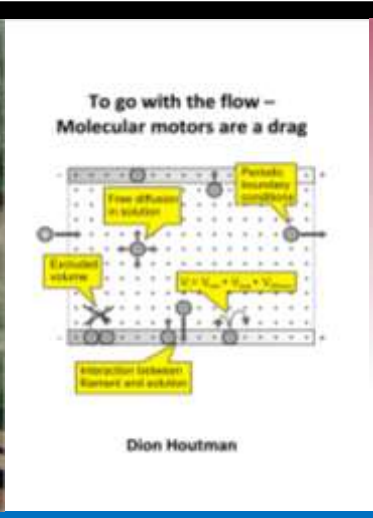
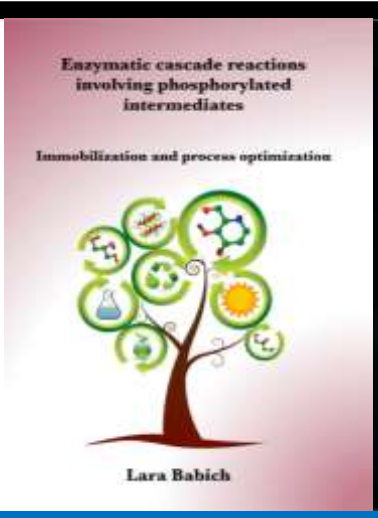
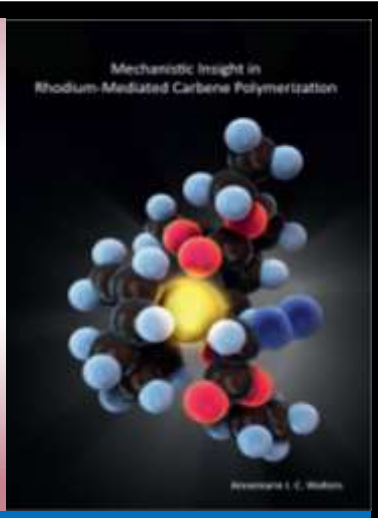
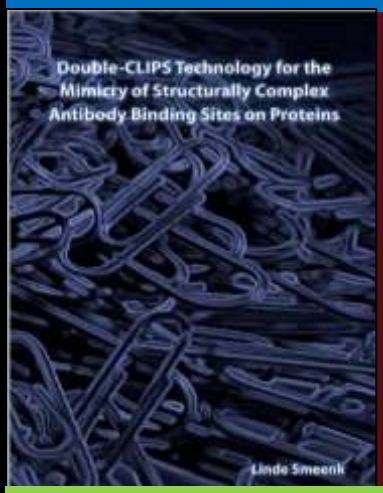
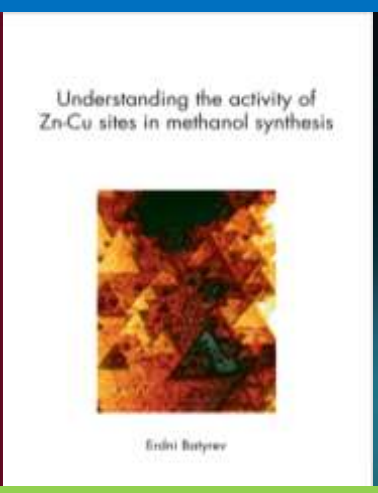


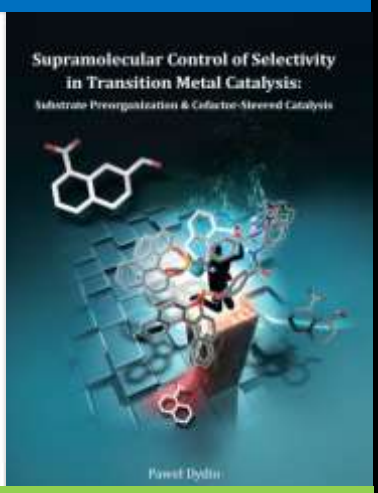




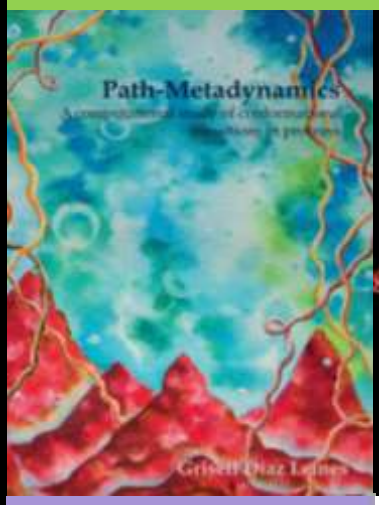
Van 't Hoff Institute for Molecular Sciences

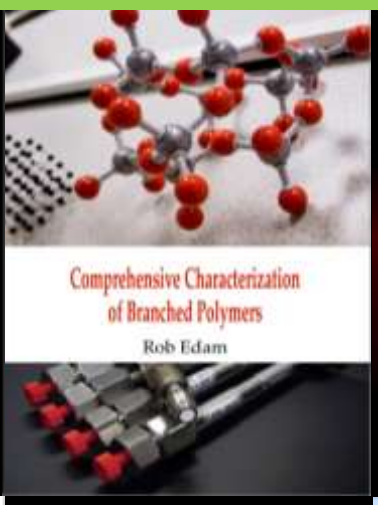


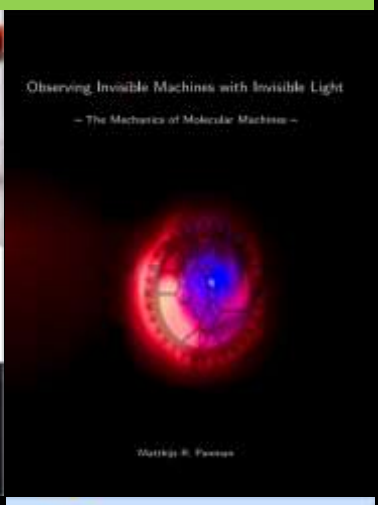


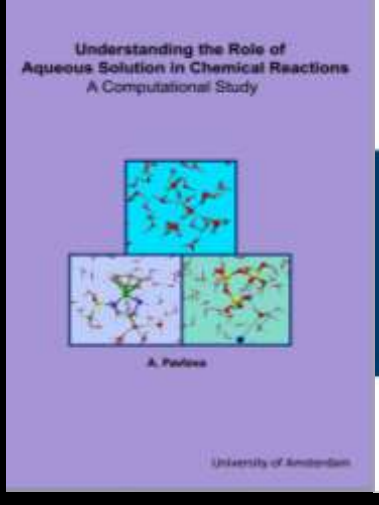


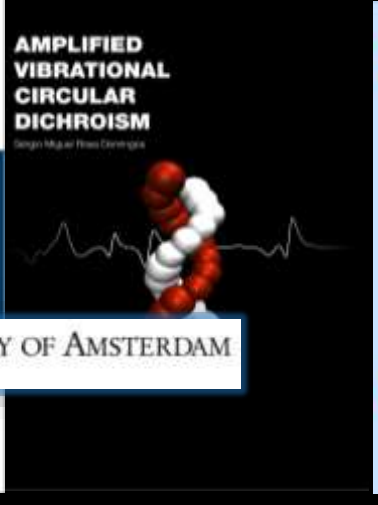
Annual Report 2013

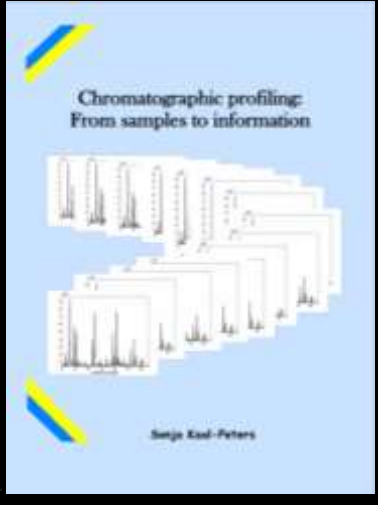












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Cover: Collage of covers of HIMS dissertations from 2013

July 2014

Preface

2013 was a hectic, but inspiring year for HIMS with our positive midterm review evaluation, election of sustainable chemistry as a UvA priority research area, our contributions to joined efforts to create AFS, and the change of director of the institute at the end of 2013. I was honored that I was appointed as the new director of HIMS in November, succeeding Prof. Aart Kleijn, who took up the position of director of the Center of Interface Dynamics for Sustainability in Chengdu, China. I thank Prof. Kleijn for his commitment to HIMS and the great institution that he entrusted to his successor.

Our researchers were very successful in acquiring external funds to start new projects and produced a record of over 200 scientific publications, including 16 PhD theses and many high impact papers. In October we had the midterm evaluation of the scientific advisory board, which was very positive. They highly appreciated the clear organization of HIMS in the four research themes, including the associated valorization programs. Besides facilitating synergy, this organization results in a better visibility of the institute. I am proud to see how these four themes each excel on their own topic as well as on collaborating with each other. That is one of the strengths of our institute.

The co-operation between the science faculties of the two Amsterdam universities became closer and many people worked hard on the creation of the Amsterdam Faculty of Science (AFS). Just before Christmas a majority of the central students council voted against the decision to start with the AFS. Although it was disappointing at that time, we have accepted this and in 2014 we will search for new possibilities to enhance the co-operation and synergy of chemists currently working at HIMS, the Swammerdam Institute for Life Sciences and Free University.

To conclude 2013 in some highlights: Sustainable Chemistry was designated as a university research priority area; three PhD students won prizes for the exceptional quality of their doctoral theses; HIMS hosted 1,500 analytical chemists from all over the world during the 39th HPLC conference; Prof. Krishna won the prestigious Eni Award; Dr Van Maarseveen was awarded the Lecturer of the Year prize; the Co van Ledden Hulsebosch Centre on forensic sciences started; HIMS participates in the Advanced Research Centre for Nano-Lithography (ARCNL) with ASML; Prof. Reek received an ERC Advanced grant and Molecular Photonics received a large ZonMW grant with the Quantivision consortium.

These and many other highlights of the institute are described in this annual report. I hope you enjoy reading.

Prof. Joost Reek
Director

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1. General considerations and highlights

1.1 Key figures of HIMS in 2013

The high level of scientific output of HIMS was maintained in 2013. HIMS published 4 papers (5 in 2012, 1 in 2011) in absolute top journals (impact factor > 15) and 9 papers (7 in 2012, 8 in 2011) in top journals (impact factor 10-15). The total number of refereed and other professional publications, patents and book(chapter)s amounted to 205 (average 2010-2012: 185). The amount of published PhD dissertations increased substantially to 16 (9 in 2012, 15 in 2011, 14 in 2010).

With a total of 6.45 M€ in external funding (excluding the own matching budget of approximately 2.6 M€) the year 2013 was very successful (average 2010-2012: 5.8 M€). These funds were acquired from funding agencies such as NWO (Chemical Sciences, *Vernieuwingsimpuls*, FOM, ZonMW), SmartMix CatchBio and ERC (one Advanced Grant), as well as from industry and other partners.

In December the Research Priority Area Sustainable Chemistry was established within HIMS. The University of Amsterdam has appointed twenty-called Research Priority Areas over the entire spectrum of science. These RPA's are among the best the UvA has to offer and are internationally renowned. HIMS received substantial additional funds from the UvA. IN 2014 HIMS will hire two promising young scientists on a tenure track basis who will set up their own research group at the Science Park Amsterdam.

1.2 Personnel

In 2013 the total staff amounted to 136.5 fte[1]. This amount is lower than the years before (158.0 in 2012 and 163.2 in 2011). The difference may be explained by a loss of temporary scientific staff (postdocs and PhD students) due to the completion of several projects and the overtaking manoeuver for promotions.

Prof. dr. Fred Brouwer has been appointed professor of Spectroscopy and Photonic Materials. Before Brouwer was professor by special appointment of Molecular Spectroscopy. Dr. Bas de Bruin has been appointed professor of Bio-inspired Sustainable Catalysis.

In September HIMS welcomed Dr Anett Schallmey who started a tenure track to full professor Biocatalysis. This was one of the open positions obtained via the *Sectorplan Natuur- en Scheikunde* (SNS). Only at the end of 2013 HIMS candidates for the other SNS-positions where in sight; a new full professor and a tenure track candidate both working on Supramolecular Separations. The appointments will have be realized early 2014.

1.3 Finances

HIMS finished the year 2013 with a positive financial result of + 258 k€. This result looks satisfactory, but one should note that a reservation was made of 466 k€ on SNS funds that were received, while the positions where not yet filled. HIMS did not yet fully adjust to the budget reduction of the structural university budgets (eerste geldstroom) of 10% (1 M€) the institute was confronted with during the years 2009-2012. On the other hand, the increased amount of acquired external funding shows that HIMS is able to stay a healthy organisation.

[1] Full time equivalents (fte), including all research, educational and general tasks over the whole year. The amount of employees on 31 December 2013 was 127 fte.

1.4 Highlights

1.4.1 Institutional highlights

Amsterdam briefly reigns as world capital of analytical chemistry
Analytical chemists at the Van 't Hoff Institute for Molecular Sciences hosted 1,500 international colleagues and numerous businesses in Amsterdam in June during the 39th International Symposium on High-Performance-Liquid-Phase Separations and Related Techniques, chaired by Prof. Peter Schoenmakers.

Prestigious Italian award for Prof. Krishna
Prof. Rajamani Krishna won the prestigious Eni Award for his research on fundamental aspects of gas separation and purification. Italy's President Giorgio Napolitano presented him with the award – a gold medal and EUR 200,000 – in Rome in June. Eni, an Italian multinational oil and gas company on a par with global corporations such as Shell, BP, ExxonMobil and Total, launched the Eni awards in 2008 as a 'Nobel Prize for energy and the environment'.

Sustainable Chemistry: University research priority area
In 2013, the Executive Board designated 'Sustainable Chemistry, from theory to application', a theme initiated by the HIMS, as a University research priority area. Structural additional funding was earmarked to expand the number of academic staff and thereby bolster research focused on better understanding chemical processes in which fuels are produced or consumed under the influence of light or electricity.

Amsterdam Center for Forensic Science and Medicine opens
The Amsterdam Center for Forensic Science and Medicine (CLHC) opened its doors on 13 September as an interdisciplinary expertise centre clustering the experience, knowledge and expertise of the HIMS, AMC-UvA and the Netherlands Forensic Institute (NFI). Prof. Adrian van Asten, professor by special appointment of Forensic Analytical Chemistry (HIMS), and Prof. Maurice Aalders, professor by special appointment of Forensic Biophysics (AMC-UvA), both delivered inaugural lectures to mark the occasion. The center is named after Co Van Ledden Hulsebosch (1877-1952), a renowned pioneer in the field of forensic sciences.

Appointments
- Prof. Bas de Bruin was named professor of Bio-inspired Sustainable Catalysis.
- Prof. Fred Brouwer was named professor of Spectroscopy and Photonic Materials. He was previously professor by special appointment of Molecule Spectroscopy, a chair endowed by Stichting John van Geuns Fonds.
- Prof. Joost Reek was appointed the new director of the HIMS effective 1 November, succeeding Prof. Aart Kleijn, who took up the position of director of the Center of Interface Dynamics for Sustainability in Chengdu, China.

1.4.2 Scientific highlights

Research at HIMS is organized in four multidisciplinary research themes - Sustainable Chemistry, Computational Chemistry, Analytical Chemistry and Molecular Photonics - covering fields in chemical sciences where in the next decade interesting new developments and important breakthroughs are anticipated. In the long term the HIMS research topics are envisaged to be pivotal for the development of a sustainable society. Below the highlights of all research groups are clustered per theme.

- Sustainable Chemistry

Homogeneous and Supramolecular Catalysis

New supramolecular enzyme-inspired strategies to control activity and selectiviy have been disclosed. Alkene substrates with carboxylate functional groups can be hydroformylated with unprecedented regioselectively using catalysts with well-defined binding sites for substrate orientation via the carboxylate (JACS, Angewandte Chemie). These hydroformylation reactions with full control of region-selectivities enables new synthetic routes to be developed for the preparation of important fine chemical intermediates. For substrates that do not have any functional groups, supramolecular cages can be used to control such regio-sectivity via the second coordination sphere; it was demonstrated for the first time that the selectivity of a metal catalyzed reaction can be controlled by only changing the second coordination sphere (Nature Commun). Encapsulation strategies have also been explored for radical type reactions. To this end, a new cubic M8L6 cages was designed that is able to host metallo-porphyrins inside. The encapsulated cobalt porphyrin catalyst shows a longer life time because it is protected by the second sphere (Chem Eur. J., front cover.) The first experimental (spectroscopic) evidence for the existence of rhodium-bound nitridyl radical (•N2-) species was disclosed (JACS). These species are expected to play an important role in future activation of elemental nitrogen (N2). The synthesis, characterization and reactivity of a rare terminal phosphido-complex of iridium was reported (Inorg. Chem.) as well as the reversible cyclometalation at iridium (Organometallics), which may open up new avenues in the context of reactive ligand design for cooperative bond activation.

Heterogeneous Catalysis and Sustainable Chemistry

Inspired by patents from the 1960's audiocassette recording industry, HCSC chemists invented new Fischer-Tropsch catalysts for making fuels from natural gas and biomass. The results were published as a VIP cover article in Angewandte Chemie. The catalyst was patented worldwide by Total S.A.

Oil companies use cobalt-based catalysts for making middle distillate fuels such as diesel and kerosene, but cobalt is expensive. In 2009, Total asked Rothenberg to design a cheaper catalyst that will perform as well as pure cobalt. This was no mean task. Gaining an economic advantage requires engineering of the particles at single-nanometer resolution, yet in a manner that can be scaled up to multi-ton scale. This rules out all chemical procedures that require high sophistication, extreme temperatures, or expensive chemicals.

