a variety of structures, such as strings, sheets and large vesicles.

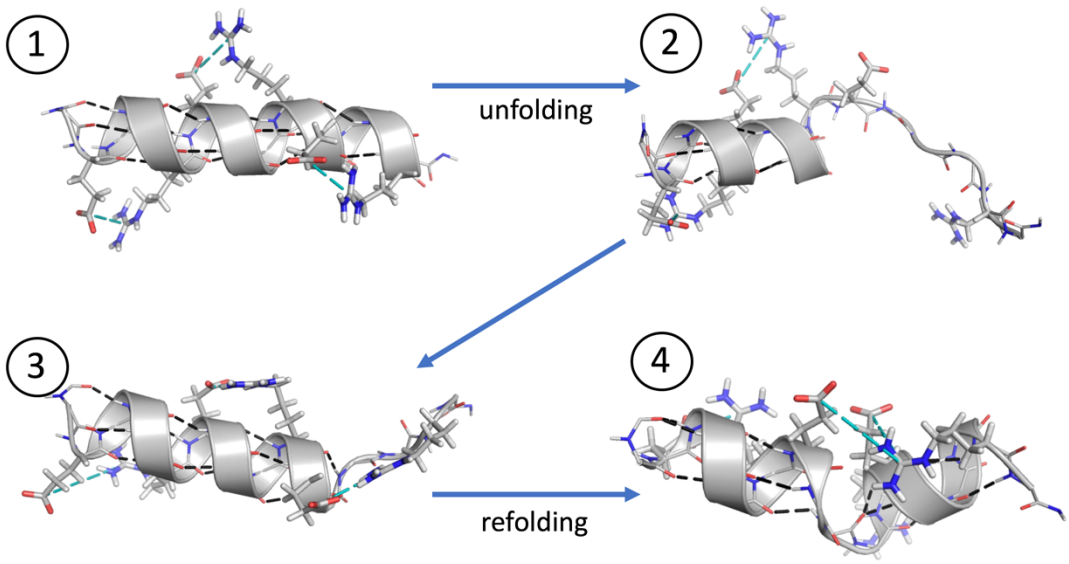


Monte Carlo simulation shows a variety of self-assembled

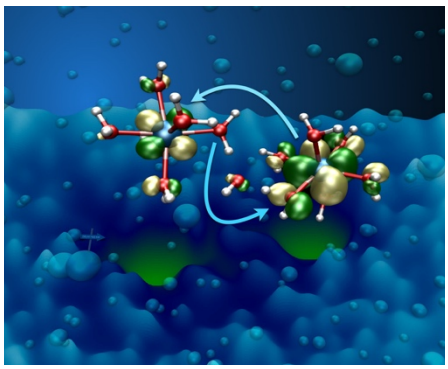
Moreover, Aniso-tropic colloids with attractive patches can self-assemble into open lattices, "colloidal" molecules, and micelles. However, to date model systems that combine mutual attraction, anisotropy and deformability have not been reported. By synthesis and simulations of colloids with these characteristics we show how this leads to self-assembled microcapsules. Mutual attraction and deformability induce directional interactions via colloidal bond hybridization. The particles contain both mutually attractive and repulsive surface groups that are flexible. In analogy to the simplest chemical bond—in which two isotropic orbitals hybridize into the molecular orbital of H_2—these flexible groups rearrange on binding. Through colloidal bond hybridization several

structures can be formed: isotropic spheres self-assemble into planar monolayers, whereas anisotropic snowman-shaped particles self-assemble into hollow monolayer microcapsules. A modest change in the building blocks yield a much greater complexity of the self-assembled structures. Hence, these relatively simple building blocks self-assemble into markedly more complex structures than do similar particles that are isotropic or non-deformable.

Protein conformations and dynamics (Researchers: Vreede)
The group of Vreede studied the effect of salt bridges on the stability and folding kinetics of model alpha-helices, in collaboration with Sander Woutersen. The picture illustrates the observed sequence of an alpha-helix unfolding and refolding:



Electron transfer in complex environment (Researcher: Ensing)

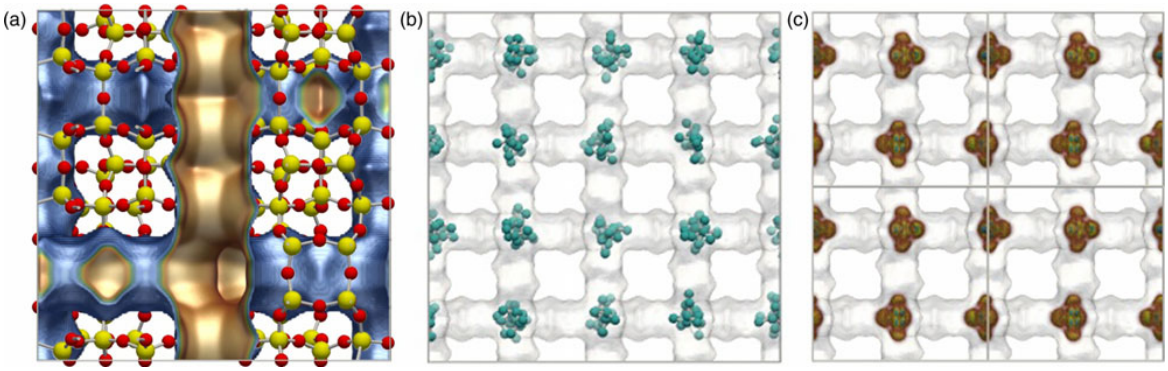


Impression of electron transfer between two Ru ions in water

A new methodological advance by the group made it possible to simulate for the first time electron transfer between a donor and an acceptor species in water solution. Until now, it was only possible to study a (redox) half-reaction at the DFT-MD level of theory, because the random motions in the water solution that drive the spontaneous transfer of an electron between two non-covalently bonded solutes is too rare to observe in a straight-forward simulation. The new technique, a modified version of Transition Path Sampling, generates a large number of independent reactive trajectories, which are analyzed to reveal the rare solvent and ligand fluctuations. For the prototypical self-exchange reaction between two $Ru^{2+/3+}$ ions in water, we discovered that the electron transfer is concerted with a proton transfer reaction from one of the water ligands of the Ru^{2+} complex to a deprotonated ligand of the Ru^{3+} complex. Hereafter, this technique can be used to

unravel the mechanistic details of electron transfer in various types of redox chemistry, including electrochemical reactions at electrode surfaces and electron transfer in enzymes and between biomolecules.

Nanoporous Materials (Researcher: Dubbeldam)
RASPA is a software package, developed in the group of Dubbeldam, for simulating adsorption and diffusion of molecules in flexible nanoporous materials is presented. The code implements the latest state-of-the-art algorithms for Molecular Dynamics and Monte Carlo in various ensembles including symplectic/measure-preserving integrators, Ewald summation, Configurational-Bias Monte Carlo, Continuous Fractional Component Monte Carlo, Reactive Monte Carlo, and Baker's minimization. Applications of RASPA include computing coexistence properties, adsorption isotherms for single and multiple

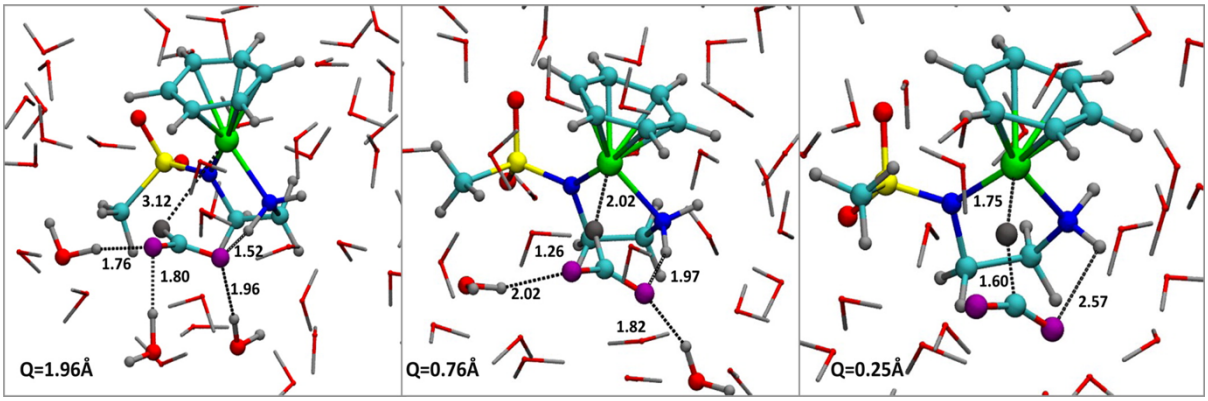


RASPA: computational package for computation and visualization of adsorption and diffusion in nanoporous materials, (a) the MFI-type zeolites consisting of oxygen (red) and silicon (yellow), (b) snapshots of adsorbing di-branched alkanes at 433K and high loading, (c) density plot.

components, self- and collective diffusivities, reaction systems, and visualization. After 10 years of development, the software is now released as open source under the GNU General Public License in 2016 and includes the methodologies developed in my VIDI project (700.10.428). The package is now in use by over 30 research groups and institutions, including groups at the University of Amsterdam, Technical University of Delft, Georgia Tech (Atlanta, USA), Northwestern University (Evanston, USA), Shell (Amsterdam), and CSIRO (Melbourne, Australia). The package is described in RASPA: Molecular Simulation Software for Adsorption and Diffusion in Flexible Nanoporous Materials by D. Dubbeldam, S. Calero, D.E. Ellis, and R.Q. Snurr, *Molecular Simulation 2016*, 42(2), 81-101.

