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1. General

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 2017. 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 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.



Prof. dr. Wybren Jan Buma
Scientific Director of the HRSMC

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 2017, nineteen 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 2017, the HRSMC has granted one proposal for PhD research written by MSc chemistry student David Klein. He was appointed at the Leiden University.

The success of this strategy, activities and efforts lead to the following results in 2017:

- ✦ On December 31 2017, **76** staff members and **163** PhD students participated in the School. Together with postdocs, technical support, and others involved in the organisation, the HRSMC had about **345** members.
- ✦ A total of **32** PhD theses have been published within the HRSMC (see chapter 3.3).
- ✦ The annual Dick Stufkens Prize was awarded to Dr. Sven Askes (UL) for the most outstanding PhD thesis within the HRSMC.
- ✦ **19** students participated in the HRSMC-NWO Excellence Master programme '*Sustainability: the Molecular Approach*'
- ✦ In 2017 the following UvA/VU/UL groups or staff members joined the HRSMC:
 - the Hybrid Solar Energy Conversion research group of Dr. E.L. von Hauff (VU),
 - the Biomolecular Simulation and Modeling group of Dr. D.P. Geerke (VU),
 - Dr. S. Castellanos Ortega (guest appointment UvA; ARCNL) within the Molecular Photonics group (UvA).

while from the RU the following groups or staff members became associated members:

- the Synthetic Organic Chemistry group of Prof. dr. F.P.T.J. Rutjes, Dr. T.J. Boltje, Dr. M.C. Feiters and Dr. J. Mecinovic,
- Prof. dr. H.M. Cuppen within the Theoretical Chemistry group.
- ✦ In 2017 the HRSMC has organised:
 - two Schools with in total **145** participants, including **83** participants from foreign or other Dutch universities, **28** MSc students and **9** industrial participants,
 - four Courses with in total **74** participants,
 - the annual HRSMC Symposium with \pm **190** attendants.
- ✦ In 2017, 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 David Klein has been appointed at the UL (three other PhD students were already appointed in 2015 and 2016),
 - **9** Fellowship applications within the HRSMC Fellowship Programme (€ 37.625), of which one is the special John van Geuns Fellowship under auspices of the HRSMC.

The HRSMC is grateful to the John van Geuns foundation for its financial support for the 'Organic Synthesis' Summer School and the John van Geuns Fellowship.

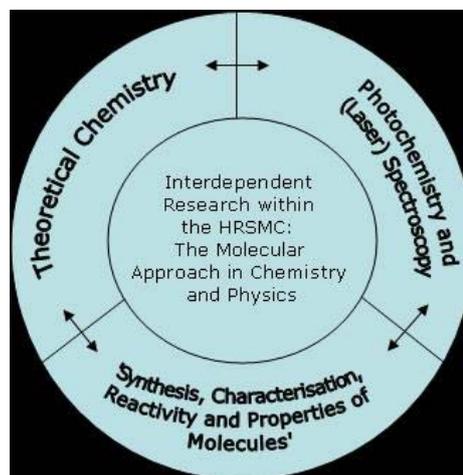
With its broad educational activities and graduate and fellowship programmes, the HRSMC offers an excellent platform for interuniversity and multidisciplinary cooperation, as well as an incentive for worldclass education and research in molecular chemistry and physics.

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. 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 SEP evaluations 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 2017, 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).

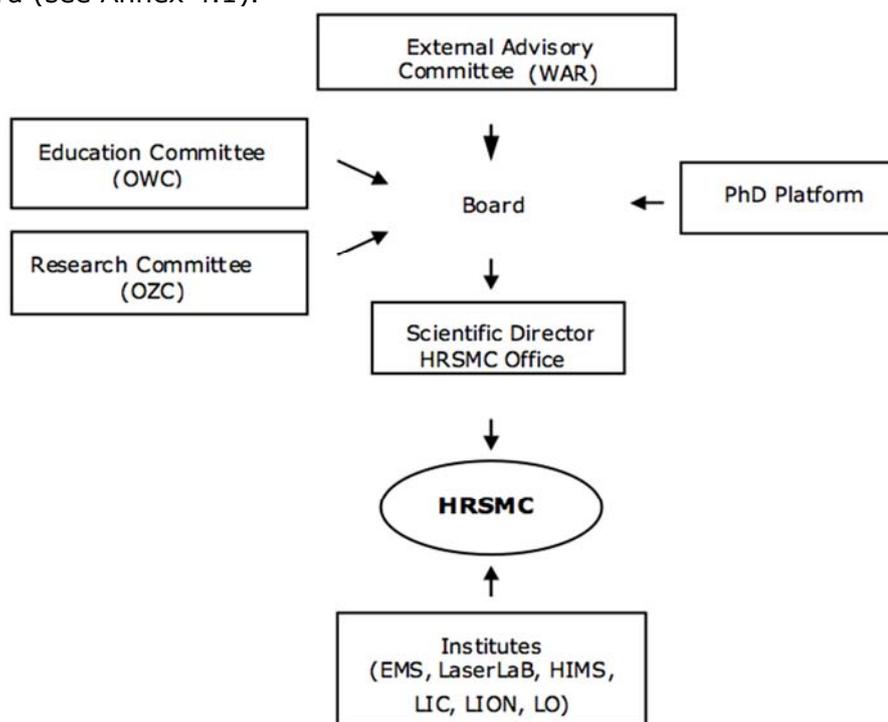


Figure 1.1 Schematic organisation of the HRSMC

The organisation of the HRSMC is schematically depicted in Fig. 1.1. On December 31 2017, 76 staff members and 163 PhD students participated in the School. Together with postdocs, technical support, and others involved in the organisation, the HRSMC had about 345 members.

1.3 General Activities and Highlights of 2017

In 2017, 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 HRSMC Symposium was held at the Amsterdam Science Park Congress Centre on 16 November, 2017. Besides the guest lecture of Prof. dr. ir. René Janssen (TU/e), there were lectures of five PhD students and three lectures by senior scientists. In addition, the Dick Stufkens prize was awarded by Prof. Jan Verhoeven (UvA, member of the HRSMC Scientific Advisory Committee) to Dr. Sven Askes (former UL 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.



At the HRSMC Symposium, Prof. dr. Jan Verhoeven (UvA) hands out the Dick Stufkens prize to Dr. Sven Askes

The symposium, which was attended by ca. 190 scientists, included poster sessions with 49 posters, mainly presented by PhD students. Further details regarding this symposium can be found in Chapter 3.2.

The HRSMC activities of 2017 consisted of:

- the two weeks Winter School 'Molecular Simulation', organized under the auspices of CECAM (January 9-20, UvA):



-
- the Course '*Physical Methods in Inorganic Chemistry*' (6 – 10 February, UvA - UL)
 - the Course '*Photophysics, Photochemistry & Photobiology*' (April 2017, UvA/VU)
 - the 4 day Scientific Writing - High Impact Writing Course, in combination with a 1 day Peer Review Survival Course (June 12 – 16, UL)
 - the Summer School '*Organic Synthesis*' (10-13 July, Kasteel Vaeshartel, Maastricht):



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 2017 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. In 2017, nineteen students participated in the HRSMC-NWO Excellence Master Graduate programme '*Sustainability: the Molecular Approach*'.

In 2017, the HRSMC has granted the proposal for PhD research written by chemistry student of David Klein, MSc. Within the NWO Graduate Programme, David Klein was appointed at the Leiden University.

More information about this programme can be found in Chapter 3.4.



David Klein, MSc.

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 2017, there have been two rounds, in April and October. Nine Fellowship applications were awarded (€ 37.625), of which one is the special John van Geuns Fellowship under auspices of the HRSMC.

In 2017 four publications appeared as a result of previous awarded Fellowships.

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 2017, while several joint applications at CW-NWO were awarded.

(Personnel) mutations

In 2017 the following UvA/VU/UL groups or staff members joined the HRSMC:

- the Hybrid Solar Energy Conversion research group of Dr. E.L. von Hauff (VU),
- the Biomolecular Simulation and Modeling group of Dr. D.P. Geerke (VU),
- Dr. S. Castellanos Ortega (guest appointment UvA; ARCNL) within the Molecular Photonics group (UvA).

while from the RU the following groups or staff members became associated members:

- the Synthetic Organic Chemistry group of Prof. dr. F.P.T.J. Rutjes, Dr. T.J. Boltje, Dr. M.C. Feiters and Dr. J. Mecinovic,
- Prof. dr. H.M. Cuppen within the Theoretical Chemistry group.

As of 1 February 2017, Associate Professor Célia Fonseca Guerra (Theoretical Chemistry, VU) has been appointed Extraordinary Professor of Applied Theoretical Chemistry at the Leiden University.

In 2016 Dr. J.C. Slootweg, Dr. A.W. Ehlers and seven co-workers moved from Vrije Universiteit Amsterdam to the HIMS premises at Amsterdam Science Park. In 2017, Dr. J.C. Slootweg was incorporated in the Synthetic Organic Chemistry group of Prof. dr. H. Hiemstra and Prof. dr. J.H. van Maarseveen, and Dr. A.W. Ehlers in the Homogeneous, Supramolecular and Bio-Inspired Catalysis group of Prof. dr. B. de Bruin and Prof. dr. J.N.H. Reek.



Posters winners at our Annual Symposium from left – right: Silvia D'Agostini (public prize), Xiaobo Sun (public prize), Hans de Bruijn (public prize) and Michelle Hammerton (official Staff jury prize & Students prize) with Prof. Wybren Jan Buma (scientific director HRSMC).

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 2017. 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 2017, which is constantly evolving and which fluctuates annually.

Table 2.1 HRSMC research themes, corresponding research groups and their staff members in 2017.

| | Group (University, institute) staff members |
|--------------------------------|---|
| T H E M E 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. A.W. Ehlers, Dr. T.J. Mooibroek, 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. W.T. Fu, Dr. D.G.H. Hettterscheid |
| | 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, Dr. J.C. Sloopweg |
| | Synthetic Organic Chemistry (RU) Prof. dr. F.P.T.J. Rutjes, Dr. T.J. Boltje, Dr. M.C. Feiters, Dr. J. Mecinovic |
| | |

| | |
|--------------------------------|---|
| T H E M E 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 |
| | Hybrid Solar Energy Conversion (VU, EMS) Dr. E.L. von Hauff |
| | Raymond and Beverly Sackler Laboratory Astrophysics and Astrochemistry (UL, LION) Prof. dr. H. Linnartz |
| | 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. ir. A. Pettrignani-Taube, Dr. R. M. Williams, Dr. H. Zhang, Guest appointment: Dr. S. Castellanos Ortega (ARCNL), Prof. dr. J. Oomens (RU) |
| | Molecular Structure and Dynamics – FELIX/Molecular and Biophysics (RU) Prof. dr. J. Oomens, Dr. J.M. Bakker, Dr. A.M. Rijs |
| | Surface Chemistry and Catalysis (UL, LIC) Prof. dr. M. Koper ¹ , Dr. W.T. Fu, Dr. I.M.N. Groot, Dr. D.G.H. Hetterscheid, Dr. L.B.F. Juurlink |
| T H E M E 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, Prof. dr. C. Fonseca Guerra, Prof. dr. P. Gori Giorgi, Dr. O. Gritsenko |
| | Biomolecular Simulation and Modeling (VU, EMS) Dr. D.P. Geerke |
| | Theoretical Chemistry (UL, LIC) Dr. J. Meyer |
| | Theoretical Chemistry (RU) Prof. dr. ir. G.C. Groenenboom, Dr. H.M. Cuppen |

¹also 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** carries out cutting-edge research at the interphase between the chemical and the biological sciences. The research mainly focuses on: the development of novel biocatalytic systems (e.g. in vitro and in vivo enzyme cascades) for the sustainable manufacturing of chemical products; the identification and characterisation of novel enzymes; the engineering of enzymes to improve existing activities or introduce new activities; the creation of artificial enzymes.

The mission of the **Heterogeneous Catalysis and Sustainable Chemistry** group at the UvA is to discover new catalysts and materials for sustainable chemistry and sustainable energy. We start from fundamental concepts and develop practical applications. These includes fuel cells and supercapacitors, CO₂ conversion, selective oxidation and porous molecular materials for a variety of applications. Our strengths are in catalyst and materials design, synthesis and testing, and characterization under real-life conditions. HCSC is interdisciplinary (organic chemists, physicists, chemical engineers, electronics experts, materials scientists, chemometricians and computational chemists), and all our projects benefit from this. Many of our projects provide direct solutions to real-life industrial challenges.

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 innovative 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. Novel reactions relevant for bio-renewable conversion as well as conventional reactions relevant for synthesis and industry receive particular attention. We also study reactions for green energy applications such as water oxidation, proton reduction, CO₂ reduction, formic acid decomposition, alcohol dehydrogenation and 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. Advanced spectroscopic methods are developed to obtain detailed insights in structure and electronics as well as reactivity and mechanisms.

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 potential applications as homogeneous catalysts, electrocatalysts for the reduction of carbon dioxide or the oxidation of water, photo-activatable antitumor drugs, models for the active sites in metalloproteins, and molecular materials.

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 as well as protein-RNA interactions. In addition, novel techniques for the stabilization of enzymes are explored. 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). In addition, molecular biology (e.g. heterologous protein expression) represents a key expertise.

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 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.

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.

The **Synthetic Organic Chemistry (RU)** at Radboud University became a guest-member in 2017 and covers a broad range of organic synthesis topics to create biologically active small molecules and to develop new reactions that can be applied at the interface of chemistry and biology to unravel biochemical processes in the cell. More specifically, areas that are studied concern the development of new click-probes for bio-orthogonal conjugation, continuous flow chemistry in microreactor systems, MS-IR measurements to study the conformation of glycosyl cations, and the physical organic chemistry of epigenetic molecular interactions. Furthermore, in collaboration with physical chemistry groups new chiral crystallization phenomena and NMR hyperpolarization techniques are studied.

Biocatalysis

Dr. F. Mutti (UvA)

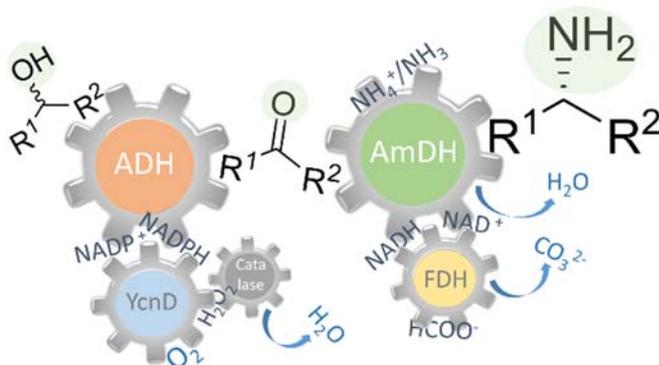
Research topics

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 2017

α -Chiral amines are key intermediates for the production of active pharmaceutical ingredients, fine chemicals and agrochemicals. Structurally simpler amines are also of interest for the production of polymers, dyes and other materials. Following its breakthrough publication in *Science* on the *asymmetric hydrogen-borrowing bioamination of alcohols*, the Biocatalysis group has elucidated further the substrate scope and catalytic properties of amine dehydrogenase enzymes (Green Chem. 2017). Additionally, the group has developed a new orthogonal biocatalytic network that enables the quantitative and stereospecific amination of alcohols (Org. Biomol. Chem. 2017). The system is based on the combination of two redox-neutral enzymatic modules. The first module, driven by NADP-dependent enzymes, oxidizes racemic alcohols to carbonyl compounds intermediates. The second module, driven by NAD-dependent enzymes, performs the asymmetric amination of the intermediate. As the two modules have a divergent co-enzyme specificity (NAD vs NADP), multiple redox reactions run simultaneously in the same vessel without the need for a physical separation. This property in chemistry is defined as "orthogonality". Orthogonal chemical reactions are very rare as traditional chemical (redox) reagents are not selective. Moreover, the orthogonal biocatalytic network for the conversion of racemic alcohols into enantiopure amines is very efficient because it consumes only O₂ and produces only stoichiometric carbonate as by-product



Key publications 2016-2017

- Knaus, T.; Böhmer, W.; Mutti, F.G.; Amine dehydrogenases: efficient biocatalysts for the reductive amination of carbonyl compounds, *Green Chem.*, **2017**, 19, 453-463.
- Knaus, T.; Cariati, L.; Masmam, M.F.; Mutti, F.G.; In vitro biocatalytic pathway design: orthogonal network for the quantitative and stereospecific amination of alcohols, *Org. Biomol. Chem.*, **2017**,15, 8313-8325.

Important Grants and Prizes in 2017

- Dr. F. Mutti: Inclusion in the top-100 list of Italian scientists (from all fields of sciences) under age of 40 (Italian Institute of Culture of Brussels, Belgium).

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
- CO₂ conversion
- Molecular Sensing
- Molecular Separations
- Asymmetric catalysis
- Fuel cells

Group highlights 2017

UvA catalyst for cleaning cyanide from wastewater goes pilot scale

A cyanide decomposition catalyst developed by Dr Paula Oulego, Dr Raveendran Shiju and Prof. Gadi Rothenberg is now being tested on an industrial pilot scale. Treating industrial wastewater continuously at a rate of 1000 liters per hour, the pilot is the last step before large-scale industrial application in areas such as gold mining, processing of precious metals, and steel production. The solid catalyst, based on a simple and cheap copper oxide, was invented in 2015. That it was developed in less than two years to an industrial pilot scale attests to the simplicity and efficiency of the process. The catalyst enables cyanide decomposition by a fast reaction of cyanide ions with hydrogen peroxide at 40 °C, under ambient pressure. This reaction is so quick that the catalyst can be used with cyanide concentrations ranging from 1 mg/liter all the way up to 10 g/liter. It can thus be used for treating a broad range of industrial wastewater flows. 500 kg of the new

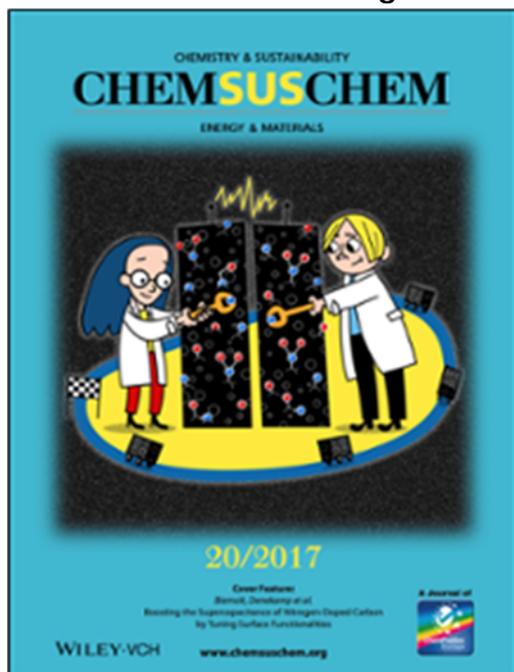
catalyst were produced industrially especially for this pilot installation.



Dr. Shiju and Prof. Rothenberg next to the first two barrels (500kg) of their industrial catalyst. (Photo: UvA)

Research highlights per staff member

Prof. Dr. Gadi Rothenberg

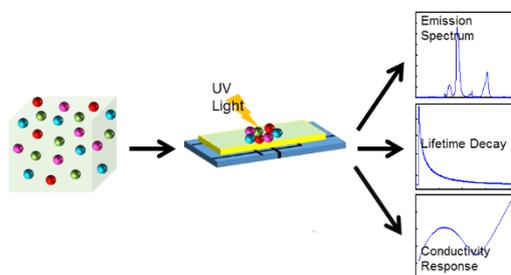


In a project that has attracted worldwide attention, HIMS MSc students Jasper Biemolt and Ilse Denekamp have tripled the specific capacitance of nitrogen-doped carbons: new materials with potential applications in fast energy storage (e.g. for regenerative braking or fast charging of cellphones). Their experiments required new pieces of equipment which were designed and produced in the lab using 3D printing. The Amsterdam students investigated the factors that govern different modes of supercapacitance in the new supercapacitor material that was invented by Prof. Gadi Rothenberg. They were able to tune the materials' surface structure and functional groups in order to maximise fast faradaic reactions at the surface, storing energy in transient chemical bonds. Their

results were published in an open-access paper in the high-impact international journal ChemSusChem, and featured on the issue cover. For this achievement, Ms. Denekamp was also awarded the Unilever Research Prize 2017.

Dr. Stefania Grecea

The research focused on the rational design of functional materials for sustainable applications has continued in molecular separations, molecular sensing and asymmetric catalysis. Grecea's subgroup has demonstrated that embedding optically active centres in a controlled fashion enables the formation of three-dimensional porous structures. The porosity of these materials facilitates the reversible storage and release of guest molecules and also allows the differential recognition of molecules. Using combined photoluminescence and impedance spectroscopy studies, it was shown that specific porous materials behave as highly effective and reliable humidity sensors, enabling dual-mode humidity detection. These materials can be scaled up and integrated into films and on specific surfaces, making them an ideal platform for designing detection devices.

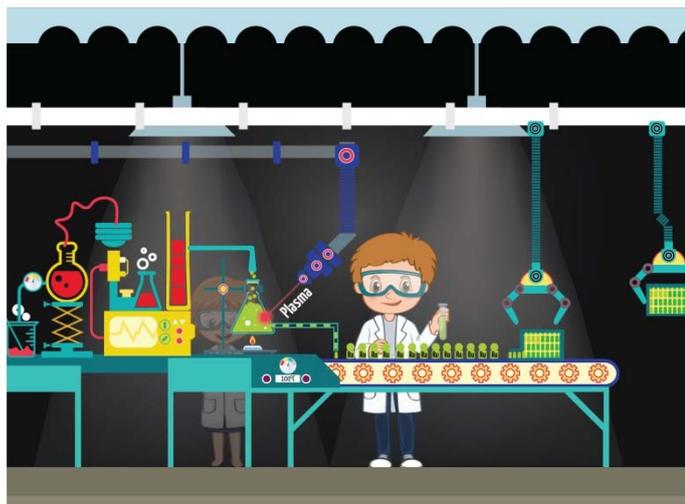


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Dr. Shiju Raveendran

In Catalysis Engineering, we were active in acquiring new knowledge and developing new catalysts in several research areas including CO₂ conversion and biomass conversion. We developed a new inexpensive catalyst that can convert CO₂ to CO efficiently under mild conditions. This catalyst performs better than those reported in the literature; thus, a patent application is filed. On the catalyst synthesis part, we showed that treating catalyst precursors with 'cold plasma' leads to efficient catalysts without the need of high

temperature calcination and reduction. This treatment also avoids the use of O_2 and H_2 . The highly uniform and small nanoparticles of metal resulting from low temperature plasma treatment perform better as chemo- and electro catalysts than those obtained by conventional treatment. This work is highlighted in the cover of *ChemCatChem* (see illustration). In biomass conversion, we achieved, with a suitable combination of catalysts,



one-pot hydrolysis–hydrogenation of hemicellulose to xylitol. A biomass-derived organic acid was used as the catalyst for the hydrolysis step, matching well with the objectives of biorefinery. Using another catalyst system, we showed that optimising the catalyst support is as important as manipulating the active species in achieving high selectivity for desired product in biomass conversion reactions.