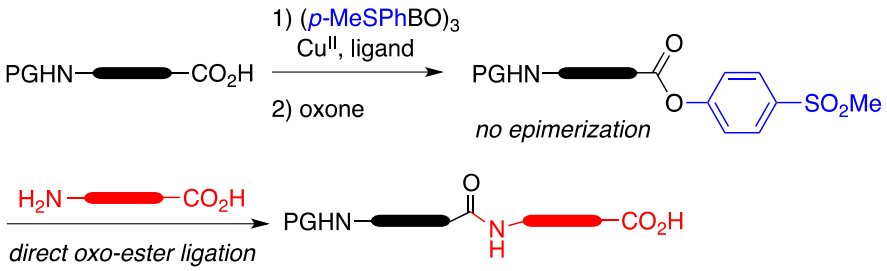
Inspired by methods patented by TDK and BASF in the 1960s for producing magnetic audio tapes, the team succeeded in inventing a cheap, reliable, efficient and, most importantly, scalable method for synthesizing spherical *core-shell* catalyst particles. The particles have an average diameter of 10 nm and consist of a 8 nm magnetite (iron oxide) core with a cobalt oxide shell of only 1 nm. These proved to be excellent Fischer-Tropsch catalysts.

Biocatalysis and Bio-organic Chemistry

We used our recently expressed, purified and characterized bacterial arylsulfate sulfotransferase (AST) from *Desulfitobacterium hafniense* as a catalytic tool to derivatize poorly soluble aromatic compounds (polyphenols). As examples we sulfated the natural occurring compounds *p*-coumaric acid, 6-hydroxyflavone, resveratrol, phloretin and quercetin . These water-soluble sulfate esters were isolated, purified and characterized. This simple enzymatic one-step sulfation method is easy to use and allows a convenient and clean production of sulfated compounds with improved solubility and availability.

Synthetic Organic Chemistry

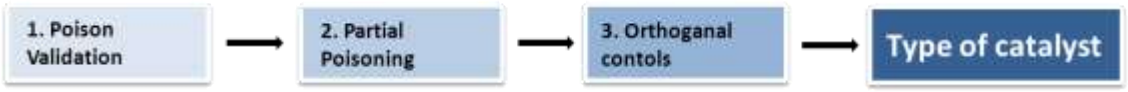
Although generally accepted as "text book chemistry", the preparation of esters, but especially amides from acids can be problematic. This is most profound in the peptide series. To avoid racemization peptides are generally elongated at the *N*-terminus, as activation of the terminal carboxyl moiety of a peptide inevitably leads to epimerization. On the other hand, methods that allow racemization-free *C*-terminal elongation of peptides are greatly desired. **Very recently we achieved epimerization-free *C*-terminal activation of peptides** via aryl esterification using the so-called Chan-Lam reaction between carboxylic acids and arylboronic acids. The new methodology will be devoted to novel peptide ligation strategies, peptide cyclization, and, ultimately, protective group free reverse peptide synthesis.



Auxiliary-mediated synthesis of ring-strained lactams (ECHO project, Rutters). This project was already concluded some time ago. Completion of the PhD thesis is expected in 2014.

Molecular Inorganic Chemistry

Many well-known reactions appear to be catalyzed by in situ generated nano-particles (NP) instead of the initially proposed molecular catalyst. Determining the type of active catalyst is important, but often neglected because distinguishing between molecular catalysts and NP catalysis is far from trivial. For this reason we have this year developed a *partial poisoning protocol* that is easy to use and gives reliable results. The method is in principle compatible with various reaction types and it provides kinetic data.



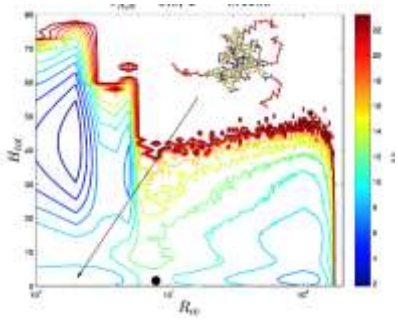
The protocol consists of three steps: poison validation, partial poisoning tests and confirmation of the viability of the method through orthogonal control experiments. Together these comprise of a comprehensive method that provides reliable results: it demonstrates that the poison is applicable, then it provides mechanistic insight and, finally, it verifies the results by excluding non-stoichiometric poisoning and resting states. We have applied this protocol to investigate palladium catalyzed semi-hydrogenation reactions. Validation took place by checking a known reaction that proceeds by molecular catalysis. Finally, we have demonstrated that tetramethyl thiourea is an excellent poison instead of the hitherto employed CS_2.

- Computational Chemistry

The Computational chemistry theme consists of the related groups Biomolecular and Molecular Simulation and the group Computational Polymer Chemistry. The latter group leads the Science for Arts activities within HIMS.

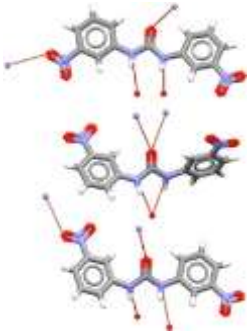
Biomolecular and Molecular Simulation

Polypeptides can self-assemble into hierarchically organized fibrils consisting of a stack of individually folded polypeptides driven together by hydrophobic interaction. Using a coarse-grained model, we systematically studied this self-assembly as a function of temperature and hydrophobicity of the residues on the outside of the building block (Ni et al., PRL 2013).



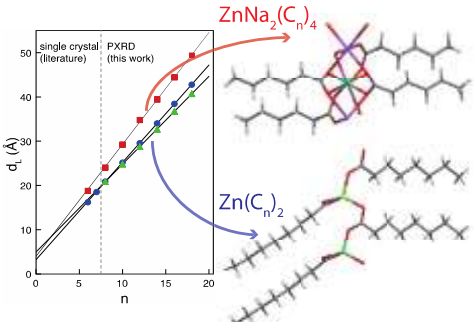
We find the self-assembly can occur via two different pathways-a random aggregation-folding route and a templated-folding process-thus indicating a strong coupling between folding and assembly. The simulation results can explain experimental evidence that assembly through stacking of folded building blocks is rarely observed, at the experimental concentrations. The model thus provides a generic picture of hierarchical fibril formation.

Molecular crystals are perfectly ordered symmetric materials. They are encountered in day-to-day products such as food, pigments, drugs or cosmetics. To form a crystal a huge number of molecules (in the order of 10 to the power of 23) have to come together. In many cases the same molecules can crystallize in more than one crystal structure. These different crystal structures are referred to as polymorphs. Polymorphs can differ considerably in their properties. From time to time molecules also change their shape (referred to as conformation) when they crystallize in different polymorphs. This phenomenon, called **conformational polymorphism**, has been the subject of a review article (Chemical Review, Cruz-Cabeza and Bernstein). The review shines a new light on the phenomenon of conformational polymorphism in Molecular Materials: it refines definitions, helps identify the phenomenon and quantifies its occurrence through a combination of database analysis, theoretical calculations and literature review. The result is an in-depth and comprehensive view of Conformational Polymorphism.



Computational Polymer Chemistry and Science for Arts

The formation of zinc palmitate and zinc stearate in ZnO-containing oil paints is an important problem for painting conservators. Besides causing the loss of pigment, the zinc alkanoates ($Zn(C_n)_2$, C_n = $CH_3(CH_2)_n$-$2COO^-$) are known to cause increased transparency that alters the appearance of the painting and their growing aggregates often weaken the entire paint layer causing craquelures and paint flaking. To improve our understanding of these degradation processes, we have investigated the exact structure and likely compositions of zinc alkanoates formed in oil paint systems. It was found that in the presence of Na^+ and K^+ ions, mixed metal soaps form in linseed oil. The molecular structure of $ZnNa_2(C_n)_4$ and $ZnK_2(C_n)_4$ complexes was elucidated by using a newly developed method that combines FTIR spectroscopy and powder-XRD, and comparing crystal spacings of homologous series of zinc soap complexes with published single-crystal data. This work provides a method for structural analysis of layered structures that do not form crystals suitable for single-crystal XRD, and highlights the potentially large variation in metal soap structures formed in oil paint systems.



Structures of zinc alkanoates and crystal spacings versus alkane length from XRD.

- Molecular Photonics

Water lubricates molecular machines (published in Nature Chemistry). During our ongoing research on the structure and dynamics of molecular machines, we discovered that these machines can be 'lubricated' by adding small amounts of co-solvent. Surprisingly, water proved to be the best lubricant by far. We used advanced spectroscopic methods (time-resolved vibrational spectroscopy and nuclear magnetic resonance) to examine translational and rotational motions in molecular machines, and found both types of motion occur much faster if a small quantity of water was added to the solvent: three percent water is enough 'lubricant' to make the movement more than twice as quick. We investigated the effect of other substances as well, but the less similar to water the substance added was, the less good its lubricating effect. Butanol, which in terms of properties is in between water and lubricating oil actually made the movement slower. The discovery is important for the design and optimization of new nano-machines. The potential applications of such machines range from molecular computers to surfaces with switchable properties. In addition, hydrogen bonds also occur in natural, biological molecular machines where water probably has a lubricating effect as well.

Helium nanodroplets are nowadays increasingly used as a novel medium to study chemical reactions at ultralow temperatures, to determine the structure of proteins, or to synthesize special metal alloys. One of the properties of such droplets that is key to such applications is the friction objects experience in such droplets. For macroscopic quantities of helium this is well known: helium becomes superfluid at low temperatures, that it, it behaves like a liquid with zero viscosity. The big question that has been floating around for a long time is whether superfluidity also arises in finite-size systems. This question was in 2013 for the first time answered in a publication in Phys. Rev. Letters which reports the results of studies on the critical Landau velocity in helium nanodroplets. These results confirm the existence of superfluidity at the nanoscale for helium nanodroplets down to a radius of 2.5 nm, containing less than a thousand helium atoms.

- Analytical Chemistry

The major event for the group in 2013 was the organization of HPLC2013, the 39th International Symposium on High Performance Liquid Phase Separations and Related Techniques, which was held from June 16 to 20 in the RAI in Amsterdam. The symposium was chaired by Peter Schoenmakers and Wim Kok, and all members of the group were heavily involved in the organization, with Petra Aarnoutse as focal point. With 200 lectures, almost 1000 posters, and well over 1500 attendees the congres was by far the largest European version ever in the series, which has been running since 1973. Also included in the program were 4 short courses and 21 tutorials, given by internationally reknown experts, on various aspects and application fields of HPLC, which provided an excellent learning opportunity for MSc and PhD students active in the group.

The HPLC2013 organization team

1.4.3 Prizes and honours

Monalisa Goswami wins 2nd prize in Very Short Introductions contest

HIMS researcher Monalisa Goswami finished as runner-up in the Very Short Introductions Competition 2013 of the SPUI25 academic-cultural centre in Amsterdam. Last Friday 29 November she presented her introduction 'That's quite radical' in front of a professional jury which awarded her the second prize. Monalisa Goswami is a PhD researcher in group of professor Bas de Bruin, she investigates catalytic systems for the synthesis of biologically and/or industrially relevant molecules.

Elena Uliyanchenko wins the I.M.Kolthoff Award

Elena Uliyanchenko received the I.M.Kolthoff Award for the best PhD thesis in Analytical Sciences from the section Analytical Chemistry of the Royal Netherlands Chemical Society (KNCV). The jury praised the scientific quality of her thesis titled 'Ultra performance polymer separations' and the balance between theory and practice. The fact that the findings have been embraced by instrument manufacturers and by major chemical industries weighed heavily.

Nicole Franssen wins DPI Golden Thesis Award

Nicole Franssen has been awarded the Dutch Polymer Institute's (DPI) Golden Thesis Award 2013. Franssen obtained her PhD at HIMS in December 2012 with research supervised by professor Bas de Bruin. Her work led to a DPI patent and seven scientific publications in excellent research journals. Franssen is currently a researcher at Shell Global Solutions in Amsterdam.

Helias Andriessen nominated for TEDxAmsterdam Award 2013

Helias Andriessen, master student at the research group Heterogeneous Catalysis and Sustainable Chemistry of professor Gadi Rothenberg and winner of the 2013 Amsterdam Sustainable Research Award for Young Scientists, became one of the 10 finalists of the TEDxAmsterdam Award 2013 with a presenation about Bioplastic.

Linde Smeenk receives Stufkens Prijs for protein mimicry

The *Dick Stufkens Prijs 2013* was awarded to Dr. Linde Smeenk for her Ph.D. thesis 'Double-CLIPS Technology for the Mimicry of Structurally Complex Antibody Binding Sites on Proteins' under supervision ofprofessor Peter Timmerman co-promotor Jan van Maarseveen. The prize is annually awarded to the best thesis of a Ph.D. student belonging to the Holland Research School of Molecular Chemistry (HRSMC). Smeenk is now a postdoc at the ETH Zürich.

Prestigious Eni prize for UvA chemistry professor R. Krishna

Prof. Rajamani Krishna has been awarded a prestigious Eni award for his research into fundamental aspects of gas separation and purification through the understanding of fundamental physical and chemical phenomena at molecular and microscopic level. The prize - in the category New Frontiers of Hydrocarbons - was presented to him on 27 June in Rome by Italian president Giorgio Napolitano. The award consists of a gold medal and a sum of 200,000 Euros.

Joost Reek elected new member of the KMWH

Prof. Joost Reek has been elected as a new member of the Royal Holland Society of Sciences and Humanities (Koninklijke Hollandsche Maatschappij der Wetenschappen, KHMW). Joost Reek was invited for this honourable membership because of his accomplishments in the fields of homegeneous catalysis and sustainable chemistry. He was welcomed as a new member at the general KHMW assembly of 25 May.

Lecturer of the Year

Jan van Maarseveen was awarded the Lecturer of the Year 2012 prize during UvA's Dies Natalis celebration on 8 January 2013. The jury found that Van Maarseveen earned this award because of his dynamic and innovative teaching style. Van Maarseveen demonstrated a unique ability to teach students about the connections that exist between different fields of science such as chemistry, physics and biology. He was successful in providing insight and clarity in the sciences, not in small part due to his toy molecules.

Nomination AVS Fellow of the Society

Prof. Aart Kleijn has been elected to the 2013 class of AVS (American Vacuum Society) Fellows. The 2013 AVS Fellows were honored during the AVS Awards Ceremony on October 30, 2013 during the 60th Annual AVS International Symposium and Exhibition in California.

Startsymposium Co van Ledden Hulsebosch Center

Prior to the 'double oration' of prof. Arian van Asten, Forensic Analytical Chemistry (HIMS) and prof. Maurice Aalders, Forensic Biophysics (AMC), a mini symposium was organized which was the official start of the Co van Ledden Hulsebosch Center (CLHC), the Amsterdam Centre for Forensic Science and Medicine. The CLHC is a joint effort of the Faculty of Science (Faculty of Science) from the University of Amsterdam, the Academic Medical Center (AMC) and the Dutch Forensic Institute (NFI).

1.4.4 Grants

HIMS researchers were extremely successful in acquiring research funding in 2013. The thirteen research proposals that were approved are listed below.

Title	**Sustainable chemistry: A must for a sustainable world**
Applicants:	Prof.dr. Joost Reek, prof.dr. Gadi Rothenberg, prof.dr. Bas de Bruin, prof.dr. Kees Elsevier, prof.dr. Henk Hiemstra
Subsidy from:	Executive Board UvA (College van Bestuur, CvB), Research Priority Area (Zwaartepunt)
Amount:	k€ 428 per annum, for two tenure track positions, postdocs and equipment

Title	**Multicyclic CLIPS-peptides: Next Generation Therapeutic Peptide Drugs**
Applicants:	Dr. Jan van Maarseveen, prof.dr. Peter Timmerman and prof.dr. Henk Hiemstra
Subsidy from:	Technology foundation STW, Open Technology Programme
Amount:	k€ 485 for two PhD students and new HPLC equipment.

Title	**Optically amplified vibrational circular dichroism**
Applicants:	Prof.dr Wybren Jan Buma and prof.dr Sander Woutersen
Subsidy from:	NWO CW, ECHO
Amount:	k€ 260 for one PhD student

Title	**Development and improvement of medical imaging**
Applicants:	Institute Quantivision (iQ), collaboration of UvA, VU, VUmc, AMC, NKI-AvL. Prof.dr. Wybren Jan Buma is member of the management team.
Subsidy from:	ZonMW
Amount:	k€ 1,500

Title	**Mimicking nature to boost transition metal catalysis**
Applicants:	Prof.dr. Joost Reek
Subsidy from:	ERC Advanced Grant
Amount:	k€ 2,500

Title	**Reacting dinitrogen**
Applicants:	Dr. Wojciech Dzik
Subsidy from:	NWO Veni
Amount:	k€ 250

Title	**Ester Hydrogenation using Cheap Base Metal Catalysts**
Applicants:	Prof.dr. Kees Elsevier, prof.dr. Bas de Bruin, dr. Jarl Ivar van der Vlugt
Subsidy from:	SmartMix programme CatchBio
Amount:	k€ 188

Title	**A scalable palladium-catalyzed reductive arylation**
Applicants:	Prof.dr. Joost Reek
Subsidy from:	SmartMix programme CatchBio
Amount:	k€ 188

Title	**Lignin**
Applicants:	Prof.dr. Gadi Rothenberg
Subsidy from:	SmartMix programme CatchBio
Amount:	k€ 282

Title	**Mechanistic insights in catalytic energy conversion processes**
Applicants:	Prof.dr. Bas de Bruin
Subsidy from:	FOM CSER
Amount:	k€ 40 + 1 phD position

Title	**Induced decay and ageing mechanisms in paintings: focus on interactions between pigments and organic binders**
Applicants:	Dr. Katrien Keune, dr. Annelies van Loon, prof.dr. Piet Iedema
Subsidy from:	NWO Joint Programming Initiative Cultural Heritage and Global Change
Amount:	k€ 50

Title	**Oxygen evolving catalysts**
Applicants:	Prof.dr. Joost Reek
Subsidy from:	Towards Biosolar cells
Amount:	k€ 102

Title	**Artificial Leaf**
Applicants:	Prof.dr. Joost Reek
Subsidy from:	Towards Biosolar cells
Amount:	k€ 300

1.4.5 Dissertations

In 2013 the following 16 PhD theses were successfully defended. One of the PhD students (Chantal Carpentier) worked in collaboration with prof. Daniel Bonn of the UvA Institute of Physics, who was her first promotor.