Chemical Reactions in Aqueous Solvent (Researcher: Meijer)
Chemical transformations in an aqueous solvent is an important field. Asymmetric transfer hydrogenation in aqueous solution catalyzed by a metal-based molecular catalyst is a prime example. Ruthenium compounds can efficiently catalyze asymmetric transfer hydrogenation. The nature of the efficiency is still not understood. In a computational study we provide novel insight for two key steps in the catalytic cycle of transfer hydrogenation cycle, using a model of Ru(p-cymene)[TsDPEN] with explicit aqueous solvent. Employing ab initio molecular dynamics simulations, the hydride transfer between formate and the protonated and deprotonated catalyst *and* the dissociation of the ruthenium-formato complex is elucidated. It is shown that solvent water molecules

play an important role, provides a significant contribution to the reaction barriers: they induce an increasing the hydride transfer barrier, while decreasing the dissociation barrier for ruthenium-formato complex, when compared with gas-phase models. These effects can be attributed to hydrogen-bond structure around the formate, which favors the formate to be in solution. Furthermore, the hydride transfer barrier was significantly higher for the deprotonated catalyst, suggesting that the catalyst protonation state is an important factor.



Ab initio molecular dynamics of ruthenium-formate hydrogen transfer in aqueous solution. Representative snapshots of key steps along the reaction pathway.

The study demonstrates that a first-principles molecular dynamics approach, incorporating a molecular description of the solvent, is able to capture the full complexity of catalytic reactions in an aqueous solution. This approach can provide an important contribution to understanding reaction mechanisms, as well as provide directions for novel catalytic systems.

Key publications 2015-2016

- Evers, C.H.J.; Luiken, J.A.; Bolhuis, P.G.; Kegel, W.G.; Self-assembly of microcapsules via colloidal bond hybridization and anisotropy, *Nature* **2016**, *534*, 364-368.
- Brotzakis, Z.F.; Bolhuis, P.G.; A one-way shooting algorithm for transition path sampling of asymmetric barriers, *Journal of Chemical Physics* **2016**, 145, 164112.
- Meuzelaar, H.; Vreede J.; Woutersen S.; Influence of Glu/Arg, Asp/Arg, and Glu/Lys Salt Bridges on α-Helical Stability and Folding Kinetics, *Biophysical Journal* **2016**, 110, 2328-2341.
- Tiwari, A; Ensing, B.; Reactive trajectories of the $Ru^{2+/3+}$ self-exchange reaction and the connection to Marcus' theory, *Faraday Discussions* **2016**, 195, 291-310.
- Van den Ende, J.A.; Ensing, B.; Cuppen, H.M.; Energy barriers and mechanisms in solid-solid polymorphic transitions exhibiting cooperative motion, *CrystEngComm*, **2016**, 1, 4420–4430.
- Balestra, S.; Bueno-Pérez, R., Hamad, S.; Dubbeldam, D.; Ruiz-Salvador, A.R.; Calero, S.; Controlling Thermal Expansion: a Metal Organic Frameworks Route, *Chemistry of Materials* **2016**, 28, 8296-8304.
- Heinen, J.; Burtch, N.; Fonseca Guerra, C.; Walton, K.S.; Dubbeldam, D.; Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials using Force Field Calculations based on Energy Decomposed Density Functional Theory, *Chemistry - A European Journal* **2016**, 22, 18045-18050.

- Pavlova, A.; Rösler, E.; Meijer, E.J.; Mechanistic Aspects of Using Formate as a Hydrogen Donor in Aqueous Transfer Hydrogenation, *ACS Catalysis* **2016**, 6, 5350–5358.
- DeWispelaere, K.; Wondergem, C.S.; Ensing, B.; Hemelsoet, K.; Meijer, E.J.; Weckhuysen, B.M.; Van Speybroeck, V.; Ruiz-Martinez, J.; Insight in the effect of water on the methanol-to-olefins conversion in H-SAPO-34 from molecular simulations and in-situ micro-spectroscopy, *ACS Catalysis* **2016**, 6, 1991-2002.

Important Grants and Prizes in 2016

Title	Identification of potential salt sensors in plants
Applicants	J. Vreede, K. de Groot, S. Spoelstra
Grant from	NWO Topsector chemistry student competition
Amount	k€ 18

Title	Upconversion mechanism of lanthanide-based nanomaterials
Applicants	E.J. Meijer, H. Zhang, T. Langping
Grant from	HRSMC and John van Geuns Fonds
Amount	k€ 18

Title	Research on Mechanism of Thermal Dissociation of Tertiary Amine Hydrochlorides Using Molecular Simulation Techniques
Applicants	E.J. Meijer, Jianguo Yu, Xingfu Song, C. Dong
Grant from	China Research Council
Amount	12 month PhD Scholarship for C. Dong

Theoretical Chemistry

Prof. dr. F.M. Bickelhaupt, Prof. dr. L. Visscher, Prof. dr. E.J. Baerends (em.), Dr. C. Guerra, Prof. dr. P. Gori Giorgi, Dr. I.A.C. Infante, Dr. K. Giesbertz (VU)

Research topics

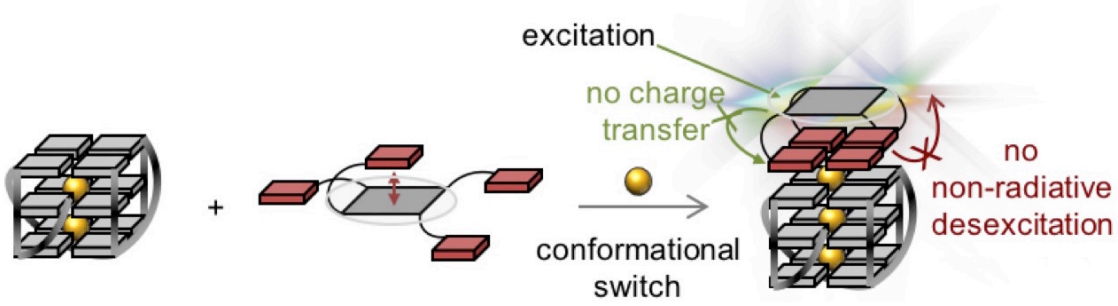
- Theoretical Organic Chemistry and Biocatalysis (Bickelhaupt)
- Quantum Chemistry and Multiscale Modeling (Visscher)
- Applied Theoretical Chemistry (Fonseca Guerra)
- Density (Matrix) Functional Theory (Gori-Giorgi)
- Density (Matrix) Functional Theory (Baerends)

Group highlights 2016

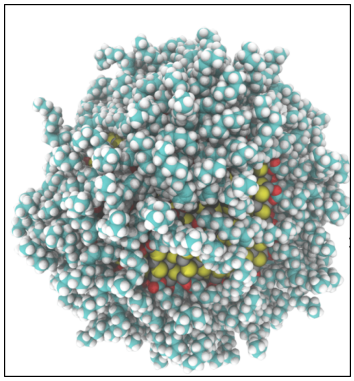
Computational understanding and experimental characterization of twice-as-smart quadruplex ligands as chemical sensors of bacterial nucleotide second messengers

J. Zhou, B. T. Roembke, G. Paragi, A. Laguerre, H. O. Sintim, C. Fonseca Guerra, D. Monchaud, *Scientific Reports* 2016, 6, 33888.

Célia Fonseca Guerra has in collaboration with Herma O. Sintim (Purdue University, USA) and David Monchaud (University of Bourgogne, France) successfully uncovered the precise photophysical mechanism that governs the fluorescence properties of twice-as-smart quadruplex ligands. These twice-as-smart ligands are able to track and label G-quadruplexes: a higher-order nucleic acid structures originating from the assembly of four guanine(G)-rich DNA or RNA strands, whose stability is imparted by the formation and the self-assembly of G-quartets. The absence of overlap between the molecular orbitals of the ligand and the quadruplex is the reason for the fluorescence to occur.



'Darker-than-Black' PbS Quantum Dots: Enhancing Optical Absorption of Colloidal Semiconductor Nanocrystals via Short Conjugated Ligands



C. Giansante, I. Infante, E. Fabiano, R. Grisorio, G.P. Suranna, G. Gigli, *Journal of the American Chemical Society* 2015, 137, 1875.

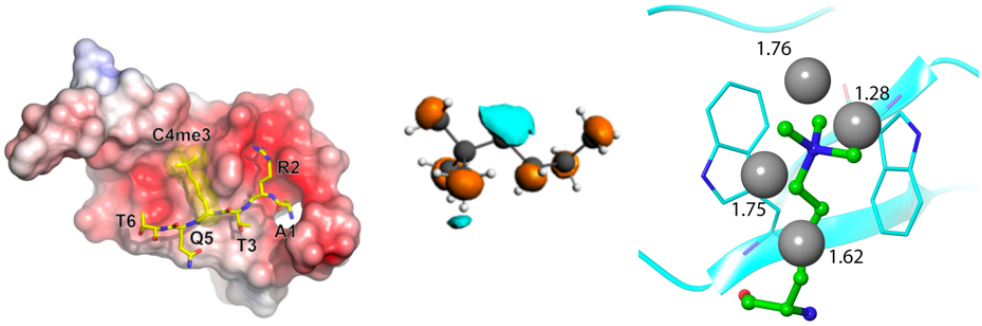
This paper has received a great deal of attention from the scientific community in the nanoscience field. This article has been cited already 42 times and was downloaded more than 3000 times from the ACS website. It was also translated in a lay-person language in the scientific divulgative blog

MappingIgnorance.org. The work combines theory and experiments and it provides a new strategy to modify the surface of colloidal nanocrystals by increasing their optical absorption cross-section and retaining colloidal stability. For these reasons, this work introduces a novel path in the design of light harvesting nanomaterials, which could find applications in photovoltaic and photo detection devices.

Chemical Basis for the Recognition of Trimethyllysine by Epigenetic Reader Proteins

J.J.A.G. Kamps, J. Huang, J. Poater, C. Xu, B.J.G.E. Pieters, A. Dong, J. Min, W. Sherman, T. Beuming, F.M. Bickelhaupt, H. Li, J. Mecinovic, *Nature Communications* 2015, *6*, 8911/1-12.