Dr. Ning Yan

2017 is another year of research success. We still kept our focuses on developing and understanding perovskite oxide and porous carbon materials for electrocatalysis. In particular, we found that the layered double perovskite can suffer surface degradation under potential bias in the electrolyte during water splitting reaction. Our advanced materials characterizations revealed that the surface decomposition caused the dopants segregation and surface amorphization. Through a combined experimental and computational investigation, we discovered that Ca substitution at the A'-site was able to suppress such degradation. Regarding the carbon research, we tailored the morphology and composition of our N-doped carbon catalyst. The developed carbon nanorods were embedded by MnO_x nanoparticles, leading to much better catalytic performances in both oxygen reduction and evolution reactions.



Key publications 2016-2017

- Biemolt, J.; Denekamp, I.M.; Slot, T.K.; Rothenberg, G.; Eisenberg, D.; Boosting the supercapacitance of nitrogen-doped carbon by tuning surface functionalities, *ChemSusChem* **2017**, 10, 4018–4024.
- Gehre, M.; Guo, Z.; Rothenberg, G.; Tanase, S.; Sustainable separations of C4 hydrocarbons using microporous materials, *ChemSusChem* **2017**, 53, 4465–4468.
- Gao, Y.; Jing, P.; Yan, N.; Hilbers, M.; Zhang, H.; Rothenberg, G.; Tanase, S.; Dual-mode humidity detection using a lanthanide-based metal-organic framework: towards multifunctional humidity sensors, *Chem. Commun.* **2017**, 53, 4465–4468.

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- Pandey, J.; Hua, B.; Ng, W.; Yang, Y.; van der Veen, K.; Chen, J.; Geels, N.J.; Luo, J.L.; Rothenberg, G.; Yan, N.; Developing hierarchically porous MnO_x/NC hybrid nanorods for oxygen reduction and evolution catalysis, *Green Chem.* **2017**, 19, 2793-2797.
 - Hua, B.; Sun, Y.-F.; Li, M.; Yan, N.; Chen, J.; Zhang, Y.-Q.; Zeng, Y.M.; Amirkhiz, B.S.; Luo, J.L.; Stabilizing Double Perovskite for Effective Bifunctional Oxygen Electrocatalysis in Alkaline Conditions, *Chem. Mater.* **2017**, 29, 6228-6237
 - Yang, Y.; Yan, N.; Understanding the cooperative atomic motion and shape change of ultrasmall Au nanoparticles below the premelting temperature, *RSC Adv.* **2017**, 7, 55807-55811.

Important Grants and Prizes in 2017

- The catalyst invented by Rothenberg and Shiju has been scaled up to industrial pilot scale (see group highlight).
- A patent has been filed in collaboration with the Analytical Chemistry group: Use of a nitrogen-doped porous carbon material for enriching phosphorylated proteins or peptides. M. Camenzuli, S. Koot and G. Rothenberg, Eur. Pat. Appl. 17172844.7, 09/2017.
- Prof. G. Rothenberg was appointed as Senior Visiting Scholar at Fudan University, one of the top five universities in China, for one year. This appointment strengthens the contacts between the UvA and Fudan, which already includes joint papers, a joint project funded by the Chinese Government, and student exchange.
- Dr. Shiju Raveendran has been appointed as visiting professor at Yangzhou University for a period of five years. This appointment creates new opportunities for collaboration, and includes funding for several postdocs to perform research in Europe.
- S. Grecea, RAPIDD access grant to the facilities at the Advanced Light Source, Berkley Laboratory.
- S. Grecea, General and inorganic chemistry lectures for the students representing the Netherlands at the 49th International Chemistry Olympiad.

Homogeneous, Supramolecular Catalysis and Spectro-electrochemistry

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

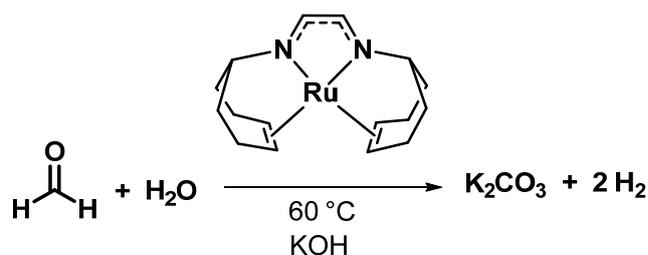
Research topics

- Development of new approaches in transition metal catalysis and catalyst recovery, including supramolecular approaches, ligand design, bioinspired approaches, controlled radical-type reactions, non-innocent 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
- Ligand radicals in catalysis
- Application of reactive ligands (redox-active, chemoresponsive) for bond functionalization and catalysis
- Coordination chemistry and catalysis with base and main group metals
- Catalysis using electrochemistry
- C1-carbene chemistry
- Development of advanced spectroscopic techniques as tools in catalysis.
- Targeting unprotected carbohydrates with tailored supramolecular organo(metallic) catalysts.
- Studies into the nature and directionality of unconventional non-covalent interactions, in particular as they manifest themselves in the solid state.

Group highlights 2017

Highlight Bas de Bruin

Small organic molecules provide a promising solution for the requirement to store large amounts of hydrogen in a future hydrogen-based energy system. Together with collaborators from the ETH Zürich we showed that diolefin-ruthenium complexes containing the chemically and redox non-innocent ligand trop₂dad catalyse the production of H₂ from formaldehyde and water in the presence of a base.

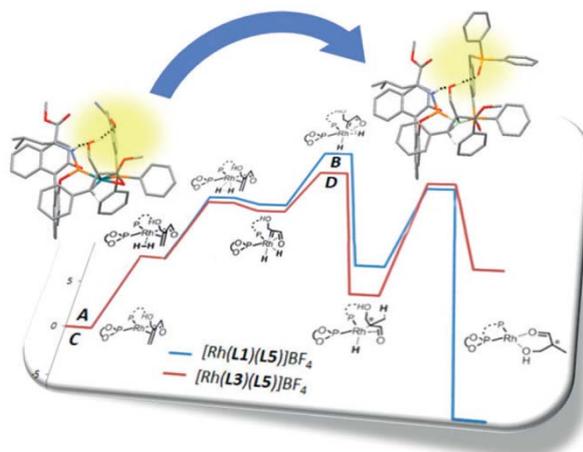


The process involves the catalytic conversion of formaldehyde to carbonate salt using aqueous solutions and is the fastest reported for acceptorless formalin dehydrogenation to date. A mechanism supported by density functional theory calculations postulates protonation of a ruthenium hydride to form a low-valent active species, the reversible uptake of dihydrogen by the ligand and active participation of both the ligand and the metal in substrate activation and dihydrogen bond formation.

Trincado, M.; Sinha, V.; Rodriguez-Lugo, R.E.; Pribanic, B.; de Bruin, B.; Grützmacher, H.; Homogeneously Catalysed Conversion of Aqueous Formaldehyde to H₂ and Carbonate, *Nature Communications* **2017**, *8*, 14990. DOI: 10.1038/ncomms14990.

Highlight Joost Reek

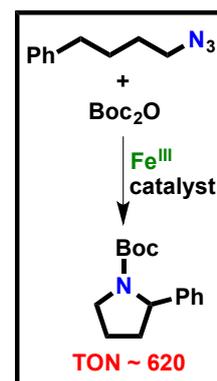
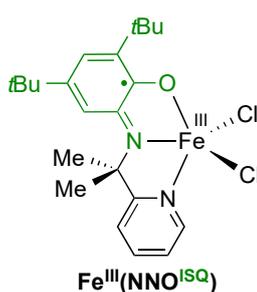
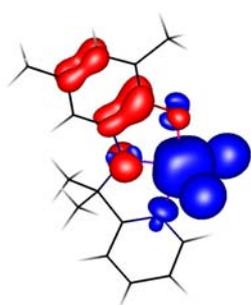
Developing new catalysts for new asymmetric conversions in general requires a lot of trial-and-error, as computational prediction of the selectivity of the catalysts is too challenging. A strategy was developed that brings chemistry one step closer to a more efficient catalyst development by rational design. At the homogeneous and supramolecular catalysis research group of professor Reek supramolecular catalysts have been developed where a rhodium complex acts as a selective catalyst for asymmetric hydrogenation. From a detailed study the Amsterdam researchers were able to establish the crucial role of hydrogen bonding between the catalyst and the substrate. The experimental data were used as input for a computational study to exactly determine the reaction pathway and the specific role of the hydrogen bonds. As it turns out, the hydrogen bonds not only lead to better pre-association of the substrate, but also lower the transition state of the rate limiting step. Based on this information a new catalyst was developed by replacing a urea group for a phosphine oxide, thus optimizing the hydrogen bonding, which resulted in a faster and more selective catalyst. With this study the researchers show that supramolecular interactions between substrate and catalyst are of crucial importance, and, importantly, catalyst can be optimized in silico by just 'zooming in' on these interactions.



Daubignard, J.; Detz, R.J.; Jans, A.C.H.; de Bruin, B.; and Reek, J.N.H. Rational Optimization of Supramolecular Catalysts for the Rhodium-Catalyzed Asymmetric Hydrogenation Reaction, *Angew Chem Int Ed* **2017**, *56*, 13056-13060.

Highlight Jarl Ivar van der Vlugt

We have disclosed a highly active and recyclable iron-based catalyst for the selective intramolecular C-H amination of a wide range of aliphatic organoazides into valuable N-heterocyclic products. This has allowed for world-record turnover numbers for this

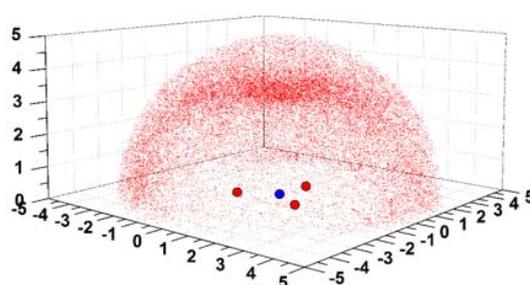
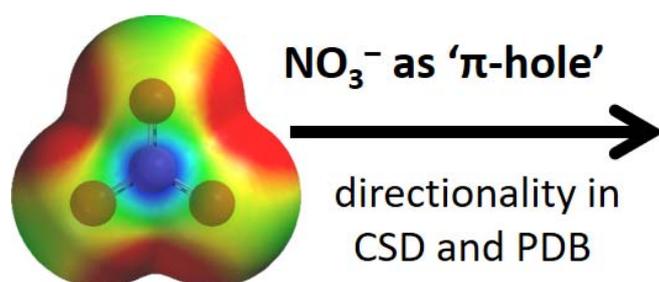


relevant transformation. The Fe^{III}-system bears a redox-active NNO-pincer ligand derived from *o*-aminophenol that was previously developed in the group. The FeCl₂(NNO) complex was fully characterized, using a combination of Mössbauer spectroscopy, magnetochemistry, Evans' method, computational analysis, UV-vis spectroscopy and single crystal X-ray crystallography.

The overall *S* = 2 spin system comes about by anti-ferromagnetic coupling of a metal-centered unpaired electron with an electron residing in the ligand backbone. The Fe-complex displayed very unusual kinetics in the C-H amination, which requires Boc₂O to release the N-heterocyclic product. In stark contrast to the few reported systems capable of converting aliphatic organoazides, the rate for the catalysis induced by this Fe-system is not affected by the substrate concentration, but rather shows first-order dependence of the Boc₂O co-reagent. This has allowed for formulation of a highly unusual pre-activation of the Fe-complex to generate the actual catalytic species.

Bagh, B.; Broere, D.L.J.; Sinha, V.; Kuipers, P.T.; van Leest, N.P.; de Bruin, B.; Demeshko, S.; Siegler, M.A.; van der Vlugt, J.I.; *J. Am. Chem. Soc.* **2017**, *139*, 5117-5124.

Highlight Tiddo Mooibroek

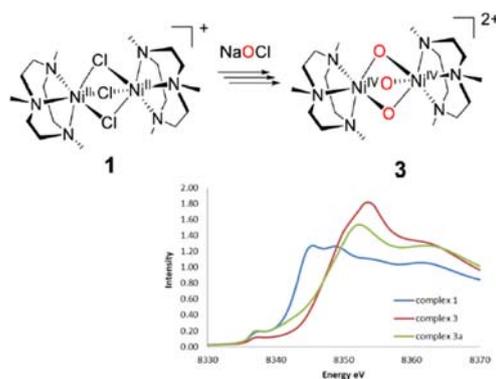


Molecules are sticky and Nature utilizes this to facilitate all kinds of processes: binding of a medicine to a protein; alignment of fatty acids to form cell walls; association of two strands of DNA to form the classical double helix, etc. An important driving force behind molecular association is electrostatic attraction. Identifying electron donating and accepting moieties is thus crucial to understanding molecular aggregation phenomena. Anions such as NO₃⁻ are typical electron donors. However, computations predict that the charge distribution of NO₃⁻ is anisotropic and minimal on N. In a recent publication in *Nature Communications* we showed that when the nitrate's charge is sufficiently

dampened by resonating over a larger area, a Lewis acidic site emerges on N that can interact favorably with electron rich partners. Surveys of the CSD and PDB reveal geometric preferences of some O- and S-containing entities around (uncoordinated) nitrate anions that are consistent with this 'n-hole bonding' geometry. A subsequent CSD survey of n-hole interactions involving *coordinated* nitrate anions (*CrystEngComm*) revealed that overlap of van der Waals shells increases with increased coordination and 84% of close contacts involve anti-electrostatic $\text{NO}_3^- \cdots \text{NO}_3^-$ interactions.

Highlight Moniek Tromp

A novel lab-based X-ray spectrometer to allow X-ray absorption and emission spectroscopy in the laboratory, on a 24/7 basis, rather than at the synchrotron, was developed in collaboration with the University of Seattle (G. Seitler, D. Mortensen). The instrument enables studies on 3d and 5d transition metals systems, for their detailed structural and mostly electronic properties.



The first publication including data on the lab spectrometer appeared in JACS [1]. Here, a reactive high-valent dinuclear nickel(IV) oxido bridged complex is reported that can be formed at room temperature by reaction of $[(\text{L})_2\text{Ni}(\text{II})_2(\mu\text{-X})_3]\text{X}$ ($\text{X} = \text{Cl}$ or Br) with NaOCl in methanol or acetonitrile (where $\text{L} = 1,4,7$ - trimethyl-1,4,7-triazacyclononane). The unusual Ni(IV) oxido species is stabilized within a dinuclear tris- μ -oxido-bridged structure as $[(\text{L})_2\text{Ni}(\text{IV})_2(\mu\text{-O})_3]^{2+}$. Its structure and its reactivity with organic substrates are demonstrated through a combination of UV–Vis absorption, resonance Raman, ^1H NMR, EPR, and X-ray absorption (near-edge) spectroscopy, ESI mass spectrometry, and DFT methods. The identification of a Ni(IV)-O species opens opportunities to control the reactivity of NaOCl for selective oxidations.

Padamati, S.K.; Angelone, D.; Draksharapu, A.; Primi, G.; Martin, D.J.; Tromp, M.; Swart, M.; Browne, W.R.; Transient Formation and Reactivity of a High Valent Nickel(IV) Oxido Complex, *J. Am. Chem. Soc.* **2017**, 139, 8718-8724.

Key Publications 2016-2017

- Jing, X.; Yang, Y.; He, C.; Chang, Z.; Reek, J.N.H.; Duan, C.; Control of Redox Events by Dye Encapsulation Applied to Light-Driven Splitting of Hydrogen Sulfide, *Angew Chem Int Ed Engl* **2017**, 56, 11759-11763.
- Wang, X.; Nurttala, S.S.; Dzik, W.I.; Becker, R.; Rodgers, J.; Reek, J.N.H.; Tuning the Porphyrin Building Block in Self-Assembled Cages for Branched-Selective Hydroformylation of Propene, *Chem. Eur. J.* **2017**, 23, 14769-14777 (inside cover).
- te Grotenhuis, C.; Das, B.G.; Kuijpers, P.F. Hageman, W.; Trouwborst, M.; de Bruin, B.; Catalytic 1,2-Dihydronaphthalene and E-Aryl-Diene Synthesis via Co(III)-Carbene Radical and o-Quinodimethane Intermediates, *Chemical Science*, **2017**, 8, 8221-8230.
- Kuijpers, P.F.; Tiekink, M.J.; Breukelaar, W.B.; Broere, D.L.J.; van Leest, N.P.; van der Vlugt, J.I.; Reek, J.N.H.; de Bruin, B.; Nitrene-radical approach to Saturated

Heterocycles; Cobalt Porphyrin Catalysed Intramolecular Ring-Closing C-H Amination of Aliphatic Azides, *Chem. Eur. J.* **2017**, *23*, 7945 –7952 (Very Important Paper; inside Front Cover).

- Devillard, M.; de Bruin, B.; Siegler, M.A.; van der Vlugt, J.I.; Transition metal-free cleavage of CO, *Chem. Eur. J.* **2017**, *23*, 13628-13632.
- de Boer, S.Y.; Korstanje, T.J.; La Rooij, S.R.; Kox, R.; Reek, J.N.H.; van der Vlugt, J.I.; Ruthenium PNN(O) complexes: Cooperative reactivity and application as catalysts for acceptorless dehydrogenative coupling reactions, *Organometallics* **2017**, *36*, 1541-1549.
- Bauza, A.; Frontera, A.; Mooibroek, T.J.; NO₃⁻ anions can act as Lewis acid in the solid state, *Nature Communications*, **2017**, *8*, 14822.
- Rios, P.; Mooibroek, T.J.; Carter, T.S.; Williams, C.; Wilson, M.R.; Crump, M.P.; Davis, A.P.; Enantioselective Carbohydrate Recognition by Synthetic Lectins in Water, *Chemical Science*, **2017**, *8*, 4056.
- Padamati, S.K.; Angelone, D.; Draksharapu, A.; Primi, G.; Martin, D.J.; Tromp, M.; Swart, M.; Browne, W.R.; Transient Formation and Reactivity of a High Valent Nickel(IV) Oxido Complex, *J. Am. Chem. Soc.* **2017**, *139*, 8718-8724.

Important Grants and Prizes in 2017

- CBBC project with AkzoNobel: Replacing Co in paint curing (Bas de Bruin)
- CBBC project with AkzoNobel: Novel catalyst for polyester formation (Joost Reek & Moniek Tromp)
- NWO-NFSC joined program on supramolecular catalysis (1PhD; two PhD's in china) (Reek/ van der Vlugt.)
- NWO materials for sustainability 2 PhD's 1 Post doc, (van der Vlugt/Reek.)
- NWO materials for sustainability 1 PhD Moniek Tromp en Petra de Jongh/Petr Ngene (UU)
- NICAS 2 projects, 1 full project with 1 PhD led by Katrien Keune, 1 seed money project led Moniek Tromp
- Joost Reek became distinguished faculty professor in 2017.
- Moniek Tromp Elected Fellow of the European Academy of Sciences, 2017.
- Moniek Tromp Winner of the NWO Athena Price 2017.

Metals in Catalysis, Biomimetics & Inorganic Materials

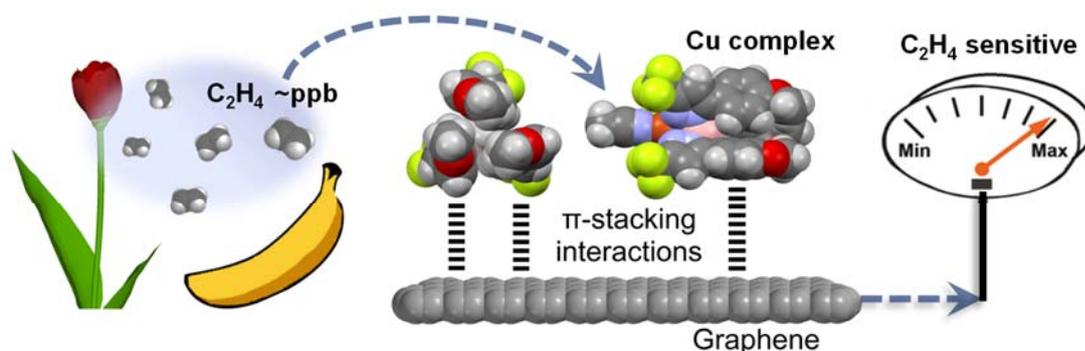
Prof. dr. E. Bouwman, Dr. S. Bonnet, Dr. D.G.H. Hetterscheid (UL)

Research topics

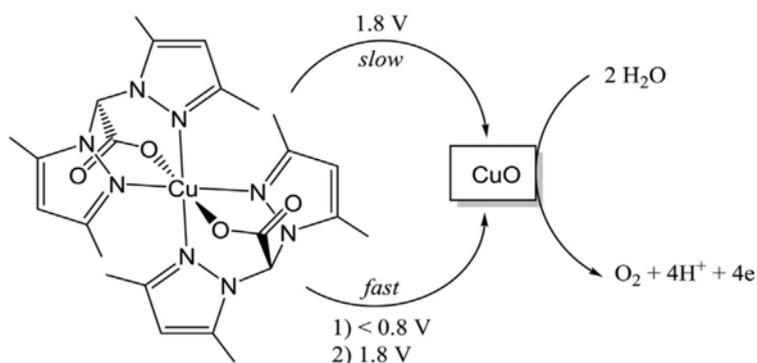
- Inorganic chemistry
- Homogeneous- and photo-catalysis (reported within NIOK)
- Biomimetic and bioinorganic chemistry
- Molecular materials

Group highlights 2017

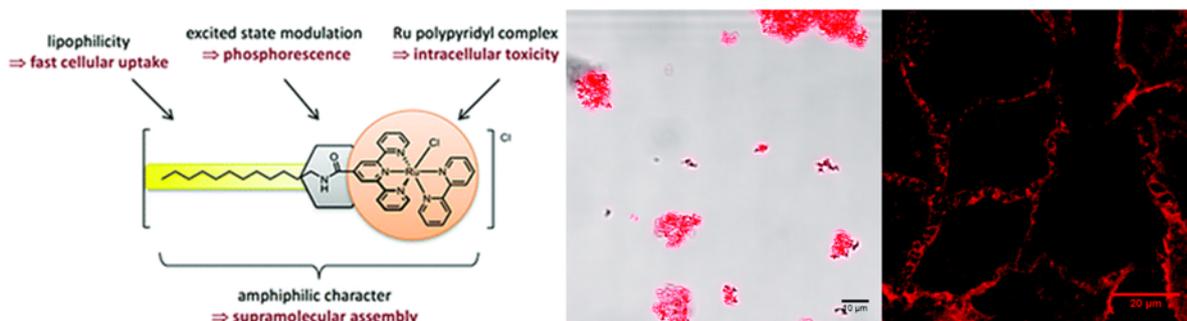
Ethene is a highly diffusive and relatively unreactive gas that induces ageing responses in plants in concentrations as low as parts per billion. Monitoring concentrations of ethene is critically important for e.g. transport and storage of food crops. We have shown that by functionalizing graphene with copper complexes biologically relevant concentrations of ethene and of the spoilage marker ethanol can be detected. Inorganic copper complexes have been combined with graphene, resulting in a GFET sensor that exhibits reproducible detection of ethene with larger sensitivity (down to 2 ppb) than existing technologies. By using a systematically engineered set of probe molecules we obtained useful information such as reaction rates and equilibrium constants, which were used to derive a plausible reaction mechanism. The use of a Langmuir adsorption isotherm allowed for the extraction of K_D and k_{-1} values, which are physically meaningful data that are very difficult to obtain otherwise. (W. Fu, T.F. van Dijkman, L.M.C. Lima, F. Jiang, G.F. Schneider, E. Bouwman. *Nano Lett.* **2017**, *17*, 7980-7988.)