A.J.C. (Annemarie) Walters, 18 December 2013
Mechanistic insight in rhodium-mediated carbene polymerization
Promotors: B. de Bruin, J.N.H. Reek
Group: Homogeneous, Supramolecular and Bio-inspired Catalysis

S.M. (Sérgio) Rosa Domingos, 11 December 2013
Amplified vibrational circular dichroism
Promotor: W.J. Buma
Co-promotor: S. Woutersen
Group: Molecular Photonics

M.R. (Matthijs) Panman, 5 December 2013
Observing invisible machines with invisible light: The mechanics of molecular machines
Promotor: W.J. Buma
Co-promotor: S. Woutersen
Group: Molecular Photonics

D. (Daniela) Peroni, 29 November 2013
Advancing GC×GC through integrated sample preparation methods and optimized column formats
Promotor: J.G.M. Janssen
Co-promotor: P.J. Schoenmakers
Group: Analytical Chemistry

P.F. (Pawel) Dydio, 22 November 2013
Supramolecular control of selectivity in transition metal catalysis: Substrate preorganization & cofactor-steered catalysis
Promotor: J.N.H. Reek
Group: Homogeneous, Supramolecular and Bio-inspired Catalysis

G. (Grisell) Díaz Leines , 15 November 2013
Path-metadynamics: A computational study of conformational transitions in proteins
Promotor: P.G. Bolhuis
Co-promotor: B. Ensing
Group: Computational Chemistry

S. (Sonja) Kaal – Peters, 12 November 2013
Chromatographic profiling: From samples to information
Promotors: J.G.M. Janssen, P.J. Schoenmakers
Co-promotor: G. Vivó-Truyols
Group: Analytical Chemistry

D. (Dion) Houtman, 11 November 2013
To go with the flow: Molecular motors are a drag
Promotor: E.J. Meijer
Co-promotor: E. Eiser
Group: Computational Chemistry

A. (Anna) Pavlova, 30 October 2013
Understanding the role of aqueous solution in chemical reactions: A computational study
Title: Understanding the role of aqueous solution in chemical reactions: A computational study
Promotor: E.J. Meijer
Group: Computational Chemistry

C.E. (Chantal) Carpentier, 26 September 2013
Three-dimensional visualization of contact networks in granular material
Promotors: D. Bonn, A.M. Brouwer
Co-promotor: P. Schall
Group: Molecular Photonics

E.D. (Erdni) Batyrev, 11 September 2013
Understanding the activity of Zn-Cu sites in methanol synthesis
Promotor: G. Rothenberg
Co-promotor: N.R. Shiju
Group: Heterogeneous Catalysis and Sustainable Chemistry

V.J.F. (Vivike) Lapoutre
Infrared spectra of strongly bound clusters: Extending the limits of action spectroscopy
Promotor: J. Oomens
Co-promotor: J.M. Bakker
Group: Molecular Photonics

A.I. (Alma) Olivos Suárez, 4 June 2013
Hypovalent substrates in transition metal catalysis: C–H bond functionalisation, ring-closing reactions & polymer synthesis
Promotor: J.N.H. Reek
Co-promotor: B. de Bruin
Group: Homogeneous, Supramolecular and Bio-inspired Catalysis

L.E.J. (Linde) Smeenk, 22 March 2013
Double-CLIPS technology for the mimicry of structurally complex antibody binding sites on proteins
Promotor: P. Timmerman
Co-promotor: J.H. van Maarseveen
Group: Synthetic Organic Chemistry

R. (Rob) Edam, 21 February 2013
Comprehensive characterization of branched polymers
Promotor: P.J. Schoenmakers
Group: Analytical Chemistry

L. (Lara) Babich, 25 January 2013
Enzymatic cascade reactions involving phosphorylated intermediates: immobilization and process optimization
Promotor: R. Wever
Group: Biocatalysis and Bio-organic Chemistry

1.4.6 Public outreach and media coverage

Spui25 lectures

HIMS researchers contributed to three popular science lectures at Spui25 in 2013:

- 14 March 2013: Zonenergie en CO_2 vastlegging. Prof. Joost Reek and prof. Klaas Hellingwerf (UvA, SILS).
- 27 November 2013: De chemie van het schilderij: dynamisch en complex. Dr. Katrien Keune (HIMS) and dr. Maartje Stols-Witlox (Conservation and Restoration).
- 16 October 2013: Waarom zijn twee linkerhanden ideaal voor een moleculenmaker? Dr. Jan van Maarseveen and prof. Ron Wever.

Radio

- On 26 March 2013 Dr. Katrien Keune, painting research scientist and chemist and project leader of Paint Alterations in Time (PAinT), gave an interview on radio program 'Hoe?Zo!'
- Sunday 24 February 2013, Swammerdam Radio over Antibiotica (Dr. J.H. van Maarseveen and dr. T. den Blaauwen)
- On 1 September 2013 Dr. Sander Woutersen was interviewed on Radio 1 about the effects of water on molecular motors.

Lectures

- de Bruin, B., UvA, 5 April 2013, Gastcollege for 3 VWO scholieren, Zaandam. Title: “Drinken Vampieren ook Blauw Bloed?”
- Brouwer, A.M. (2013, October 3) Lecture “Luminescentie”, Vrije Universiteit, Profielwerkstukbegeleiding.
- Williams, R.M.: Practicum Proefstuderen, 30 January 2013;, 10 December 2013.
- Dr. J.H. van Maarseveen
    - 5 March, onderwijsdebat “Videocolleges”, Kohnstamhuis
    - 14 March, lezing “Making complex molecules, the past, current and future”, symposium “Lab of the Future”, ESTEC Noordwijk
    - 28 March, lezing Dies, FNWI “Samenwerken met studenten en moleculen”.
    - 22 May: lezing basisschooldocenten NEMO “Hoe smaken Moleculen?”
    - 31May: Lezing BKO deelnemers “Teacher of the year: the recipe”
    - 1 June: Lezing Universiteitsdag “Grote problemen oplossen op kleine schaal. Een fascinatie voor moleculen”.
    - 18 June: lezing Junior Chamber International, Amsterdam “Molecules”
    - 22 August: Lezing “Academic Climate at the UvA”, new foreign master students, Oudemanhuispoort.
    - 30 August, Lezing “Van de Oerknal naar het Leven”, Intreeweek, Artis.
    - 6 October: Broodje Wetenschap NRC, NRC café Rokin
- Prof. dr. P. Timmerman
    - 15 October, Web-college in de serie “Cyttron-lectures”, Universiteit Leiden.
    - 26 November, Master-college “Fighting Cancer”, Hogeschool Arnhem/Nijmegen.
    - 28 November, HRSMC/KNCV carrière-adviesmiddag

Miscellaneous

- The projects of the Heterogeneous Catalysis and Sustainable Chemistry group attracted much attention in the media in 2013, especially the discovery of the Fischer-Tropsch catalysts (see highlight in section 1.4.2) and the discovery and application of the bioplastic.
- Prof. Kees Elsevier gave Ad hoc consultancy for a company and assisted a VWO pupil concerning a project about molten salt for reactor cooling and synthesis of a ternary eutectic mixture of salts.
- Interview with professor Arian van Asten on the occasion of the erection of the Co van Ledden Hulsebosch Center on 13 September 2013. Published in Het Parool and in Folia.

2. Research

Research at HIMS is organized in four multidisciplinary research themes - Sustainable Chemistry, Computational Chemistry, Analytical Chemistry and Molecular Photonics - covering fields in chemical sciences where in the next decade interesting new developments and important breakthroughs are anticipated. In the long term the HIMS research topics are envisaged to be pivotal for the development of a sustainable society. Below the annual reports of all research groups are clustered per theme.

2.1 Sustainable Chemistry

Sustainable chemistry is the largest theme within HIMS. This theme covers all relevant catalysis sub-disciplines and was acknowledged a University Research Priority Area ('onderzoekszwaartepunt') in 2013. All research groups within HIMS participate in this area and two new tenure track candidates will be hired in 2014. This paragraph contains the reports of the following groups:

- Homogeneous and Supramolecular Catalysis
- Heterogeneous Catalysis and Sustainable Chemistry
- Synthetic Organic Chemistry
- Molecular Inorganic Chemistry
- Biocatalysis and Bio-organic Chemistry

Group:	Homogeneous and Supramolecular Catalysis		
Group leader:	Prof. Dr. J.N.H. Reek		
Academic staff:	Prof. dr. B. de Bruin Dr.Ir. J.I. van der Vlugt		
Support staff:	Z. Abiri (temp) ing. F. Ait El Maate A.M. van der Burg E. Duin Berteling C. Mahabiersing		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. W.I. Dzik Dr. D. Hetterscheid Dr. T.R.M. Besset Dr. M. Otte Dr. V. Lyaskovskyy Dr. P. Li Dr. S. Mandal Dr. Y. Gloaguen Dr. N.D. Paul Dr. R. Detz Dr. T.J. Korstanje Dr. P. Dydio Dr. A.M. Shultz Dr. R. Gramage Doria Dr. P. Gualco	01-11-2012 01-02-2010 01-10-2012 15-08-2012 01-02-2011 01-07-2012 01-04-2013 01-11-2010 01-08-2012 01-09-2012 15-08-2013 01-07-2013 01-09-2011 01-11-2011 01-06-2013	31-10-2016 31-01-2013 31-03-2013 31-10-2013 31-01-2013 30-06-2014 31-07-2013 14-05-2013 21-12-2013 31-12-2015 14-08-2015 31-12-2013 31-08-2013 30-04-2014 31-05-2014
PhD students:	Drs. A.I. Olivos Suarez Drs. P. Dydio Drs. A.J.C. Walters Drs. Y. Gumrukcu Drs. F.G. Terrade	15-01-2009 01-07-2009 01-08-2009 01-11-2009 15-11-2009	14-01-2013 30-06-2013 15-09-2013 31-10-2013 14-11-2013

	Drs. B. van den Bosch	01-05-2010	30-04-2014
	Drs. S. Oldenhof	01-10-2010	30-09-2014
	Drs. J.J.M. Daubignard	01-01-2011	31-12-2014
	Drs. Z. Tang	01-01-2011	31-12-2014
	Drs. J.M. Koelewijn	01-02-2011	31-01-2015
	Drs. S.Y. de Boer	15-08-2011	14-08-2015
	Drs. P. Boulens	01-10-2011	30-09-2014
	Drs. S.H.A.M. Leenders	01-10-2011	30-09-2015
	Drs. L.S. Jongbloed	15-02-2012	14-02-2016
	Drs. R. Becker	01-03-2012	28-02-2016
	Drs. V. Vreeken	01-05-2012	30-04-2016
	Drs. D.L.J. Broere	15-05-2012	14-05-2016
	Drs. A. Chirila	01-09-2012	31-08-2016
	Drs. P.F. Kuijpers	01-10-2012	30-09-2016
	Drs. R. Zaffaroni	01-11-2012	31-10-2016
	Drs. F.F. van de Watering	01-11-2012	31-10-2016
	Drs. M. Goswami	01-08-2013	31-07-2017
	Drs. C. Rebreyend	01-08-2013	31-07-2017
	Drs. C. te Grotenhuis	01-08-2013	31-07-2017
	Drs. E.C.F. Schippers	01-11-2013	31-10-2017
MSc students:	Richard van Heck Rogier Kox Lambert Baij Dirk Zant Renee Haver Maarten van Ham Melanie Chevry Esther Schippers		

Mission of the group:
The mission of the research group is the development of supramolecular and bio-inspired tools to enhance the field of transition metal catalysis. Eventually these new tools should lead to the discovery of new catalyst systems that display unrivaled selectivities and activities for reactions that are relevant to the fine chemical or bulk industry, or contribute to societal challenges such as the transition to alternative energy sources or bio-based economy.

Research results per sub project

ERC advanced Grant J.N.H. Reek
Title: Nature Inspired catalysis (NATCAT). PhD student 2013: Drs. E.C.F. Schippers (PhD).
This project started in November 2013. Initial focus is on the preparation of cage compounds and the isolation of the Nitrogenase co-factor. This involves a collaboration with Prof Seefeldt (Utah, USA). A Bruker X-ray machine has been ordered and will be operational early 2014.

NWO TOP Grant J.N.H. Reek
Title: Enzyme inspired transition metal catalysis
PhD students and postdocs 2013: Pawel Dydio (PD), Drs. S.H.A.M. Leenders (PhD), Drs. S. Oldenhof (PhD), Drs. J.J.M. Daubignard (PhD).
This project is half-way and program proceeds as planned. Several new complexes based on METAMORPhos have been established, including one based on iridium. This complex was demonstrated to be a good catalyst for the base-free dehydrogenation of formic acid, which is important in light of the use of formic acid as energy storage (*Chem. Eur. J*). In the area of substrate

orientation as a tool to control asymmetric hydrogenation we made a lot of progress. Several intermediates have been isolated and characterized, and we are now converging to a clear picture of the operational mode of the supramolecular catalysts used in this reaction. Several cages have been synthesized and explored as host for transition metal catalysts, and we are currently looking at various catalytic transformations with these systems.

Applied Catalysis J.N.H. Reek

Title: Supramolecular catalysts for applied hydroformylation (Eastman) and oligomerization catalysts (IFP). PhD students and postdocs 2013: Tatiana Besset (PD), Pierre Boulens (PhD). Eastman project was successfully concluded in 2013 and one publication has been published so far. IFP project is proceeding as planned. Results are confidential.

NRSCC group program J.N.H. Reek, B. de Bruin and J.I van der Vlugt

Title: new catalytic processes.

PhD students and postdocs 2013: Drs. P. Dydio (PhD), Drs. F.G. Terrade, (PhD), Drs. S.Y. de Boer (PhD), R. Gramage Doria (PD). Dydio graduated Cum Laude in November 2013. His thesis on DIMPhos, a new bidentate ligand with an intergrated anion binding pocket that can be used to control selectivity in transition metal catalysis in a new manner (see highlight, JACS, ACIE). Frederic Terrade almost finished his thesis, which deals on the use of METAMORPhos ligands in coordination and catalysis. One of the highlights is the observation of non-linear effects when chiral (non enantiopure) ligands are used in asymmetric hydrogenation by dinuclear rhodium complexes (Chem. Eur. J.). De Boer is working on new ligand concepts in which the ligands actively participate in the catalytic event.

Catalysis for green energy applications: BioSolarCells/FOM/NWO/NRSCC J.N.H. Reek, B. de Bruin and J.I van der Vlugt

Title: several programs around energy.

PhD students and postdocs 2013: Drs. B. van den Bosch (PhD), Drs. J.M. Koelewijn, (PhD), Drs. R. Becker (PhD), Drs. F.F. van de Watering (PhD), Drs. R. Zaffaroni (PhD), Dr. A.M. Shultz (PD, Dr. P. Li (PD), Dr. R. Detz (PD), Dr. D Hetterscheid (PD), Dr. W. Dzik (PD). This is a strong program in our group in which we study all facets related to storages of solar energy in chemical bonds. One of the major goals is the fabrication of solar to fuel devices based on molecular components. Towards this goal we have made several catalysts for water oxidation and several for proton reduction. In addition, we can immobilize the catalysts and chromophores on electrodes. It is expected that next year we will have the first working (half)devices. In addition to hydrogen, we also look into the activation of CO_2 and N_2, to generate formic acid, methanol and amonia as energy carriers. This program involves collaboration with national networks (BioSolarCells, NRSCC) as well as European networks (EUROCORE).

CatchBio project Prof. J.N.H. Reek & B. de Bruin

Title: New reactions to chiral amines from alcohols and ketones. PhD student 2013: Yasemin Gumrukcu. Project has ended december 2013 and the PhD student is currently writing the thesis. A supramolecular catalyst system has been developed for the activation of allyl alcohols, and the further conversion to form C-C and C-N bonds. In addition, an unusual coupling between allyl alcohols and styrene derivatives has been found. For both reactions, detailed kinetics and DFT calculations reveal the mechanism of these reactions. Several papers are expected in the next period.

ERC starting Grant B. de Bruin

Title: Catalytic Carbene Insertion Reactions (CatCIR). PhD students and postdocs 2013: Volodomyr Lyaskovskyy (PD), Yann Gluoaguen (PD), Matthias Otte (PD), Alma Olivos Suarez (PhD), Annemarie Walters (PhD). This project ended August 2013. Both PhD students got their PhD. The project led to 8 publications in 2013. The project proceeded as planned. New carbene polymers were characterized in detail, showing unexpected 3D helical structure parameters explaining LC behavior. Several new carbene insertion reactions were explored, among which catalytic ketene synthesis.

NWO-VICI Grant B. de Bruin
Title: Radicals in Catalysis; Selective Metal-Mediated Radical-Type Transformations
PhD students and postdocs 2013: Monalisa Goswami (PhD), Paul Kuipers (PhD), Andrei Chirila (PhD), Christophe Rebreyend (PhD), Colet te Grotenhuis (PhD), Nanda Dulal Paul (PD), Pauline Gualco (PD), Sutanuva Mandal (PD). Project is proceeding as planned. The project has already led to several publications in 2013. Several new radical-type reactions are being explored. Several different techniques to control these radical-type reactions are under investigation, among which reactions in cages, metallo-radical control, redox non-innocent ligand control. A Bruker EPR machine was purchased and has been made operational.

NWO-ECHO Grant B. de Bruin
Title: Cooperative ligands in hydrogenation, dehydrogenation and dehydrogenative couplings
PhD student 2013: Zhou Tang. Project is proceeding as planned. After a period of synthesizing new complexes they are now tested as catalysis in several new reactions. Several papers are expected in the next period.