A large number of structurally-diverse epigenetic reader proteins specifically recognize methylated lysine residues on histone proteins. In this paper, we describe comparative thermodynamic, structural and computational studies on the recognition of the positively-charged natural trimethyllysine and its neutral analogues by reader proteins. This work provides strong experimental and theoretical evidence that reader proteins predominantly recognize trimethyllysine *via* a combination of favorable cation–π interactions and the release of the high-energy water molecules that occupy the aromatic cage of reader proteins upon the association with the trimethyllysine side chain. These results have implications in rational drug design by specifically targeting the aromatic cage of readers of trimethyllysine.



Key publications 2015-2016

- Goesten, M.G.; de Lange, M.F.; Olivos Suarez, A.I.; Bavykina, A.V.; Serra-Crespo, P.; Krywka, C.; Bickelhaupt, F.M.; Kapteijn, F.; Gascon, J.; The Oscillatory Growth of Zirconium and Hafnium Based UiO-66: A Solid-State Clock Reaction, *Nature Communications* **2016**, 7.
- Vengut-Climent, E.; Lucas, R.; Peñalver, P.; Gomez-Pinto, I.; Aviño, A.; Muro-Pastor, A.M.; Fonseca Guerra, C.; Bickelhaupt, F.M.; Eritja, R.; Gonzalez, C.; Morales, J.C.; Glucose-Nucleobase Pseudo Base Pairs as a New Binding Motif in a DNA Context, *Angewandte Chemie International Edition* **2016**, 55.
- Laloo, J.Z.A.; Rhyman, L.; Ramasami, P.; Bickelhaupt, F.M.; de Cozar, A.; Ion-Pair SN2 Substitution: Activation Strain Analyses of Counter-Ion and Solvent Effects, *Chemistry - A European Journal* **2016**, 22 (cover).

- Schlüns, D.; Klahr, K.; Mück-Lichtenfeld, C.; Visscher, L.; Neugebauer, J.; Subsystem-DFT potential-energy curves for weakly interacting systems, *Physical Chemistry Chemical Physics* **2015**, 17.
- Rüger, R.; Niehaus, T.; van Lenthe, E.; Heine, T.; Visscher, L.; Vibrationally Resolved UV/Vis Spectroscopy with Time-Dependent Density Functional Based Tight Binding, *The Journal of Chemical Physics* **2016**, 145.
- Vuckovic, S.; Irons, T.; Savin, A.; Teale, A.M.; Gori-Giorgi P.; Exchange-correlation functionals via local interpolation along the adiabatic connection, *Journal of Chemical Theory and Computation* **2016**, 12 (ACS Editor's choice).
- Malet, F.; Mirtschink, A.; Mendl, C.B.; Bjerlin, J.; Karabulut, E.O.; Reimann, S.M.; Gori-Giorgi, P.; Density functional theory for strongly-correlated bosonic and fermionic ultracold dipolar and ionic gases**,** *Physical Review Letters* **2015**, 115 (Editor's suggestion).
- Zaccaria, F.; Paragi, G.; Fonseca Guerra, C.; The Role of Alkali Metal Cations in the Stabilization of Guanine Quadruplexes: Why K+ is the best, *Physical Chemistry Chemical Physics* **2016**, 18 (cover DFT Developm. Themed Issue).
- Zhou, J.; Roembke, B.T.; Paragi, G.; Laguerre, A.; Sintim, H.O.; Fonseca Guerra, C.; Monchaud, D.; Computational understanding and experimental characterization of twice-as-smart quadruplex ligands as chemical sensors of bacterial nucleotide second messengers, *Scientific Reports* **2016**, 6.
- ten Brinck, S.; Infante, I.; Surface Termination, Morphology, and Bright Photoluminescence of Cesium Lead Halide Perovskite Nanocrystals, *ACS Energy Letters* **2016**, 1.
- Giansante, C.; Infante, I.; Fabiano, E.; Grisorio, R.; Suranna, G.P.; Gigli, G.; 'Darker-than-Black' PbS Quantum Dots: Enhancing Optical Absorption of Colloidal Semiconductor Nanocrystals via Short Conjugated Ligands, *Journal of the American Chemical Society* **2015**, 137.
- Giesbertz, K.J.H.; Invertibility of the retarded response functions for initial mixed states: application to one-body reduced density matrix functional theory**,** *Molecular Physics* **2016**, 114.
- Giesbertz, K.J.H.; Avoiding the 4-index transformation in one-body reduced density matrix functional calculations for separable functionals, *Physical Chemistry Chemical Physics* **2016**, 18.

Important Grants and Prizes in 2016

Bickelhaupt selected Member *Advanced Research Center Chemical Building Blocks* (ARC-CBBC).

Theoretical Chemistry

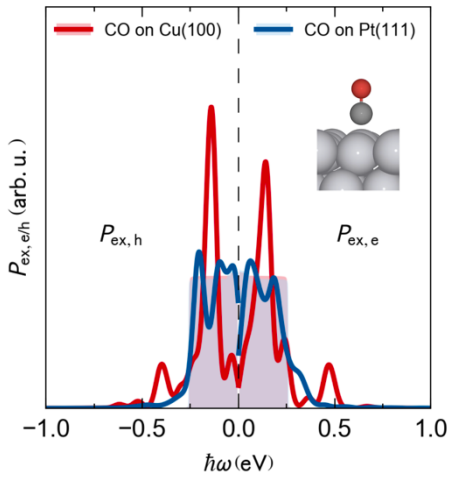
Dr. J. Meyer (UL)

Research Topics

- Modelling of energy exchange at interfaces
- Non-adiabatic dynamics at metal surfaces (electronic friction and beyond)
- Phonons of bulk and surfaces

Group highlights 2016

There is an increasing number of experiments on surface dynamical phenomena involving metal substrates that can only be understood by breaking with the ubiquitous Born-Oppenheimer approximation and thus considering a non-adiabatic coupling of nuclear adsorbate motion to electron-hole (eh) pair excitations in the substrate. However, high-level non-adiabatic calculations are either conceptually challenging or computationally intractable for extended metal surfaces, which is why molecular dynamics with electronic friction has attracted significant interest. Within this numerically very efficient approach to account for the concomitant energy loss in the nuclear dynamics, a fundamental understanding of the underlying eh-pair excitations remains inaccessible. We have thus developed a perturbative approach rooted in time-dependent density functional theory which allows to explicitly evaluate eh-pair excitation spectra (see [1], and references therein). For the presumably well understood case of non-adiabatic vibrational damping of the CO stretch mode on metal surfaces this questions the neglect of electronic coherence as intrinsically assumed within electronic friction theory.



[1] Meyer J.; Reuter, K.; New Journal of Physics 2011, 13, 085010.

Key publications 2015-2016

- Wijzenbroek, M.; Helstone, D.; Meyer, J.; Kroes, G.-J.; Dynamics of H2 Dissociation on the Close-Packed (111) Surface of the Noblest Metal: H2 + Au(111), *Journal of Chemical Physics* **2016**, *145* (14), 144701.

- Rittmeyer, S.P.; Meyer, J.; Juaristi, J.I.; Reuter, K.; Electronic Friction-Based Vibrational Lifetimes of Molecular Adsorbates: Beyond the Independent-Atom Approximation, *Physical Review Letters* **2015**, *115* (4), 046102.

Important Grants and Prizes in 2016

Travel funding (short term scientific mission) within COST action MP1306 'EUSpec' for a two weeks visit of Simon Rittmeyer, working with Prof. Reuter at TU München, Germany.

Theoretical Chemistry

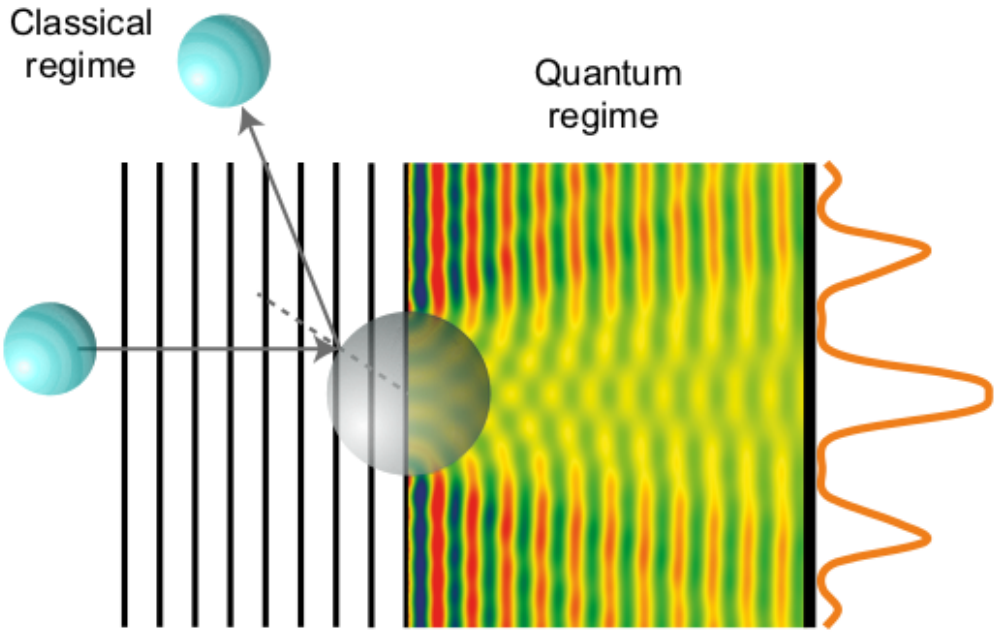
Prof. dr. ir. G.C. Groenenboom (RU)

Research Topics

- Electronic structure and quantum dynamics of molecules

Group highlights 2016

Collisions of atoms and molecules in the gas phase can result in chemical reaction or energy transfer. More subtly, the directions in which the particles move, and the orientation of the axes around which they rotate can change. Measurements of these so called vector properties reveal details of reaction mechanisms and intermolecular interactions. The stereodynamics of collisions can often be understood from inspecting classical trajectories. In a joint theoretical and experimental study with the group of Bas van de Meerakker on the collision of NO radicals with rare-gas atoms we discovered a purely quantummechanical stereodynamics phenomenon, which we could reproduce in quantum scattering calculations and fully explain in an analytical 'Fraunhofer' model. The figure shows backward scattering, which can be understood classically, and forward scattering, which gives rise to diffraction oscillations and our newly identified quantum stereodynamics (see J. Onvlee et al., Nature Chem. 2016, 9, 226).