The activation processes of [Cu(bdmpza)₂] in the water oxidation reaction was investigated using cyclic voltammetry and chronoamperometry. Two different paths wherein CuO is formed were distinguished. [Cu(bdmpza)₂] can be oxidized at high potentials to form CuO, which was observed by a slight increase in catalytic current over time. When [Cu(bdmpza)₂] is initially reduced at low potentials, a more active water oxidation catalyst is generated, yielding high catalytic currents from the moment a sufficient potential is applied. This work highlights the importance of catalyst pre-treatment and choice of the experimental conditions in water oxidation catalysis using copper complexes. Published in *Catalysis Today* 290 (2017) 33–38.



Next to catalysis, metal compounds are also used for their biological properties. Ruthenium-based light-activated anticancer compounds are developed at MCBIM. One of the problems of this family of compounds is their inherent “invisibility” in cells: while many ruthenium compounds are phosphorescent and can be imaged in living cells, or even used for bioimaging, photoactivated chemotherapeutic compounds are usually not emissive, precisely because they are photoreactive. Recently, we found that light-activated compounds of the $[\text{Ru}(\text{terpy})(\text{bpy})\text{Cl}]^+$ family can be fine-tuned using amide groups in the 4' position on the terpyridine ligand, which provides both light activation and phosphorescence. The amide group borne by the ruthenium compound was a long C12 alkyl chain, which also gave the complex amphiphilic properties. Because of its emissive properties the fate of this complex in cancer cells was followed by emission microscopy, which showed that the molecule first attacks the cell membrane, before being internalized further and killing the cell. Published in *Chem. Commun* 53 (2017), 11126-11129.



Key publications 2016-2017

- Terrade, F.G.; van Krieken, J.; Verkuijl, B.J.V.; Bouwman E.; Catalytic cracking of lactide and poly(lactic acid) to acrylic acid at low temperatures, *ChemSusChem*, **2017**, *10*, 1904-1908.
- Limburg, B.; Gloaguen, Y.; de Bruijn, H.M.; Drent, E.; Bouwman, E.; Palladium-Catalyzed Isomerization/(Cyclo)carbonylation of Pentenamides: a Mechanistic Study of the Chemo- and Regioselectivity, *ChemCatChem*, **2017**, *9*, 2961-2971.
- van der Ham, C.J.M.; Işık, F.; Verhoeven, W.G.M.; Niemantsverdriet, J.W.; Hetterscheid, D.G.H.; Activation pathways taking place at molecular copper precatalysts for the oxygen evolution reaction, *Catalysis Today* **2017**, *290*, 33-38.
- Hetterscheid, D.G.H.; In Operando Studies on the Electrochemical Oxidation of Water Mediated by Molecular Catalysts, *Chem. Commun.*, **2017**, *53*, 10622-10631.

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- Lameijer, L.N.; Ernst, D.; Hopkins, S.L.; Meijer, M.S.; Askes, S.H.C.; Le Dévédec, S.E.; Bonnet, S.; Efficient red light activated NAMPT inhibition in hypoxic cancer cells using water-soluble ruthenium complexes, *Angew. Chem. Int. Ed.* **2017**, *56*,11549–11553.
 - Askes, S.H.C.; Gandra, U.R.; Wyrwa, R.; Bonnet, S.; Schiller, A.; Red light-triggered CO release from $\text{Mn}_2(\text{CO})_{10}$ using triplet sensitization in polymer non-woven fabrics, *J. Am. Chem. Soc.* **2017**, *139*, 15292–15295.

Important Grants and Prizes in 2017

- S. Bonnet: ERC Proof-of-Concept grant (2017-2018), HypoRuLight, 150 k€

Organic and Peptide Chemistry

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

Research topics

- Peptidomimetics
- Proximity-induced reactions
- Inhibition of protein-protein interactions
- Inhibition of protein-RNA interactions

Group highlights 2017

Kerstin Wallraven, PhD student in the group, receives a poster prize for her contribution at the German Peptide Symposium.

In collaboration with the groups of Oliver Koch (TU Dortmund) and Sven Hennig (VU Amsterdam) we developed a computational workflow that allows the docking and scoring of large and flexible macrocycles as inhibitors of protein-protein interactions (published in *J. Med. Chem.*).

Key publications 2016-2017

- Krüger, D.M.; Glas, A.; Bier, D.; Pospiech, N.; Wallraven, K.; Dietrich, L.; Ottmann, C.; Koch, O.; Hennig, S.; Grossmann, T.N.; Structure-based design of non-natural macrocyclic peptides that inhibit protein-protein interactions, *J. Med. Chem.* **2017**, 60, 8982–8988.
- Glas, A.; Wamhoff, E.C.; Krüger, D.M.; Rademacher, C.; Grossmann, T.N.; Increased conformational flexibility of a macrocycle–receptor complex contributes to reduced dissociation rates, *Chem. Eur. J.* **2017**, 23, 16157–16161 (inside cover).
- Dietrich, L.; Rathmer, B.; Ewan, K.; Bange, T.; Heinrichs, S.; Dale, T.C.; Schade, D.; Grossmann, T.N.; Cell permeable stapled peptide inhibitor of Wnt signaling that targets β -catenin protein–protein interactions, *Cell Chem. Biol.* **2017**, 24, 958–968.
- Stiller, C.; Krüger, D.M.; Brauckhoff, N.; Schmidt, M.; Janning, P.; Salamon, H.; Grossmann, T.N.; Translocation of an intracellular protein via peptide-directed ligation, *ACS Chem. Biol.* **2017**, 12, 504–509.

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 2017

Predicting reactivity in multicomponent reactions (MCRs) is extremely difficult. These reactions proceed *via* multiple pathways and are inherently associated with a large potential variation of reactants and functional groups. To date, theoretical chemistry has been used in hindsight to verify experimental observations. However, its use in the early stages of a (multicomponent) reaction development process can prevent laborious and time-consuming optimization studies by pinpointing the most relevant parameter(s) in reactivity thus focusing the experimental efforts. In collaboration with the Theoretical Chemistry group at the VU (Bickelhaupt) we now truly integrate theoretical and synthetic chemistry and unravel in full detail the complex and intricate reaction characteristics of a novel versatile MCR of α -acidic isothiocyanates, amines and aldehydes to access densely functionalized imidazoline-2-(thi)ones (*Eur. J. Org. Chem* 2017).

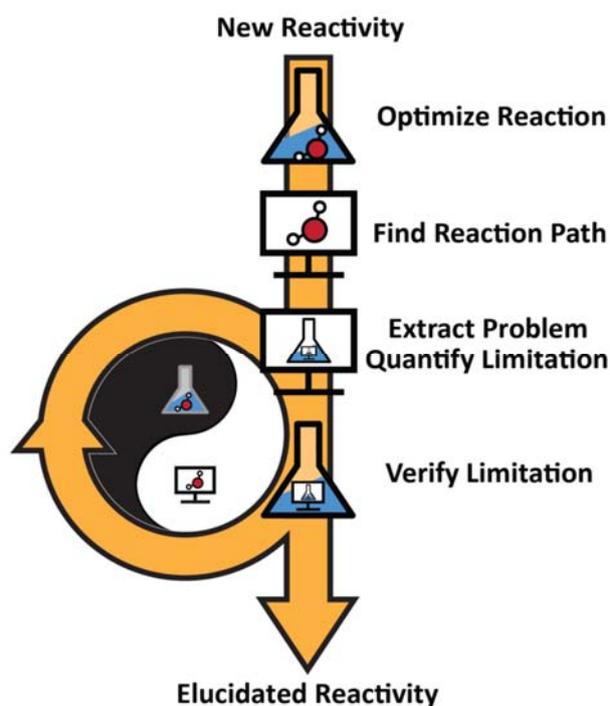


Figure: Our integrative methodology for iterative theory-experiment driven multicomponent reaction exploration

Key publications 2016-2017

- Turrini, N.G.; Cioc, R.C.; van der Niet, D.J.H.; Ruijter, E.; Orru, R.V.A.; Hall, M.; Faber, K.; Biocatalytic access to nonracemic γ -oxo esters via stereoselective reduction using ene-reductases, *Green Chem.* **2017**, 19, 511-518.
- Thomas, B.; Rombouts, J.A.; Oostergetel, G.T.; Gupta, K.B.S.S.; Buda, F.; Lammertsma, K.; Orru, R.V.A.; de Groot, H.J.M.; A Hybrid Solid State NMR and Electron Microscopy Structure Determination Protocol for Engineering Advanced Paracrystalline Optical Materials, *Chem. Eur. J.* **2017**, 23, 3280-3284.
- Mampuys, P.; Neumann, H.; Sergeyev, S.; Orru, R.V.A.; Jiao, H.; Spannenberg, A.; Maes, B.U.W.; Beller, M.; Combining Isocyanides with Carbon Dioxide in Palladium-Catalyzed Heterocycle Synthesis: N3-Substituted Quinazoline-2,4(1H,3H)-diones via a Three-Component Reaction, *ACS Catal.* **2017**, 7, 5549-5556.
- Kruithof, A; Mulder, J.R.; Ruiz, J.M.; Janssen, E.; Mooijman, M.; Ruijter, E.; Fonseca Guera, C.; Bickelhaupt, F.M.; Orru, R.V.A.; Integrative Theory/Experiment-Driven Exploration of a Multicomponent Reaction towards Imidazoline-2-(thi)ones, *Eur. J. Org. Chem.* **2017**, online.

Important Grants and Prizes in 2017

- Our group received two NWO-CW ECHO-grants and a NWO-TTW NACTAR grant (Antibiotic Resistance in collaboration with Wilbert Bitter of VUmc)

Synthetic Organic Chemistry (UvA)

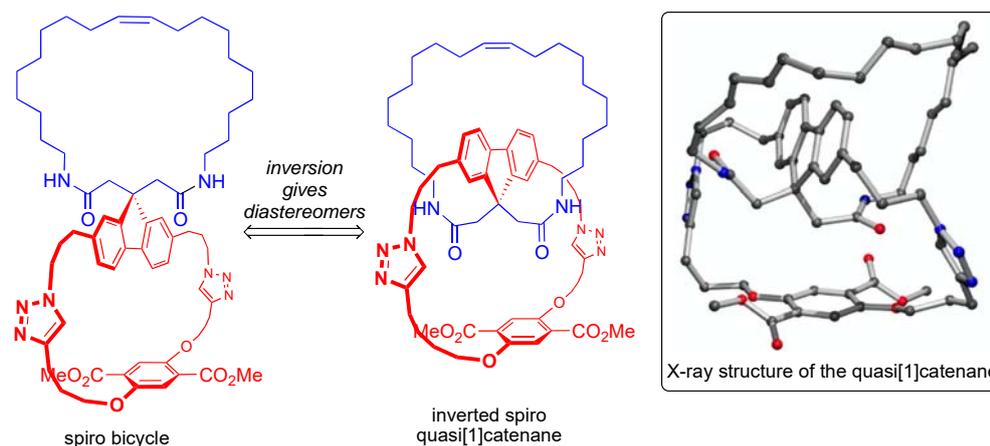
Prof. dr. H. Hiemstra, Prof. dr. P. Timmerman, Prof. dr. J.H. van Maarseveen, Dr. M.A. Fernández Ibáñez (UvA), Dr. S. Ingemann, Dr. J.C. Slootweg

Research topics

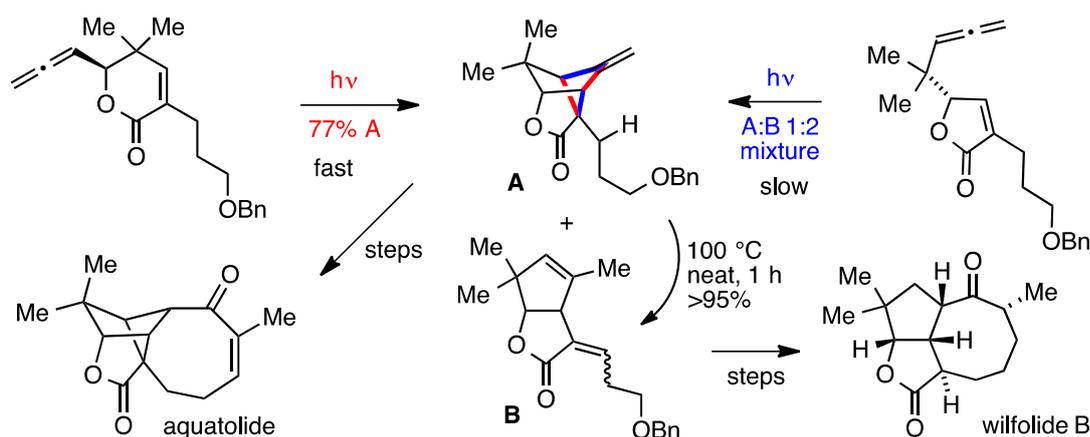
- Synthetic methodology development
- Target-oriented synthesis
- Organocatalysis
- Bioi-organic chemistry
- C-H activation
- Main group chemistry
- Sustainable phosphorous chemistry

Group highlights 2017

Van Maarseveen: Since unravelling their fascinating architecture some fifteen years ago, the microorganism-derived lasso peptides attract the synthetic community. Five years ago we started the development of new covalent template-mediated methodology aimed at precise folding of a macrocycle over a molecular thread. This resulted in the first synthesis of a spirocyclic compound with an inverted geometry at the connecting carbon atom coined as a quasi[1]catenane by us. Also the stereoisomer with regular spiro geometry was prepared and, uniquely, although only one stereocenter is present, both compounds have a diastereomeric relationship. By the introduction of scissile bonds at the central carbon atom this methodology should lead to [2]catenanes and [2]rotaxanes and, in the far future, eventually to the lasso peptide series (*Nature Communications*, 2017, 8, 15392).

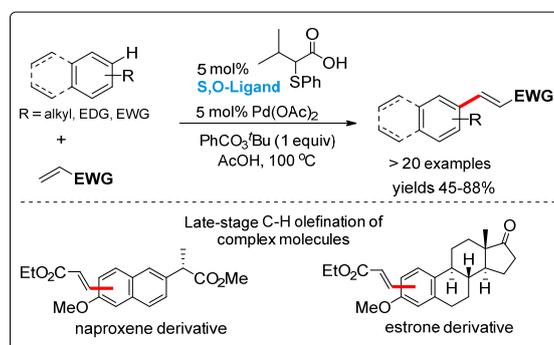


Hiemstra: The key [2+2]-photocycloaddition step in the total synthesis of the sesquiterpene lactone aquatolide was further investigated. It appeared that route A was far more efficient than route B for reasons that still have to be clarified. **A** was thermally converted into **B** in high yield. From **B** the first total synthesis of racemic wilfolide B was achieved.

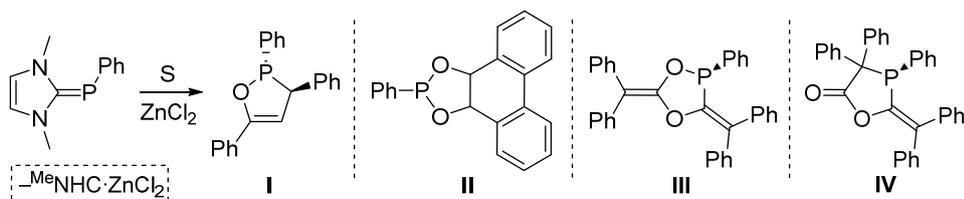


Unequivocal determination of complex molecular structures using anisotropic NMR measurements (*Science* 356, 2017).

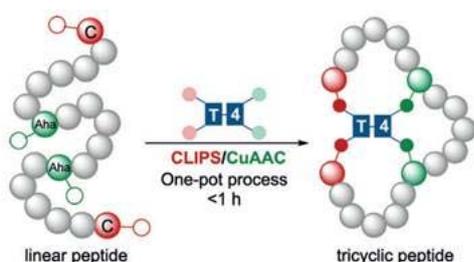
Fernández-Ibáñez: A new class of structurally readily accessible S,O-ligands, namely thioethercarboxylic acids, have been developed that enable non-directed Pd-catalyzed C-H olefination reactions of non-prefunctionalized arenes. These S,O-ligands show higher activity and stronger influence on the site selectivity than the previously described catalytic systems for the oxidative Heck reaction of arenes. The new catalytic system can be applied efficiently to sterically congested, electron rich and poor arenes. In addition, the new methodology is also successful in preparative scale and in late-stage functionalization of complex molecules (*ACS Catal.* 2017, 7, 6342-6346).



Slootweg: On the chemistry of N-heterocyclic carbene (NHC)-phosphinidene adducts it was a possible application was demonstrated of the sterically accessible carbene-phosphinidene adduct $\text{Me}^e\text{NHC}=\text{PPh}$ as phenylphosphinidene transfer agent upon functionalization with ZnCl_2 . This Lewis acid protection enabled the synthesis of the new uncomplexed phosphorus heterocycles I-IV upon treatment with the electron-poor heterodienes (S) 9,10-phenanthrenequinone, diphenylketene and trans-chalcone, while ZnCl_2 trapped the remaining carbene as an insoluble coordination polymer (*Angew. Chem. Int. Ed.* 2017, 56, 7948-7951).



Timmerman: We report a one-pot ligation/cyclization technology for the rapid and clean conversion of linear peptides into tricyclic peptides that is based on using tetravalent scaffolds containing two benzyl bromide and two alkyne moieties. These react via CLIPS/CuAAC reactions with cysteines and azides in the peptide. Flexibility in the scaffolds is key to the formation of isomerically pure products as the flexible scaffolds **T4**₁ and **T4**₂ mostly promote the formation of single isomeric tricycles while the rigid scaffolds **T4**₃ and **T4**₄ do not yield clean products. There seems to be no limitation to the number and types of amino acids present as 18 canonical amino acids were successfully implemented. We also observed that azides at the peptide termini and cysteine residues in the center gave better results than compounds with the functional groups placed the other way round (Angew. Chem. **2018**, 57(2), 501-505).



Key publications 2016-2017

- Steemers, L.; Wanner, M.J.; Lutz, M.; Hiemstra, H.; Van Maarseveen, J.H.; Synthesis of spiro quasi[1]catenanes and quasi[1]rotaxanes via a templated backfolding strategy, *Nature Communications* **2017**, 8, 15392.
- Steemers, L.; Wanner, M.J.; Ehlers, A.W.; Hiemstra, H.; Van Maarseveen, J.H.; A short covalent synthesis of an all-carbon ring [2]rotaxane, *Org. Lett.* **2017**, 19, 2342-2345.
- Liu, Y.; Sauri, J.; Mevers, E.; Pecuh, M.W.; Hiemstra, H.; Clardy, J.; Martin, G.E.; Williamson, R.T.; Unequivocal determination of complex molecular structures using anisotropic NMR measurements, *Science* **2017**, 356.
- Naksomboon, K.; Valderas, C.; Gomez-Martinez, M.; Alvarez-Casao, Y.; Fernández Ibáñez, M.A.; S,O-Ligand-Promoted Palladium-Catalyzed C-H Functionalization Reactions of Nondirected Arenes. *ACS Catal.* **2017**, 7, 6342-6346.
- Naksomboon, K.; Valderas, C.; Maciá, B.; Fernández Ibáñez, M.A.; Synthesis of α -Substituted Diphenylphosphinocarboxylic Acids and Their Palladium Complexes. *Synlett* **2017**, 28, 221-224.
- Borger, J.E.; Ehlers, A.W.; Lutz, M.; Slootweg, J.C.; Lammertsma, K.; Selective [3+1] Fragmentations of P₄ by "P" Transfer from a Lewis Acid Stabilized [RP₄]⁻ Butterfly Anion, *Angew. Chem. Int. Ed.* **2017**, 56, 285-290.

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- Habraken, E.R.M.; Mens, L.C.; Nieger, M.; Lutz, M.; Ehlers, A.W.; Slootweg, J.C.; Reactivity of the geminal phosphinoborane $t\text{Bu}_2\text{PCH}_2\text{BPh}_2$ towards alkynes, nitriles, and nitrilium triflates, *Dalton Trans.* **2017**, *46*, 12284–12292.