ERC Starting Grant J.I. van der Vlugt
Title: Smart Systems for Small Molecule Activation and Sustainable Homogeneous Catalysis (*EuReCat*)
PhD students 2013: Linda Jongbloed, Vincent Vreeken and Danny Broere. This project, aimed at the development of mono- and dinuclear systems bearing reactive ligands for metal-ligand bifunctional activation of small molecules and cooperative catalysis, is proceeding as planned. Highly unusual phenomena with both proton-responsive and redox-noninnocent ligand based complexes have been observed and applied for selective bond activation processes. An MBraun glovebox was purchased and has been operational. Three papers were published in 2013 and several papers are expected in the next period.

Collaborations J. Reek 2013:
- Prof. Kroutil, University of Gratz (Austria).
- Prof. Bonn, Max Planck Institute (Germany).
- Prof. Sander Woutersen (HIMS)
- Prof. Fred Brouwer (HIMS)
- Prof. Ivanovic-Burmazovic, University of Erlangen (Germany).
- Prof. M. Fujita, University of Tokyo (Japan).
- Dr. Bourbigou/dr. Breuil IFP Lyon France.
- Dr. Lutz (UU).

In 2013, Joost Reek was scientific director of the spinoff company InCatT.

Collaborations B. de Bruin 2013:
- Prof. Sven Schneider, University of Göttingen (Germany).
- Prof. Robert Wolf, University of Regensburg (Germany).
- Prof. Sander Woutersen & Prof. Wybren-Jan Buma (HIMS)
- Prof. Xuefeng Fu, University of Peking (China).
- Prof. Hansjörg Grützmacher, ETH Zürich (Switzerland).
- Prof. Theo Dingemans, TU Delft.

Collaborations J.I. van der Vlugt 2013:
- Dr. Jorge Gascon, Prof. Freek Kapteijn (TU Delft).
- Prof. Evamarie Hey-Hawkins (Leipzig, Germany)
- Dr. Maxime Siegler (JHU, Baltimore).
- Dr. Martin Lutz (Utrecht).
- Prof. Fred Brouwer (HIMS).

Key publications per academic staff member

Prof. Dr. JNH Reek

- P. Dydio J.N.H. Reek* 'Supramolecular Control of Selectivity in Hydroformylation of Vinyl Arenes: Easy Access to Valuable Beta-Aldehyde Intermediates ' *Angew. Chem. Int. Ed.*, **2013**, *52*, 3878. ***Highlighted in Nature Chemistry.***
- P. Dydio, R. Detz, J.N.H. Reek***** *"*Precise Supramolecular Control of Selectivity in the Rh-Catalyzed Hydroformylation of Terminal and Internal Alkenes*" J. Am. Chem. Soc.* **2013** *135*, 10817.
- V. Bocokic, A. Kalkan, M. Lutz, A.L. Spek, D.T. Gryko & J.N.H. Reek***** "Capsule-controlled selectivity of a rhodium hydroformylation catalyst" *Nature Communications* **2013**, *4*, 2670.

Prof. Dr. B. de Bruin

- Nitrogen-Centred Ligand Radical Complexes; Classification, Spectroscopic Features, Reactivity and Catalytic Applications. Olivos Suarez, A.I.; Lyaskovskyy, V.; Reek, J.N.H.; van der Vlugt, J.I.; de Bruin, B.*; Angew. Chem. Int. Ed., 2013, 52, 12510–12529.
- Encapsulation of Metallo-Porphyrins in a Self-Assembled Cubic M8L6 Cage – A new Molecular Flask for Cobalt-Porphyrin Catalyzed Radical-type Reactions. Otte, M.; Kuijpers, P. F.; Troeppner, O.; Ivanović-Burmazović, I.; Reek, J. N. H.; de Bruin, B.*; Chem. Eur. J., 2013, 19, 10170 – 10178.
- Synthesis and Reactivity of a Transient, Terminal Nitrido Complex of Rhodium. Scheibel, M. G.; Wu, Y.; Stückl, A. C.; Krause, L.; Carl, E.; Stalke, D; de Bruin, B.*; Schneider, S.*, J. Am. Chem. Soc., 2013, 135, 17719.

Dr.Ir. JI van der Vlugt

- Y. Gloaguen, W. Jacobs, B. de Bruin, M. Lutz, J.I. van der Vlugt* "Reactivity of a mononuclear IrI species bearing a terminal phosphido fragment embedded in a triphosphorus ligand" Inorg. Chem. 2013, 52, 1682-1684.
- Y. Gloaguen, L.M. Jongens, J.N.H. Reek, M. Lutz, B. de Bruin, J.I. van der Vlugt* "Reductive elimination at an orthometalated IrIII hydride bearing a tripodal tetraphosphorus ligand" Organometallics 2013, 32, 4284-4291.
- A. Perrier, M. Ferreira, J.N.H. Reek, J.I. van der Vlugt* "Regioselective Pd-catalyzed hydroamination of substituted dienes" Catal. Sci. Technol. 2013, 3, 1375-1379.

Dissertations

Dydio, P.F. (22 November 2013). *Supramolecular control of selectivity in transition metal catalysis: Substrate preorganization & cofactor-steered catalysis.* Universiteit van Amsterdam (200 pag.). Prom./coprom.: prof.dr. J.N.H. Reek.

Olivos Suárez, A.I. (4 June 2013). *Hypovalent substrates in transition metal catalysis: C–H bond functionalisation, ring-closing reactions & polymer synthesis.* Universiteit van Amsterdam (199 pag.). Prom./coprom.: prof.dr. J.N.H. Reek & prof.dr. B. de Bruin.

Walters, A.J.C. (18 December 2013). *Mechanistic insight in rhodium-mediated carbene polymerization.* Universiteit van Amsterdam (186 pag.). Prom./coprom.: prof.dr. B. de Bruin & prof.dr. J.N.H. Reek.

Grants and prizes

- Bruin, B. de (2013). project 'Mechanistic insights in catalytic energy conversion processes'. Shell/NWO/FOM programma 'Computational sciences for energy research'
- Franssen, N.M.G. (2013). DPI Golden Thesis Award.
- Goswami, M. (2013). 2nd prize Very Short Introductions Competition 2013 of SPUI25.
- Reek, J.N.H. (2013). elected member of the Koninklijke Hollandsche Maatschappij der Wetenschappen (KMWH).
- Reek, J.N.H. (2013). ERC Advanced Grant.

Invited lectures

- De Bruin, B., SILQCOM/2013 (Simposio Latinoamericano de Quimica de Coodinacion y Organometalica), Oaxaca, Mexico, October 13-17, 2013, Title: Catalytic Radical-Type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'. Plenary Lecture.
- De Bruin, B., Seminar at the Chemistry Department of University of South Florida. Host: X. Peter Zhang. October 10, 2013. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.
- De Bruin, B., Seminar at the University of Zaragoza, September 19-20, 2013. Invited lecture, Title: Catalytic Radical-type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.
- De Bruin, B., 2013 Physical Organic Chemistry Gordon Research Conference, New Hampshire (USA), June 23-28, 2013. Title: Bio-Inspired Catalytic Radical-Type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'. Plenary Lecture.
- De Bruin, B. 6th Pacific symposium on Radical Chemistry, Vancouver (Canada), June 16-20, 2013. Title: Bio-Inspired Catalytic Radical-Type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'. Plenary Lecture.
- De Bruin, B. 171st Dies Symposium TU Delft 'Structure in Catalysis', January 10, 2013. Delft, The Netherlands. Title: Bio-Inspired Catalytic Radical-type Transformations.
- Reek, J.N.H. (2013, January). *Supramolecular strategies in Transition metal catalysis.* Stuttgart, Gemany, Faculty symposium University of Stuttgart.
- Reek, J.N.H. (2013, March). *Supramolecular strategies to control selectivity in hydroformylation.* New Orleans, USA Invited lecture Hydroformylation Symposium at ACS.
- Reek, J.N.H. (2013, May). *Supramolecular strategies in Transition metal catalysis.* Agde, France, Invited lecture Gecom-Concoord.
- Reek, J.N.H. (2013, May). *Supramolecular strategies in Transition metal catalysis.* Tokio, Japan, Invited lecture Gratama conference
- Reek, J.N.H. (2013, June). *Supramolecular strategies in Transition metal catalysis.* Aachen, Germany, Invited lecture Honorary symposium Noble prize winners 2010.
- Reek, J.N.H. (2013, July). *Supramolecular strategies in Transition metal catalysis.* Marseille, France, Invited lecture 18th European Symposium on Organic Chemistry (ESOC 2013).
- Reek, J.N.H. (2013, september). *Supramolecular strategies in Transition metal catalysis.* Padova, Italy, Invited lecture 2013 Italian Supramolecular meeting.
- Reek, J.N.H. (2013, september). *Supramolecular strategies in Transition metal catalysis.* Lausanne, Invited lecture Swiss Chemical Society meeting.
- Reek, J.N.H. (2013, september). *Supramolecular strategies in Transition metal catalysis.* Groningen, Invited lecture supramolecular systems meeting.
- Reek, J.N.H. (2013, November). *Supramolecular strategies in Transition metal catalysis.* Strasbourg, Faculty symposium ISIS Strasbourg.
- Reek, J.N.H. (2013 November). *Supramolecular strategies in Transition metal catalysis.* Leiden, The Netherlands, Invited lecture HRSMC symposium.
- Reek JNH Plenary Lecture NIOK-KNAW symposium "catalysis for the catalysis " New strategies in Transition metal catalysis" November 2013.
- Vlugt, J.I. van der (2013 September). *Design of Reactive Ligands for Cooperative Activation of Small Molecules.* Leipzig, Germany, Minisymposium, Graduate School BuildMoNa, invited lecture.
- Vlugt, J.I. van der (2013 December). *Organometallic Cooperative Ligands: Avenues for Bifunctional Bond Activation and Catalysis.* Xcaret, Mexico, Zing Conference Coordination Chemistry, invited lecture.

Patents and utilization

Reek, J.N.H. (2013) *Nouveau complexe à base de nickel et son utilisation dans un procédé d'oligomérisation des oléfines*.

Committee & Management Activities 2013

- de Bruin, B., UvA coordinator new UvA-VU Master Track 'Science for Energy and Sustainability'.
- de Bruin, B., Member of the Chemistry Education Committee (Onderwijscommissie Scheikunde, OCS) UvA-VU (since 09-2008). (Co)chair of the committee since 2012.
- de Bruin, B., Member of the NWO-CW TOP/ECHO selection committee 2013.
- Reek Boardmember KNCV since 2009
- Reek Member (Chair 2013-2016) UOC UvA
- Reek Director of research priority area sustainable chemistry UvA (since 2013)
- Reek, Director Van 't Hoff Institute for Molecular Science (HIMS) (Sep 2013-now)
- Reek Chair of NWO work group Coordination and Catalysis since 2008

Editorial Board Activities 2013:

- de Bruin, B., Editorial board European Journal of Inorganic Chemistry (member since 01-2008). Chair of the Board since March 1, 2013
- de Bruin, B., Editorial Advisory Board Organometallics since January 2014.
- Reek Advisory Board Eur. J. Inorg Chem. Since 2008
- Reek Advisory Board ChemPlusChem since 2011

Group:	Heterogeneous Catalysis and Sustainable Chemistry		
Group leader:	Prof. dr. G. Rothenberg		
Academic staff:	Dr. N.R. Shiju Dr. S. Grecea		
Support staff:	ing. P.F. Collignon ing. N.J. Geels Dr. M.C. Mittelmeijer- Hazeleger		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Drs. A.H. Alberts Dr. H.L. Castricum Dr. N. Mandaan - Jaso Dr. M.J. Louwerse Dr. ir. E.V. Ramos Fernandez Dr. A.G. Maldonado Dr. A.L. Dantas Ramos	01-01-2012 01-04-2010 01-12-2012 01-10-2009 01-03-2012 n/a (Solvay) 01-03-2013	31-12-2014 31-03-2013 30-11-2014 30-09-2014 28-02-2014 n/a (Solvay) 01-03-2014
PhD students:	Drs. Z.I. Strassberger Drs. B. Coskuner	01-01-2010 Erasmus fellow	31-12-2013 Erasmus fellow
MSc students:	Drs. R. Beerthuis Drs. H.A.A. Andriessen Drs. C. Hernandez-Mejia Drs. S. Boeree		

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

Research results per sub project
Title: Hydrothermally stable organosilica-based hybrid membranes for molecular separations (funded by STW)
Researchers: Dr. H.L. Castricum
2013 was the final year of this project, a collaboration with Twente University and ECN. We continued with the synthesis of hybrid membranes and their applications. The results were published in a full paper (published online in 2013): Tuning the nanopore structure and separation behavior of hybrid organosilica membranes. H.L. Castricum, G.G. Paradis, M.C. Mittelmeijer-Hazeleger, W. Bras, G. Eeckhaut, J.F. Vente, G. Rothenberg and J.E. ten Elshof, *Micropor. Mesopor. Mater.*, **2014**, 185, 224-234.

Title: Synthesis and testing of novel mixed oxides for solar fuel thermocatalysis (funded by NRSC-C)
Researchers: Dr. E.V. Ramos-Fernandez
This project centres on the understanding of the reduction mechanism of CO_2 to CO at high temperatures catalysed by doped ceria. We succeeded in explaining the mechanism and thereby pinpointing the optimal dopants and their formulation on the surface. The results were presented in international conferences and published (paper appeared in 2014). Also on the strength of these achievements, Dr. Ramos-Fernandez was appointed to a permanent position in Spain.

Title: New catalytic routes to 1,3-butadiene (funded by LANXESS)
Researchers: Dr. N. Madaan
This project is proceeding according to plan. A press release was published, see http://www.uva.nl/en/about-the-uva/organisation/faculties/content/faculteit-der-natuurwetenschappen-wiskunde-en-informatica/shared-content/news/2012/07/uva-chemists-sign-agreement-with-synthetic-rubber-company-lanxess.html Further, a paper has been accepted for publication on the project results (will appear in 2014).

Title: Catalytic valorization of lignin to key phenols and aromatics (funded by CatchBio)
Researchers: Drs. Z. Strassberger
This project ended in December 2013 and Zea Strassberger submitted her PhD thesis to the reading committee (defence expected summer 2014). By using a variety of monomeric and dimeric model compounds as well as real lignin feedstocks, we showed that catalytic removal of labile groups is feasible. The results were published in several per-reviewed articles and presented in various national and international conferences. Due to the promising results obtained in this project, Catchbio granted its continuation for another 3 years. A postdoc will be appointed in 2014.

Title: Strategic collaboration with Solvay on predictive modelling (funded by Solvay)
Researchers: Dr. M.J. Louwerse; Dr. A.G. Maldonado
In this project HCSC provides solutions to problems raised by Solvay's business units worldwide. The solutions centre on a combined modelling/experimentation workflow developed by our group. Apart from funding, this project also gives direct access to important industrial business units, and to the questions that these units must solve.

Title: Synthesis and properties of new metal organic-frameworks
Researchers: Dr. A. L. Ramos Dantas (senior fellowship funded by CAPES foundation, Programme "Science without borders")
This project focused on the selective separation of water from water/alcohols mixtures, one of the thornisest practical problems in many industrial processes. We designed a new lanthanide MOF with a highly stable microporous structure. It has hydrophilic 1D tetragonal channels with a window size appropriate for accommodating water molecules. Unlike most MOFs, it is also hydrothermally stable at high temperatures. This is the first lanthanide MOF showing highly selective water adsorption. It opens exciting opportunities for developing desiccants for removing small amounts of water from water/alcohol mixtures as well as wet gases. The results are submitted for publication and presented in national/international conferences.

Title: Degradation of cyanides in waste water by solid catalysts
Researcher: Paula Oulego Blanco (visiting PhD student, University of Oviedo, Spain)
Waste waters generated by many industrial processes, *e.g.* metallurgical, steel, rubber, gold and silver mining, usually contain free and complex cyanides. Since these are toxic for living organisms, proper treatment before they are discharged into the water ways is very important. In this project, a number of solid catalysts were tested for oxidative destruction of the cyanides using H_2O_2. Copper and niobium oxides were found to be most active and stable.

Title: Heterogeneously catalysed hydrogenation of levulinic acid to γ-valerolactone
Researcher: Bilge Coşkuner (visiting PhD student-Erasmus Mundus scheme, Yildiz Technical University, Turkey). The hydrogenation of biomass-derivable levulinic acid (LA) and its esters to γ-valerolactone (GVL) is a key reaction in developing biorenewable routes to chemicals and fuels. Precious metals such as ruthenium catalyses this hydrogenation using molecular H_2. However, there are many unresolved issues, such as the stability of the catalysts and dependence of activity on the support properties. This project aims to develop new heterogeneous catalysts for LA hydrogenation to GVL and to establish structure-activity correlations.

Title: Understanding the activity of Zn-Cu sites in methanol synthesis (funding: STW)
Researcher: Dr. Erdni Batyrev
Dr. Batyrev successfully defended his PhD thesis in September 2013. His thesis deals with the Cu/ZnO interaction in activated methanol synthesis catalysts. A combination of classical characterization techniques and surface science techniques was applied to probe the dynamic modification of catalyst structure upon the activation in hydrogen. Based on the findings, the active sites of the Cu/ZnO methanol catalysts were proposed. The results were also published in *J. Phys. Chem. C.*

Collaboration project:
Title: Direct conversion of ethane to acetic acid in aqueous phase over solid catalysts
Researcher: Rie Indo (Collaboration with Prof. T. Ishihara, Department of Applied Chemistry, Faculty of Engineering, Kyushu University, Japan)
Ethane is the second-largest component of natural gas. Thus, its selective conversion into useful oxygenated products, e.g. acetic acid, is of significant importance. However, ethane is also one of the least reactive hydrocarbons, which limits its practical use. The high temperatures needed to achieve reasonable conversion decrease the selectivity. This project aims the direct oxidation of ethane to acetic acid at moderate temperatures, using aqueous H_2O_2 as oxidant over solid catalysts.