Key publications 2015-2016

- Onvlee, J.; Gordon, S.D.S.; Vogels, S.N.; Auth, T.; Karman, T.; Nichols, B.; van der Avoird, A.; Groenenboom, G.C., Brouard, M.; van de Meerakker, S.Y.T.; Imaging quantum stereodynamics through Fraunhofer scattering of NO radicals with rare gas atoms, *Nature Chemistry* **2016**, 9, 226.

- Schewe, H.C.; Zang, D.; Meijer, G.; Field, R.W.; Sartakov, B.G.; Groenenboom, G.D.; van der Avoird, A.; Vanhaecke, N.; Stark-interference of electric and magnetic dipole transitions in the A - X band of OH, *Physical Review Letters* **2016***,* 116, 153001.

Important Grants and Prizes in 2016

- Dutch Astrochemistry Network II, 1 PhD position, Rotation-vibration inelastic collision rates of polyatomic molecules (EUR 250.000).
- 1st prize KNCV Golden Master, Boy Lankhaar.

2.4 HRSMC Co-operations

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
Artificial metalloenzyme for the selective C-H alkenylation of arenes	Mutti/Fernández-Ibáñez	1	UvA
Artizymes	Lammertsma/Overhand	1	VU/UL
Circular dichroism in plants	Buma/Ariese	2	UvA/VU
Asymmetric catalysis	Grecea/Woutersen/vdVlugt	1	UvA
Calculations on Multicomponent Syntheses	Bickelhaupt/Orru/Fonseca Guerra	1.3	VU
Catalysis in confined spaces	Reek/deBruin/vMaarseveen/ Rothenberg/Gracia/vdVlugt	1	UvA
Chemistry Behind CuII-μ-thiolate and CuI-disulfide complexes	Bouwman/Fonseca Guerra/Bickelhaupt	1.3	UL/VU
Cyclizations in confined spaces	Van Maarseveen/Reek	1	UvA
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
Enantioselective biocatalysis	Van Maarseveen/Mutti	1	UvA
Enzymatic C-H Functionalization of non-activated arenes	Fernández-Ibáñez/Mutti	1	UvA
Early stage dynamics of protein folding	Woutersen/Bolhuis	2.3	UvA
Electrocatalysis of immobilized molecular catalysts for water oxidation	Koper/Reek/Hetterscheid/Tromp	2.3	UL/UvA
Electronic structure calculations on organometallic complexes	Baerends/Lammertsma	1.3	VU
Electronic structure of phosphinidine complexes	Baerends/Lammertsma	1.3	VU
Enzyme cascade reactions	Wever	1	UvA
Ester hydrogenolysis and (de) hydrogenations using first-row transition metals	Elsevier/deBruin/vdVlugt/vMaarseveen	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 Maarseven	1.2	UvA
IR spectroscopy of PAHs	Buma / Rijs / Oomens	2	UvA, RU
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	1.2	UL
Measuring and simulating chemistry in cometary processes	Bickelhaupt/Linnartz	3.2	VU, UL
Mechanism of oxygen-induced long-tissue damage	Bickelhaupt/van Maarseveen	1	VU/UvA
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
PAHs in the laboratory and in space	Buma/Ubachs/Linnartz	2	UVA/VU/UL
Pd-Catalyzed Z-Selective Semihydrogenation of Alkynes: Determining the Type of Active Species	Elsevier/deBruin	1	UvA
Photocatalysis	Brouwer/Reek/Hartl/vdVlugt	1.2	UvA
Photocatalysis	Reek/vdVlugt/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/deBruin	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/vdVlugt/Woutersen	1.2	UvA
Spectroscopy of chiral molecules	Buma/Janssen	2	UvA/VU
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
Use of phosphatases and sulfatases in enantioselective reactions	Wever	1	UvA
Various Synthetic products	Hiemstra/Orru/vMaarseveen	1	UvA/VU
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

2.5 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. In 2016, there have been 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.

Awarded Fellowships – 3rd 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 – 4th 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. Vreede (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.

3. Education and Research Training

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 annually in the study guide on the HRSMC website. The management of the school administers the credit points obtained by the PhD students and presents HRSMC certificates to those students who have fulfilled the Education Programme (see Annex 4.5).

3.1 HRSMC Education Programme

The HRSMC offers PhD students a broad programme of inter-university courses and schools.

HRSMC Courses (2-3 ECTS)

- Molecular Modelling (every two or three years, HRSMC theme 2 and 3)
- Physical Methods in Inorganic Chemistry (biannually, HRSMC theme 1)
- Photophysics, Photochemistry, and Photobiology (every three years, HRSMC theme 2)
- Molecular Simulation (yearly, HRSMC theme 3)
- Synthetic Chemistry problem sessions (HRSMC theme 1)

Character:

- Courses are given at UvA, UL or VU (or in combinations).
- Participants are mostly from HRSMC, a few from other Dutch universities or from Dutch chemical companies. The Molecular Simulation course has a lot of participants from abroad.
- Lecturers are mainly from Holland.

HRSMC Schools (2-3 ECTS)

- Summer School on Photochemistry (every 4 years, HRSMC theme 2)
- Tulip School 'Modern Developments in Spectroscopy' (every 3 years, HRSMC theme 2)
- Summer School 'Synthetic Bio-organic Chemistry' (every 4 years, HRSMC theme 1)
- Autumn School on Metal-organic Chemistry and Catalysis (every 2 years, HRSMC theme 1)

Character:

- More like a conference with lectures, discussion sessions and poster sessions.
- The schools are given at an external location.
- Participants come partly from the HRSMC. Many participants come from other Dutch universities and from abroad.
- Lecturers come mostly from abroad.

Activities of 2016:

- The two weeks HRSMC School *'Molecular Simulation'*, organized under the auspices of CECAM (4-15 January 2016, UvA)
- HRSMC Lab visit at the LaserLaB VU for the UvA/UL groups (22 April 2016)
- HRSMC Course HRSMC Course Molecular Modeling (6-17 June, 2016, VU)
- HRSMC Summer School *'Photochemistry, Fundamentals and Applications'* (27 – 31 August, 2016, Kasteel Vaeshartel, Maastricht)
- HRSMC – HIMS Sustainability workshop (23 September 2016, Amsterdam, WCW Congreszalen)

Details of courses that were specifically developed for the HRSMC by its members were:

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 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 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)

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.

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

Progamme 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

3.2 Symposium

The annual HRMSC Symposium was held at Leiden University on 17 November, 2016. The symposium, which was attended by ca. 190 scientists, also included poster sessions with 40 posters, mainly presented by PhD students. The format of previous symposia was also used for this symposium: less posters (about three posters per group selected by the work group leaders) per session, and more and shorter lectures.

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"

3.3 PhD Graduations (in order of graduation date)

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
Copromotor: Prof. dr. B. de Bruin
March 11, 2016

Wolters, L.P.
Chemical Bonding and Catalysis. Molecular Orbital Perspectives on Catalyst Design and Halogen Bonds
Promotor: Prof. dr. F.M. Bickelhaupt
March 22, 2016

Kolb, M.J.
Water related adsorbates on stepped platinum surfaces
Promotor: Prof. dr. M.T.M. Koper
Co-Promotor: Dr. L.B.F. Juurlink
March 23, 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
April 28, 2016

Torres Knoop, A.
Entropy driven separations in nanoporous materials
Promotor: Prof. dr. E.J. Meijer
Co-promotor: D. Dubbeldam
April 28, 2016

Graaff, C. de
Cascade Reactions with a Twist - Chemoenzymatic Synthesis of Biologically Relevant Heterocycles
Promotor: Prof. dr. ir. R.V.A. Orru
Co-promotor: Dr. E. Ruijter
May 2, 2016

Dijkman, T.F. van
Copper trispyrazolylborate complexes for ethene detection
Promotor: Prof. dr. E. Bouwman
Co-Promotor: Dr. S. Bonnet
May 12, 2016

Broere, D.L.J.
New avenues for redox-active ligands: Non-classical reactivity with late transition metals facilitated by o-aminophenol derived architectures
Promotor: Prof. dr. J.N.H. Reek
Co-promotor: Dr. 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
Co-promotor: Dr. L. Juurlink
June 9, 2016

Boer, S.Y. de
Proton-responsive pyridine-based ligands: Synthesis, coordination chemistry and catalysis
Promotor: Prof. dr. J.N.H. Reek
Co-promotor: J.I. van der Vlugt
June 28, 2016

Liu, X.
Luminescence and applications of lanthanoid coordination polymers
Promotor: Prof. dr. E. Bouwman
Co-Promotor: Dr. S. Bonnet
June 30, 2016

Becker, R.
[FeFe]hydrogenase mimics for proton reduction catalysis: Supramolecular proton reduction catalysts with appended redox-active and proton-responsive ligands towards application in a molecular artificial leaf
Promotor: Prof. dr. J.N.H. Reek
Co-promotor: Dr. J.I. van der Vlugt
September 14, 2016

Jongbloed, L.S.
Fundamental reactivity of the Metal-Carbon bond in cyclometalated PNC-complexes
Promotor: Prof. dr. J.N.H. Reek
Co-promotor: Dr. J.I. van der Vlugt
September 28, 2016

Thomas, B.
Towards artificial photosynthesis: resolving supramolecular packing of artificial antennae chromophores through a hybrid approach
Promotor: Prof. dr. H.J.M. de Groot
Co-promotor: Dr. W.J. de Grip
November 10, 2016

Badan, C.
Surface-structure dependence of water-related adsorbates on platinum
Promotor: Prof. dr. M.T.M. Koper
Co-promotor: Dr. J.B.F. Juurlink
November 22, 2016