Important Grants and Prizes in 2017

Grants:

- Van Maarseveen: NWO-ECHO grant "A scaffold-directed backfolding approach towards the lasso peptide series".
- Slootweg: Shell sponsors a 2 yr-postdoc (318 k€) on the metal-free activation and functionalization of methane.
- Slootweg: STW Take-off grant (NWO grant no 16041) for the development of a circular phosphorus economy (40 k€)

Prizes:

- Hiemstra: Lecture Award at the 17th International Conference on Heterocycles in Bioorganic Chemistry, Galway, Ireland (Event), 29 May 2017 – 31 May 2017

Synthetic Organic Chemistry (RU)

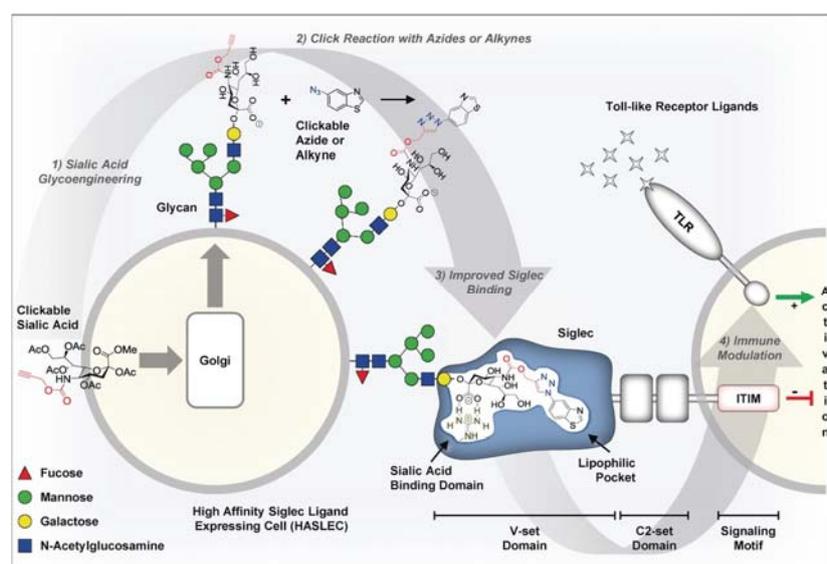
Prof. dr. F.P.J.T. Rutjes, Dr. T.J. Boltje, Dr. M.C. Feiters, Dr. J. Mecinovic (RU)

Research topics

- Small molecule synthesis
- Click chemistry
- Continuous flow chemistry
- Carbohydrate chemistry
- Chemical epigenetics
- Viedma ripening
- NMR hyperpolarization

Group highlights 2017

Boltje group: Sialic acid sugars that terminate cell-surface glycans form the ligands for the sialic acid binding immunoglobulin-like lectin (Siglec) family, which are immunomodulatory receptors expressed by immune cells. Interactions between sialic acid and Siglecs regulate the immune system, and aberrations contribute to pathologies like autoimmunity and cancer. Sialic acid/Siglec interactions between living cells are difficult to study owing to a lack of specific tools. Here, we report a glycoengineering approach to remodel the sialic acids of living cells and their binding to Siglecs. Using bioorthogonal chemistry, a library of cells with more than sixty different sialic acid modifications was generated that showed dramatically increased binding toward the different Siglec family members. Rational design reduced cross-reactivity and led to the discovery of three selective Siglec-5/14 ligands. Furthermore, glycoengineered cells carrying sialic acid ligands for Siglec-3 dampened the activation of Siglec-3⁺ monocytic cells through the NF- κ B and IRF pathways (*Angew. Chem. Int. Ed.* **2017**, *56*, 3309-3313).



Key publications 2016-2017

- Al Temimi, A. H. K.; Boltje, T. J.; Zollinger, D.; Rutjes, F. P. J. T.; Feiters, M. C., Peptide-Appended Permethylated beta-Cyclodextrins with Hydrophilic and Hydrophobic Spacers. *Bioconjugate Chemistry* **2017**, *28* (8), 2160-2166.
- Al Temimi, A. H. K.; Reddy, Y. V.; White, P. B.; Guo, H.; Qian, P.; Mecinovic, J., Lysine Possesses the Optimal Chain Length for Histone Lysine Methyltransferase Catalysis. *Scientific Reports* **2017**, *7*.
- Bernar, I.; Fiser, B.; Blanco-Ania, D.; Gomez-Bengo, E.; Rutjes, F. P. J. T., Pd-Catalyzed Hydroamination of Alkoxyallenes with Azole Heterocycles: Examples and Mechanistic Proposal. *Organic Letters* **2017**, *19* (16), 4211-4214.
- Bull, C.; Collado-Camps, E.; Kers-Rebel, E. D.; Heise, T.; Sondergaard, J. N.; den Brok, M. H.; Schulte, B. M.; Boltje, T. J.; Adema, G. J., Metabolic sialic acid blockade lowers the activation threshold of moDCs for TLR stimulation. *Immunology and Cell Biology* **2017**, *95* (4), 408-415.
- Bull, C.; Heise, T.; van Hilten, N.; Pijnenborg, J. F. A.; Bloemendal, V.; Gerrits, L.; Kers-Rebel, E. D.; Ritschel, T.; den Brok, M. H.; Adema, G. J.; Boltje, T. J., Steering Siglec-Sialic Acid Interactions on Living Cells using Bioorthogonal Chemistry. *Angewandte Chemie-International Edition* **2017**, *56* (12), 3309-3313.
- Cavina, L.; van der Born, D.; Klaren, P. H. M.; Feiters, M. C.; Boerman, O. C.; Rutjes, F. P. J. T., Design of Radioiodinated Pharmaceuticals: Structural Features Affecting Metabolic Stability towards in Vivo Deiodination. *European Journal of Organic Chemistry* **2017**, (24), 3387-3414.
- Gilissen, P. J.; Blanco-Ania, D.; Rutjes, F. P. J. T., Oxidation of Secondary Methyl Ethers to Ketones. *Journal of Organic Chemistry* **2017**, *82* (13), 6671-6679.
- Padial, J. S.; Poater, J.; Nguyen, D. T.; Tinnemans, P.; Bickelhaupt, F. M.; Mecinovic, J., Stabilization of 2,6-Diarylanilinum Cation by Through-Space Cation-pi Interactions. *Journal of Organic Chemistry* **2017**, *82* (18), 9418-9424.

Important Grants and Prizes in 2017

- T.J. Boltje: ERC Starting Grant

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 detection of microplastics, Raman-based medical diagnosis and depth analysis through non-transparent 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.

The **Hybrid Solar Energy Conversation group** (VU) studies organic, hybrid, and nanostructured semiconductors for solar energy applications. We are known for our expertise in impedance spectroscopy. With this technique we investigate the electrical transport properties of semiconducting films as a function of chemical structure, film composition, and morphology. Further, we combine impedance spectroscopy with modelling to identify relevant interfacial phenomena, thereby gaining insight into design parameters for more efficient and stable solar cell architectures. We recently developed a new approach that couples vibrational and impedance spectroscopies in a single measurement. This allows us to elucidate structure-function relationships semiconducting and electroactive materials in-situ.

In the **Raymond and Beverly Sackler Laboratory for Astrophysics** (UL) experimental studies are performed that focus on simulating the chemical processes in

the inter- and circumstellar 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. A recent focus has been on extending the Leiden Database for Ice to provide the spectra needed to search for ice spectra that will be recorded with the James Webb Space Telescope (launch 2021). 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. A main focus has been on the formation of so called iCOMs (interstellar complex organic molecules) under dark core, i.e, prestellar conditions and for settings that are needed to understand the physical and chemical processes in protoplanetary disks.

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 group at FELIX (RU)** aims 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 sustainable 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-uv 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 Spectroscopy

Dr. F. Ariese (VU)

- Pico-second time-gated Raman spectroscopy for analyzing non-transparent 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
- Raman-based medical diagnosis

Group highlights 2017

Our home-built setup for stimulated Raman scattering (SRS) was used within the framework of several interesting and highly relevant interdisciplinary studies. Miriam Moester could visualize in a non-invasive way the number, shape and size of adipocytes (fat cells) in zebrafish embryos. It was found that the development of these cells is strongly influenced by the diet received during the first days of their lives.

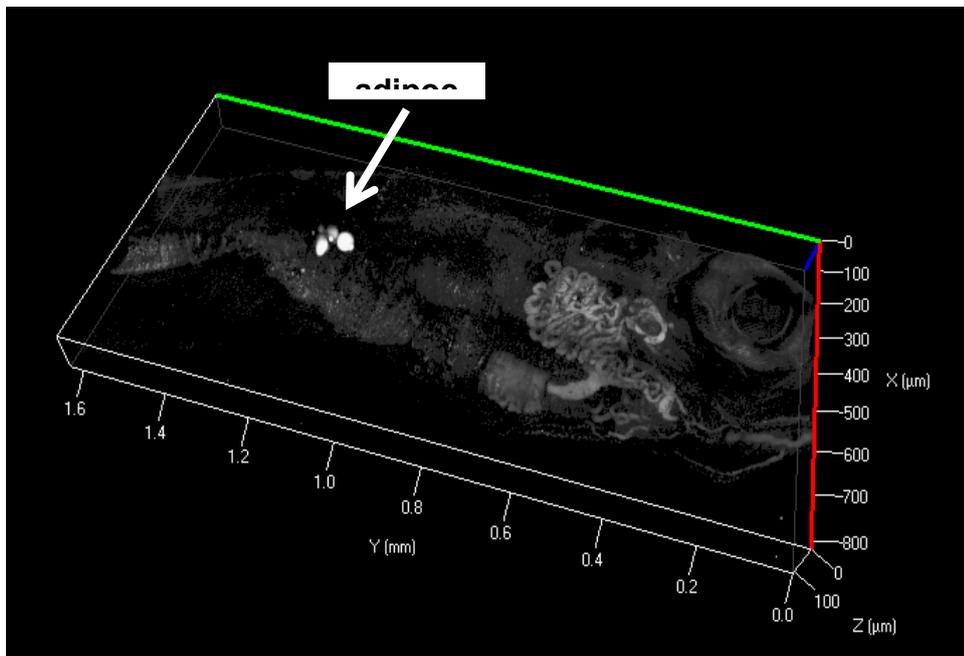


Figure: Stimulated Raman scattering detects the presence of adipocytes (fat cells) inside a zebrafish embryo. Target wavenumber: 2845 cm^{-1} (CH_2 stretch).

In a separate project, Liron Zada used SRS to detect and identify microplastic particles in sediment samples from the Rotterdam harbour area. Using density separation, filtration, SRS at 6 specific wavenumber combinations and a multiplexing algorithm, five different types of polymers could be detected.

Key publications 2016-2017

- Broeder, M.J.; Moester, M.J.B.; Kamstra, J.H.; Cenijn, P.; Davidoiu, V.; Kamminga, L.M.; Ariese, F.; de Boer, J.F.; Legler, J.; Altered adipogenesis in zebrafish larvae

following high fat diet and chemical exposure is visualised by Stimulated Raman Scattering Microscopy *Environ. Health Persp.* **2017**, 18, art # 894.

- van Hoorn, C.H.; Wessels, C.; Ariese, F.; Mank, A.J.G.; Fast high resolution screening method for reactive surfaces by combining atomic force microscopy and surface enhanced Raman scattering, *Appl. Spectrosc.* **2017**, 71, 1551-1559.

Important Grants and Prizes in 2017

- STW-Open Technologie program: Toolbox for studying the Chemistry Of Light-induced Degradation (TooCOLD), in collaboration with Maarten van Bommel (PI), Peter Schoenmakers, Pim de Voogt (UvA) en Govert Somsen (VU), total project costs 935 kE for 2 AIOs and 1 PD.

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

Group highlights 2017

NMR and TEM structure determination of a light-harvesting compound

Hybrid magic-angle spinning (MAS) NMR spectroscopy and TEM were demonstrated for *de novo* structure determination of para-crystalline materials with a bioinspired fused naphthalene diimide (NDI)–salphen–phenazine prototype light-harvesting compound. Starting from chiral building blocks with C_2 molecular symmetry, the asymmetric unit was determined by MAS NMR spectroscopy, index low-resolution TEM diffraction data, and resolve reflection conditions, and for the first time the ability to determine the space group from reciprocal space data using this hybrid approach was shown. Refinement with heteronuclear distance constraints confirmed the racemic $P2/c$ packing that was scaffolded by molecular recognition of salphen zinc in a pseudo-octahedral environment with bromide and with alkyl chains folding along the phenazine. The NDI light-harvesting stacks ran orthogonal to the intermolecular electric dipole moment present in the solid. Finally, the orientation of flexible lamellae on an electrode surface was determined.

Simulations of large-scale systems for applications in nanotechnologies

We have extended an existing hybrid MD-SCF simulation technique that employs a coarsening step to enhance the computational efficiency of evaluating non-bonded particle interactions. This technique is conceptually equivalent to the single chain in mean-field (SCMF) method in polymer physics. In contrast to SCMF, however, MD-SCF evolves particle coordinates by the usual Newton's equation of motion. Since collisions are seriously affected by the softening of non-bonded interactions, we have devised a way to reinsert the effect of collisions on the structural evolution by merging MD-SCF with multi-particle collision dynamics (MPCD). The resulting hybrid MD-SCF/MPCD method was validated for a particular coarse-grained model of phospholipids in aqueous solution. Our results show that efficiency is improved, as properly accounting for hydrodynamic interactions considerably speeds up the phase separation dynamics. This new method enables realistic simulations of large-scale systems that are needed to investigate the applications of self-assembled structures of lipids in nanotechnologies.

An Arabidopsis mutant with high operating efficiency of Photosystem II

The overall light energy to biomass conversion efficiency of plant photosynthesis is generally regarded as low. Forward genetic screens in *Arabidopsis* have yielded very few mutants with substantially enhanced photochemistry. Here, we report the isolation of a novel *Arabidopsis* mutant with a high operating efficiency of Photosystem II and low chlorophyll fluorescence from a library of lines harboring T-DNA constructs encoding artificial transcription factors. This mutant was named Low Chlorophyll Fluorescence 1 (LCF1). Only a single T-DNA insertion was detected in LCF1. Although LCF1 plants had decreased rosette surface area and biomass under normal growth conditions, they

contained more starch per gram fresh weight. The growth defect of LCF1 was alleviated by low light and short day conditions, and growth could even be enhanced after a period of dark-induced senescence, showing that the plant can utilize its excess photosynthetic conversion capacity as a resource when needed.

A.Quantum-mechanical Study of the Binding Pocket of Proteorhodopsin

Proteorhodopsin is a light-driven proton pumping membrane protein related to bacteriorhodopsin. It contains an all-trans retinal chromophore covalently bound to a lysine residue via a protonated Schiff base (PSB). We exploited DFT calculations to investigate the retinal binding pocket in the dark state and after photoisomerization. The model of the binding pocket is constructed incrementally by adding the residues near the retinal that are necessary to ensure a stable PSB. The presence of a few water molecules near the Schiff base turns out to be an essential feature of the model. The absorption properties studied using time-dependent DFT (TDDFT) further validate the structural model. TDDFT results reproduce the main experimental absorption peak accurately and quantitatively determine the spectral shift induced by substituting the native all-trans retinal chromophore with different retinal analogues. *Ab initio* molecular dynamics simulations of our models before and after isomerization provide insight into experimental FTIR difference spectra.

Key publications 2016-2017

- Sevink, G.J.A.; Schmid, F.; Kawakatsu, T.; Milano, G.; Combining cell-based hydrodynamics with hybrid particle-field simulations: efficient and realistic simulation of structuring dynamics, *Soft Matter* **2017**, 13, 1594-1623.
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- Thomas, B.; Rombouts, J.; Sai Sankar Gupta, K.B.; Orru, R.V.A.; Lammertsma, K.; de Groot, H.J.M.; Determination of Controlled Self-Assembly of a Paracrystalline Material by Homology Modelling with Hybrid NMR and TEM, *Chemistry - A European Journal* **2017**, 23, 9346 – 9351.
- Ganapathy, S.; Venselaar, H.; Chen, Q.; de Groot, H.J.M.; Hellingwerf, K.J.; de Grip, W.J.; Retinal-Based Proton Pumping in the Near Infrared, *Journal of the American Chemical Society* **2017**, 139, 2338-2344.
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- Van Tol N.; Rolloos A.M.; Augustijn D.; Alia A.; de Groot H.J.M.; Hooykaas P.J.J.; van der Zaal E.J.; An Arabidopsis mutant with high operating efficiency of Photosystem II and low chlorophyll fluorescence, *Scientific Reports* **2017**, 7, 3314.
- Monti, A.; de Ruiter, J.M.; de Groot, H.J.M.; Buda, F.; A Dynamic View of Proton-Coupled Electron Transfer in Photocatalytic Water Splitting, *Journal of Physical Chemistry C* **2016**, 120, 23074–23082.
- 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, 7340-7349.

Important Grants and Prizes in 2017

- FOM/NWO-I Pilot project within 'Towards BioSolarCells'-TBSC, nr. 115; Title: 'Myleaf: fase 1' awarded in 2017.
- NWO Top Sector Chemistry Student Competition 2017 entitled "An Interdisciplinary Screening Of Proteorhodopsin Mutants For Near Infrared Proton Pumping Systems", awarded in May 2017.

Hybrid Solar Energy Conversion

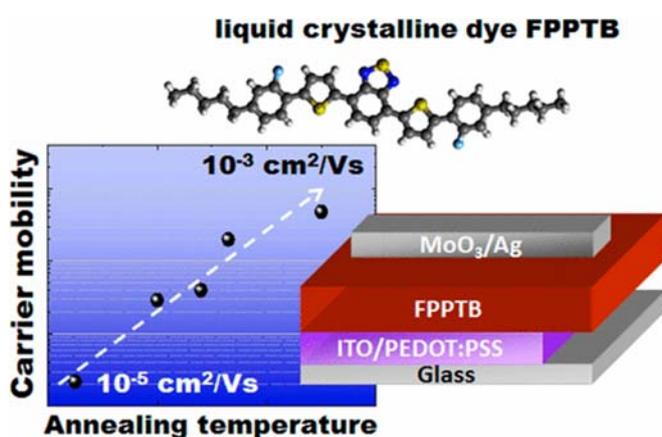
Dr. E.L. von Hauff (VU, EMS)

Research topics

- Solar energy conversion
- Organic and hybrid semiconductors
- Interfacial phenomena
- Spectroscopy

Group highlights 2017

In 2016 - 2017 the Hybrid Solar Energy group published 10 papers. One of our key publications was on results together with our cooperation partner Merck Chemicals, in which we demonstrated new insights into electrical transport properties in liquid crystalline semiconductors. Further, in this time, 1 PhD graduate and 10 undergraduates



completed lab projects in the group. The PI obtained funding from the NWO to establish a new measurement approach. The technique involves coupling impedance and Raman spectroscopies in a single measurement setup. A PhD was hired to build the setup and perform first measurements. We are currently preparing a publication based on new results.

From the publication ACS Appl. Mater. & Interfaces 9 (2017) 6228-6236: together with Merck Chemicals we studied the molecular properties of liquid crystalline dyes, and demonstrate how their unique packing properties can be exploited to realise high mobility semiconducting films for opto-electronics.

Key publications 2016-2017

- Tchamba Yimga, N.; Ramanan, C.; Borchert, H.; Parisi, J.; Untenecker, H.; Kirsch, P.; von Hauff, E.; Interplay between long range crystal order and short range molecular interactions tunes carrier mobility in liquid crystal dyes, *ACS Applied Materials & Interfaces* **2017**, 9, 6228–6236,
- MacKenzie, R.C.I.; Balderrama, V.S.; Schmeisser, S.; Stoof, R.; Greedy, S.; Pallarès, J.; Marsal, L.F.; Chanaewa, A.; von Hauff, E.; Loss mechanisms in high efficiency polymer solar cells, *Adv. Energy Mater.* **2016**, 6, 1501742.

Important Grants and Prizes in 2017

- NWO ECHO Grant *Good vibrations in organic semiconductors: a new approach to correlate molecular dynamics with carrier transport.*

Raymond and Beverly Sackler Laboratory Astrophysics and Astrochemistry

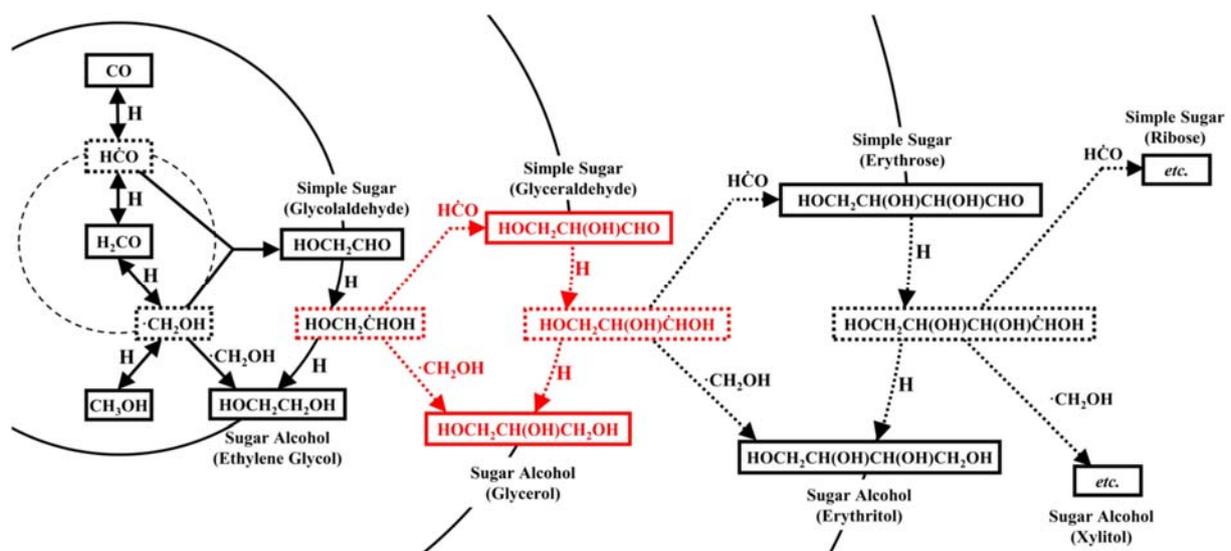
Prof. dr. H. Linnartz, Dr. J. Bouwman (UL)

Research topics

- Laboratory astrophysics and astrochemistry
- High resolution IR (2500-4000 cm^{-1}) and UV/VIS (200-1000 nm) spectroscopy of molecular transients of astrophysical interest
- Interstellar ice: spectroscopy and molecular dynamics
- Astronomical observations (ALMA, Very Large Telescope, Hubble Space Telescope, James Webb Space Telescope)

Group highlights 2017

The identification of interstellar complex organic molecules (i-COMs) in prestellar cores, i.e., cold environments in which thermally induced chemistry can be excluded and radiolysis is limited to cosmic-ray induced UV photons, is particularly important as this stage sets up the initial chemical composition from which ultimately stars and planets evolve. Recent laboratory results from our lab (MNRAS 448 (2015) 1288) demonstrate that molecules as complex as glycolaldehyde and ethylene glycol are efficiently formed on icy dust grains via nonenergetic atom addition reactions between accreting H atoms and CO molecules, a process that dominates surface chemistry during the "CO freeze-out stage" in dense cores. In 2017 we were able to extend this reaction network with the formation of the biologically relevant molecule glycerol, a three-carbon-bearing sugar alcohol necessary for the formation of membranes of living cells (Astrophys. J. 842 (2017) A5), see figure. So far all astronomical observations are fully consistent with this scheme.