Other activities
The group has several strong collaborations with the chemical industry, centred on our core competence of catalyst and materials discovery and development. Our scientific staff invests a substantial fraction of their time in developing these collaborations, which in many cases lead to industrially-funded projects.

In 2013, we hosted several visiting PhD students and Postdocs on Erasmus and EU-funded research visits, typically for 3-month or 6-month periods: Drs. Bilge Coskuner, Drs. Paula Oulego Blanco, Ms. Karolin Dietrich, Drs. Piera Demma Cara.

Conference organising and chairing:
- N.R. Shiju: Co-Chair, Heterogeneous Catalysis session, XIVth Netherlands' Conference on Chemistry and Catalysis, Noordwijkerhout, Netherlands, 2013.
- N.R. Shiju: Session Chair, Adsorption and Separation; 66th Annual Session of Indian Institute of Chemical Engineers (IIChE) and joint Indo-US symposium, ICT, Mumbai, India, 2013.

Key publications per academic staff member
Dr. S. Grecea (Tanase)
- Catalytic cleavage of lignin ß-O-4 link mimics using copper on alumina and magnesia-alumina. Z. Strassberger , A.H. Alberts , M.J. Louwerse , S. Tanase and G. Rothenberg,Green Chem., 2013, 15, 768-774.
- Poly(vinylidene fluoride)/nickel nanocomposites from semicrystalline block copolymer precursors. V.S.D. Voet, M. Tichelaar, S. Tanase, M.C. Mittelmeijer-Hazeleger, G. ten Brinke and K. Loos, Nanoscale, 2013, 5, 184-192.
- Synthesis, characterization and testing of a new V2O5/Al2O3−MgO catalyst for butane dehydrogenation and limonene oxidation. Z. Strassberger, E.V. Ramos-Fernandez, A. Boonstra, R. Jorna, S. Tanase and G. Rothenberg, Dalton Trans., 2013, 40, 5546-5553.

Dr. N.R. Shiju
- Hemicellulose hydrolysis catalysed by solid acids. P. Demma Carà, M. Pagliaro, A. Elmekawy, D.R. Brown, P. Verschuren, N.R. Shiju and G. Rothenberg, Catal. Sci. Technol.,2013, 3, 2057-2061.
- Efficient three-component coupling catalysed by mesoporous copper-aluminum based nanocomposites. J. Dulle, K. Thirunavukkarasu, M.C. Mittelmeijer-Hazeleger, D.V. Andreeva, N.R. Shiju and G. Rothenberg, Green Chem., 2013, 15, 1238-1243.

- De novo design of nanostructured iron-cobalt Fischer-Tropsch catalysts. V.R. Calderone, N.R. Shiju, D. Curulla Ferré, S. Chambrey, A. Khodakov, A. Rose, J. Thiessen, A. Jess and G. Rothenberg, Angew. Chem. Int. Ed.,2013, 52, 4397-4401.

Prof. Dr. G. Rothenberg

- Modeling catalyst preparation: The structure of impregnated-dried copper chloride on γ-alumina at low loadings. M.J. Louwerse and G. Rothenberg, ACS Catal., 2013, 3, 1545-1554.
- Predicting adsorption on metals: Simple yet effective descriptors for surface catalysis. E.J. Ras, M.J. Louwerse, M.C. Mittelmeijer-Hazeleger and G. Rothenberg, Phys. Chem. Chem. Phys., 2013, 15, 4436-4443.
- Kinetics of Propane Dehydrogenation over Pt-Sn/Al2O3. S. Gómez-Quero, T. Tsoufis, P. Rudolf, M. Makkee, F. Kapteijn and G. Rothenberg, Catal. Sci. Technol., 2013, 3, 962-971.

Dissertations

Batyrev, E.D. (11 September 2013). *Understanding the activity of Zn-Cu sites in methanol synthesis.* Universiteit van Amsterdam (141 pag.). Prom./coprom.: prof.dr. G. Rothenberg & dr. N.R. Shiju.

Grants and prizes

Andriessen, H.A.A. (2013). 2013 Amsterdam Sustainable Research Award for Young Scientists of the University of Amsterdam and nominated for TEDxAmsterdam Award 2013.

Invited lectures

- G. Rothenberg: A new type of plastic made from plants. Ben-Gurion University, Israel, May 2013 (Dean's Podium lecture);
- G. Rothenberg: And now for something completely different. Albemarle Technology Day, Amsterdam, June 2013 (Plenary lecture);
- G. Rothenberg: Heterogeneous Catalysis and Sustainable Chemistry in Amsterdam, TEI Chalkida, Greece, September 2013 (invited lecture);
- G. Rothenberg: From weird ideas to practical applications: New catalysts for making synthetic fuels; Departmental Seminar, Chemistry, the Technion, Israel, October 2013 (invited lecture);
- G. Rothenberg: From old ideas to new innovations - the invention of practical Fischer-Tropsch catalysts; Departmental Seminar, Chemistry and Materials Engineering, Fudan University, Shanghai, China, November 2013 (invited lecture);
- N. R. Shiju: Heterogeneously catalysed conversion of biomass derivatives to chemicals; 66th Annual Session of Indian Institute of Chemical Engineers (IIChE) and joint Indo-US symposium, ICT, Mumbai, India, 2013, (invited lecture).
- N. R. Shiju: Catalytic conversion of hemicellulose to sugars and sugar alcohols; XIth European Congress on Catalysis, Lyon, France, 2013 (contributed lecture).
- S. Grecea: Short-range correlations in d-f cyanide-bridged assemblies; Joint European Magnetic Symposia, Rhodes, Greece, 2013 (contributed lecture).

Patents and utilization

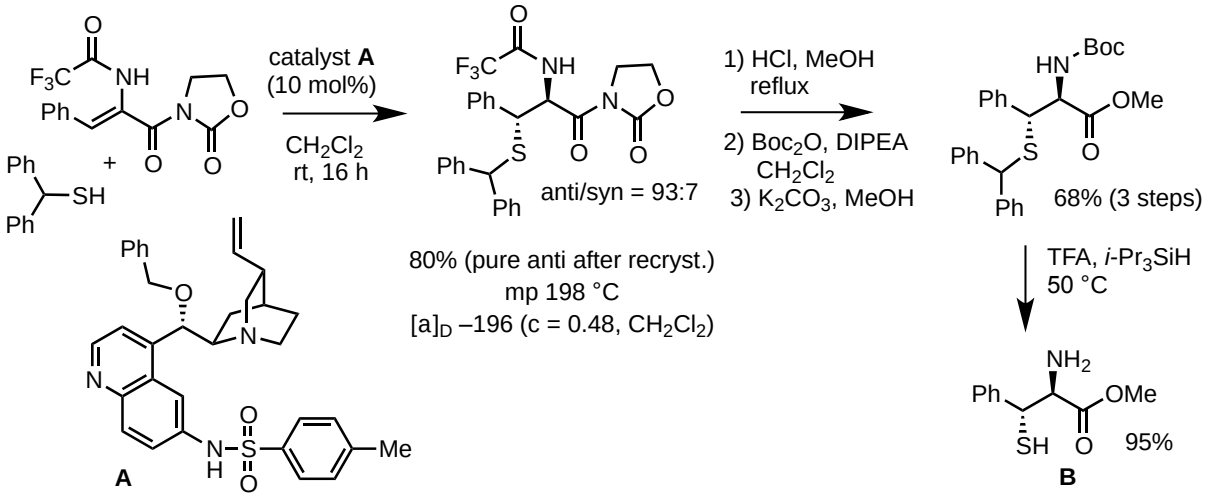
- The group did not file new patent applications in 2013. However, four patent applications submitted in 2011 were published, entering the national registration phase. The patent on the new Fischer-Tropsch catalysts (project funded by Total Gas & Power) was registered worldwide by Total, and a new industrial project is in the making based on it.
- The bioplastic project has made much progress in 2013 towards valorisation, and we foresee that it will be spun out as an independent company in the first half of 2014.
- Core-shell particles with catalytic activity. V.R. Calderone, N.R. Shiju, G. Rothenberg and D. Curulla-Ferre, WO 2012/163969 (May 30, 2011).
- Composite material comprising synthetic filler and specific polymer. A.H. Alberts and G. Rothenberg, EP 2511326; WO 2012/140239 (April 14, 2011).

- Laminate comprising carrier and coating polymer. A.H. Alberts and G. Rothenberg, WO 2012/140238 (April 14, 2011).
- Composite material comprising bio-filler and specific polymer. A.H. Alberts and G. Rothenberg, WO 2012/140237 (April 14, 2011).

Group:	Synthetic Organic Chemistry		
Group leader:	Prof. dr. H. Hiemstra		
Academic staff:	Dr. J.H. van Maarseveen Dr. S. Ingemann Jorgensen Prof. dr. P. Timmerman (BHGL)		
Support staff:	R.A. Kleinnijenhuis M.J. Wanner *Vacancy, filled since Jan 16th 2014*		
Temporary staff		Start date	(Foreseen) end date
Postdocs:			
PhD students:	Drs. J.P.A. Rutters Drs. A.C. Breman Drs. S. Popovic Drs. G.J.J. Richelle Drs. L. Steemers	01-10-2007 01-11-2009 01-02-2010 01-11-2013 01-09-2012	31-03-2012 31-10-2013 31-01-2014 31-10-2017 31-07-2016
MSc students:	M.W.E. (Elma) Mons Jelmer A.A. Koole Nabil Tahiri Medea Kosean Camille l'Epine (Marseille) Dieuwertje E. Streefkerk Jordy Saya Martien Würdemann Jamie I. Scott (Edinburgh) Charlotte E. Wilson (Edinburgh) Nikos Kyriakou	01-01-2013 01-01-2013 01-01-2013 01-12-2012 01-02-2013 01-09-2013 01-09-2013 01-10-2013 01-10-2013 01-10-2013 01-11-2013	30-09-2013 30-09-2013 31-10-2013 30-09-2013 31-07-2013 31-03-2014 31-05-2014 30-06-2014 30-06-2014 30-06-2014 31-07-2014
HBO stagiairs	Nick de Vries Jelle O. Streefkerk	01-01-2013 01-09-2013	30-06-2013 31-03-2014

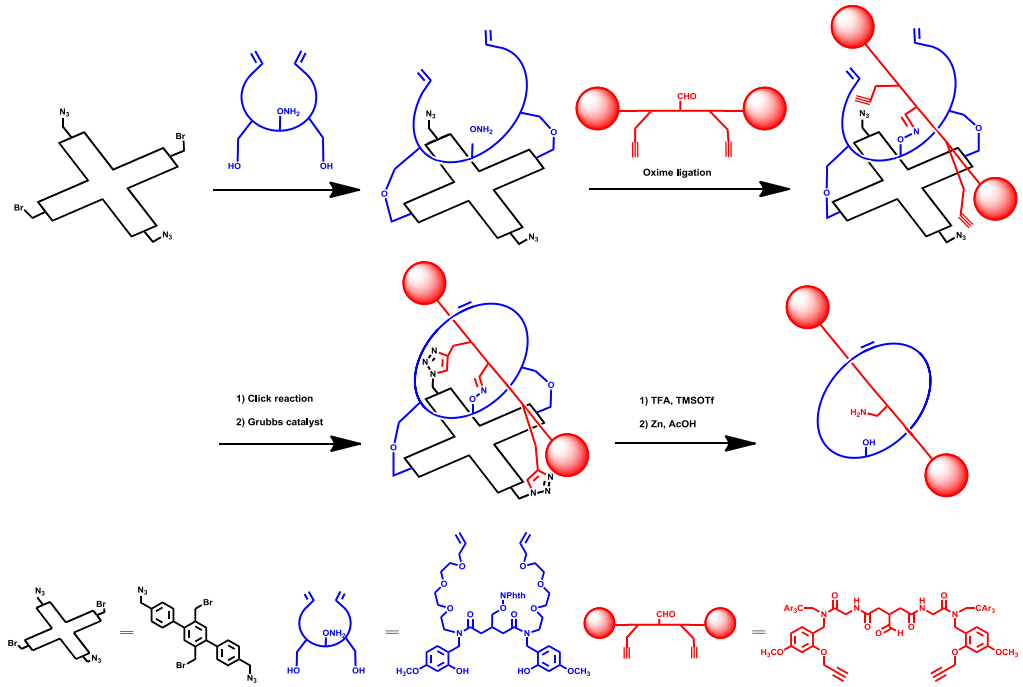
Mission of the group:
The research in the Synthetic Organic Chemistry group is directed at the development of efficient and selective, diversity-oriented synthetic methodology, in particular organocatalytic procedures, and target-oriented preparation of molecules of relevance in chemistry, biology and medicine. The main target molecules are novel enantiopure organocatalysts, indole and tetrahydro-isoquinoline 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.

Research results per sub project
Organocatalysis (NRSCC project, Breman, D. Streefkerk, Scott). In this project *Cinchona* alkaloids and derivatives are explored as enantioselective catalysts for primarily the sulfa-Michael addition in order to prepare analogues of cysteine. A highly selective catalyst (**A**, see drawing below) was prepared with a *p*-toluenesulfonylamide moiety connected to the quinoline ring providing □-phenylcysteine (**B**) in high yield and purity. Furthermore, the quinuclidine part of quinidine was modified in order to probe its influence on asymmetric induction in conjugate addition. The project will be concluded with the appearance of Breman's thesis in about August 2014.

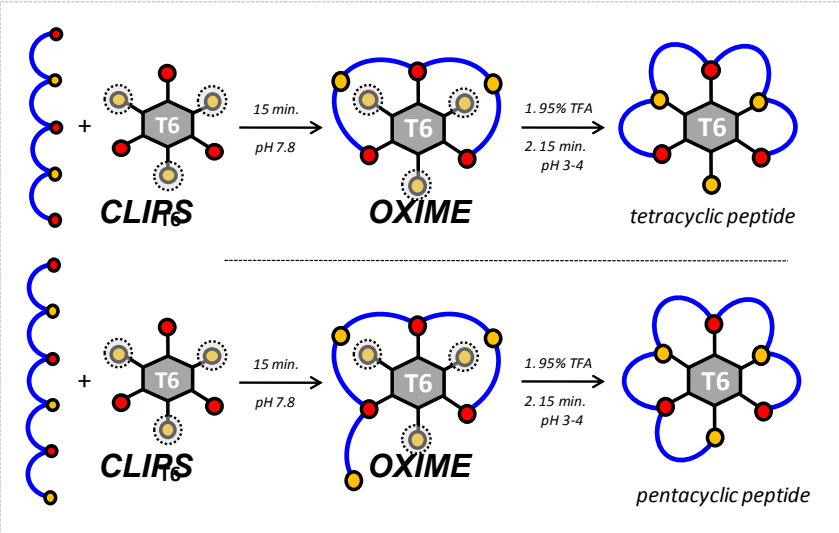


Organocatalysis (NRSCC project, Popovic, l'Epine, De Vries, Koole, Wilson). The most important result of this work was put as highlight above. The epimerization-free *C*-terminal peptide elongation is now applied in the synthesis of several biologically interesting cyclic peptides such as gramicidin S. This work will also be concluded with a thesis to appear later this year.

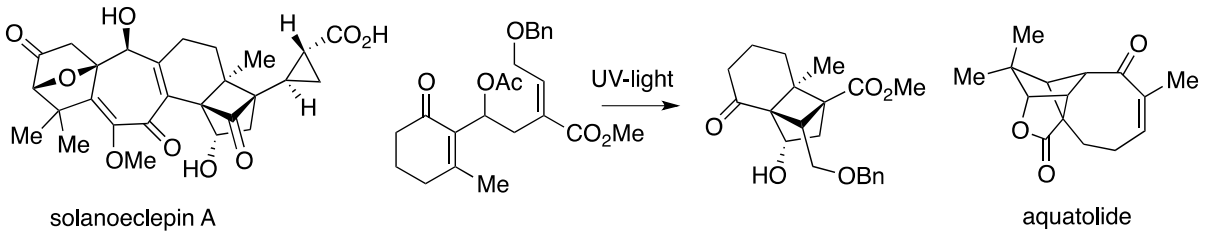
A scaffold-directed clipping approach towards the lasso peptide series (ECHO project, Steemers, J. Streefkerk, Kosian, Kyriakou). Peptide rotaxanes are a class of naturally compounds that have been discovered recently. We aim at the synthesis of this challenging compound class by developing a template-mediated clipping method to wrap a peptide around another peptide thread followed by ring closure. Currently the synthesis of the ring and thread fragments are under investigation.



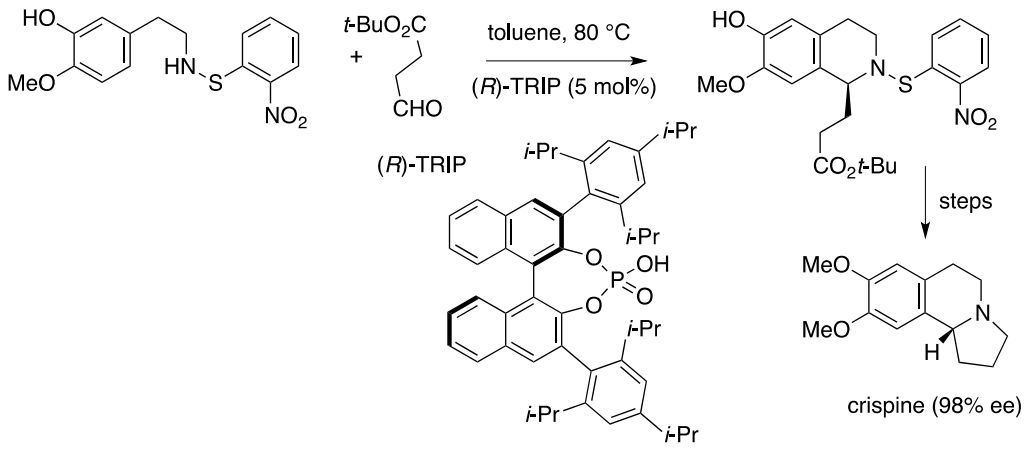
Multicyclic peptides: next generation therapeutic drugs (STW project, Richelle). The successful ECHO project of Dr. Smeenk on protein mimics (PhD in 2013) led to this follow-up STW project. It should lead to more advanced multicyclic mimics. To this end, scaffolds will be prepared incorporating two types of anchors with orthogonal chemical reactivities, one of which is the proven Pepscan-developed CLIPS-reaction. Around these scaffolds peptides will be wrapped providing several loops that mimic proteins in an advanced fashion.