Askes, S.H.C.
Upconverting nanovesicles for the activation of ruthenium anti-cancer prodrugs with red light
Promotor: Prof. dr. E. Bouwman
Co-promotor: Dr. S. Bonnet
November 24, 2016

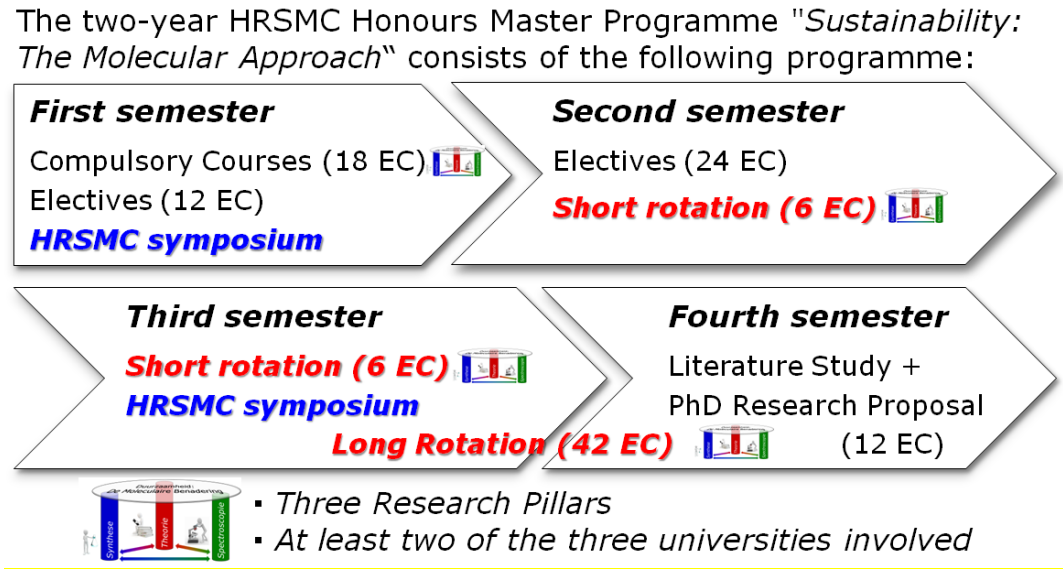
Vreeken, V.
PNP pincer ligands in late transition metal nitrido chemistry and gold catalysis
Promotor: Prof. dr. J.N.H. Reek
Co-promotor: Dr. J.I. van der Vlugt
December 1, 2016

3.4 HRSMC Excellence Master '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. On 31 December 2016, seven MSc students participated in this Excellence Program and three students graduated in the period of August-October 2016.
As mentioned before, in the summer of 2016, the HRSMC has granted one proposal for PhD research written by MSc chemistry student Tessel Bouwens. She was appointed at the University of Amsterdam.

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 Top Master Track (e.g. progress and choice of internships). This special 'Advisory Committee' consists of Dr. Eelco Ruijter (VU), Dr. Sylvestre Bonnet (UL) and Dr. Célia Fonseca Guerra (VU).



On 31 December 2016, seven MSc students participated in this the HRSMC Excellence programme Sustainability, the Molecular Approach", of which two students started in September 2016, four students in September 2015 and one in September 2013.

Selected PhD proposal in HRSMC/NWO excellence programme

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). Tessel Bouwens wrote her proposal as part of the special HRSMC master's programme for talented chemistry students and defended her proposal before a broad panel of experts consisting of Prof. dr. G. van Koten (UU), as external member, as well as HRSMC Board members and the chair of the HRSMC Research Committee. She started her PhD research in November 2016, financed by the Netherlands Organisation for Scientific Research NWO.

The NWO Graduate Programme has stopped recently and there have been no possibilities for the HRSMC to obtain alternative funding to finance PhD positions within the Graduate Programme. As a consequence, the members of the cohort that started in 2016 still have to write their own research proposal in the final stage of this master, but cannot compete directly for PhD positions. However, students that write a high quality research proposal in the final stage of this master are supported by the HRSMC Board to obtain PhD positions from other funding sources, preferentially within the HRSMC but otherwise elsewhere.

Nevertheless, the HRSMC Excellence Master Programme is a unique, challenging programme that is greatly appreciated by potential candidates because of its interdisciplinary and interuniversity aspects. Indeed, former students have encouraged the HRSMC Board to continue with this programme:

"It is hard work but you get a lot in return: more involvement in HRSMC Courses and you get into much closer contact with Research groups during your Master than normally would be the case. It is good for your personal development and networking."

4. Annexes

4.1 Annex 1 - HRSMC Organisation

Organisation Structure
The interuniversity research school HRSMC is a collaboration between the University of Amsterdam (UvA), the Vrije Universiteit Amsterdam (VU), Leiden University (UL) and the Radboud University (RU), as explained in chapter 1.2. The University of Amsterdam legally represents 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

4.2 Annex 2 - Financial Account 2016

Income		**Expenses**	
Contribution UvA 2016 - faculty[1]	150.000	Donation HIMS Institute[1]	150.000
Contribution UvA 2016 - HIMS[1]	150.000	Personnel Costs	69.400
Photochemistry School (fee and sponsoring[2])	44.224	Photochemistry School	51.659
Fellowship (reservation 2016)	11.000	Fellowship Programme	67.125
Fellowship – JvGeuns[2]	10.000	Symposium	7.026
Sustainability Workshop (contribution HIMS en sponsoring) [2]	4.395	Sustainability Workshop	6.025
Molecular Modeling Course	840	Bureau Costs	2.885
Correction 2015	351	Molecular Modeling Course	1.547
Interest	334	PhD activity	2.012
		Board	1.579
		Annual Report 2015	1.226
		Dick Stufkens PhD prize	1.000
		Graduate Programme[3]	676
		Lab Visit VU	632
		Reservation for 2017-2019[4]	8.356
	€ 371.145		**€ 371.145**

Income minus Expenses **€ 0**

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) has become 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 is 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) The HRSMC is grateful to **the John van Geuns foundation** for its financial support for the Photochemistry School, the Sustainability Workshop and the John van Geuns Fellowship.
3) 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.
   Estimation for the personnel costs covered by the HRSMC for the three PhD in 2016:
   € 8.3 kEuro (2/48 x 200 keuro) for Tessel Bouwerns
   € 50 kEuro (12/48 x 200 keuro) for Kaj van Vliet
   € 50 kEuro (12/48 x 200 keuro) for Hans de Bruijn



John van Geuns foundation

These costs (in total approx. **108.3 kEuro**) are compensated by the NWO grant of **800 kEuro**.

4) Reservation for the Fellowship Programme and the HRSMC Lustrum Symposium.

4.3 Annex 3 - Staff and Temporary Personnel 2016

Theme 1

Biocatalysis	Wever		R.	Emeritus		
	Mutti		F.	HGL		
	Knaus		T.	PD	01/01/15	01/01/19
	Böhmer		W.	PhD	01/09/15	01/09/19
	Tseliou		V.	PhD	01/10/15	01/10/19
	Vilim		J.	PhD	01/10/15	01/10/19
	Pham		L.C.	OBP		
Organic and Peptide Chemistry	Grossmann		T.N.	HGL		
Metals in Catalysis, Biomimetics and Inorganic Materials	Drent		E.	Emeritus	01/09/10	31/12/99
	Reedijk		J.	Emeritus	01/11/09	31/12/99
	Bouwman		E.	HGL	01/04/10	31/12/99
	Bonnet		S.B.	Tenure Tracker	01/10/09	31/12/99
	Hetterscheid		D.G.H.	Tenure Tracker	01/02/13	01/02/17
	Higgins		S.L.H.	PD	01/09/13	31/12/16
	Siewert		B.	PD	01/09/13	31/12/16
	Askes		S.H.C.	PhD	01/10/12	01/10/16
	Bruijn	de	H.	PhD	01/11/15	01/11/19
	Busemann		A.	PhD	08/12/14	08/12/18
	Cuello-Garibo			PhD	17/06/13	17/06/17
	Geest	van	E.	PhD	01/09/15	01/09/19
	Gezer		G.	PhD	15/07/13	15/10/17
	Jiang		F.	PhD	01/04/14	01/04/18
	Kottrup		K.	PhD	01/07/13	01/07/17
	Lameijer		L.N.	PhD	01/07/13	01/07/17
	Langerman			PhD	01/01/15	01/01/19
	Liu		X.	PhD	21/09/12	21/09/16
	Luo		S.	PhD	01/09/13	01/09/17
	Meijer		M.S.	PhD	01/01/14	01/01/16
	Rixel	van	V.	PhD	01/02/13	01/02/17
	Sk		A.	PhD	01/05/15	01/05/19
	Smits		N.	PhD	01/01/16	01/01/20
	Snellenberg		Y	SECR	15/09/81	31/12/99
Biophysical Organic Chemistry	Groot	de	H.J.M.	HGL		
	Alia		A.	UD		
	Buda		F.	UD		
	Ganapathy		S.	PD	15/05/12	31/10/17

	Sevink		G.J.A.	UHD		
	Thomas		B.	PD	31/01/12	16/07/16
	Augustijn		D.	PhD	01/08/14	31/07/18
	Roy		U.	PhD	01/01/12	31/01/16
	Ruiter	de	J.M.	PhD	01/09/13	31/05/18
	Schadewijk	van	R.	PhD	01/02/14	31/01/18
	Sun		Z.	PhD	02/09/14	31/08/18
	Menzel		J.P.	PhD	31/05/18	31/05/18
	Sai sankar Gupta		K.B.	OBP		
	Shao		Y.	PhD	13/09/16	31/08/20
	Velden	van der	E.	SECR		
Heterogeneous Catalysis And Sustainable Chemistry	Rothenberg		H.G.	HGL		
	Yan		N	Tenure Tracker		
	Grecea-Tanase		S.	UD		
	Shiju		N.R.	UD		
	Guo		Z.	PhD	01/01/15	01/01/19
	Narani		D.	PD	01/06/15	31/05/16
	Pandey		J.	PD	01/07/15	30/06/16
	Prinsen		P.L.K.	PD	01/02/14	31/01/16
	Solomon Raja		E.G.K.	PD	01/07/14	30/06/16
	Eisenberg		D.	PhD	01/01/15	01/01/19
	Gao		Y.	PhD	01/01/14	01/01/18
	Gheorghe		A.	PhD	01/01/16	01/01/20
	Rees		L.	PhD	01/01/15	01/01/19
	Ronda Lloret		M.	PhD	01/01/17	01/01/21
	Tang		Y.	PhD	01/10/15	01/10/19
	Zhang		W.	PhD	01/10/15	01/10/19
	Collignon		P.F.	OBP		
	Mittelmeijer-Hazeleger		M.	OBP		
Homogeneous, Supramolecular Catalysis and Spectro-electrochemistry	Bruin	de	B.	HGL		
	Reek		J.N.H.	HGL		
	Zwaan	van der	B.	HGL-BZ		
	Tromp		M.	Tenure Tracker		
	Vlugt	van der	J.I.	UHD		
	Hartl		F.	Guest	01/04/05	31/12/99