Key publications 2016-2017

- Spieler, S.; Kuhn, M.; Postler, J.; Simpson, M.; Wester, R.; Scheier, P.; Ubachs, W.; Bacalla, X.; Bouwman, J.; Linnartz, H.; C₆₀⁺ and the diffuse interstellar bands; an independent laboratory check, *ApJ* **2017**, 846, 168.
- Fedoseev, G.; Chuang, K.-J.; Ioppolo, S.; Qasim, D.; van Dishoeck, E.F.; Linnartz, H.; Formation of glycerol through hydrogenation of CO ice under prestellar core conditions, *ApJ* **2017**, 842 (2017) A52.
- De Haas, A.J.; Oomens, J.; Bouwman, J.; Facile pentagon formation in the dissociation of polyaromatics; *PCCP* 19 (2017) 2974.
- Zhen, J.; Castellanos, P.; Bouwman, J.; Linnartz, H.; Tielens, A.G.G.M.; Infrared spectra of hexa-peri-hexabenzocoronene cations: HBC⁺ and HBC²⁺, *ApJ* **2017**, 836, A28.
- Bouwman, J.; de Haas, A.J.; Oomens, J.; Spectroscopic evidence for the formation of pentalene(+) in the dissociative ionization of naphthalene, *Chem. Comm.* **2016**, 52, 2636.
- Kuhn, M.; Renzler, M.; Postler, J.; Ralser, S.; Spieler, S.; Simpson, M.; Linnartz, H.; Tielens, A.G.G.M.; Cami, J.; Mauracher, A.; Wang, Y.; Alcamí, M.; Martín, F.; Beyer, M.K.; Wester, R.; Lindinger, A.; Scheier, P.; Atomically resolved phase transition of fullerene cations solvated in helium droplets, *Nature Communications* **2016**, 7, 13550.
- 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, *MNRAS* **2016** 455, 1702.

Important Grants and Prizes in 2017

- Dr. J. Bouwman: VIDI grant
- Three PhD grants within context of Dutch Astrochemistry Network

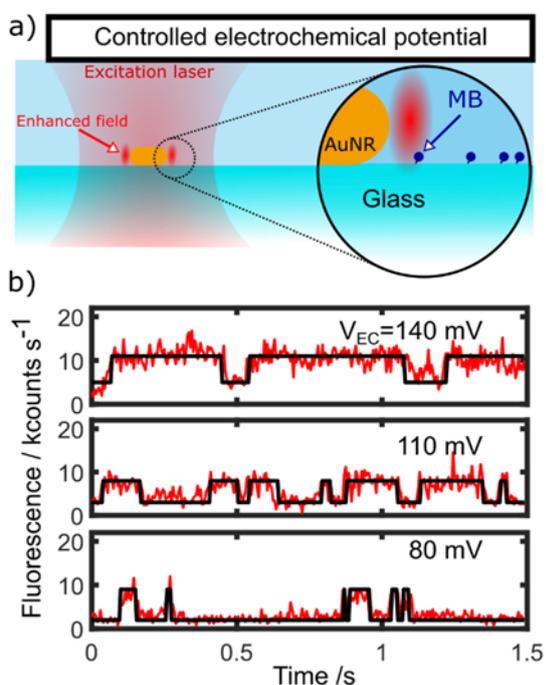
Molecular Nano-Optics and Spins

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).
- Single-molecule fluorescence and absorption spectroscopy, microscopy of single metal nanoparticles, optical trapping and diffusion of single nanoparticles.

Group highlights 2017



Highlight: Single-Molecule Electrochemistry
Fluorescence enhancement by single gold nanorods makes it possible to monitor weakly fluorescent single molecules. We have applied it to methylene blue, a molecule with a quantum yield of only 4% in its colored state, too weak to measure in standard single-molecule microscopes. Thanks to plasmonic enhancement, we have followed single methylene blue molecules as a function of the applied redox potential, as shown in the Figure hereby. From blinking single-molecule fluorescence trace, we determined the mid-point potential for each molecule. This potential depends on local electrostatic conditions at the molecule's binding site on the surface. This result was published in *Angewandte Chemie*.

Key publications 2016-2017

- Hou, L.; Adhikari, S.; Tian, Y.; Scheblykin, I.G.; Orrit, M.; Absorption and Quantum Yield of Single Conjugated Polymer Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) Molecules, *NanoLett.* **2017**, 17, 1575-1581.
- Zhang, W.; Caldarola, M.; Pradhan, B.; Orrit, M.; Gold Nanorod Enhanced Fluorescence Enables Single-Molecule Electrochemistry of Methylene Blue, *Angew. Chem. Int. Ed.* **2017**, 56, 3566-3569.
- Gast, P.; Groenen, E.J.J.; EPR Interactions: g-Anisotropy, *eMagRes* **2016**, 5, 1435-1444.

Important Grants and Prizes in 2017

- Michel Orrit: Spinoza prize (NWO) 2017

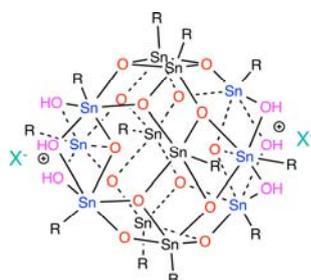
Molecular Photonics

Prof. dr. W.J. Buma, Prof. dr. A.M. Brouwer, Prof. dr. S. Woutersen, Dr. ir. A. Petrignani, 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

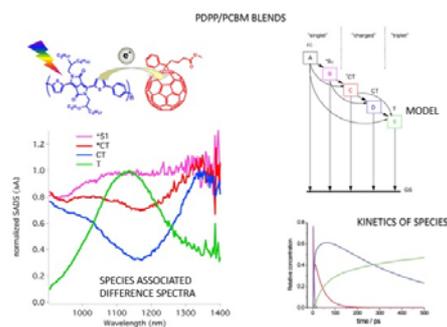
Group highlights 2017



Nanolithography In 2017 the nanophotochemistry research at the Advanced Research Center for Nanolithography has begun to bear fruit. Several papers have been published on the chemistry and patterning performance of tin-oxo cage compounds. In order to establish our position in the research community we deliberately chose specialist journals in the field instead of broader materials chemistry journals. These tin cages are potential photoresists for application with extreme ultraviolet

(EUV) light, and in some aspects resemble commercial materials that are in the test phase for application in ASML's lithography machines. We found that irradiation with UV light led to the cleavage of the tin-carbon bonds, albeit with a low quantum efficiency. Also patterning by means of EUV interference lithography was carried out successfully. We found that contrary to the previously reported results, heating of the exposed photoresist gave rise to improved sensitivity. Moreover, the sensitivity was much better than reported before.

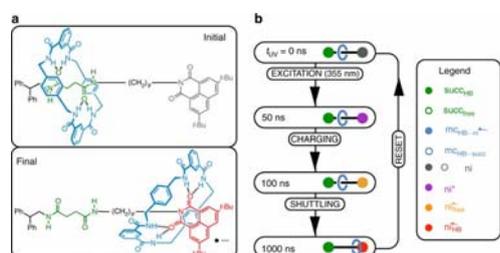
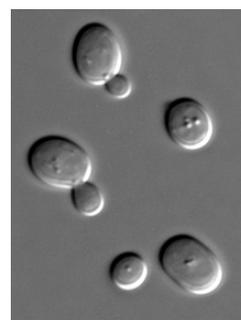
Organic Photovoltaic Materials In 2017 the work with TuE on "Ultrafast Charge and Triplet State Formation in Diketopyrrolopyrrole Low Band Gap Polymer/Fullerene Blends: Influence of Nanoscale Morphology of Organic Photovoltaic Materials on Charge Recombination to the Triplet State" was finalized. Femtosecond transient absorption spectroscopy of thin film blends of two types of morphologies is presented and indicates triplet state formation by charge recombination, an important loss channel in organic photovoltaic materials. The rate of triplet state formation is influenced by the nanoscale morphology, which not only influences interfacial area and conduction of holes and electrons but also influences the mechanism of intersystem crossing (ISC).



Photolysis induced D/H enrichment Understanding the D/H fractionation gives us insight into the evolution of the universe. The deuterium fractionation in the Universe is mainly determined by its formation during the Big Bang nucleosynthesis era and its

subsequent destruction in stellar nuclear fusion. However, in the interstellar medium (ISM), there are local variations that are not understood, even when taking dust into account as sink. PAHs, observed via their IR emission bands to be ubiquitous, could be major players if a selective processes leading to enrichment would take place. We studied the photolysis of protonated, perdeuterated PAHs (or H⁺-PADs) and deuterated PAHs (or D⁺-PAHs) at the FELIX Laboratory in Nijmegen using both UV and IR multiple photon dissociation (IRMPD) spectroscopy, recording both mass and infrared spectra. The resulting spectra showed the molecules to undergo scrambling before dissociation, removing preferentially H atoms over D atoms.

Ultrafast dynamics of “living” water We have used time-resolved spectroscopy to study water inside living organisms in real time (i.e. on the picosecond time scale). This has enabled us to test the hypothesis of ‘biological water’: the controversial but widely held view that intracellular water would be different from bulk water (see e.g. *Cells, Gels and the Engines of Life* by Gerald Pollack). We have studied different organisms, and find that in all of them the majority of intracellular water exhibits exactly the same picosecond dynamics as bulk water. This holds both for the random motion of individual water molecules (which we probe with femtosecond-IR spectroscopy), and—importantly—also for collective motion of water molecules (which we probe with dielectric-relaxation spectroscopy). A small but significant fraction of the water shows slower dynamics, because it is situated in the hydration layer of proteins or buffer ions inside the cell.

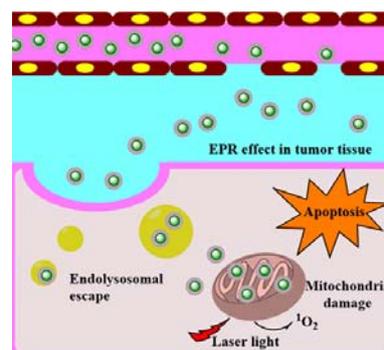


Molecular nanotechnology Molecular machinery that can be addressed optically continues to be of primary interest. In the past year we have shown how two-dimensional infrared (T2DIR) spectroscopy has allowed us to observe directly how the components of a ‘molecular shuttle’ move with respect to each other, and how their spatial

structure changes during this motion. We furthermore have been involved in gas-phase studies unravelling the exact structure of the tiny molecular motor of chemistry Nobel laureate Ben Feringa. Rotational spectroscopy revealed in this case just how the individual parts of the motor are constructed and arranged with respect to each other. Currently, the motor is the largest molecule ever successfully investigated with microwave spectroscopy. Finally, a novel class of photoswitches operating in the red part of the spectrum and based on Donor–acceptor Stenhouse adducts has been studied using ultrafast visible and IR pump–probe spectroscopies as well as quantum chemical calculations. These studies have elucidated the switching mechanism and identified key factors for improving switching characteristics.

Nanotechnology assisted photodynamic therapy

Recent advances in upconversion nanophotosensitizers (UCNPs-PS) excited by near-infrared (NIR) light have led to substantial progress in improving photodynamic therapy (PDT) of cancer. For a successful PDT, subcellular organelles are promising therapeutic targets for reaching a satisfactory efficacy. It is of vital importance for these nanophotosensitizers to reach specifically the organelles and to perform PDT with precise time control. To do so, we have traced the dynamic subcellular distribution, especially in organelles such as lysosomes and mitochondria, of the poly(allylamine)-modified and dual-loaded nanophotosensitizers. The apoptosis of the cancer cells induced by PDT demonstrated the dependence of the distribution status of the nanophotosensitizers in organelles, which has provided an in-depth picture of intracellular trafficking of organelle-targeted nanophotosensitizers, which shall facilitate the improvement of nanotechnology assisted photodynamic therapy of cancers.



Key publications 2016-2017

- Chang, Y.; Li, X.; Zhang, L.; Xia, L.; Liu, X.; Li, C.; Zhang, Y.; Tu, T.; Xue, B.; Zhao, H.; Zhang, H.; Kong, X.; Precise photodynamic therapy of cancer via subcellular dynamic tracing of dual-loaded upconversion nanophotosensitizers, *Sci. Rep.* **2017**, 45633, 1-10
- Di Donato, M.; Lerch, M.M.; Lapini, A.; Laurent, A.D.; Iagatti, A.; Bussoti, L.; Ihrig, S.P.; Medved, M.; Jacquemin, D.; Szymański, W.; Buma, W.J.; Foggi, P.; Feringa B.L.; Shedding light on the photo-isomerization pathway of donor-acceptor Stenhouse adducts, *J. Am. Chem. Soc.* **2017**, 139, 15596-15599.
- Domingos, S.R.; Cnossen, A.; Buma, W.J.; Browne, W.R.; Feringa, B.L.; Schnell, M.; Cold snapshot of a molecular rotary motor captured by high-resolution rotational spectroscopy, *Angew. Chem. Int. Ed.* **2017**, 56, 11209-11212.
- Panman, M.R.; van Dijk, C.N.; Huerta-Viga, A.; Sanders, H.J.; Bakker, B.H.; Leigh, D.A.; Buma, W.J.; Brouwer, A.M.; Woutersen, S.; Transient two-dimensional vibrational spectroscopy of an operating molecular machine, *Nat. Commun.* **2017**, 8, 2206.
- Tros, M.; Zheng, L.; Hunger, J.; Bonn, M.; Bonn, D.; Smits, G.; Woutersen, S.; Picosecond orientational dynamics of water in living cells, *Nat. Commun.* **2017**, 8, 904.
- 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, *Sci. Adv.* **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, *J. Phys. Chem. Lett.* **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, *Chem. Eur. J.* **2016**, 22, 5489-5493.

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- 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., *Nat. Commun.* **2016**, 7, 12633.
 - Maltseva, E.; Petrigani, A.; Candian, A.; Mackie, C.J.; Huang, X.; Lee, T.J.; Tielens, A.G.G.M.; Oomens, J.; Buma, W.J.; High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons in the 3- μ m region: Role of periphery, *Astrophys. J.* **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, *Chem. Eur. J.* **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? *J. Phys. Chem. Lett.* **2016**, 7, 4285-4290.

Important Grants and Prizes in 2017

Prizes

- Brouwer: Honda-Fujishima award of Japanese Photochemistry Association

Grants

- Buma, Rijs: *High-resolution vibrational and electronic spectroscopy of the isolated aromatic universe*, NWO Astrochemistry DAN-II, k€ 214 (1 PhD student)
- Petrigani: *The reaction dynamics of ionic and neutral PAHs*, NWO Astrochemistry DAN-II, k€ 214 (1 PhD student)
- Reek, Koch, Detz, Brouwer, Sinke, Garnett: *Redox Mediators in Dye-sensitized Photoelectrochemical Cells for CO₂-reduction*, NWO Solar to Products, k€ 557.
- ELENA Consortium (Brouwer member): *ELENA Low energy electron driven chemistry for the advantage of emerging nano-fabrication methods*, European Commission, HORIZON 2020 program, k€ 1067 (k€ 255, 1 PhD student at ARCNL; defence at UvA).
- Buma, Janssen (MassSpecpecD BV): *Thermo-elevated PiezoValve*, NWO-KIEM, k€ 19 (3 months postdoc).
- CANCER consortium (Zhang member): *CANCER (Immunotherapy Approaches To Improving Cancer Outcome and Quality of Life)*, H2020-MSCA-RISE-2017, No 777682, k€ 1067 (24 months PhD students at UvA).

Molecular Structure and Dynamics – FELIX

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

Research topics

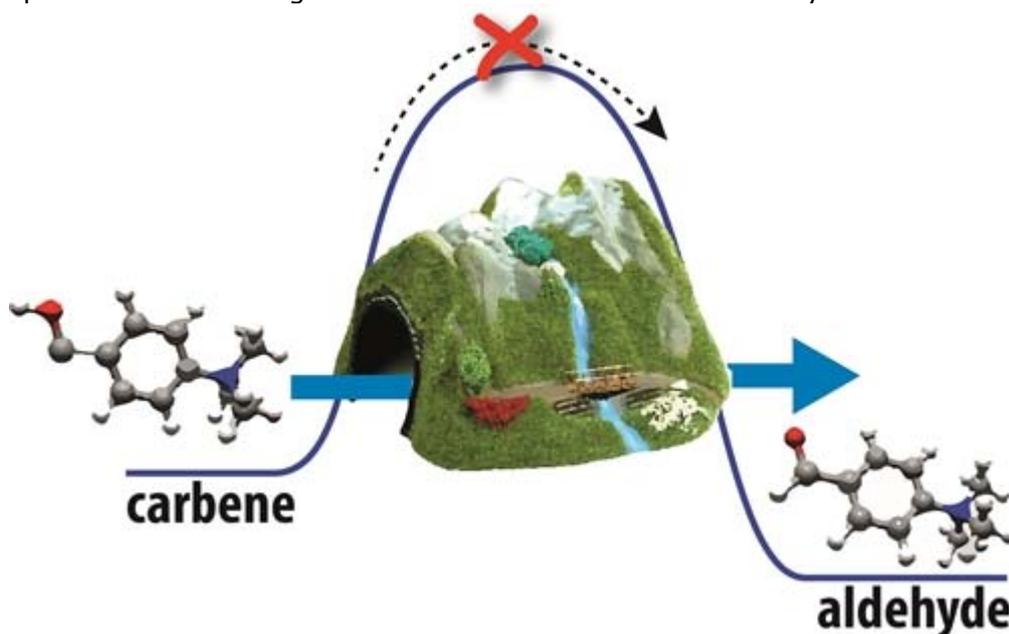
- Structure of peptides
- Far-Infrared Spectroscopy to probe Hydrogen Bond Signatures
- Biomarker discovery via IR ion spectroscopy (IRIS)
- Ion Chemistry
- Astrochemistry

Group highlights 2017

Observation of hydrogen tunneling in an isolated system at room temperature

Tunneling is a quantum-mechanical phenomenon where a particle proceeds from one side of a potential barrier to the other even though it possesses an energy that is lower than the barrier height, a process that is classically strictly forbidden. This phenomenon is postulated to play a crucial role in low temperature chemistry, for instance in astrochemistry, where thermal reactivity is inherently low. Various electron transfer processes in biochemistry and catalysis at room temperature have also been attributed to tunneling. In collaboration with researchers from the universities of Cologne (D) and Sheffield (UK), a particularly clear example of room-temperature tunneling of a hydrogen atom in an isolated system was uncovered.

The researchers prepared a molecular ion possessing a hydroxycarbene moiety and mass-isolated it in an ion trap mass spectrometer. The molecular structure of the ion is established by its in-situ recorded IR spectrum facilitated by use of the tunable IR radiation from the free electron laser. Varying the storage time of the ions in the trap, the IR spectrum recorded after different delay times is observed to change, indicating the spontaneous rearrangement of the carbene ion to its aldehyde isomer.



Key publications 2016-2017

Selective C–H Bond Cleavage in Methane by Small Gold Clusters.

S.M. Lang, T.M. Bernhardt, V. Chernyy, J.M. Bakker, R.N. Barnett, U. Landman.
Angew. Chem. Int. Ed., 2017, 56, 13406-13410.

Mapping gas phase dipeptide motions in the far-infrared and terahertz domain.

J. Mahe, D.J. Bakker, S. Jaeqx, A.M. Rijs, M.-P. Gaigeot
Phys. Chem. Chem. Phys. 2017, 19, 13778-13787.

Preparation of Labile Ni⁺(cyclam) Cations in the Gas Phase Using Electron-Transfer Reduction through Ion–Ion Recombination in an Ion Trap and Structural Characterization with Vibrational Spectroscopy

M.U. Munshi, S.M. Craig, G. Berden, J. Martens, A.F. DeBlase, D.J. Foreman, S.A. McLuckey, J. Oomens, M.A. Johnson
J. Phys. Chem. Lett. 2017, 8, 5047-5052.