Synthetic studies toward solanoeclepin A and related compounds (Kleinnijenhuis, Tahiri, Saya). Solanoeclepin A is the hatching agent of potato cyst nematodes. Synthetic studies toward this complex terpene have relevance for the treatment of this agricultural pest. The key photochemical reaction to produce the key right hand substructure has now been secured. Model studies to attach the left hand ring have seen good progress (Tahiri). The synthesis of the structurally related natural product aquatolide is also under investigation (Saya). The key step is the [2+2]-photocycloaddition of an allene, which successfully produced the skeleton.



Organocatalytic (enantioselective) alkaloid synthesis (Wanner, Mons, Würdemann).
Several indole and isoquinoline alkaloids are important synthetic targets because of their interesting pharmacological properties. Such compounds are accessed by enantioselective Pictet-Spengler cyclisations catalyzed by chiral phosphoric acids. Crucial for success in the tetrahydroisoquinoline series is the use of the o-nitrophenylsulfenyl substituent on nitrogen for good yield and enantioselectivity.



Other activities

Prof. H. Hiemstra

- Elected Member of the Royal Holland Society of Sciences (KHMW)
- Member of the Editorial Board of the European Journal of Organic Chemistry.
- Member International Scientific Committee European Symposia on Organic Chemistry (ESOC)
- Member of the International Advisory Board of the Organic division of the Czech Chemical Society
- Chairman of the organizing committee of the HRSMC summer school on New Vistas for Organic Synthesis in Maastricht 1-4 July 2013.
- Member of the Management Committee of the COST Action CM0905 (Organocatalysis).

Dr. J. H. van Maarseveen

- Member of the NWO-CW VIDI selection committee
- Expert member, panel W&T4 Fonds Wetenschappelijk Onderzoek, Flanders, Belgium
- Member of the Management Committee of the COST Action CM0905 (Organocatalysis).
- Chairman of a scientific conference of the COST Action in Amsterdam, 18-20 April 2013.
- Member of the organizing committee of the HRSMC summer school on New Vistas for Organic Synthesis in Maastricht 1-4 July 2013.

Key publications per academic staff member

- Total synthesis of the spirocyclic oxindole alkaloids corynoxine, corynoxine B, corynoxeine, and rynchophylline, M. J. Wanner, S. Ingemann, J. H. van Maarseveen, H. Hiemstra *Eur. J. Org. Chem.* **2013**, 1100-1106.
- Cinchonas and Cupreidines, S. Ingemann, H. Hiemstra Comprehensive Enantioselective Organocatalysis, Volume 1: Privileged Catalysts, Chapter 6, p. 119-160; Ed. P. I. Dalko, Wiley-VCH: Weinheim, 2013.
- Folding Dynamics of the Trp-Cage Miniprotein: Evidence for a Native-Like Intermediate from Combined Time-Resolved Vibrational Spectroscopy and Molecular Dynamics Simulations,
- H. Meuzelaar, K. A. Marino, A. Huerta-Viga, M. R. Panman, L. E. J. Smeenk, A. J. Kettelarij, J. H. van Maarseveen, P. Timmerman, P. G. Bolhuis, S. Woutersen, *J. Phys. Chem. B* **2013**, *117*, 11490-11501.
- Epimerization-free C-terminal peptide activation, S. Popovic, H. Bieräugel, R. J. Detz, A. M. Kluwer, J. A. A. Koole, D. E. Streefkerk, H. Hiemstra, J. H. van Maarseveen, *Chem. Eur. J.* **2013**, *19*, 16934-16937.

Dissertations

Smeenk, L. E. J. (22 March 2013). *Double-CLIPS technology for the mimicry of structurally complex antibody binding sites on proteins.* Universiteit van Amsterdam (200 pages). Promotor/copromotor: prof. dr. P. Timmerman & dr. J. H. van Maarseveen.

Grants and prizes

- Kerschgens, I. P. (2013). Golden Master Award 2012.
- Maarseveen, J. H. van (2013). University of Amsterdam Lecturer of the Year 2012 Award.
- Maarseveen, J. H. van, Timmerman, P. & Hiemstra, H. (2013). STW grant for the project entitled “Multicyclic CLIPS-peptides: Next Generation Therapeutic Peptide Drugs”.
- Smeenk, L. E. J. (2013). Dick Stufkens Prijs 2013.

Invited lectures

- Hiemstra, H. (2013, September 19th). Adventures in Total Synthesis. Ghent, Belgium, Symposium on the occasion of the retirement of Prof. P. de Clercq, Tales and Careers in Organic Synthesis, plenary lecture, on invitation.
- Hiemstra, H. (2013, October 18th). Recent adventures in natural product synthesis. Groningen, The Netherlands, University of Groningen, invited lecture.

- Hiemstra, H. (2013, December 13th). Recent adventures in natural product total synthesis. Twelfth Symposium on Recent Advances in Synthesis & Chemical Biology, Trinity College, Dublin, Ireland, plenary lecture, on invitation.
- Maarseveen, J.H. van (2013, December 05th). Cu(II)-PROMOTED EPIMERIZATION-FREE C-TERMINAL PEPTIDE ACTIVATION. Blankenberge (Belgium), 17th SIGMA-ALDRICH Organic Synthesis Meeting, plenary lecture, on invitation.
- Maarseveen, J.H. van (2013, October 25th). EPIMERIZATION-FREE C-TERMINAL PEPTIDE ACTIVATION. Utrecht, The Netherlands, Van 't Hoff Symposium, Universiteit Utrecht, plenary lecture, on invitation.
- Timmerman, P. (2013, April 12th). "3D-Structured Peptides as Real Mimics of Protein Surfaces using (double)-CLIPS technology", KNCV Organic Section Symposium in Wageningen. KEYNOTE/INVITED.
- Timmerman, P. (2013, May 13-15th) "Peptide Lead Finding & Optimization using CLIPS Peptide Arrays", TIDES-symposium, IBC Life Sciences, Boston (MA/USA). INVITED.
- Timmerman, P. (2013, June 7th)"3D-Structured Peptides as Real Mimics of Protein Surfaces using a.o. CLIPS technology", Medicinal Chemistry, University Utrecht, invited by Dr. Johan Kemmink.
- Timmerman, P. (2013, June 28th)"Peptide Lead Finding & Optimization using CLIPS Peptide Arrays; Discovery & Optimization of CLIPS-constrained Peptides", Medical Immunology, Radboud UMC Nijmegen, invited by Prof. Harry van Goor.
- Timmerman, P. (2013, August 29th) "Peptide Lead Finding & Optimization using Pepscan Technologies", Symposium on the occasion of the 50th anniversary of SENN Chemicals AG, Dielsdorf, Switzerland. INVITED
- Timmerman, P. (2013 September 2-4th) "The use of CLIPS-technology in PEPSCAN's Peptide Arrays", Microarray Conference, Edinburgh, Scotland. INVITED
- Timmerman, P. (2013, September 24th) "2-CLIPS Peptides for Affinity Purifications", Kennisnetwerk "NL-GUTS", Breda. INVITED
- Timmerman, P. (2013, November 16-18th) "2-CLIPS Peptides, a Novel Class of Biopharmaceuticals", Oligonucleotide & Peptide Therapeutics Congress, San Diego (CA/USA). INVITED.
- Timmerman, P. (2013, November 22th) "2-CLIPS Peptides, a Novel Class of Biopharmaceuticals", MedChem Conference, Johnson & Johnson, Beerse, Belgium. INVITED.

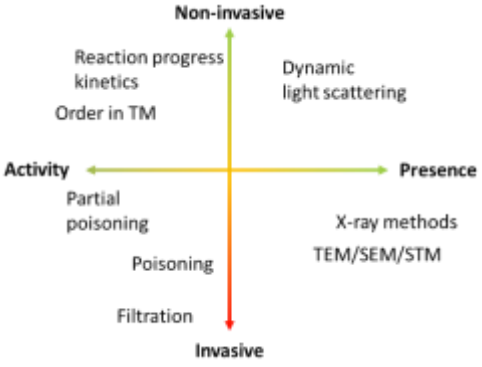
Group:	Molecular Inorganic Chemistry		
Group leader:	Prof. dr. C.J. Elsevier		
Academic staff:			
Support staff:	J.M. Ernsting Drs. D.S. Tromp		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. T.J. Korstanje	15-08-2013	15-08-2015
PhD students:	Drs. S.N. Sluijter Drs. E. Jansen Drs. R.M. Drost	01-06-2011 01-04-2009 01-04-2010	31-05-2015 30-09-2013 31-03-2014
MSc students:	S. Beerents L. Jongkind	01-09-2013 01-10-2013	01-06-2014 01-07-2014

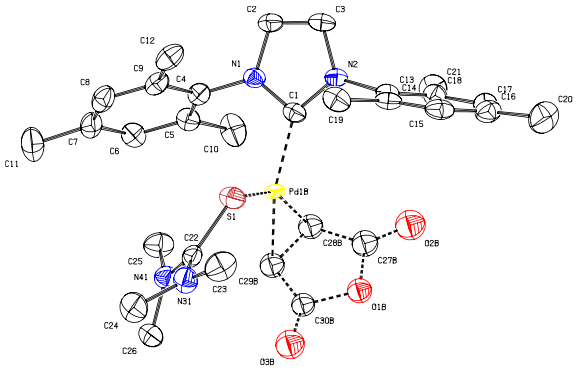
Mission of the group:
The Molecular Inorganic Chemistry group is involved in fundamental research in Coordination and Organometallic Chemistry, which resides at the basis of most catalytic processes. Focus is on the synthesis, characterization and application of organometallic compounds in homogeneous catalysis. The approach is through rational design of (pre-) catalysts, by studying single steps and constituting new catalytic cycles from these building blocks. We also contribute to solutions of employing bio- and waste materials in a sustainable way, for instance by studying conversions of 'platform molecules' into useful and re-usable chemicals. Importantly, careful analysis of the mechanism of homogeneous catalytic, metal-mediated reactions is carried out as a necessary step-up to the discovery of solutions to problematic chemical transformations as well as detailed understanding, hence improvement of processes. Spectroscopic studies are an integral part of our studies, partly in order to evaluate and understand the reaction and intermediates under conditions similar to those in the catalytic reactions studied.
Currently, we focus on important hydrogenation and alkylation reactions involving transition-metal-poly-phosphine, N-heterocyclic carbene (NHC) and heteroditopic bis-carbene complexes.

Research results per sub project

Title: Conversion of Bio-platform molecules (CatchBio)
Researchers: E. Jansen MSc (aio)., T.J. Korstanje PhD (PD)
E. Jansen: The research has focused on hydrogenolysis of esters using various transition metals (TM) and on direct alkylation reactions. The structural investigation and application of TM complexes that contain bidentate N-heterocyclic carbenes (NHCs) and primary amine moieties of the type [M(arene)Cl(L)] where M = Ru, Ir, or Rh; arene = p-cymene or Cp*; L=1-(2-aminophenyl)-3-(n-alkyl)imidazol-2-ylidine have been finalized. The complexes are quite active catalysts for hydrogenation reactions. Notably, structural variations in the chelate ring size of the heteroditopic ligand revealed that smaller chelate ring sizes in combination with ring conjugation in the ligand are beneficial for the activity of this type of catalyst. Part of the project studied by E. Jansen was carried out in collaboration with prof.dr. D. Cole-Hamilton (St. Andrews, UK) and prof.dr. B. de Bruin (HomKat). It has been finalized with two published papers, a doctoral dissertation and two papers are in preparation.
T. Korstanje: The project is carried further by T. Korstanje (in collaboration with prof.dr. B. de Bruin), who managed to implement the difficult hydrogenolysis of esters by using first row transition metals like cobalt in combination with the triphos ligand that the group has been using (with more expensive Ru in catalysts) for previous studies of ester hydrogenolysis. This finding holds promise for future directed utilization of more readily available and cheaper first row transition metals for this industrially challenging reaction.

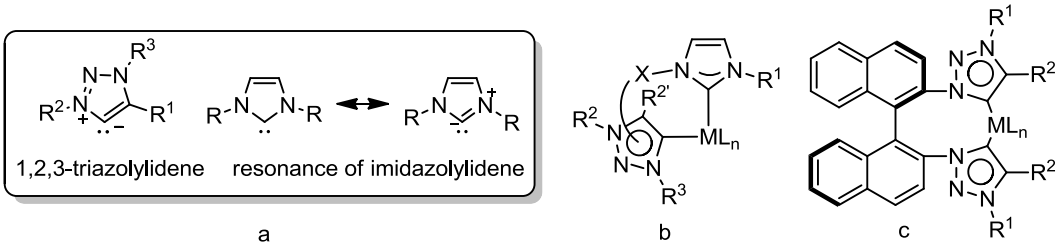
Title: Metal-carbene complexes for catalytic hydrogenation and alkylation reactions (NRSC-C)
Researchers: R.M. Drost MSc, S.N. Sluijter MSc.
R.M. Drost: Emphasis has this year been on developing a "partial poisoning protocol" in order to conclusively distinguish between molecular and nano-particle catalysts. Over the last decade it has appeared that several well-known homogeneous reactions are in fact catalyzed by nano-particles (NP) generated under the conditions of the reaction rather than by the initially proposed molecular catalyst. Determination of the type of active catalyst is crucial for design and rational catalyst development; for instance, ligand design is of limited use if the catalytic reaction proceeds via NPs, which are often devoid of ligands. Determining the type of active catalyst is therefor of prime importance, but is often neglected because distinguishing between molecular catalysts and NP catalysis is far from trivial. For this reason we have developed a partial poisoning protocol that is easy to use and gives reliable results. The method is in principle compatible with various reaction types and it provides kinetic data.





This protocol consist of three steps: Poison validation, partial poisoning and confirmation of the viability of the method through orthogonal control experiments. Together they form a comprehensive method that gives reliable results: it demonstrates that the poison is applicable, then it provides mechanistic insight and, finally, it verifies the results by excluding non-stoichiometric poisoning and resting states. We have applied this protocol to investigate palladium catalyzed semi-hydrogenation reactions: catalysis by particles was observed when hydrogen gas is applied, but molecular catalysis for transfer hydrogenation using e.g. formic acid as the hydrogen carrier. Simultaneously, we have demonstrated that tetramethylthiourea is an excellent poison instead of CS_2, it has a similar performance but is less toxic and less volatile.

S.N. Sluijter: Chelating heteroditopic di-NHC complexes in catalytic hydrogenation. Several zero-and di-valent palladium complexes with chelating di(NHC) ligands were obtained through transmetallation using silver(I) precursors. In contrast to the transfer semihydrogenation, in which only low activity was observed, complex some of these showed activity and selectivity comparable to their monodentate counterparts in the semihydrogenation of alkynes with molecular hydrogen.
Furthermore, a large number of late transition metal complexes (b) involving mesoionic carbene moieties (a) in bidentate heteroditopic NHC-MIC ligands have been prepared and were succesfully employed in catalytic hydrogenation and alkylation reactions.
A start has been made (with L. Jongkind, student) in the design and synthesis of enantiopure atropisomeric metal-di-carbene species (c) for enantioselective hydrogenations, hydrosilations and alkylations. Moderate but encouraging levels of enantioselectivity have been observed in hydrogenations of several ketones and enones.



Employing expanded-ring N-heterocyclic carbenes (erNHC's: bulky, strong sigma-donor ligands that impart a highly constrained geometry on the complexes) has enabled, in collaboration with prof. K. Cavell (Cardiff), the isolation of coordinatively and electronically unsaturated Pd complexes. Significantly enhanced catalytic activity in the selective transfer hydrogenation of certain alkynes toward (Z)-alkenes was observed using these [Pd(erNHC] complexes as precatalysts.

Other activities

Cooperation with: HomKat staff (de Bruin, Reek, v.d. Vlugt) on general aspects of organometallic chemistry and catalysis, sharing of equipment and work discussions; discussions and collaboration with prof. P. Braunstein (Strassbourg) concerning metal carbene chemistry; with prof.dr. C. Coperet (Lyon) about metal catalysts on carriers and NMR of catalysts in action.
Collaboration with dr. B. Milani (Trieste) concerning co-polymerization and development of molecular catalysts.

Key publications per academic staff member

- Hauwert, P., Dunsford, J. J., Tromp, D.S., Weigand, J.J., Lutz, M., Cavell, K.J. & Elsevier, C.J. (2013). Zerovalent [Pd(NHC)(Alkene)(1,2)] Complexes Bearing Expanded-Ring N-Heterocyclic Carbene Ligands in Transfer Hydrogenation of Alkynes. *Organometallics, 32*(1), 131-140.
- Jansen, E., Jongbloed, L.S., Tromp, D.S., Lutz, M., Bruin, B. de & Elsevier, C.J. (2013). Ligand Effects on the Hydrogenation of Biomass-Inspired Substrates with Bifunctional Ru, Ir, and Rh Complexes. *ChemSusChem, 6*(9), 1737-1744.
- Sluijter, S.N., Warsink, S., Lutz, M. & Elsevier, C.J. (2013). Synthesis of palladium(0) and -(II) complexes with chelating bis(N-heterocyclic carbene) ligands and their application in semihydrogenation. *Dalton Transactions, 42*(20), 7365-7372.