Becker		R.	PD	01/03/16	15/04/17
Bheeter		C.B.	PD	01/09/16	01/09/18
Das		B.G.	PD	01/07/15	30/06/16
Detz		R.J.	PD	01/09/12	01/09/16
Devillard		M.	PhD	01/01/15	01/01/19
Dzik		W.I.	PD	01/11/11	01/05/17
Gonell Gomez		S.	PD	01/05/15	30/04/16
Jongbloed		L.S.	PD	01/10/16	01/01/17
Kluwer		A.M.	PD Guest	01/01/09	01/01/18
Koelewijn		J.M.	PD	01/02/16	02/05/16
Mathew		S.	PD	01/09/15	01/09/16
Raoufmoghaddam		S.	PD	01/02/14	01/02/16
Wang		X.	PD	01/05/14	01/11/16
Bagh		B.	PhD	01/01/15	01/01/19
Bai		S.	PhD	01/09/15	01/09/19
Becker		R.	PhD	01/03/12	01/03/16
Boer	de	S.Y.	PhD	15/08/15	28/06/16
Bouwens		T.	PhD	01/11/16	01/11/20
Broere		D.L.J.	PhD	15/05/12	07/06/16
Chirila		A.	PhD	01/09/12	01/09/16
Coskuner		B.	PhD Guest	01/01/12	01/01/16
Daubignard		J.J.M.	PhD Guest	01/01/15	01/01/16
Goswami		M.	PhD	01/08/13	01/09/17
Hartendorp		A.P.T.	PhD	01/09/15	01/09/19
Heim		L.	PhD Guest	01/10/16	01/12/16
Hessels		J.	PhD	01/10/15	01/10/19
Jongbloed		L.S.	PhD	15/02/12	01/10/16
Jongkind		L.J.	PhD	01/09/14	01/09/18
Karns		A.S.	PhD Guest	15/09/16	15/12/16
Kuijpers		P.F.	PhD	01/10/12	01/03/17
La Rosa		A.	PD	01/01/16	15/04/16
Leest	van	K.	PhD	01/09/16	01/09/20
Linnebank		P.R.	PhD	15/02/16	15/02/20
Martin		D.J.	PD	01/10/15	01/10/16
Mooibroek		T.J.	PhD	01/06/16	01/08/21
Mouarrawais		V.	PhD	01/02/16	01/02/20
Nurttila		S.S.	PhD	01/06/14	01/06/18
Oudsen		J.P.H.	PhD	01/09/15	01/09/19
Plessius		R.	PhD	01/10/15	01/10/19
Poole		D.A.	PhD Guest	01/10/16	01/08/17
Rebreyend		C.	PhD	01/08/13	01/08/17
Schippers		E.C.F.	PhD	01/11/13	01/11/17
Sun		B.	PhD	01/10/15	01/10/19
Te Grotenhuis		C.	PhD	01/08/13	01/08/17
Venderbosch		B.	PhD	01/11/15	01/11/19
Vreeken		V.	PhD	01/05/12	01/12/16
Watering	van de	F.F.	PhD	01/11/12	01/02/17
Zaffaroni		R.	PhD	01/12/12	01/12/16

	Abiri		Z.	OBP Guest		
	Ait El Maate		F.	OBP		
	Burg	van den	A.M.	OBP		
	Duin-Berteling		E.	OBP		
	Ernsting		J.M.	OBP		
	Geels		N.J.	OBP		
	Mahabiersing		C.	OBP		
	Tromp		D.S.	OBP		
Molecular Inorganic Chemistry	Vrieze		K.	Emeritus		
	Elsevier		C.J.	HGL		
	Gruter		G.J.M.	HGL-BZ		
	Oskam		A.	Emeritus		
Organic and Organometallic Chemistry	Lammertsma		K.	Emeritus		
	Ehlers		A.W.	UD		
	Borger		J.E.	PhD	15/12/13	15/12/16
	Habraken		E.R.M.	PhD	15/12/14	15/12/18
	Krachko		T.	PhD	01/09/13	01/09/17
	Nicolas		E.C.	PhD	01/08/13	01/08/16
Synthetic & Bio-organic Chemistry	Orru		R.V.A.	HGL		
	Ruijter		E.	UD		
	Braun		J.	PhD	11/11/14	11/11/18
	Cioc		R.	PhD	15/11/12	15/11/16
	Collet		J.	PhD	01/01/15	01/01/19
	Estévez Closas		V.	PD	01/05/13	01/05/17
	Heijden	van der	G.	PhD	01/11/12	01/11/16
	Mampuys		P.	PhD Guest	01/09/13	01/09/17
	Saya		J.M.	PhD	01/12/14	01/12/18
	Vicente Garcia		E.	PD	01/03/13	01/03/17
	Janssen		A.C.	OBP		
Synthetic Organic Chemistry	Hiemstra		H.	HGL		
	Maarseveen	van	J.H.	HGL		
	Timmerman		P.	HGL-BZ		
	Fernández-Ibáñez		M.A.	Tenure Tracker		
	Ingemann Jørgensen		S.	UHD		
	Slootweg		J.C.	UHD		
	Alvarez Casao		Y.	PD	01/10/16	01/03/18
	Gajewski		P.	PD	01/04/16	01/04/17
	Steemers		L.	PD	01/09/16	01/09/18
	Valderas Cortina		C.	PD	01/05/15	01/11/16

	Boom		D.H.A.	PhD	01/11/16	01/11/17
	Botez		L.	PhD Guest	01/11/16	01/08/17
	Holtrop		F.	PhD	01/11/16	01/09/19
	Jia		W.L.	PhD	01/01/16	01/10/20
	Naksomboon		K.	PhD	01/09/15	01/09/19
	Richelle		G.J.J.	PhD	01/11/13	01/11/17
	Schmidt		M.	PhD Guest	15/09/16	15/09/20
	Streefkerk		D.E.	PhD	01/06/14	01/06/18
	Wijsman		L.	PhD	01/09/15	28/02/19
	Bieraugel		H.	OBP Guest	01/03/14	01/09/16
	Boer	de	M.A.	OBP		01/02/17
	Jong	de	G.B.	OBP		01/02/17
	Klein Nijenhuis		R.A.	OBP		
	Wanner		M.J.	OBP		
	Zuidinga		E.	OBP		
	Rutjes		F.P.J.T.	HGL		
Theme 2						
Biophotonics & Medical Imaging	Ariese		F.	UHD		
	Mooij		B.	PhD	01/10/15	01/10/19
	Zada		L.	PhD	01/11/14	01/11/18
Laboratory Astrophysics and Astrochemistry	Linnartz		H.V.J.	HGL		
	Doney		K.D.	PhD	07/01/14	30/06/18
Molecular Nano-optics and Spin	Groenen		E.J.J.	HGL		
	Orrit		M.	HGL		
	Gast		P.	UD		
	Huber		M.	UD		
	Caldarola		M.	PhD	01/01/15	01/01/19
	Carattino		A.	PhD	01/02/13	01/02/16
	Hou		L.	PhD	15/08/12	15/08/16
	Kumar		P.	PhD	15/06/12	15/06/16
	Nami		F.	PhD	01/03/12	01/03/16
	Panarelli		E.G.	PhD	01/09/13	01/06/18
	Pradhan		B.	PhD	01/02/14	31/01/18
	Verhart		N.R.	PhD	09/07/12	09/07/16
	Zhang		W.	PhD	01/09/14	31/08/18
	Zurlo		E.	PhD	01/02/15	31/01/19
	Leeuwen		H.C.M.	SECR		
Molecular Photonics	Schenk		H.	Emeritus		
	Verhoeven		J.W.	Emeritus		
	Aalders		M.C.G.	HGL BZ		
	Brouwer		A.M.	HGL		
	Buma		W.J.	HGL		