Molecular identification in metabolomics using infrared ion spectroscopy

J. Martens, G. Berden, R.E. van Outersterp, L.A.J. Kluijtmans, U.F. Engelke, C.D.M. van Karnebeek, R.A. Wevers, J. Oomens
Scientific Reports 2017, 7, 3363

Hydrogen Tunneling above Room Temperature Evidenced by Infrared Ion Spectroscopy

M. Schäfer, K. Peckelsen, M. Paul, J. Martens, J. Oomens, G. Berden, A. Berkessel, A.J.H.M. Meijer
J. Am. Chem. Soc., 2017, 139, 5779–5786

Combined Liquid Chromatography-Infrared Ion Spectroscopy for Identification of Regioisomeric Drug Metabolites

J. Martens, V. Koppen, G. Berden, F. Cuyckens, J. Oomens,
Anal. Chem. 2017, 89, 4359–4362

Important Grants and Prizes in 2017

- NWO TTW Open Technology Program (15769): *IRIS: a new dimension in mass spectrometry* (Oomens)
- NWO Dutch Astrochemistry Network (Rijs, Oomens)

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)

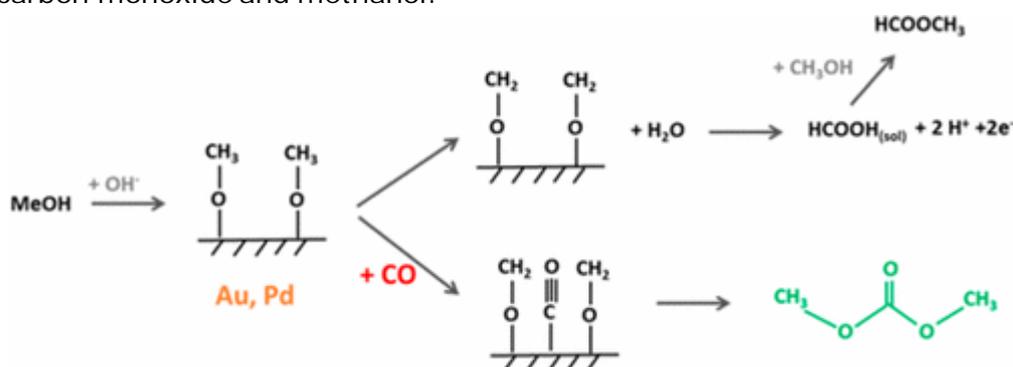
Research topics

- 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 2017

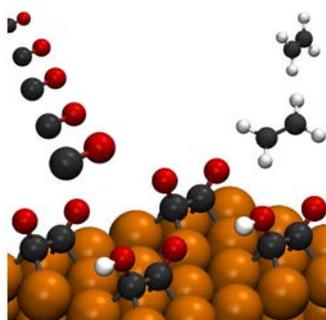
Electrochemical synthesis of dimethylcarbonate in JACS

Marta Figueiredo, in collaboration with colleagues from Covestro in Germany, has elucidated the mechanism by which dimethylcarbonate can be formed electrochemically from carbon monoxide and methanol:



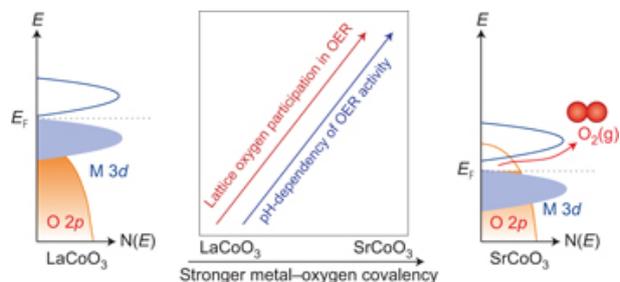
Spectroscopic evidence for CO dimer during CO reduction on copper

A paper by Elena Perez-Gallent in *Angewandte Chemie* gives spectroscopic evidence for CO dimerization during electrocatalytic CO reduction on copper electrodes.



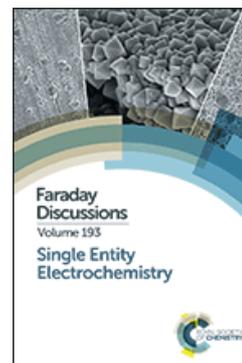
New oxygen evolution mechanism in Nature Chemistry

A collaborative paper between MIT and our group gives experimental and computational evidence for a new mechanism for oxygen evolution on perovskite electrodes in alkaline media.

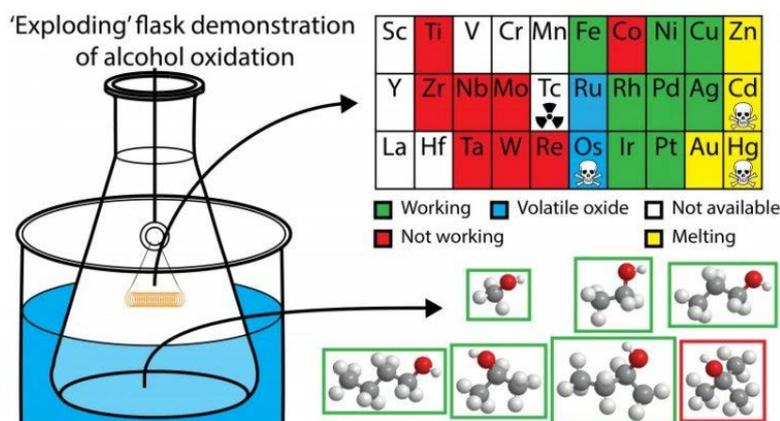


Cathodic corrosion of gold and rhodium on the cover of Faraday Discussions

A paper by Thom Hersbach features on the cover of the Faraday Discussions issue on “Single Entity Electrochemistry”



Leon Jacobse en Ludo Juurlink hebben met een groep BSc studenten van de opleiding MST twee artikelen gepubliceerd over een bekende chemische demonstratie in the Journal of Chemical Education. Op één van de artikelen is Rick Spierenburg, zelf nog BSc student, zelfs eerste auteur. De demonstratie laat zien hoe methanol katalytisch oxideert op een platina draad, die gaat gloeien door de vrijkomende reactiewarmte. Er kunnen zelfs kleine explosies bij ontstaan. In hun LO3 onderzoeksproject hebben de studenten variaties op de demonstratie en de chemisch achtergrond ervan onderzocht. Ze kwamen tot de conclusie dat er veel fouten in voorgaande literatuur staan. In één artikel laten ze zien dat de demonstratie ook werkt met veel andere overgangsmetalen en veel andere kleinere alcoholen. In het andere artikel laten ze zien dat, in tegenstelling tot eerdere suggesties, de oxidatie niet vooral verloopt door vorming van methanal, maar dat oxidatie door gaat tot vorming van CO en CO₂. Daarbij wordt ook H₂ gevormd wat waarschijnlijk de oorzaak is van de explosies. De publicatie van deze twee artikelen illustreert hoe met vrij eenvoudige middelen en ideeën BSc studenten uitstekend kunnen bijdragen aan wetenschappelijk onderzoek.



Cum laude voor begrijpen katalysator bij extreme omstandigheden

Fysisch chemicus Rik Mom ontwikkelde een revolutionaire manier om katalysatoren in actie tot in detail te onderzoeken. Voor zijn werk kreeg hij tijdens zijn verdediging op 29 juni de onderscheiding cum laude.

Key publications 2016-2017

- Grimaud, A.; Diaz-Morales, O.; Han, B.; Hong, W.T.; Lee, Y.-L.; Giordano, L.; Stoerzinger, K.A.; Koper, M.T.M.; Shao-Horn, Y.; Activating lattice oxygen redox reactions in metal oxides to catalyze oxygen evolution, *Nature Chemistry* **2017**, 9, 457-465.
- Ledezma-Yanez, I.; Wallace, W.D.Z.; Sebastian-Pascual, P.; Climent, V.; Feliu, J.M.; Koper, M.T.M., Interfacial water reorganization as a pH-dependent descriptor of the hydrogen evolution rate on platinum electrodes, *Nature Energy* **2017**, 2, 17031.
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- Perez-Gallent, E.; Figueiredo, M.C.; Calle-Vallejo, F.; Koper, M.T.M.; Spectroscopic observation of a hydrogenated CO dimer intermediate during CO reduction on Cu(100) electrode, *Angewandte Chemie International Edition* **2017**, 57, 3621-3624.
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- Walsh, A.; van Lent, R.; Auras, S.; Gleeson, M.A.; Berg, O.T.; Juurlink, L.B.F.; Step-type and step-density influences to CO adsorption probed by Reflection Absorption Infrared Spectroscopy (RAIRS) using a curved Pt(111) surface, *Journal of Vacuum Science and Technology A* **2017**, 35, 03E102, DOI: 10.1116/1.4976617.
- van Spronsen, M.A.; Frenken, J.W.M.; Groot, I.M.N.; Observing the oxidation of platinum, *Nature Communications* **2017**, 8, 429.
- van Spronsen, M.A.; Frenken, J.W.M. Groot, I.M.N; Surface science under reaction conditions: CO oxidation on Pt and Pd model catalysts, *Chemical Society Reviews* **2017**, 46, 14, 4347-4374.
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Important Grants and Prizes in 2017

- The Electrochemistry Group of the Royal Society of Chemistry has awarded Marc Koper the 2017 Faraday Medal for his "significant contributions to various areas of electrochemistry, ranging from fundamental science to application, including theory and experiments at the highest levels."
- Yuvraj Birdja was awarded a poster prize at the 68th Annual Meeting of the International Society of Electrochemistry for his poster "The Importance of Cannizzaro-Type Reactions during Electrocatalytic Reduction of Carbon Dioxide".

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- Cathodic corrosion of gold and rhodium on the cover of Faraday Discussions: A paper by Thom Hersbach features on the cover of the Faraday Discussions issue on “Single Entity Electrochemistry”.
 - Marc Koper is one of the 26 new members of the Royal Netherlands Academy of Arts and Sciences (KNAW) in 2017.

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 Bickelhaupt, Visscher, Gori-Giorgi and Fonseca Guerra (VU) 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 wavefunction-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.

The **Theoretical Chemistry** group of Dr. J. Meyer (UL) aims at a better fundamental understanding of energy conversion at interfaces by combining existing as well as developing new computational techniques. Within this scope one particular focus is on non-adiabatic dynamics of molecules on metal surfaces, another on phonons surfaces and adsorbed overlayer structures.

The **Theoretical Chemistry group** of Prof. dr. ir. Gerrit C. Groenenboom at the RU works on explaining and predicting properties of molecules, clusters, and molecular solids. They use quantum mechanical, semiclassical, classical, and statistical mechanical methods. The approach is computational, new methods and software are developed when necessary, and they work in close collaboration with experimental groups. Research questions arise from astrochemistry and atmospheric chemistry and we study quantum phenomena in ultracold molecular collisions. The work on molecular solids is also inspired by industrial applications.

The **Biomolecular Simulation and Modeling group** of Dr. Daan P. Geerke joined HRSMC in 2017 as well. Research in the group of Daan Geerke focuses on rationalizing and predicting wanted and unwanted ligand binding to proteins, with a special focus on flexible drug-metabolizing enzymes such as Cytochrome P450s. In addition the group works on *in silico* mutagenesis of biocatalytically and pharmaceutically relevant enzymes, and there is a strong focus on developing (automated) free energy methods and polarizable force fields for use in biomolecular simulation.

Computational Chemistry

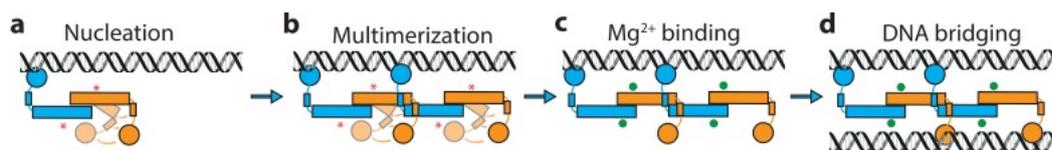
Prof. dr. P.G. Bolhuis, Prof. dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede (UvA)

Research topics

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

Group highlights 2017

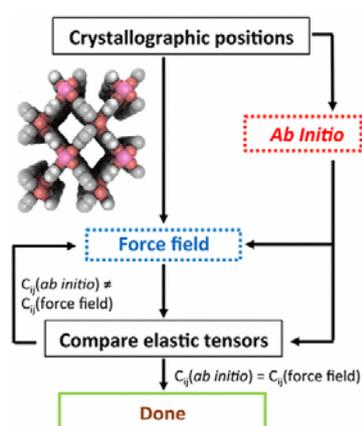
Regulating proteins (Jocelyne Vreede): Bacteria frequently need to adapt to altered environmental conditions. Adaptation requires changes in gene expression, often mediated by global regulators of transcription. The nucleoid-associated protein H-NS is a key global regulator in Gram-negative bacteria and is believed to be a crucial player in bacterial chromatin organization via its DNA-bridging activity. H-NS activity in vivo is modulated by physico-chemical factors (osmolarity, pH, temperature) and interaction partners. Mechanistically, it is unclear how functional modulation of H-NS by such factors is achieved. Here, we show that a diverse spectrum of H-NS modulators alter the DNA-bridging activity of H-NS. Changes in monovalent and divalent ion concentrations drive an abrupt switch between a bridging and non-bridging DNA-binding mode. Similarly, synergistic and antagonistic co-regulators modulate the DNA-bridging efficiency. Structural studies suggest a conserved mechanism: H-NS switches between a 'closed' and an 'open', bridging competent, conformation driven by environmental cues and interaction partners.



Model of H-NS complex assembly on DNA, based on tethered particle motion experiments, DNA bridging assays and molecular dynamics simulations.

(a) H-NS nucleates at preferred DNA sequences in the genome. (b) H-NS laterally multimerizes laterally along the DNA in the 'closed' conformation. (c) In the presence of Mg²⁺ or other H-NS modulators such as Hha, H-NS switches to the 'open', bridging capable conformation. (d) H-NS forms DNA bridges in trans. The red asterisk indicates the buckle location. Mg²⁺ ions are shown as green orbs.

Modeling Metal Organic Frameworks (David Dubbeldam): Constructing functional forms and their corresponding force field parameters for the metal–linker interface of metal–organic frameworks is challenging. We propose fitting these parameters on the

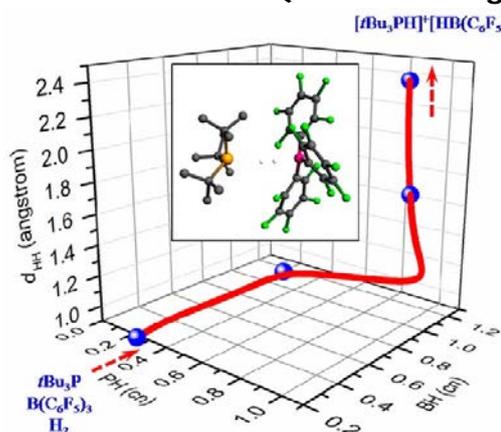


elastic tensor, computed from ab initio density functional theory calculations¹. The advantage of this top-down approach is that it becomes evident if functional forms are missing when components of the elastic tensor are off. Another advantage of this approach is that the construction of flexible force fields for *functionalized* MOFs should be straightforward. If the parent material reproduces the elastic constants well, then one can use functional forms and parameters from generic organic force fields to include the flexible modes of the substituted organic linkers. As a proof-of-concept, a new flexible force field for MIL-47(V) is derived. Negative thermal expansion is observed and framework

flexibility has a negligible effect on adsorption and transport properties for small guest molecules. We believe that this force field parametrization approach can serve as a useful tool for developing accurate flexible force field models that capture the correct mechanical behavior of the full periodic structure.

CO₂ capture and hydrogen activation by Frustrated Lewis Pairs (Bernd Ensing):

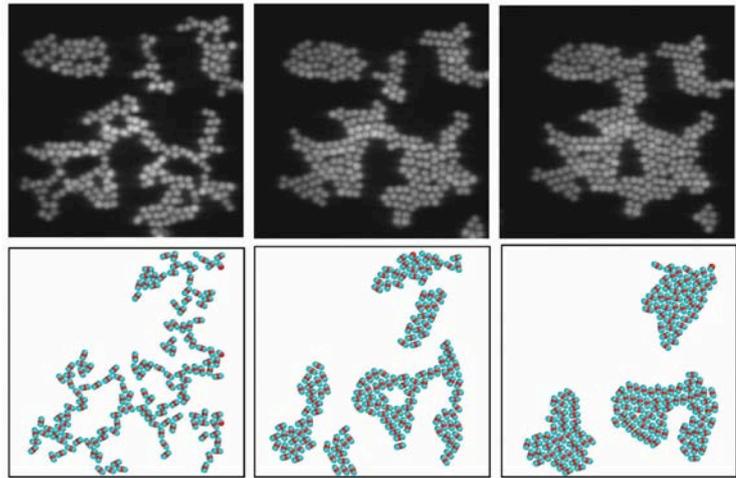
Frustrated Lewis pairs have great potential as metal-free catalysts, for example, for the activation of molecular hydrogen. However, rational design of improved catalysts is hampered because the catalytic reaction mechanisms still remain largely unclear. In this study, we present a density-functional-theory-based metadynamics study of the hydrogen activation by a typical frustrated Lewis pair, *t*Bu₃P/B(C₆F₅)₃. The computed free-energy landscape reveals a different reaction path compared with the ones in the literature. We found different roles of the Lewis acid and base centres in the hydrogen activation. The rate-determining step is the hydride transfer to the Lewis acid, and the overall reaction is found to be exothermic once the proton transfer to the Lewis base step is accomplished. Frustrated Lewis pairs (FLPs) are also known for their ability to capture CO₂. Our metadynamics simulations have now revealed the complete reaction path for the capture of CO₂ by the *t*Bu₃P/B(C₆F₅)₃ pair. In our recent publication, we propose a rule of thumb for future synthesis of FLP-based catalysts for the capture of CO₂.



Critical Casimir forces in suspensions of anisotropic particles (Peter Bolhuis)

Colloidal particles suspended in a binary liquid mixture experience an effective attraction when the temperature is raised from below towards the coexistence line of the binary mixture. This universal attraction between colloids, that occurs close to the critical point of the binary liquid, is commonly referred to as the critical Casimir force. For anisotropic

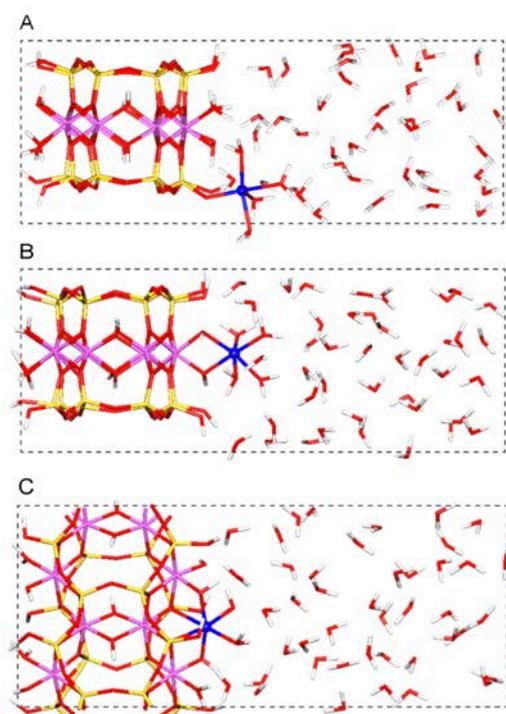
colloids this interaction becomes directional, which leads to rich phase behavior. While experimental imaging and particle tracking techniques allow determination of isotropic effective potentials via Boltzmann inversion, the modeling of effective interaction in anisotropic systems is non-trivial precisely because of this directionality. Here we extract effective interaction potentials for non-spherical dumbbell particles



from observed radial and angular distributions, by employing reference interaction site model (RISM) theory and direct Monte Carlo simulations. For colloidal dumbbell particles dispersed in a binary liquid mixture and interacting via induced critical Casimir forces, we determine the effective site–site potentials for a range of experimental temperatures. Using these potentials to simulate the system for strong Casimir forces, we reproduce the experimentally observed collapse, and provide a qualitative explanation for this behavior. The figures shows how simulations (lower part) mimic the formation of a compact, collapsed structure observed in experiments (upper part).

Metal-ion adsorption on clay surfaces (Evert Jan Meijer)

Clay minerals play important roles in the migration and retardation of heavy metal elements in nature. Because of their high adsorptive capacity, low cost, and chemical stability, clay materials are extensively used in environmental engineering. The molecular ar-scale adsorption mechanism of heavy metal cations on clay minerals is crucial for understanding the relevant interface geochemistry and developing efficient environmental materials. In this context, we used first-principles molecular dynamics (FPMD) simulations to investigate the structures, free energies and acidity constants of Ni(II) complexes adsorbed on edge surfaces of 2:1 phyllosilicates. We considered (A) mono-, (B) bi- and (C) tetra-dentate complexes, and characterized these in detail. Computed free energy values indicate that the tetradentate complex is significantly more stable than the other two. Computed free energy values indicate that the tetradentate complex is significantly more stable than the other two. The calculated acidity constants indicate that the tetradentate complex ($pK_a = 8.4$) can get deprotonated at the ambient conditions whereas the other two hardly deprotonate due to extremely high pK_a



values. This study forms a physical basis for understanding the transport and fixation of heavy metal elements in a large variety of geologic environments.

Key publications 2016-2017

- Meuzelaar, H.; Vreede, J.; Woutersen, S.; Influence of Glu/Arg, Asp/Arg, and Glu/Lys Salt Bridges on α -Helical Stability and Folding Kinetics, *Biophys. J.* **2016**, 110, 2328.
- Van der Valk, R.A.; J. Vreede, J.; Qin, L.; Moolenaar, G.F.; Hofmann, A; Goosen, N.; Dame, R.T.; Mechanism of environmentally driven conformational changes that modulate H-NS DNA-bridging activity, *eLIFE* **2017**, 6: e27369.
- Dubbeldam, D.; Calero, S.; Ellis, D.E.; Snurr, R.Q.; RASPA: Molecular Simulation Software for Adsorption and Diffusion in Flexible Nanoporous Materials, *Mol. Simulat.* **2016**, 42, 81-101.
- Heinen, J.; N.C. Burtch, N.C.; Walton, K.S.; Dubbeldam, D.; Flexible Force Field Parameterization through Fitting on the Ab Initio derived Elastic Tensor, *J. Chem. Theory. Comput.* **2017**, 13, 3722-3730.
- Tiwari, A; Ensing, B.; Reactive trajectories of the Ru^{2+/3+} self-exchange reaction and the connection to Marcus' theory, *Faraday Discuss.* **2016**, 195, 291-310.
- Liu, L.; Lukose, B.; Ensing, B.; Hydrogen activation by frustrated Lewis pairs revisited by metadynamics simulations. *J. Phys. Chem. C* **2017**, 121, 2046 – 2051.
- Pavlova, A.; Rösler, E.; Meijer, E.J.; Mechanistic Aspects of Using Formate as a Hydrogen Donor in Aqueous Transfer Hydrogenation, *ACS Catal.* **2016**, 6, 5350–5358.
- Zhang, C.; Liu, X.; Lu, X.; He, M.; Meijer, E.J.; Wang, R.; Surface complexation of heavy metal cations on clay edges: insights from first principles molecular dynamics simulation of Ni(II), *Geochim. Cosmochim. Acta* **2017**, 203, 54–68.
- 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.
- Newton, A. C.; Nguyen, T. A.; Veen, S. J.; Kraft, D. J.; Schall, P., Bolhuis, P. G.; Modelling critical Casimir force induced self-assembly experiments on patchy colloidal dumbbells, *Soft Matter* **2017**, 13, 4903-4915.