Invited lectures

- Elsevier, C.J., Drost, R.M. & Sluijter, S.N. (2013, December 02). *Labile palladium species and applications in catalysis.* Rennes, France, Institut de Chimie; Université Rennes-1, invited lecture.
- Elsevier, C.J., Drost, R.M., Hauwert, P., Jansen, E., Sluijter, S.N., Tromp, D.S. & Warsink, S. (2013, september 05). *Labile palladium species and applications in catalysis.* Parma, Italy, Annual meeting Inorganic Division of Soc Chim Ital. On invitation; plenary lecture.

Group:	Biocatalysis and Bio-organic Chemistry		
Group leader:	Dr. A. Schallmey (per September 2013)		
Academic staff:	Prof.dr. R. Weber (Emeritus)		
Support staff:	A.F. Hartog		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. L. Babich Dr. M. van der Horst	01-10-2012 01-07-2012	31-01-2013 31-01-2013

Mission of the group:
The research topics studied in the Biocatalysis group are highly relevant for society. The aim of the group is to replace existing chemical synthetic procedures by more sustainable biocatalytic procedures. A number of procedures been developed in which enzymatic procedures are used that may successfully replace classical organic synthetic procedures and that offer green alternatives.

Research results per sub project
Most projects were stopped with the retirement of the group leader in 2012 and the end of the contracts of the two postdoc's. Only the work on arylsulfotransferase was continued and publication will be submitted soon.

Other activities
Due to the retirement of the group leader in 2012 most of the external collaborations had to be discontinued.

Key publications per academic staff member
- Marhol, P., Hartog, A.F., Horst, M.A. van der, Wever, R., Purchartova, K., Fuksova, K., Kuzma, M., Cvacka, J., Kren, V. (2013). Preparation of silybin and isosilybin sulfates by sulfotransferase from Desulfitobacterium hafniense. *Journal of Molecular Catalysis B-Enzymatic, 89*, 24-27.
- Wever, R., Horst, M.A. van der (2013). The role of vanadium haloperoxidases in the formation of volatile brominated compounds and their impact on the environment. *Dalton Transactions, 42* (33), 11778-11786.
- Babich, L., Peralta J. L. V. M., Hartog, A.F, Wever, R. (2013). Phosphorylation by alkaline phosphatase: immobilization and synthetic potential. *International Journal of Chemistry*, *5*, (3), 87-98

Dissertations
Babich, L. (25 January 2013). *Enzymatic cascade reactions involving phosphorylated intermediates: immobilization and process optimization.* UvA Universiteit van Amsterdam (150 pag.). Prom.: prof.dr. R. Wever.

2.2 Computational Chemistry

The Computational chemistry theme consists of the related groups Biomolecular and Molecular Simulation and the group Computational Polymer Chemistry. The latter group leads the Science for Arts activities within HIMS.

Group:	Biomolecular and Molecular Simulation		
Group leaders:	Prof. dr. P.G. Bolhuis and Prof. dr. E.J. Meijer		
Academic staff:	Dr. D. Dubbeldam Dr. B. Ensing Dr. C.P. Lowe Dr. J. Vreede Prof. R. Krishna (Emeritus) Prof. dr. S.O. Nielsen (BHGL, till 15-06-2013) Prof. dr. A. Fasolino (till 30-04-2013)		
Support staff:	-		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. A.J. Cruz Cabeza Dr. D. Sun Dr. R. Ni	01-11-2011 21-10-2013 01-09-2012	31-10-2014 20-10-2015 28-02-2014
PhD students:	W Du, MSc K. Singhal, MSc J. Luiken, MSc A. Kumar, MSc F. Brotzakis, MSc A. Newton, MSc M. Nowosielski, MSc R. Zeiler, MSc G. Diaz Leines, MSc W. Homsi Brandeburgo, MSc M. Kilic, MSc A. Pavlova, MSc A. Teterin, MSc A. Torres Knoop, MSc D.D. McKendric, MSc	01-08-2009 15-05-2010 01-10-2010 01-09-2010 01-09-2012 15-04-2012 15-04-2011 01-12-2009 01-11-2008 15-01-2011 01-11-2008 15-11-2008 01-02-2012 01-03-2012 01-09-2011	31-10-2013 14-05-2014 30-09-2014 31-08-2014 31-08-2016 14-04-2016 14-04-2015 14-04-2014 30-04-2013 14-01-2015 28-02-2013 14-02-2013 31-07-2013 29-02-2016 28-02-2013
MSc students:	J. Heinen	01-11-2013	31-08-2014

Mission of the group:

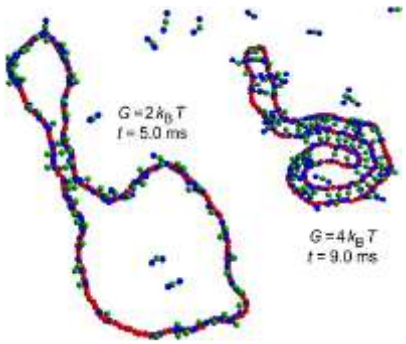
The research of the group focuses on the study of complex chemical, physical, and biological systems using multiscale modeling. Development and application of novel computational techniques and connection with experimental observations are essential parts of the research program.

Research results per sub project

Biomolecular Systems and (Bio)materials

Researchers: Staff: Bolhuis, Ensing, Lowe, Vreede; PhD's/PD's: Brotzakis, Diaz-Leines, Du, Kumar, Luiken, Newton, Ni, Nowosielski, Singhal, Zeiler

The **histone-like nucleoid structuring protein** (H-NS) is a nucleoid-associated protein, which is involved in DNA compaction. H-NS can bind to DNA in two different ways: in trans, by binding to two separate DNA duplexes, or in cis, by binding to different sites on the same duplex. To get more insight into the compaction mechanism, we constructed a coarse-grained model. These simulations highlight the fact that DNA compaction is extremely sensitive to the difference in binding energies of the cis and trans configurations (Zhu et al., PLoS Comput Biol. 2013). This publication was selected for New and Notable in the same issue of Biophysical Journal (Biophys J 2013; 104).



Snapshots of the coarse grained simulations at different bending energies G for H-NS. DNA is shown in red, H-NS is shown in green and blue, with blue the DNA-binding particles.

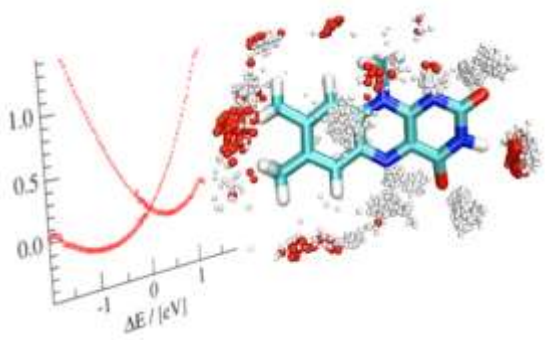
We published a molecular dynamics and metadynamics study on the HAMP signal relay domain, occurring in prokaryotic sensor proteins. To date, it is unclear how HAMP can relay signals from one domain to another, although several models exist. Our results indicate that HAMP can access additional conformational states characterized by helical piston motions, which are accompanied by a change in helical tilt angle, thus revealing that HAMP exhibits a collective motion. Our results provide insights into the conformational changes that underlie the signaling mechanism involving HAMP (Joyeux and Vreede, Biophys J. 2013).

Trigger factor (TF) is a bacterial chaperone that interacts with nascent polypeptide chains to suppress aggregation. While its crystal structure has been resolved, the solution structure and dynamics are largely unknown. We performed molecular dynamics simulations on Trigger factor in solution, and show that isolated TF typically adopts a collapsed state, with the formation of domain pairs. This collapse of TF in solution is induced by hydrophobic interactions and stabilized by hydrophilic contacts. To determine the nature of the domain interactions, we analyzed the hydrophobicity of the domain surface and found that the formation of domain pairs changes the hydrophobic map of TF. These insights into the dynamics and interactions of the TF domains are important to eventually understand chaperone-substrate interactions and chaperone function (Singhal et al., PLoS One 2013).

Chemical processes in complex environment

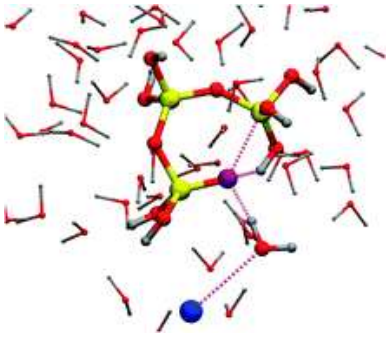
Researchers: Ensing and Meijer; PhD's/PD's: Brandeburgo, Kilic, Pavlova, Sun

Flavins are ubiquitously found in nature as cofactors in proteins that regulate electron and proton transfer reactions. The electron and proton affinities of flavins are modulated by their molecular environment. Using density functional theory based molecular dynamics simulations, Kilic and Ensing have studied the first and second reduction reactions of the prototypical flavin named lumiflavin in aqueous solution. They find that the reduction potential, calculated using free energy perturbation simulations, has the typical parabolic shape as predicted by Marcus' theory of electron transfer. The water solvent structure undergoes significant changes within the first coordination shell upon lumiflavin reduction. These structural changes account largely for the reorganization free energy term in the measured redox



potential. However, in the second reduction reaction, from semiquinone to fully reduced lumiflavin, also the inner-sphere reorganization contributes significantly via the increased "butterfly" bending of the flavin. This butterfly bending causes a remarkable deviation from the linear response approximation that underlies Marcus' theory of electron transfer.

Silica oligomerization is the key reaction in zeolite synthesis. NaOH is a common additive in thezeolite synthesis that decreases the reaction rate of smaller silica oligomers and also affects the final structure of the zeolite. We studied the role of sodium in the inital stages of **silica oligomerization** by *ab initio* molecular dynamics simulations using explicit aqueous solution (Pavlova and Meijer, PCCP 2013). The study confirms that sodium decreases the reaction rates of oligomerization for smaller silica chains. Analysis of the molecular dynamics trajectories shows that sodium does not increase the reaction barriers by direct coordination to the silica. However, sodium is often present in the second solvation shell of the reactive atoms. Correlation between sodium presence in the first or the second shell of the reactive oxygen and a decrease in hydrogen bonding for that oxygen was found for the first reaction step. Therefore, the presence of sodium could contribute to an increase in reaction barriers for silica oligomerization by some rearrangement of the hydrogen bond network of water solution around the reactants.

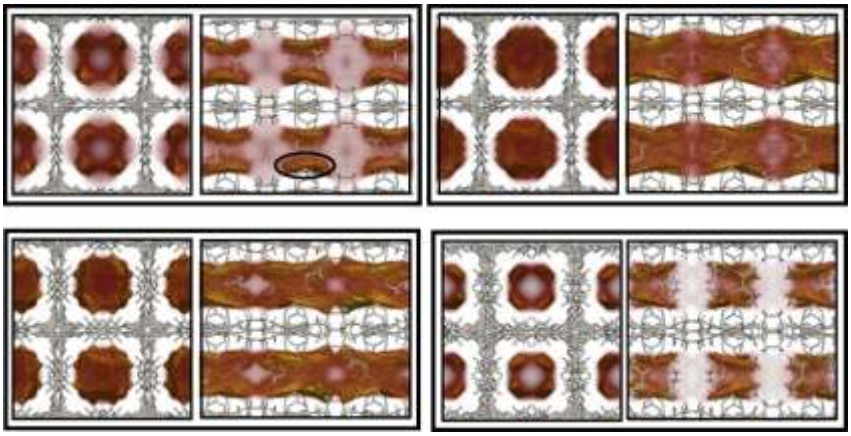


In the group of de Bruin (HIMS theme Catalysis), Fransen synthesised novel **syndiotactic polycarbene polymers** that show interesting unexpected properties, such as liquid crystal behaviour and a linear structuring shown by STM. Although molecular mechanics calculations performed in the group of De Bruin indicated that the polymer chains form a helical structure, molecular dynamics simulations by Ensing showed that these helical chains by themselves are too flexible to exhibit liquid crystal behaviour. However, computer simulations of several polycarbene polymers showed that the chains self-assemble into triple-helix structures, which behave as a rigid rod and explain the surprising liquid-crystal behavior. The paper featured on the cover of Chem. Eur. J. and was highlighted in ChemViews Magazine.

Hard Materials

Researchers: Staff: Cabeza-Cruz, Dubbeldam, Fasolino, Krishna, Meijer; PhD's/PD's: McKendric, Teterin, Torres-Knoop

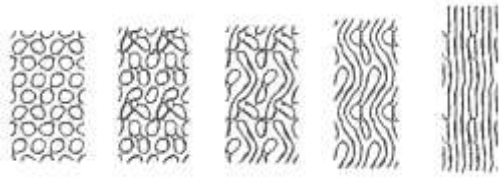
Fundamental insight into how low pressure adsorption properties are affected by chemical functionalization is critical to the development of next-generation porous materials for postcombustion CO_2 capture. We developed a systematic approach to understanding low pressure CO_2 affinity in isostructural **metal–organic frameworks** (MOFs) using molecular simulations and apply it to obtain quantitative, molecular-level insight into interesting experimental low pressure adsorption trends in a series of pillared MOFs (Dubbeldam et al, JACS 2013).



CO2 density distributions at infinite dilution and 298 K. The x–y and x–z planes of DMOF (top left), DMOF-TF (top right), DMOF-DM (bottom left), and DMOF-TM (bottom right) are shown. The black oval on the y–z plane of the parent DMOF structure highlights the concentrated adsorbate density around its strongest 0 K binding site.

Our experimental results show that increasing the number of nonpolar functional groups on the benzene dicarboxylate (BDC) linker in the pillared DMOF-1 [$Zn_2(BDC)_2(DABCO)$] structure is an effective way to tune the CO_2 Henry's coefficient in this isostructural series. Through a combined experimental and simulation approach, we demonstrate how subtle, structure-specific differences in CO_2 affinity induced by functionalization can be understood at the molecular-level through classical simulations. This work also illustrates how structure–property relationships resulting from chemical functionalization can be very specific to the topology and electrostatic environment in the structure of interest. Given the excellent agreement between experiments and simulation, predicted CO_2 selectivity's over N_2, CH_4, and CO are also investigated to demonstrate that methyl groups also provide the greatest increase in CO_2 selectivity relative to the other functional groups. These results indicate that methyl ligand functionalization may be a promising approach for creating both water stable and CO_2 selective variations of other MOFs for various industrial applications.

Metal-organic frameworks can offer pore geometries that are not available in zeolites or other porous media, facilitating distinct types of shape-based molecular separations. We have studied $Fe_2(BDP)_3$ (BDP^{2-} = 1,4-benzenedipyrazolate), a highly stable framework with triangular channels that effect the separation of hexane isomers according to the degree of branching (Krishna and co workers, Science 2013). We found an adsorption selectivity order of *n*-hexane > 2-methylpentane > 3-methylpentane > 2,3-dimethylbutane ≈ 2,2-dimethylbutane. This is consistent with the varying abilities of the isomers to wedge along the triangular corners of the structure, adsorption isotherms and calculated isosteric heats. A breakthrough experiment performed at 160°C with an equimolar mixture of all five molecules confirms that the dibranched isomers elute first from a bed packed with $Fe_2(BDP)_3$, followed by the monobranched isomers and finally linear *n*-hexane. Configurational-bias Monte Carlo simulations confirm the origins of the molecular separation.

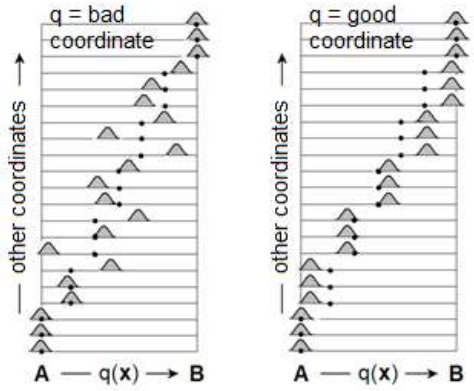


We determined the stability and the transformation mechanism of (5,5) and (10,10) **single-walled carbon nanotube bundles** up to 20 GPa and 4000 K, using Monte Carlo simulations and a the state-of-the-art reactive potential LCBOPII (Colonna, Fasolino, Meijer; PRB 2013). At low temperature, upon increasing pressure, large (10,10) nanotubes first collapse and then coalesce, yielding almost perfect graphitic structures. In contrast, small (5,5) nanotubes do not collapse, but coalesce and transform to graphite via a mixed graphite-tube structure. At high temperature (above~2000 K), for both (10,10) and (5,5) nanotubes, coalescence dominates the transformation to graphitic structures. We argue that the sp3-interlinking defects appearing at coalescence can act as seed and facilitate the transformation to diamond structures.

Method Development

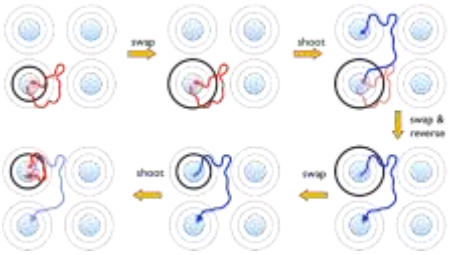
Researchers: All

In collaboration with the groups of Peters and Shea in Santa Barabara (Peters et al, JCP 2013) we have developed a method for **identifying accurate reaction coordinates** among a set of trial coordinates. The method applies to special cases where motion along the reaction coordinate follows a one-dimensional Smoluchowski equation. In these cases the reaction coordinate can predict its own short-time dynamical evolution, i.e., the dynamics projected from multiple dimensions onto the reaction coordinate depend only on the reaction coordinate itself.



The method is illustrated for three model free energy landscapes with anisotropic diffusion.

We have developed a new single **replica transition interface path sampling** algorithm (Du and Bolhuis, JCP 2013) that samples rare transitions between many metastable states using a Wang-Landau approach or, alternatively, a fixed bias. We illustrated the method on several model systems: a particle diffusing in a simple 2D potential, isomerization in a small Lennard Jones cluster, and isomerization of the alanine dipeptide in explicit water. The method dramatically speeds up the convergence of the sampling.