		Oomens		J.	HGL-BZ	
		Woutersen		S.	HGL-BZ	
		Zhang		H.	UHD	
		Williams		R.M.	UD	
		Bakker		J.M.	Guest	01/01/94	31/12/99
		Bloem		R.	PD	03/07/15	01/07/16
		Castellanos Ortega		S.	PD Guest	01/02/16	01/02/18
		Ijgosse-Werner		C.T.M.	PD Guest	16/09/16	16/06/17
		Nicu		V.P.	PD	01/06/15	01/06/19
		Petrignani		A.	PD	01/03/16	01/03/21
		Roeterdink		W.G.	PD	01/05/16	01/05/18
		Shen		S.	PD	01/05/15	01/05/16
		Song		L.T.	PD	01/07/16	01/07/17
		Chen		H.C.	PhD Guest	01/09/11	01/02/16
		Cota		R.O.	PhD	01/06/15	01/06/19
		Feng		Y.	PhD	01/03/16	01/03/20
		Gutierrez Cota		R.O.	PhD	01/06/15	01/06/19
		Haitjema		J.	PhD	15/09/15	15/09/19
		Jing		P.	PhD	01/08/15	01/01/16
		Koenis		M.A.J.	PhD	01/09/15	01/09/19
		Lugier		O.C.M.	PhD Guest	10/02/16	01/11/20
		Maltseva		E.O.	PhD Guest	01/08/12	01/11/17
		Petrova		D.	PhD	01/04/15	01/04/19
		Raeisolsadati Oskouei		M.	PhD Guest	01/10/15	01/02/17
		Rocha Martins		B.M.	PhD	01/11/14	01/11/18
		Roeters		S.J.	PhD Guest	15/10/11	01/12/17
		Suhina		T.	PhD	01/09/12	01/09/16
		Wiersma		S.D.	PhD	01/01/16	01/09/20
		Wu		L.	PhD Guest	16/09/16	16/09/20
		Wu		Y.	PhD	01/09/16	01/09/20
		Zhang		Y.	PhD	01/01/15	01/01/19
		Zheng		D.	PhD	01/09/14	01/09/18
		Bakker		B.H.	OBP	
		Bebelaar		D.	OBP	
		Groeneveld		M.M.	OBP Guest	01/05/14	01/05/16
		Hilbers		M.F.	OBP	
		Ramesdonk	van	H.J.	OBP Guest	01/04/08	01/04/16
		Reinders		P.P.	OBP	
		Sanders		H.J.	OBP	
	Molecular Structure and Dynamics - FELIX / Molecular and Biophysics	Oomens		J.H.	HGL	
		Bakker		J.	UD	
		Rijs		A.M.	UD	
2	Surface Chemistry	Kleijn		A.W.	HGL-BZ	

and Catalysis

Koper		M.T.M.	HGL		
Groot		I.M.N.	Tenure Tracker		
Hetterscheid		D.G.H.	Tenure Tracker		
Fu		W.T.	UHD		
Juurlink		L.B.F.	UHD		
Bondü		C.J.	PD	04/07/16	03/07/17
Calle Vallejo		F.	PD	01/04/15	30/03/18
Deng		X.	PD	22/09/16	21/09/17
Feng		J.	PD	18/04/16	17/04/17
Figueiredo		M.C.	PD	01/11/14	30/04/17
Göttle		A.J.	PD	01/09/14	14/03/17
Huang		Y.	PD	16/10/13	31/03/17
Walsh		A.J.	PD	01/06/14	17-8-2016
Aranzalas Ochoa		D.M.	PhD	01/08/16	31/07/20
Auras		S.	PhD	15/12/15	15/12/19
Badan		C.	PhD	16/07/12	31/07/17
Birdja		Y.Y.	PhD	16/12/13	15/12/17
Bremmer		G.M.	PhD	01/10/13	30/09/17
Cao		K.	PhD	01/09/14	31/08/18
Chen		X.	PhD	01/09/15	31/08/19
D'Agostini		S.	PhD	01/12/14	30/11/18
Diaz Morales		O.A.	PhD	01/06/11	31/08/16
Dijk	van	B.	PhD	01/01/16	31/12/20
Fuchs		Y.D.E.	PhD	01/01/17	31/12/20
Granda Marulanda		L.P.	PhD	01/01/17	31/12/20
Ham	van der	C.J.M.	PhD	01/09/13	31/08/17
Hersbach		T.J.P.	PhD	01/10/14	30/09/18
Jacobse		L.	PhD	16/09/13	16/09/17
Kolb		M.J.	PhD	01/01/12	01/05/16
Ledezma Yanez		I.D.	PhD	28/11/11	31/05/16
Lent	van	R.	PhD	01/05/14	30/04/18
Mom		R.	PhD	01/01/13	31/12/16
Perez Gallent		E.	PhD	16/11/13	15/11/17
Plas	van der	M.	PhD	22/04/14	23/04/18
Prabhu		M.K.	PhD	15/06/16	16/06/17
Raaijman		S.J.	PhD	01/01/17	31/12/20
Rossius		S.G.H.	PhD	01/11/11	30/11/16
Spronsen		M.	PhD	01/01/12	31/03/16
Vos		J.	PhD	01/05/15	30/04/19

		Wenzel	S.	PhD	01/02/17	31/01/21
		Dijkzeul	J.C.M.	SECR		
Theme 3						
3	Computational Chemistry	Bolhuis	P.G.	HGL		
		Meijer	E.J.	HGL		
		Dubbeldam	D.	UD		
		Ensing	B.	UHD		
		Lowe	C.P.	UHD		
		Riccardi	E.	Guest	01/12/16	01/03/17
		Vreede	J.	UHD		
		Ni	R.	PD	01/09/12	31/08/17
		Perez de Alba Ortiz	A.	PD Guest	01/12/16	01/03/17
		Rudavskyi	A.	PD	01/10/15	01/10/16
		Sun	D.	PD	21/10/13	21/04/17
		Swenson	D.W. H.	PD	01/03/16	01/03/18
		Tu	L.	PD Guest	01/09/16	01/02/17
		Yaghini, N.	N.	PD Guest	15/04/15	01/05/16
		Arjun	A.	PhD	01/07/16	01/07/20
		Brotzakis	Z.F.	PhD	01/09/12	01/09/16
		Dong	Ch.	PhD	01/09/16	01/09/17
		Govindarajan	N.	PhD	15/02/16	14/02/20
		Heinen	J.	PhD	01/09/14	31/08/18
		Homsi Brandeburgo	W.H.	PhD Guest	15/07/15	01/07/17
		Meyer de	T.R.	PhD Guest	01/09/15	01/01/16
		Newton	A.C.	PhD	15/04/12	15/10/16
		Putenkhalathil	R.C.	PhD	01/04/16	31-04-20
		Rodriguez-Gomez	S.	PhD Guest	01/05/16	01/07/16
		Tiwari	A.	PhD	01/01/15	01/01/19
		Torres Knoop	A.	PhD	01/03/12	28/04/16
		Vijaykumar	A.	PhD Guest	01/06/13	01/06/17
		Groot de	L.K.	OBP		
		Spoelstra	S.E.	OBP		
		Kumar	A.	PhD	01/09/10	31/01/16
3	Theoretical Chemistry RU	Groenenboom	G.C.	HGL		
		Cuppen	H.	UHD		
3	Theoretical Chemistry UL	Meyer	J.	HGL		
		Nattino	F.	PD	01/01/15	01/11/19
		Rasti	S.	PhD	01/01/16	31/12/20
		Seal	S.	PhD	01/01/16	01/01/20
		Spiering	P.	PhD	01/09/15	01/09/19
3	Theoretical Chemistry VU/EMS	Baerends	E.J.	Emeritus		

	Bickelhaupt		F.M.	HGL		
	Gori Giorgi		P.	HGL		
	Visscher		L.	HGL		
	Fonseca Guerra		C.	UHD		
	Gritsenko		O.V.	UD		
	Infante		I. A. C.	UD		
	Cosseddu		S.M.	PD	01/02/15	01/02/17
	Giesbertz		K.J.H.	PD	09/01/12	09/01/18
	Lani		G.	PD	01/04/13	01/04/16
	Malet Giralt		F.	PD	01/03/12	01/06/16
	Paragi		G.T.	PD	01/05/13	01/02/16
	Boughlala		Z.	PhD	01/08/13	01/08/17
	Cózar Ruano	de	A.	PD	01/09/15	01/09/17
	Franchini		M.	PhD	01/01/14	01/01/16
	Gangarapu		S.	PhD	01/01/15	01/01/19
	Grossi		J.	PhD	01/09/15	01/09/19
	Gvozdetsky		E.	PhD	01/09/16	01/09/20
	Handzik		M.	PhD	01/01/15	01/01/19
	Hernandez Fernandez		F.	PhD	01/01/16	01/06/16
	Juliaci Rocha		M.V.	PhD	01/01/15	01/01/19
	López-Tarifa		P.	PhD	01/01/15	01/01/19
	Lubbe	van der	S.	PhD	01/01/16	31/12/20
	Narsaria		A.K.	PhD	01/07/16	01/07/19
	Rüger		R.	PhD	01/01/15	01/01/19
	Sun		X	PhD	01/11/14	01/11/18
	Vuckovic		S.	PhD	01/01/13	01/01/17
	Zaccaria		F.	PhD	01/09/14	01/09/18
	Zapata		F.	PhD	01/01/15	01/01/19
Graduate Programme "Sustainability, the Molecular Approach”	Doorn	van	I.	Excellence Master Student	01/01/15	01/01/17
	Modder		D.	Excellence Masterstudent	01/09/16	01/09/18
	Schaap		I.L.	Excellence Master Student	01/10/13	01/10/17
	Venne		M.	Excellence Master Student	01/09/13	01/09/16
	Zwart	de	F.	Excellence Masterstudent	01/09/16	01/09/18
	Bouwens		T.	Excellence Master	01/01/14	01/01/19
	Heuvel	van de	N.	Excellence	01/09/15	01/09/17

	Keijer		T.	Master Student Excellence	01/09/15	01/09/17
	Klein		D.	Master student Excellence	01/09/15	31/12/19
	Landman		I.	Master Student Excellence	01/01/14	03/01/17
	Opdam		L.	Master Student Excellence	01/09/15	01/09/17
	Stroek		W.	Master Excellence	01/09/16	01/09/18
HRSMC Office	Weijer		R.	SECR		
	Zwaan-van der Plas		H.E.	OBP		
Scientific Advisory Board	Baerends		E.J.			
	Hage		R.			
	Reedijk		J.			
	Verhoeven		J.W.			
	Vogt		E.			
	Vries	de	J.G.			

4.4 Annex 4 – The HRSMC Education Programme

The management of the school administers the credit points obtained by the PhD students and 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
- When the following Courses and Schools were followed with a validation of 3 EC according to the old rating (instead of 2 according to the new validation):
  - HRSMC Course: Physical Methods in Inorganic Chemistry (2011, 2013)
  - HRSMC Summer School on Photochemistry (2012)
  - HRSMC Tulip School 'Modern Developments in Spectroscopy' (2012)
  - HRSMC Summer School Synthetic Bio-organic Chemistry (2013)
  - HRSMC Autumn School Advanced Metal-Organic Chemistry (2012)

For each of these Courses with a validation of 3 EC instead of 2, one extra EC should be done for the total ECs for the certificate.
E.g. if you have followed the 2012 Tulip School for 3 EC, you should have 16 ECs in total.