Important Grants and Prizes in 2017

- Alberto Pérez de Alba Ortíz and B. Ensing: Modeling chemical processes in solution (Mexican Science Council), 48 months PhD scholarship
- Enrico Riccardi and Jocelyne Vreede: Simulating the binding modes of the bacterial DNA organizing protein HLNS to DNA (HRSMC Fellowship Program), 3 months visiting scholarship
- Jurn Heinen: Separation by nano-porous materials (UvA 385 Anniversary Scholarship), €3.000 travel scholarship

Theoretical Chemistry (VU)

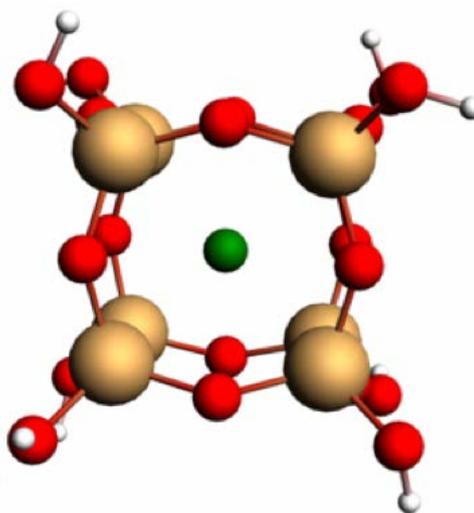
Prof. dr. F.M. Bickelhaupt, Prof. dr. L. Visscher, Prof. dr. E.J. Baerends (em.), Prof. Dr. C. Fonseca Guerra, Prof. dr. P. Gori Giorgi, Dr. I.A.C. Infante, Dr. K. Giesbertz (VU)

Research topics

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

Group highlights 2017

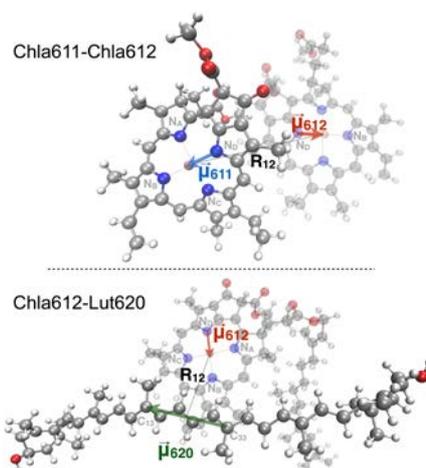
In an international collaboration (see Goesten et al., below), we have shown that a fluoride anion inside a silicate double 4-ring can form chemical bonds to the eight surrounding silicon atoms. This finding, which was published in PNAS and also highlighted in *Science*, constitutes hypervalent fluoride of exceptionally high coordination number (see illustration). Certain zeolites bind fluoride at the center of a box motif with silicons at each of eight vertices (see illustration). Using the Amsterdam Density Functional (ADF) program and Kohn-Sham MO theory, we show that all eight engage in stabilizing Si-F orbital interactions. This finding



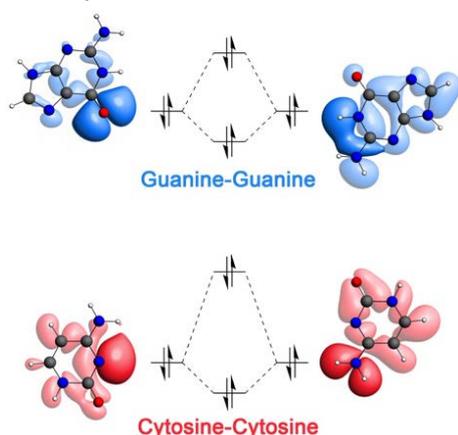
is nicely in line with, and augments our earlier findings of stable, electron-rich hypervalent carbon species that are normally transition states in S_N2 reactions.

Density functional theory (DFT) is the workhorse of theoretical and computational chemistry and solid-state physics. Although exact in principle, in practice DFT has to rely on approximations. The investigation of the exact limit of infinite electron-electron interaction of DFT put forward by the group of Gori-Giorgi, has revealed a mathematical structure completely different from that of the standard approximations used in DFT. Instead of the local density, gradients, or Kohn-Sham orbitals, in this limit certain integrals of the density play a crucial role. By rescaling and simplifying this mathematical structure, the group has proposed a new way to construct DFT approximations, which can overcome several of the present limitations of DFT. The group has also explored several different features of the strong-interaction limit, as well as other way to use the special non-locality discovered in these studies.

In a PCCP publication postdoc Pablo Lopez Tarifa investigates the accuracy of the ideal point dipole approximation (IDA) to model the interactions between chromophores in the light harvesting complexes. By comparing with supermolecular time dependent DFT calculations, he showed that IDA is accurate enough for predicting chlorophyl Coulomb couplings. However, the IDA largely overestimates chlorophyl–carotenoide interactions and should be replaced with a more detailed transition density model.



In a publication in Chem. Eur J., we demonstrated that the Pauli repulsion can be a decisive factor for relative hydrogen bonding strengths and lengths. Our study on DNA base pairs highlights the complex nature of hydrogen bonds, which are an interplay between steric, electrostatic, covalent, cooperative and π -resonance interactions, and emphasizes the importance of state-of-the-art quantum chemical analysis to shed light on their bonding mechanism. This work has been awarded the front cover and an author profile (see van der Lubbe and Fonseca Guerra).



Key publications 2016-2017

- Bickelhaupt, F.M.; Houk, K.N.; Distortion/Interaction-Activation Strain Model to Analyze Reaction Rates, *Angew. Chem. Int. Ed.* **2017**, 56, 10070-10086 (Frontispiece & Cover).
- Goesten, M.G.; Hoffmann, R.; Bickelhaupt, F.M.; Hensen, E.J.M.; 8-Coordinate Fluoride in a Silicate Double-4-Ring, *Proc. Nat. Acad. Sci.* **2017**, 114, 828-833 (highlighted in Science 2017, 355, 592-593).
- Paragi, G.; Fonseca Guerra, C.; Cooperativity in the Self-Assembly of the Guanine Nucleobase into Quartet and Ribbon Structures on Surfaces, *Chem. Eur. J.* **2017**, 23, 3042-3050 (Cover).
- Van der Lubbe, S.C.C.; Fonseca Guerra, C.; Hydrogen-Bond Strength of CC and GG Pairs Determined by Steric Repulsion: Electrostatics and Charge Transfer Overruled, *Chem. Eur. J.* **2017**, 23, 10249-10253 (Cover).
- Vuckovic, S.; Gori-Giorgi, P.; Simple Fully Nonlocal Density Functionals for Electronic Repulsion Energy, *J. Phys. Chem. Lett.* **2017**, 8, 2799 (highlighted in Spotlights).
- Grossi, J.; Kooi, D.P.; Giesbertz, K.J.H.; Seidl, M.; Cohen, A.J.; Mori-Sanchez, P.; Gori-Giorgi, P.; Fermionic Statistics in the Strongly Correlated Limit of Density Functional Theory, *J. Chem. Theory Comput.* **2017**, 13, 6089.

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- Schlüns, D.; Franchini, M.; Götz, A.W.; Neugebauer, J.; Jacob, C.R.; Visscher, L.; Analytical gradients for subsystem density functional theory within the Slater-function-based Amsterdam density functional program, *J. Comp. Chem.* **2017**, 38, 238.
 - Lopez-Tarifa, P.; Liguori, N.; Van den Heuvel, N.; Croce, R.; Visscher, L.; Coulomb couplings in solubilised light harvesting complex II (LHCII): challenging the ideal dipole approximation from TDDFT calculations, *Phys. Chem. Chem. Phys.* **2017**, 19, 18311-18320.

Important Grants and Prizes in 2017

- Bickelhaupt: Selected Member of Advanced Research Center CBBC
- Bickelhaupt: NWO Dutch Astrochemistry Network II research grant
- Visscher: NWO LIFT research grant
- Visscher: NWO JCER eScience grant
- Gori-Giorgi: NWO VICI research grant
- Gori-Giorgi: Marie Curie Intra European Fellowship (Host for Z. Musslimani)
- Gori-Giorgi: Marie Curie Intra European Fellowship (Host for A. Gerolin)

Theoretical Chemistry

Dr. J. Meyer (UL)

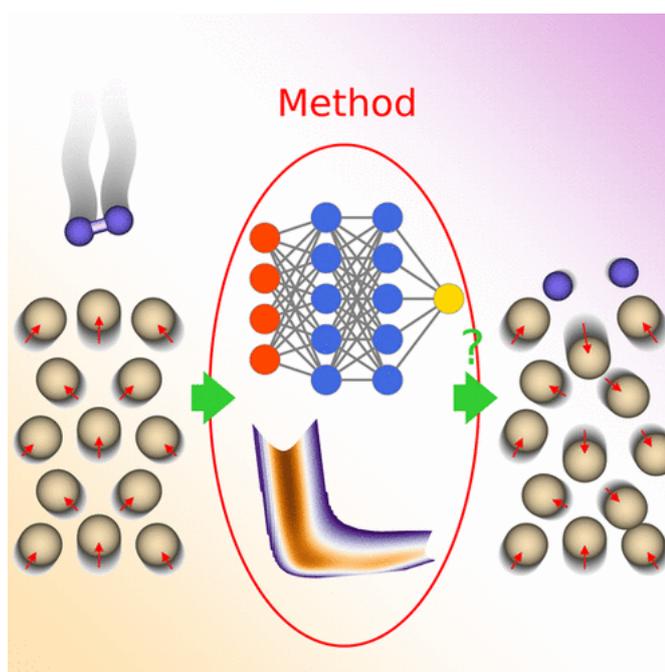
Research Topics

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

Group highlights 2017

J. Phys. Chem. Lett. **8**, 2131 (2017), Accurate Neural Network Description of Surface Phonons in Reactive Gas–Surface Dynamics: $\text{N}_2 + \text{Ru}(0001)$

Ab initio molecular dynamics (AIMD) simulations enable the accurate description of reactive molecule–surface scattering especially if energy transfer involving surface phonons is important. However, presently, the computational expense of AIMD rules out its application to systems where reaction probabilities are smaller than about 1%. Here we show that this problem can be overcome by a high-dimensional neural network fit of the molecule–surface interaction potential, which also incorporates the dependence on phonons by taking into account all degrees of freedom



of the surface explicitly. As shown for $\text{N}_2 + \text{Ru}(0001)$, which is a prototypical case for highly activated dissociative chemisorption, the method allows an accurate description of the coupling of molecular and surface atom motion and accurately accounts for vibrational properties of the employed slab model of $\text{Ru}(0001)$. The neural network potential allows reaction probabilities as low as 10^{-5} to be computed, showing good agreement with experimental results.

Key publications 2016-2017

- Shakouri, K.; Behler, J.; Meyer, J.; Kroes, G.-J.; Accurate Neural Network Description of Surface Phonons in Reactive Gas–Surface Dynamics: $\text{N}_2 + \text{Ru}(0001)$, *J. Phys. Chem. Lett.* **2017**, *8*, 2131.
- Rittmeyer, S.P.; Meyer, J.; Reuter, K.; Nonadiabatic Vibrational Damping of Molecular Adsorbates: Insights into Electronic Friction and the Role of Electronic Coherence, *Phys. Rev. Lett.* **2017**, *119*, 176808.

Theoretical Chemistry

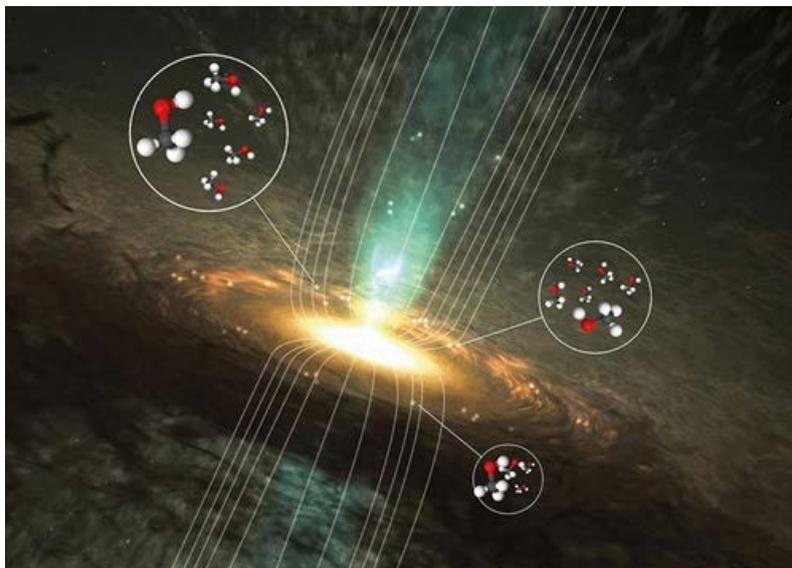
Prof. dr. ir. G.C. Groenenboom, Prof. dr. H. Cuppen, Dr. G. de Wijs, Prof. dr. A. van der Avoird (em.), Prof. dr. F.M. Bickelhaupt (by special appointment) (RU)

Research Topics

- Electronic structure and quantum dynamics of molecules

Group highlights 2017

Methanol Masers have been observed by astronomers for decades. The circular polarization of these maser carries information on the strength and orientation of the magnetic field. These fields play an important role in star formation. However, attempts to measure the magnetic properties of methanol in the lab have not been successful and the interpretation of methanol maser spectra has remained speculative. Using ab initio calculations and by quantum mechanical modeling of the rotation, internal rotation, and hyperfine structure, we have been able to determine the magnetic properties of methanol. We also discovered that different hyperfine states can have very different Landé g-factors, and this has resolved the mystery of seemingly contradictory signals from nearby methanol masers. The work was published together with the astronomers in *Nature Astronomy*.



Key publications 2016-2017

- Karman, T.; van der Avoird, A.; Groenenboom, G.C.; Line-shape theory of the $X^3\Sigma_g^- \rightarrow a^1\Delta_g, b^1\Sigma_g^+$ transitions in O_2-O_2 collision-induced absorption, *J. Chem. Phys.* **2017**, 147, 084307.
- Klein, A.; Shagam, Y.; Skomorowski, W.; Żuchowski, P.S.; Pawlak, M.; Janssen, L.M.C. Moiseyev, N.; van de Meerakker, S.Y.T.; van der Avoird, A.; Koch, C.P.; Narevicius, E.; Directly probing anisotropy in atom-molecule collisions through quantum scattering resonances, *Nature Phys.* **2017**, 13, 35.

Biomolecular Simulation and Modeling

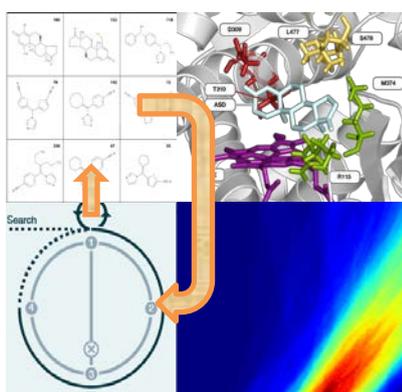
Dr. D.P. Geerke (VU, EMS)

Research Topics

- Molecular modeling and simulation of proteins to study, understand and predict ligand binding, protein activation or inhibition, and drug metabolism
- Methods for binding free energy computation
- Development of polarizable force fields for biomolecular simulation
- Automation of molecular dynamics simulation, force field parameterization and free energy calculations

Group highlights 2017

We used Molecular Dynamics (MD) simulations to rationalize impaired anticoagulant binding to blood factor FXa and to direct mutation studies towards design of first antidotes for already marketed and widely prescribed drugs (key publication 1 below). In our work on polarizable force field development we now use data from quantum and combined QM/MM calculations to derive transferable parameters for model compounds of biomolecular building blocks (*cf.* key publication 2). Another highlight (key publication 3) has been a collaboration with Bayer in which we deployed MD simulation and Linear Interaction Energy theory to infer reliable affinity models and their applicability and parameter space for industrially relevant sets of protein binders. Thereby we make profit from our efforts in automating free-energy calculations (key publication 4) that we are currently generalizing in our NLeSC-ASDI eScience project, in which we develop the *MDStudio* platform for flexible integration of molecular simulation and modeling workflows (ixa.amsia.nl/marc-van-dijk)



Key publications 2016-2017

- Verhoef, D.; Visscher, K.; Vosmeer, C.R.; Cheung, K.L.; Reitsma, P.H.; Geerke, D.P.; Bos, M.H.A.; Engineered factor Xa variants retain procoagulant activity independent of direct factor Xa inhibitors, *Nature Commun.* **2017**, *8*, 528.
- Visscher, K.M.; Vosmeer, C.R.; Luirink, R.A.; Geerke, D.P.; A systematic approach to calibrate a transferable polarizable force field parameter set for primary alcohols, *J. Comput. Chem.* **2017**, *8*, 508-517.
- Van Dijk, M.; ter Laak, A.M.; Wichard, J.D.; Capoferri, L.; Vermeulen, N.P.E.; Geerke, D.P.; Comprehensive and automated Linear Interaction Energy based binding-affinity

prediction for multifarious Cytochrome P450 Aromatase inhibitors, *J. Chem. Inf. Mod.* **2017**, *57*, 2294-2308.

- Capoferri, L.; van Dijk, M.; Rustenburg, A.S.; Wassenaar, T.A.; Kooi, D.P.; Rifai, E.A.; Vermeulen, N.P.E.; Geerke, D.P.; *eTOX ALLIES*: an automated pipeLine for Linear Interaction Energy-based simulations, *J. Cheminf.* **2017**, *9*, 58.

Important Grants and Prizes in 2017

VU-HPC grants:

- Vectorizing MD++
- Going GPU
- Bulk Synchronous Parallel Computing

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/FonsecaGuerra/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 |
| Asymmetric catalysis | Grecea/Woutersen/vdVlugt | 1 | UvA |
| Biomolecular recognition | Bickelhaupt/Mecinovic | 1.3 | VU, RU |
| Calculations on Multicomponent Syntheses | Bickelhaupt/Orru/Fonseca Guerra | 1.3 | VU |
| Catalysis in confined spaces | Reek/deBruin/vMaarseveen/ Rothenberg/Gracia/vdVlugt | 1 | UvA |
| Cation pi-interactions | Bickelhaupt/Mecinovic | 2.1 | VU/RU |
| Chemistry Behind Cu ^{II} -μ-thiolate and CuI-disulfide complexes | Bouwman/Fonseca Guerra | 1.3 | UL/VU |
| Circular dichroism in plants | Buma/Ariese | 2 | UvA/VU |
| Combined classical and quantum mechanical modelling studies on methyl transferase inhibition | Geerke/Fonseca Guerra | 3 | VU |
| Combined QM/MM computation of Cytochrome P450 binding spectra | Visscher/Ariese/Geerke | 2,3 | VU |
| Cyclizations in confined spaces | Van Maarseveen/Reek | 1 | UvA |
| Cycloaddition reactions | Bickelhaupt/Rutjes | 2.1 | VU/RU |
| 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 |
| Dispersion description in polarizable force fields | Gori-Giorgi/Geerke | 3 | VU |
| Early stage dynamics of protein folding | Woutersen/Bolhuis | 2.3 | UvA |
| Enantioselective biocatalysis | Van Maarseveen/Mutti | 1 | UvA |
| Enzymatic C-H Functionalization of non-activated arenes | Fernández-Ibáñez/Mutti | 1 | 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 |
| Heterogeneous catalysis | Ensing/Rothenberg/Shiju | 1.3 | UvA |

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|---|---------------------------------|-------|-----------|
| Heterogeneous nucleation | Meijer/Rothenberg | 1.3 | 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 |
| IR spectroscopy of PAHs | Buma/Rijs/Oomens | 2 | UvA, RU |
| IR spectroscopy of metal clusters | Bakker/Buma/Oomens/Visscher | 2.3 | RU/UvA/VU |
| Isotope-labeled peptides | Woutersen/Van Maarseven | 1.2 | UvA |
| 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 |
| Molecular understanding of homogeneous carbonylation catalysts | Bouwman/Bickelhaupt | 1.3 | UL/VU |
| Multi-component reactions as tools for peptide modification | Orru/Grossmann | 1 | VU |
| Nano-particle upconversion | Zhang/Meijer/Buma | 2.3 | UvA |
| 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 |
| Protein crystallography of modified enzymes | Mutti/Grossmann | 1 | UvA/VU |
| 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 |
| Solar Fuels | Buda / de Groot / Visscher | 2.3 | UL/VU |
| 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 |
| Termogravimetric analysis of ruthenium-functionalized upconverting nanoparticles | Bonnet/Grecea | 1.2 | UL/UvA |
| Theory/Experiment-Driven Multicomponent Reaction Development | Bickelhaupt/Orru/Fonseca Guerra | 1.3 | VU |
| Theory/Experiment-Driven Cycloaddition Reaction Development | Bickelhaupt/Rutjes | 1.3 | VU, RU |

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| 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 2017, 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.

Publications

The following publications appeared in 2017 as a result of previous Fellowships:

- Formation of glycerol through hydrogenation of CO ice under prestellar core conditions; G. Fedoseev, K.-J. Chuang, S. Ioppolo, D. Qasim, E.F. van Dishoeck, H. Linnartz, *the Astrophysical Journal*, **2017**, 842, 52 .
- Pengtao Jing, Dong Han, Di Li, Ding Zhou, Ligong Zhang, Hong Zhang, Dezhen Shen, Songnan Qu; Origin of Anisotropic Photoluminescence in Heteroatom-Doped Carbon Nanodots, *Adv Optical Mater.* **2017**, 1601049.
- Yuan Gao, Pengtao Jing, Gadi Rothenberg, M. Hilbers, Ning Yan, Hong Zhang, Stefania Tanase; Dual-mode humidity detection using a lanthanide-based metal-organic framework: towards the development of multifunctional humidity sensors, *Chem. Commun.* 53 (**2017**) 4465"
- Garcia A.C., Birdja Y.Y., Tremiliosi-Filho G. & Koper. M.T.M.; Glycerol electro-oxidation on bismuth-modified platinum single crystals, *Journal of Catalysis* 346 (**2017**) 117–124.

Awarded Fellowships – 5th Call, April 2017:

Developing design rules for a biomimetic di-iron hydrogenase catalyst

Guest: Dr. Mihajlo Etinski (University of Belgrade, Serbia); hosted by Dr. Ir. Bernd Ensing (UvA), Prof. dr. Joost Reek (UvA) and Dr. M. Tromp (UvA).

A visit of four weeks.

Origin of Diastereoselectivity in Interrupted Ugi Cascade Cyclizations

Dr. Israel Fernandez (Universidad Complutense de Madrid, Spain); hosted by Prof. dr. Matthias Bickelhaupt (VU), Prof. dr. ir. Romano Orru (VU) and Dr. Eelco Ruijter (VU).

A visit of one month.

Paramagnetic States in Solar Cell Materials by Electron Paramagnetic Resonance

Guest: Prof. Bolesław Kozankiewicz (Institute of Physics of the Polish Academy of Sciences, Warsaw, Poland); hosted by Dr. Martina Huber (Leiden University) and Prof. dr. Michel Orrit (Leiden University).

A visit of six weeks.

Photo-induced bi-stable transition metal functional molecule-based magnetic complex

Guest: Prof. dr. Daopeng Zhang (Shandong University of Technology, China); hosted by Dr. Sylvestre Bonnet (UL).

A visit of 2 months.

Awarded Fellowships – 6th Call, October 2017:

Observing Single Artificial Molecular Machines under strain

Guest: Dr. Syoji ITO (Osaka University, Japan); hosted by Prof. dr. Fred Brouwer (UvA) and Prof. dr. Michel Orrit (UL). This Fellowship is awarded by the John van Geuns Fonds.

A visit of 10 weeks, co-sponsored by the Stichting John van Geund fonds, under auspices of the HRSMC.

From Ice Grains to Planets: The Chemical Evolution of Complex Molecules in Space

Guest: Dr. Sergio Ioppolo (Queen Mary University of London, UK); hosted by Prof. dr. Harold Linnartz (Leiden University) and Dr. Herma Cuppen (Radboud University).

Four 1 week visits with a total duration of one month.

Simulating the binding modes of the bacterial DNA organizing protein HLNS to DNA

Guest: Dr. Enrico Riccardi (Norwegian University of Science and Technology NTNU, Trondheim, Norway); hosted by Dr. Jocelyne Vreede (University of Amsterdam).

A visit of 3 months.

Targeted Light-activated Metallodrugs: Synergistic Effect and Multimodal Approach

Guest: Dr. Ashis K. Patra (Indian Institute of Technology Kanpur, India); hosted by Dr. Sylvestre Bonnet (UL).

A visit of 3 months.

Controlling the properties and stability of atomically dispersed metal catalysts with adjacent ligands

Guest: Prof. Will Medlin (University of Colorado, USA); hosted by Prof. dr. Gadi Rothenberg (UvA), and Dr. David Dubbeldam (UvA).

A visit of one month.

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)
- Targeted Synthesis Challenges (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.

The HRSMC educational activities of 2017 consisted of:

- the two weeks Winter School '*Molecular Simulation*', organized under the auspices of CECAM (January 9-20, UvA)
- the Course '*Physical Methods in Inorganic Chemistry*' (6 – 10 February, UvA - UL)
- the Course '*Photophysics, Photochemistry & Photobiology*' (April 2017, UvA/VU)
- the 4 day Scientific Writing - High Impact Writing Course, in combination with a 1 day Peer Review Survival Course (June 12 – 16, UL)
- the Summer School '*Organic Synthesis*' (10-13 July, Kasteel Vaeshartel, Maastricht)

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

HRSMC Course 'Understanding Molecular Simulation', Molsim 2017 (January 9-20, 2017, UvA)

Coordinators: Dr. B. Ensing (UvA), Prof. dr. E.J. Meijer (UvA) en I. Weijer
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: 88 participants (21 UvA MSc students, 21 Dutch PhD students (2 of them were HRSMC members) and 46 participants came from foreign universities)

HRSMC Course Physical Methods in Inorganic Chemistry – PhMIC 2017 (6 – 10 February 2017, UvA - UL)

Organisation: Prof. dr. E. Bouwman (UL), Dr. S. Bonnet (UL), Prof. dr. B. de Bruin (UvA), Dr. M. Tromp (UvA), R. Weijer and drs. H.E. Zwaan
HRSMC Lecturers: Dr. S. Bonnet (UL), Prof. dr. E. Bouwman (UL), Prof. dr. A.M. Brouwer, Prof. dr. B. de Bruin (UvA), Dr. A. Ehlers (UvA), Dr. I. Groot (UL), Dr. D.G.H. Hetterscheid (UL) and Dr. M. Tromp (UvA)
Guest Lecturers: Dr. H. Kooijman (Shell)
Participants: 25 participants, of which:

- 5 MSc students (3 UvA-VU, 2 UL; 4 students passed the exam)
- 19 PhD students (11 UvA, 6 UL, 2 ARCNL)
- 1 Postdoc (UL).

Photophysics, Photochemistry & Photobiology, PPP2017 April 2017, UvA/VU

Coordinators: Dr. René Williams (UvA), Ineke Weijer (HRSMC) and drs Hilde Zwaan (HRSMC)
Lecturers: Dr. Freek Ariese (VU), Prof. dr. Fred Brouwer (UvA), Dr. Francesco Buda (UL), Dr. René Williams (UvA) and Dr. Gert van der Zwan (VU)
Guest Lecturers: Prof. dr. Maurice Aalders and Dr. Ivo van Stokkum
Course schema: 20 h of lectures, sometimes combined with excesses/tutorials. On the final day, participants gave a presentation about a scientific article with was handed out on the first day.
Participants: 11 participants; 10x PhD and 1x MSc (8x UvA, 1x ARCNL, 1x RU, 1x UL)

4 day Scientific Writing - High Impact Writing Course, in combination with a 1 day Peer Review Survival Course (June 12 – 16, UL)

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

Guest Lecturer: Prof. dr. Ulrike Muller and Dr. Otto Berg (both California State University Fresno, USA)

Participants High Impact Writing Course: 24 participants; 22 PhD students and 2 postdocs (16x UvA, 1x UvA-ARCNL, 5x UL and 2x VU).

Participants Peer Review Course: 14 participants; 13 PhD students and 1 postdoc (10x UvA, 2x VU and 2x UL)

HRSMC Summer School 'Organic Synthesis'

10-13 July, 2017, Kasteel Vaeshartel, Maastricht

Coordinators: Dr. M.Á. Fernández-Ibáñez (UvA), Prof. dr. T. Grossmann (VU), Prof. dr. H. Hiemstra (UvA), Dr. J.H. van Maarseveen (UvA), Prof. dr. ir R.V.A. Orru (VU), Dr. E. Ruijter (VU, chair), M. Smits-Weijers (UvA - HRSMC), R. Weijer (UvA - HRSMC), Drs. H. Zwaan-vd Plas (UvA - HRSMC).

Lecturers: Prof. dr. Albrecht Berkessel (Universität zu Köln, Germany), Prof. dr. Janine Cossy (CNRS, ESPCI Paris Tech, France) Prof. dr. Darren J. Dixon (University of Oxford, UK), Prof. dr. Wolfgang Kroutil (Karl Franzens Universität Graz, Austria) Prof. dr. Paul Knochel (Ludwig-Maximilians-Universität, München, Germany), Prof. dr. Richmond Sarpong (University of California - Berkeley, USA).
With evening lectures of Dr. G.J. Gruter (Avantium) and Dr. J.P. Seerden (Syncom).

Participants: 57; 41 PhD students (18 HRSMC PhD students, 16 PhD students from other Dutch universities, 7 PhD students from foreign universities), 9 participants from the industry and 7 MSc students.

3.2 Symposium

The annual HRMSC Symposium was held at the Amsterdam Science Park Congress Centre on 16 November, 2017. The symposium, which was attended by ca. 190 scientists, also included poster sessions with 49 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. Francesco Mutti (UvA)
One-pot and Atom-Efficient Conversion of Alcohols to Enantiopure Amines via Biocatalytic Cascades
- PhD/PostDoc Lecture: Evi Habraken (UvA)
Comparing Frustrated Lewis Pair Chemistry to Metal-Ligand Cooperativity
- PhD/PostDoc Lecture: Lucien Lameijer (UL)
Efficient red light-activation of a NAMPT inhibitor under hypoxia using water-soluble ruthenium complexes

Theme 2 'Physical Chemistry and Spectroscopy'

- Dr. Dennis Hetterscheid (UL)
Biomimetic Copper Systems as Catalysts for the Oxygen Reduction Reaction
- PhD/PostDoc Lecture: Sandra Wiersma (RU/UvA)
Deuterium versus Hydrogen in astronomical Polycyclic Aromatic Hydrocarbons
- PhD/PostDoc Lecture: Liron Zada (VU)
Detection of Environmental Microplastics with Stimulated Raman Scattering Microscopy

Theme 3 'Theoretical Chemistry'

- Prof. dr. Matthias Bickelhaupt
Rational Design of Chemical Reactions
- PhD/PostDoc Lecture: Ambuj Tiwari (UvA)
What drives an electron transfer: extracting order parameters from an ensemble of dft-md trajectories

Guest Lectures:

- Prof. dr. ir. René Janssen (Eindhoven University of Technology)
Organic and Hybrid Thin Film Solar Cells
- Dr. Sven Askes, winner Dick Stufkens prize 2017 (UL, currently working at AMOLF)
TBA on the work in his award winning thesis

3.3 PhD Graduations (in order of graduation date)

Newton, A.C.

Self-assembly via anisotropic interactions

Promotor: Prof. dr. P.G. Bolhuis

Co-promotor: Prof. dr. P. Schall

January 26, 2017

First job after graduation: Consultant Data Management

Brotzakis, Z.F.

Hydration layer dynamics and association mechanisms of food and antifreeze proteins

Promotor: Prof. P.G. Bolhuis

March 7, 2017

First job after graduation: Postdoctoral researcher

Nami, F.

Enzymatic reduction of oxygen by small laccase: a rapid freeze-quench EPR study

Promotors: Prof. dr. E.J.J. Groenen, Prof. dr. G.W. Canters

March 7, 2017

First job after graduation: Postdoc Solid-state NMR group Leiden Institute of Chemistry

Carattino, A.

Gold nanorod photoluminescence: Applications to imaging and temperature sensing

Promotor: Prof. dr. M. Orrit

March 9, 2017

First job after graduation: Heads his own company Uetke (<https://www.uetke.com/>)

Kuijpers, P.

Controlling radical-type reactivity with transition metals and supramolecular cages

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

April 19, 2017

First job after graduation: Technology & Application Consultant, Mettler-Toledo

Oskouei, M.

Fluorogenic organocatalytic reactions

Promotors: Prof. dr. A.M. Brouwer, Prof. dr. H. Hiemstra

April 25, 2017

Martinez, J.P.

Reactivity of Fullerenes, Endohedral Metallofullerenes, and Nanotubes, and their Possible Application in Solar Energy Conversion

Promotors: Prof. dr. F.M. Bickelhaupt, Prof. dr. M. Solà

Co-promotors: Prof. dr. C. Fonseca Guerra, dr. S. Osuna Oliveiras

17 May 2017

First job after graduation: Postdoc

Tchamba Yimga, N.

The role of molecular packing on carrier transport in liquid crystalline dyes

Promotor(s): Prof. dr. J. Parisi

Co-promotor(s): Dr. E.I von Hauff, Prof. dr. V. Wagner

May 31, 2017

First job after graduation: Post Doc at IMEC, Belgium

Van Hoorn, C.H.

Spectroscopy at the nanometer scale

Promotor: Prof. dr. D. Iannuzzi

Co-promotors: Dr F. Ariese; Dr. A.J.G. Mank

June 7, 2017

First job after graduation: Researcher at AkzoNobel

Gao, J.

Laboratory spectroscopy of ionized polyaromatic hydrocarbon derivatives of astrophysical interest

Promotor: Prof. dr. J. Oomens

Co-promotor: Dr. G. Berden

June 8, 2017

First job after graduation: PostDoc at DIFFER Institute, Eindhoven

Van de Watering, F.

N₂ fixation and dehydrogenation of methanol and formic acid with late transition metal complexes

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

Co-promotor: Dr. W. Dzik

June 15, 2017

First job after graduation: Project-engineer Witteveen+Bos

Zaffaroni, R.

Second coordination sphere effects in [FeFe]-Hydrogenase mimics

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

Co-promotors: Prof. dr. B. de Bruin, Dr. R.J. Detz

June 15, 2017

First job after graduation: 6 months post-doc and then E-Stone

Cioc, R.

Off the Beaten Path: Atypical Products of Ugi and Passerini Reactions

Promotor: Prof. dr. R.V.A. Orru

Co-promotor: Dr. E. Ruijter

June 16, 2017

First job after graduation: Process R&D Chemist, Alcami Corporation

Pieters, B.

Write, Read, Erase, Repeat: Investigating the fundamental chemical-biological interactions behind the readout process of the epigenetic histone trimethyllysine mark

Promotor: Prof. dr. G.J.M. Pruijn

Co-promotor: Dr. J. Mecinovic

June 16, 2017

First job after graduation: Bioprocess scientist at Batavia Biosciences

Kumar, P.

Parkinson's protein α -synuclein: membrane interactions and fibril structure

Promotor: Prof. dr. E.J.J. Groenen

Co-promotor: Dr. M.I. Huber

June 27, 2017

First job after graduation: Postdoc at Department of Medical Biochemistry and Biophysics, Umea University, Umea, Sweden

Rossius, S.G.H.

'Q-wires': Synthesis, electrochemical properties and their application in electro-enzymology

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

September 26, 2017

Stemers, L.

Covalent template-assisted synthesis of mechanically interlocked molecules.

Promotor: prof. dr. J.H. van Maarseveen

Co-promotor: prof. dr. H. Hiemstra

October 3, 2017

First job after graduation: PostDoc

Pereira Orenha, R.

Computational Study of Ruthenium–Nitrosyl Compounds

Promotors: Prof. dr. F.M. Bickelhaupt, Prof. dr. S.E. Galembeck

5 October 2017

First job after graduation: Postdoc

Gezer, G.

Biomimetic Models of [NiFe] Hydrogenase for Electrocatalytic Hydrogen Evolution

Promotor: Prof. dr. E. Bouwman

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

October 10, 2017

First job after graduation: Intellectual Property Analyst at Tenaris (Amsterdam)

Luo, S.

Transition metal compounds with S/N functionalized NHC ligands: Structures, redox properties and electrocatalytic activity

Promotor: Prof. dr. E. Bouwman

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

October 17, 2017

First job after graduation: Assistant Editor at the publisher MDPI (China)

Van Rixel, V.H.S.

Toward Selective Anticancer Metallodrugs

Promotor: Prof. dr. E. Bouwman

Co-promotor: Dr. S. Bonnet

October 19, 2017

First job after graduation: Autoriteit Nucleaire Veiligheid en Stralingsbescherming (ANVS)

Vijaykumar, A.

Multi-Scale simulations of reaction-diffusion systems

Promotor: Prof. dr. P.G. Bolhuis

Co-promotor: Prof. dr. P.R. ten Wolde

October 24, 2017

First job after graduation: Data and Algorithm Scientist

Maltseva, E.

Probing potential energy surfaces with high-resolution spectroscopy: From the Universe's carbon locker to molecular machines

Promotors: Prof. dr. W.J., Prof. dr. J. Oomens

October 25, 2017

First job after graduation: Financial analyst

Chirila, A.

Manipulating radicals. Using cobalt to steer radical reactions

Promotor: Prof. dr. B. de Bruin

Co-promotor: Dr. W. Dzik

November 2, 2017

First job after graduation: Postdoc University of Washington

Goswami, M.

Open shell nitrene- and carbene-complexes of cobalt: characterisation and reactivity

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

November 2, 2017

First job after graduation: 6 months post-doc and then CEO HIMS spin-off company Spark904

Bakker, D.J.

Far infrared spectroscopic methods for molecular beams. Fingerprints of hydrogen bond interactions

Promotor: Prof. dr. J. Oomens

Co-promotor: Dr. A.M. Rijs

November 13, 2017

First job after graduation: Energy consultant, Cornelissen Consulting Services BV

Vuckovic, S.

Fully Nonlocal Exchange-Correlation Functionals from the Strong-coupling limit of Density Functional Theory

Promotor: Prof. dr. P. Gori Giorgi

Co-promotor(s): dr. M.W.J. Seidl

14 November 2017

First job after graduation: Postdoc

Ganapathy, S.

Improvisations in phototrophy

Promotors: Prof. dr. H.J.M. de Groot; Prof. dr. W.J. de Grip

December 12, 2017

First job after graduation: postdoc position at TU Delft starting April 2018

Mampuys, P.

Multicomponent Chemistry with Thiosulfonate and Isocyanide Building Blocks: Challenges and Opportunities for Green Chemistry

Promotors: Prof. Dr. R.V.A. Orru & Prof. Dr. B.U.W. Maes

December 12, 2017

First job after graduation: Post-doc, university of Antwerp

Lameijer, L.N.

The synthesis and biological applications of photo-activated ruthenium anticancer drugs

Promotor: E. Bouwman

Co-promotor: S. Bonnet

December 14, 2017

First job after graduation: Postdoctoral researcher, RU Groningen

Niels Ligterink

The astrochemical factory: a solid base for interstellar reactions

Promotors: Prof. dr. E. van Dishoeck/ Prof. dr. H. Linnartz

December 18, 2017

First job after graduation: Postdoc University of Bern

Cuello Garibo, J.A.

Caging ruthenium complexes with non-toxic ligands for photoactivated chemotherapy

Promotor: Prof. dr. E. Bouwman

Co-promotor: Dr. S. Bonnet

December 19, 2017

First job after graduation: travelling

3.4 HRSMC Excellence Master 'Sustainability: the Molecular Approach'

Organisation Structure

The interuniversity research school 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. In 2017, nineteen MSc students participated in this Excellence Program. Two of them graduated in the period of August-December 2017.

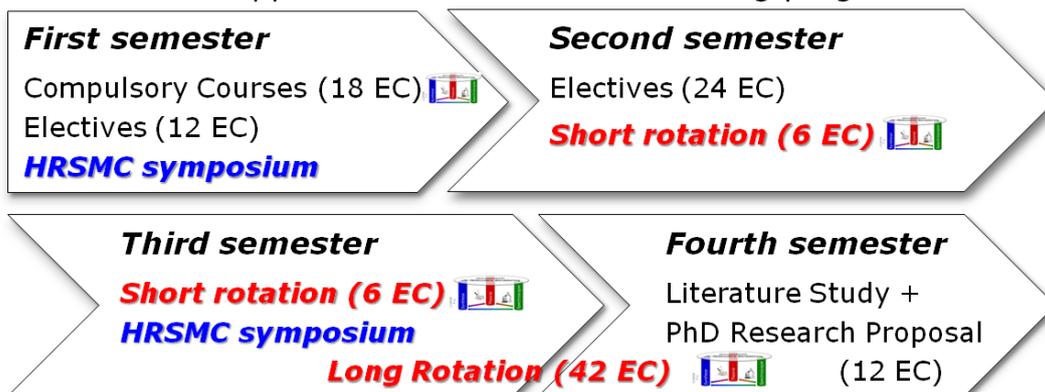
As mentioned before, in the summer of 2017, the HRSMC has granted one proposal for PhD research written by MSc chemistry student David Klein. He was appointed at the Leiden University.

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).

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



- Three Research Pillars
- At least two of the three universities involved

Selected PhD proposal in HRSMC/NWO Graduate Programme

In 2017, the HRSMC has granted the proposal of David Klein (UL): *Unidirectional electron transfer across lipid bilayers for artificial water splitting using transmembrane peptide-photosensitizer conjugates and liposomes*; Promotores: Prof. dr. E. Bouwman (UL) and Prof. dr. A. M. Brouwer (UvA); Co-promotor: Dr. S. (Sylvestre) Bonnet (UL). David Klein wrote his proposal as part of the special HRSMC master's programme for talented chemistry students and defended his proposal before a broad panel of experts consisting of Prof. dr. G. van Koten (UU) and Prof. dr. D. Wiersma (RUG), as external members, as well as HRSMC Board members and the chair of the HRSMC Research Committee. He started his PhD research in December 2017, 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

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. Ariese (VU, research theme 2)
- Dr. F. Buda (UL, research theme 2/3) *until 5 October 2017*
- Prof. dr. H. Hiemstra (chairman, UvA, research theme 1) *until 5 October 2017*
- Prof. dr. E. Bouwman (UL, research theme 1) *will replace Prof. H. Hiemstra as chair as of 5 October 2017*
- Prof. dr. E.J. Meijer (UL, research theme 3) *will replace Dr. F. Buda as of 5 October 2017*

Education Committee (OWC)

- Dr. D.G.H. Hettterscheid, (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)
- T. Bouwens, MSc (UvA, research theme 1, PhD student) *will replace E. Schippers, MSc as of November 2017*

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

-
- 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; C. te Grotenhuis, MSc; T. Bouwens, MSc and Xander Schaepkens; 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; PhD students in the Organophosphorus, Organometallic and Computational Chemistry group at VU
 - M. Faltracco, MSc; PhD student in the Synthetic and Bio-organic Chemistry group at the VU.

4.2 Annex 2 - Financial Account 2017

| Income | | Expenses | |
|---|------------------|---|------------------|
| Contribution UvA 2017 - faculty ¹⁾ | 150.000 | Donation HIMS Institute ¹⁾ | 150.000 |
| Contribution UvA 2017 - HIMS ¹⁾ | 150.000 | Personnel Costs | 79.318 |
| Synthesis School (fee and sponsoring) | 55.990 | Synthesis School | 50.579 |
| Fellowship – JvGeuns ²⁾ | 5.875 | Fellowship Programme | 37.625 |
| Ulrike Muller Cursus – fee | 1.680 | Ulrike Muller Cursus | 9.530 |
| Interest | 117 | Symposium | 10.237 |
| | | PhMIC, PPP course | 1.979 |
| | | Board | 1.166 |
| | | Bureau Costs | 1.046 |
| | | Annual Report 2016 | 968 |
| | | Dick Stufkens PhD prize | 1.000 |
| | | Graduate Programme ³⁾ | 888 |
| | | Reservation for 2018-2019 ⁴⁾ | 19.326 |
| | € 363.662 | | € 363.662 |
| 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 Synthesis School 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, one in PhD student in 2016 and one in PhD student in 2017. These finances are not included in this overview.



John van Geuns foundation

Estimation for the personnel costs covered by the HRSMC for the four PhD in 2017:

€ 4.2 KEuro (1/48 x 200 keuro) for David Klein

€ 50 KEuro (12/48 x 200 keuro) for Tessel Bouwens

€ 50 KEuro (12/48 x 200 keuro) for Kaj van Vliet

€ 50 KEuro (12/48 x 200 keuro) for Hans de Bruijn

These costs (in total approx. **154.2 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 – 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.