15 points is a minimum and can, of course, be exceeded.

4.5 Annex 5 - Major specialised equipment / expertise

Group	Equipment
Biocatalysis (UvA, HIMS) Dr. F. Mutti	2 UV-VIS spectrophotometers with thermostate.
	3 Medium speed centrifuges (up to 18000 rpm)
	2 HPLC systems (one autosampler).
	1 Akta purifier (LC for protein purification)
	1 Laminar Flow cabinet.
	2 GC-FID with hydrogen generator
	1 GC-MS
	1 high-capacity glove-box for biochemistry and bioorganic chemistry in anoxic conditions
	2 PCR machines
	1 nanospectrophotometer
	1 Gel Doc EZ Imaging System (for rapid visualization of protein and DNA electrophoresis gels)
	Various equipment for protein and DNA electrophoresis
	5 incubators for cultivation of microbial cultures
	1 sonication system for cell membrane disruption
	1 freeze-dryer
Heterogeneous Catalysis and Sustainable Chemistry (UvA, HIMS) Prof. dr.G. Rothenberg[1], Dr. S. Grecea, Dr. N.R. Shiju, Dr. N. Yan	Rigaku Miniflex powder X-ray diffractometer Cu-Kα source (range 5°-50°).
	Varian 660 FTIR spectrometer (4000-400 cm^{-1}) equipped with a Gladi ATR device.
	STA 449 F3 Jupiter® (NETZSCH Instrument) unit calorimetry for TGA and DSC.
	Thermo Scientific Surfer instrument for nitrogen adsorption measurements.
Homogeneous, Supramolecular and Bio-Inspired Catalysis (UvA, HIMS) Prof. Dr. B. De Bruin[1], Prof. Dr. J.N.H. Reek[1], Prof. dr. C.J. Elsevier, Dr. T.J. Mooibroek, Dr. M. Tromp, Dr. Ir. J.I. van der Vlugt	Thermonicolet NXR 9650 FT-Raman spectrometer and Renishaw inVia dispersive Raman microscope equipped with several UV and visible laser sources
	Varian Cary Eclipse spectrofluorimeter with a multi-cell temperature control unit, a stopped-flow module with rapid mixing (8 ms) and fibre optics dip probe for in situ measurements.
	Optically transparent and reflection spectro-electrochemical cells (UV-VIS-NIR-MIR-FIR, Raman, ECL, VCD, 2D-IR (no laser light scattering) and (bi)potentiostats-galvanostats (EG&G PAR, Ametek, Eco-Chemie, EKOM). RRDE.
	Vacuum-tight three-electrode tubular EPR spectroelectrochemical cell.
	UV-Vis-NIR-IR-FIR spectro(photo)meters (Bruker Vertex 70v, Nicolet, Varian, Perkin Elmer)
	Perkin Elmer 100 FTIR spectrometer interfaced to a

	Spotlight 400 imaging system (special resolution down to 10 microns); an ATR attachment and Atmospheric Vapour Compensation (AVC)
	Diode-array UV-Vis spectrophotometers (HP and Scinco S3100)
	EPR spectrometer (Bruker EMX plus) at X-band, equipped with He-temp control system.
	Time resolved Circular-dichroism/Uv-vis spectrometer with stop-flow equipment
	CHemspeed robot
	Amtec robot for parallel reaction and gas-uptake profiling for kinetics.
	Stopped flow system SFM400/QS (Biologic, Grenoble, France) with an optical fibre UV-visible spectrometer (MCS–UV–VIS–NIR 1/500-3 Fast Diode Array Detector, BioLogic, France).
	Potentiostat and electrochemical cell (BioLogic, France)
	UV-Vis probe (USB4000, Ocean Optics, Netherlands)
	Diverse custom designed X-ray Absorption spectroscopy cells and set-ups for operando hetero-, homo- and electrocatalysis (incl. battery and fuel cells)
	Lab-based X-ray Absorbtion and Emission Spectrometer
Metals in Catalysis, Biomimetics & Inorganic Materials (UL, LIC) Prof. dr. E. Bouwman[1], Dr. S. Bonnet, Dr. D. Hetterscheid	ICP-OES for metal trace analysis
	Electrochemistry: computer-aided Autolab PGstat 10 potentiostat controlled by GPES4 software and connected to a GC for quantitative analysis of O2 or H2.
	IR ATR probe Bruker for in situ IR spectroscopic measurements in solution, 500-2500 cm-1
	PDT lasers (630 nm/2 W, 800 nm/5 W, 980 nm/5 W)
	Cell light irradiation setup under controlled atmosphere for PDT (455 nm, 528, 617 nm, 50-150 mW)
	UV-vis probe Avantes for in situ UV-vis spectroscopic measurements in solution, 300-1100 nm
	Avantes integrating sphere for UV-Vis diffuse reflectance and absolute luminescence or upconversion quantum yield determination
	Electrochemistry: two computer controlled Autolab PGstat potentiostats controlled by NOVA 2.0 software and equipped with a Pine RRDE setup and and EQCM module
	Bruker Tensor 27 infrared spectrometer with probe for in situ IR determination
Organic and Organometallic Chemistry (VU, EMS) Dr. A.W. Ehlers, Dr.	32-node Linux cluster.
	250, 400 and 500 MHz NMR equipped with cryoprobes.
	Advanced LC and LC-MS machines including preparative LC-MS.
	Bruker Daltonics MicroQTOF MS.

J.C. Slootweg	FT-IR.
	Parallel synthesis equipment, microwave synthesizer, ozonolysis, gloveboxes and other standard synthesis equipment.
Organic and Peptide Chemistry (VU, EMS) Prof. dr. T.N. Grossmann	LC and LC-MS machines including semi-preparative
	Plate reader (including fluorescence polarization readout)
	250, 400 and 500 MHz NMR equipped with cryoprobes
	Equipment required for heterologous protein expression and protein purification (incubators, FPLC, fluidizer)
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	Several analytical HPLC instruments and one preparative HPLC instrument.
	LC-MS instrument. GC instrument.
	Polarimeter.
	Usual equipment for synthetic (organic) research, including ozonolysis apparatus and photochemical equipment.
	NMR narrow bore spectrometers frequency range (1H) 400 - 500 MHz.
	FT IR instrument.
	Prelude™ Parallel Fully Automated Peptide synthesizer
	Freeze dryer.
Biomolecular Spectroscopy (VU, EMS) Dr. F. Ariese	Picosecond time-resolved Raman spectrometer with gated ICCD detection.
	High-resolution low-temperature (5 K) fluorescence spectrometer.
	Raman microscope with 532 and 785 nm excitation.
	Raman microscope with 413 and 514 nm excitation and electrochemical cells.
	Stimulated Raman Scattering microscopy
	AFM+SNOM setup
Biophysical Organic Chemistry (UL, LIC) Prof. dr. H.J.M. de Groot, Dr. Alia, Dr. F. Buda, Dr. G.J.A. Sevink	High and Ultra High Field Magic Angle Spinning NMR Spectrometer 400MHz. 600 MHz, 759 MHz.
	Magnetic Resonance Microscopy at 750 MHz, 400 MHz.
	The group owns a Beowulfcluster with 144 cores in total.
Raymond and Beverly Sackler Laboratory Astrophysics and Astrochemistry (UL,	UHV and cryogenic (10K) equipment
	FTIR-RAIRS and TPD-QMS detection
	Atom sources
	Supersonic plasma facilities
	Cavity enhanced and spectrometric (QMS, TOF Ion trap)

LION) Prof. dr. H. Linnartz	detection techniques
	High resolution IR and UV/VIS lasers
	UHV and cryogenic (10K) equipment
	FTIR-RAIRS and TPD-QMS detection
Molecular Structure and Dynamics – FELIX/Molecular and Biophysics (RU) Prof. dr. J. Oomens, Dr. J.M. Bakker, Dr. A.M. Rijs	Molecular beam time-of-flight mass spectrometer equipped with laser desorption source (2x)
	Nanosecond Nd;YAG laser to pumpdye lasers (3x)
	ArF excimer laser (193 nm)
	Bruker ion trap modified for ion spectroscopy
	FTICR-MS with optical access
	CO2 laser
	Tunable IR OPO
	FELIX free electron aser
Molecular Nano-Optics and Spins (UL, LION) Prof. dr. E.J.J. Groenen, Prof. dr. M. Orrit, Dr. P. Gast, Dr. M. I. Huber	cw/pulsed EPR/ENDOR spectrometers at 9, 95, and 275 GHz for experiments on solutions, powders and crystals in the temperature range of 2 to 300 K.
	Single-molecule microscopes equipped with: liquid-helium cryostats, single-frequency lasers (dye and titanium-sapphire), tunable pulsed (200 fs) laser with high repetition rate (70 MHz) and OPO with intracavity doubling, sensitive photon detectors, CCD. Optical trap with fiber laser, 5 W 1064 nm for single gold nanoparticles.
	Absorption, fluorescence and fluorescence excitation spectrometers for experiments from 0.3 to 300 K.
	Confocal microscope for simultaneous photothermal and fluorescence imaging.
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 (Radboud University)	
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. Juurlink	
Computational Chemistry (UvA,	Compute facility consisting of Clusters of Linux PCs with in total ca 2000 cores.

HIMS) Prof. dr. P.G. Bolhuis, Prof. dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede	Performance ca. 10TFLOP. The facility consists of two parts, one maintained and by the computational chemistry group at the UvA and a second part that is maintained by the ACMM, together with associated groups.
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	Compute servers consisting of Clusters of Linux Workstations.
Theoretical Chemistry (UL, LIC) Dr. J. Meyer	Linux-based compute cluster for shared use within the group with several first-principles codes (including proper licenses) available
Theoretical Chemistry (RU) Prof. dr. ir. G.C. Groenenboom	