Other activities

Collaborations:

- Krishna – Karger (Leipzig)
- Bolhuis – Kegel (Utrecht), Dellago (Vienna), Cohen Stuart(Wageningen), Tans (FOM-Amolf)
- Meijer – van Santen (Eindhoven), Rijs (Nijmegen), Bakker (AMOLF), Van Speybroeck (Gent), Sprik (Cambridge), Liu (Nanjing)
- Lowe – Pagonabaragga (Barcelona)
- Ensing - Bakker (FOM-Amolf), Woutersen (UvA/HIMS), Nielsen (Texas), Moore (Philadelphia), Branduardi (Frankfurt, Germany).
- Dubbeldam – Snurr (Northwestern), van Erp (Leuven), Calero (Sevilla), Vlugt (Delft University)
- Vreede – Hellingwerf (UvA), Dame (Leiden), Groot (VU-Amsterdam), Joyeux (Grenoble, France), Naverre (Toronto, Canada)
- Cruz-Cabeza – Aakeroy (Kansas, USA), Bernstein (NYU-Abu Dhabi, UAE), Fabbiani (Gottingen, Germany)

Memberships:

Bolhuis:

- Member Physics of Life werkgemeenschap FOM
- Member Werkgemeenschap Supercomputers
- Member FOM BRM program committee
- Member committee FOM/Shell program Computational Science

Krishna

- Fellow of the Indian Academy of Sciences
- Fellow of the Indian Academy of Engineering
- Fellow of the Indian Institution of Chemical Engineers

Meijer

- UvA representative Scientific Council CECAM.
- Member Scientific Committee International Erasmus Mundus program ATOSIM
- Member NWO/CW Study group "Spectroscopy and Theoretical Chemistry"

Ensing

- Member NWO/CW Study group "Spectroscopy and Theoretical Chemistry"
- Member of educational board of the Holland Research School of Molecular Chemistry (HRSMC)

Organized conferences/schools:

- Bolhuis and Vreede - Bolhuis – ACMM Spring and Fall symposia (Amsterdam)
- Ensing – Winterschool Theoretical Chemistry and Spectroscopy, December 2013 (Han-sur-Lesse)
- Meijer, Ensing, Dubbeldam – CECAM/ACMM winterschool on “Understanding Molecular Simluation (MolSim 2013)” (Amsterdam)
- Lowe – “Write it Right”, International workshops on writing scientific papers (multiple editions)

Key publications per academic staff member

- J.A. Luiken and P.G. Bolhuis, *Anisotropic aggregation in a simple model of isotropically polymer-coated nanoparticles*, Phys. Rev. E 88, 012303 (2013).
- L. Zhu, P.G. Bolhuis and J. Vreede, *The HAMP signal relay domain adopts multiple conformational states through collective piston and tilt motions*, PLoS Comput. Biol. 9(2), e1002913 (2013).
- K. Singhal, J. Vreede, A. Mashaghi, S. Tans, and P.G. Bolhuis, *Hydrophobic Collapse of Trigger Factor Monomer in Solution*, PLoS One 8, e59683 (2013).
- R. Ni, S. Abeln, M. Schor, M.A. Cohen Stuart and P. G. Bolhuis, *Interplay between Folding and Assembly of Fibril-Forming Polypeptides*, Phys. Rev. Lett. 111, 058101 (2013).
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- N. Burtch, H. Jasuja, D. Dubbeldam and K. Walton, *Molecular-level Insight into Unusual Low Pressure CO2 Affinity in Pillared Metal-Organic Frameworks*, J. Am. Chem. Soc. 135, 7172 (2013).
- D. Dubbeldam, A. Torres-Knoop, and K.S. Walton, *Review: On the Inner Workings of Monte Carlo Codes , Mol. Sim. (special issue on Monte Carlo)* 39, 1253 (2013).
- K. Epa, C. Aakeroy, J. Desper, S. Rayat, K. Chandra and A.J. Cruz-Cabeza , *Controlling Molecular Tautomerism Through Supramolecular Selectivity*, Chem. Commun. 49, 7929 (2013).
- Z.R. Herm, B.M. Wiers, J.M. van Baten, M.R. Hudson, P. Zajdel, C.M. Brown, N Maschiocchi, R. Krishna, and J.R. Long, *Separation of Hexane Isomers in a Metal-Organic Framework with Triangular Channels*, Science 340, 960 (2013).
- A. Pavlova, T.T. Trinh, R.A. van Santen, and E.J. Meijer, *Clarifying the role of sodium in the silica oligomerization reaction*, Phys. Chem. Chem. Phys. 15, 1123 (2013).
- F. Colonna, A. Fasolino, and E.J. Meijer, *Graphitization of single wall carbon nanotube bundles at extreme conditions: collapse or coalescence route* , Phys. Rev. B88, 165416.

Dissertations

Houtman, D. (11 November 2013). *To go with the flow: Molecular motors are a drag.* Universiteit van Amsterdam (vi, 149 pag.). Prom./coprom.: prof.dr. E.J. Meijer & dr. E. Eiser.

Pavlova, A. (30 Oktober 2013). *Understanding the role of aqueous solution in chemical reactions: A computational study.* Universiteit van Amsterdam (vi, 112 pag.). Prom.: prof.dr. E.J. Meijer.

Diaz Leines, G (15 November 2013). *Path-Metadynamics, A computational study of conformational transitions in proteins*. Universiteit van Amsterdam (x, 184 pag.). Prom./coprom. Prof.dr. P.G. Bolhuis & B. Ensing.

Grants and prizes

- Krishna, ENI Award 2013 (Presented by the Italian President).
- Vreede et al., Computing Resources on National Canadian Facilities
- Meijer and Ensing, MolSim2013, CECAM Grant

Invited lectures

Bolhuis

- *Winter school "Phase stability and phase transitions in soft and hard materials", St. Christoph, Austria, February 25, 2013 to March 1, 2013. Title: "Simulation of Rare Events"*

- *CUSO Winter school "Phase stability and phase transitions in soft and hard materials", Villars, Switzerland, Feb 4, 2013 to Feb 8, 2013. Title: "Transition path sampling"*
- *The liquid-solid interface in crystal nucleation, CECAM workshop Lausanne 22-24 May 2013.*
- *Single replica multiple state transition interface sampling, SIAM meeting, Philadelphia 9-13 June*
- *Title: "Understanding the action of proteins", E-science symposium Amsterdam, 5 July 2013*
- *Enhanced path sampling of the equilibrium kinetic network of small polypeptides, Molecular kinetics workshop, Berlin 2 – 5 sept 2013, Title: "Understanding the action of proteins", Fritz Haber Institute Berlin, 20 September 2013*
- *Title: "Enhanced molecular simulation of protein folding, conformational change and self-assembly", International conference on molecular simulation, Kobe, Japan, 18-20 november 2013, Title:" Enhanced sampling of unbiased trajectories"*
- *Workshop "Five pieces and a do in computational physics, chemistry, biology, mathematics and engineering", 18-20 december 2013, Rome*

Ensing

- *Invited lecture at the colloquium of the Institute of Computational Physics at the University of Stuttgart, Germany, January 24, 2013.*
- *Invited talk at the conference on"Hybrid Particle-Continuum Methods in Computational Materials Physics (Hybrid2013)" at the Supercomputing Centre in Jülich, Germany, March 4-7, 2013.*
- *Invited talk at the Faculty of Chemistry and Biochemistry of the Ruhr-Universität Bochum, Bochum, Germany, June 3, 2013.*
- *Invited talk at the "8th Congress of the International Society of Theoretical Chemical Physics (ISTCP-VIII)" in Budapest, Hungary, August 25-31, 2013.*
- *Invited talk at the "Symposium for Theoretical Chemistry (STC 2013)" in Erlangen, Germany, September 22-26, 2013.*
- *Invited talk at the Department of Physics and Astronomy, University of Padova, Padova, Italy, October 25, 2013.*
- *Invited talk at the NDNS+ Workshop "Stochastic Modeling of Multiscale Systems" in the Eindhoven Multscale Institute, Eindhoven, The Netherlands, December 2-6, 2013.*

Cruz-Cabeza

- *"Molecular Materials by Design", NYU-AD, Mar 2014, "Conformational Polymorphism", American Crystallographic Association Meeting (ACA), Honolulu (Hawaii), July 2013*

Meijer

- *Towards a molecular understanding of solvent effects in chemical reactions*, Computational Chemistry Seminar, Ecole Normale Superieure Lyon, February 13, 2013.
- *Modeling chemical reactions in hydrogen-bonded liquids*, Physics Seminar, University of Groningen April 19, 2013.
- *Modeling of Catalysis in Solution,* Conference on "Challenges in Computational Homogeneous Catalysis", Stockholm, Dalian, Sweden, June 13-14, 2013.
- *Simulation of Catalysis in Solution,* Institute Seminar, Dalian Institute of Chemical Physics, Dalian, China, June 28, 2013.
- *Realistic Modeling of Catalysis in Solution*, Annual Global Congress of Catalysis-2013, Dalian, China, June 29-July 01, 2013.
- *Simulation of Catalysis in Solution,* Chemistry Seminar, Hong Kong University of Science and Technology, Hong Kong, China, July 3, 2013.
- *Realistic Modeling of Catalysis in Solution*, XIth European Congress on Catalysis, Lyon, France, September 01-06, 2013.
- *Modeling chemical reactions in hydrogen-bonded solvent*, CPMD-Meeting 2013 Matter, life, light from ab initio molecular dynamics simulations, University of Leipzig, September 02-06, 2013.

Theme:	Computational Polymer Chemistry and Science for Arts		
Group:	Physical Technology		
Group leader:	Prof. dr. P. Iedema		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. K. Keune Dr. A. van Loon	01-08-2012 01-08-2012	31-07-2016 31-07-2016
PhD students:	Drs. J. Kryven Drs. N. Yaghini Drs. J. Hermans	01-09-2010 15-05-2010 01-12-2012	31-08-2014 14-05-2014 30-11-2016

Mission of the group:
The group aims at fundamental understanding of chemical and physical processes in a wide range of polymer systems, from oil paint layers to industrially produced compounds, covering polymerization and long-term degradation.

Research results per sub project
Science4Arts (Annelies van Loon, Katrien Keune, Joen Hermans)
Painting studies
The concentric rings in *Couple with Clouds in their Heads* by Dalí (1936, Boijmans van Beuningen), the raised paint and the tunnels inside the paint in the *Evolution* by Mondrian (*c.*1911, Gemeentemuseum Den Haag), and the white haze on the surface of Rembrandt's *Homer* (1663, Mauritshuis) are three examples of metal-soap related degradation phenomena occurring in oil paintings that have been investigated by the PAinT team. In the *Couple*, the zinc white pigment has been reacted away by acids deriving from the oil as well as from the wooden frame. This has resulted in a thick transparent surface layer rich in zinc carboxylate salts. The tunnels in the *Evolution* manifested in areas where the paint was also rich in zinc white. The zinc white has formed zinc carboxylates (soaps), which has resulted in a loss of cohesion of the paint. Synchrotron-based FTIR, XRF and XANES studies (at Synchrotron Soleil, Paris) on paint samples from the *Homer* and related paint samples have provided a deeper insight into the lead soap formation and migration that have caused the white haze on the painting's surface. The formed lead soaps occur as amorphous species in the paint, that can travel through the layered paint system and form new complex salts after reaction with atmospheric compounds.

Similar synchrotron-based techniques (at ESRF, Grenoble and at SSRL, USA) have been used to identify new degradation products of the red/orange pigment realgar (As_4S_4) in *Still Life with Five Apricots*, a painting by Coorte (1704, Mauritshuis). Realgar is known to photo-oxidize via various intermediate phases and pararealgar into arsenic trioxide (As_2O_3). Our measurements showed that besides the presence of arsenic trioxide also calcium and iron-containing arsenates (As5+) have formed as degradation products in paintings.

The importance of the past/previous analytical work on the mechanism of darkening of red vermilion pigment by Keune was stated in *Nature* by D. Castelvecchi dd. October 4, 2013.

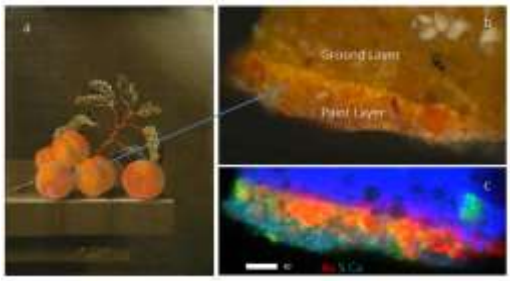
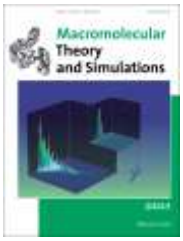


Figure 1: a) Adriaen Coorte, *Still Life with Five Apricots,* Mauritshuis; b) Paint cross-section from the region indicated, c) Composite elemental map– red = As, green = S, and blue = Ca (micro-XRF data, SSRL).

Computational Polymer Chemistry (Nazila Yaghini, Ivan Kryven)
The controlled degradation of non-branched PE is an intriguing process, since it features both scission of polymer chains as branching. Until now, no satisfactory model could explain these phenomena. We could finally attribute the branching to coupling of vinyl ends of PE to secondary radical sites on PE backbones, yielding tertiary radical sites that undergo termination by disproportionation. The Monte Carlo approach of this problem and the verification of the model with SEC-MALS data by Sabic has been published in Polymer. This project has been carried in collaboration with the chemical company Sabic (Geleen).The deterministic model of PE degradation, a higher-dimensional population balance model, has been constructed by Ivan Kryven and this work has been published in Macromolecular Theory and Simulations.
Further multi-dimensional modeling studies have been performed and published in the area of AB_2 condensation polymerization and radical crosslinking polymerization. Concerning the former we found that the branching distribution has a broad non-trivial shape that is non-symmetrical for substitution cases. The degree of branching is strongly dependent on the substitution factor, while chain length is mainly determined by cyclisation rate. (Low cyclisation rate provokes small amount of molecules with long cycle length and wise verse, high cyclisation causes more molecules to have cycles, but shorter in length.) Regarding crosslinking polymerization a new pseudo-distribution approach is applied and compared to Monte Carlo (MC) simulations. Surprisingly, taking the number of free pending double bonds as the main distribution variable enabled finding a rigorous solution of the three leading moments of the molecular size distribution. Well within the sol regime perfect agreement with data of methyl methacrylate/ethylene glycol dimethacrylate copolymerization is found, but near the gelpoint larger discrepancies appear, probably due to multiradicals not (yet) taken into account.

Cover page of Macromol. Theory Simul. 22, 2013 representing the 2-dimensional distributions of chain length and branch points from Monte Carlo simulations and deterministic model for Polyethylene after reactive processing (Ref. 2).



Key publications per academic staff member

- Keune, K. and Boon, J.J., (2013). Degradation of Emerald green in oil paint and its contribution to the rapid change in colour of the Descente des vaches (1834-35) painted by Théodore Rousseau, Studies in Conservation, 58 (3), p. 199-210.
- Kryven, I., Iedema, P.D. (2013). A novel approach to population balance modelling of reactive polymer modification leading to branching, Macromol. Theory Simul. 22, 89–106.
- Kryven, I., Berkenbos, A., Melo, P.A., Kim, D.-M., Iedema, P.D. (2013). Modeling crosslinking polymerization in batch and continuous reactors. Macromolecular Reaction Engineering, 7, 5, 205-220.
- Kryven, I., Iedema, P.D. (2013). Predicting multidimensional distributive properties of hyperbranched polymer resulting from AB(2) polymerization with substitution, cyclization and shielding. Polymer 54, 3472-3484.
- Iedema, P.D., Remerie, K., Van der Ham, M., Biemond, E. (2013). Development of MWD and branching during peroxide modification of High-Density Polyethylene by SEC-MALS and Monte Carlo simulation, Polymer 54, 4093-4104.

Invited lectures

Kryven, I. & Iedema, P.D. (2013, mei 21). *Modelling of Distributive Properties for AB2 Hyperbranched Polymer. Substitution, cyclization, shielding.* Hamburg, The 11th International Workshop on Polymer Reaction Engineering.

2.3 Molecular Photonics

Groups:	Molecular Spectroscopy; Spectroscopy and Photonic materials; Time Resolved Vibrational Spectroscopy		
Group leaders:	Prof. dr. A.M. Brouwer Prof. dr. W.J. Buma		
Academic staff:	Prof. dr. M.C.G. Aalders (BHGL) Prof. dr. H.J. Bakker (BHGL) Prof. dr. J. Oomens (BHGL) Dr. R.M. Williams Prof. dr. S. Woutersen (BHGL) Dr. H. Zhang		
Support staff:	Drs. ing. M.F. Hilbers Ing. P.P. Reinders Drs. H.J. Sanders		
Temporary staff		Start date	(Foreseen) end date
Visiting scholars:	Prof. dr. X. Hong Prof. dr. X.M. Liu Prof. dr. Y.L. Zhang	01-08-2012 01-04-2013 01-12-2012	28-02-2013 31-10-2013 30-04-2013
Postdocs:	Dr. S. Amirjalayer Dr. M.R. Panman Dr. C.N. van Dijk Dr. P. Zou	01-02-2012 01-04-2013 01-07-2011 01-02-2013	31-12-2013 30-06-2014 30-11-2013 31-10-2013
PhD students:	H.C. Chen, MSc. Drs. C.E. Carpentier F. Cao, MSc. Y. Ding, MSc. A. Huerta Viga, MSc. T.S. Kumpulainen, MSc. K. Liu, MSc. E. Maltseva, MSc. Drs. H. Meuzelaar Drs. S.J. Roeters S.M. Rosa Domingos, MSc. E.M.M. Tan, MSc. Drs. T.H. van der Loop M. Raeisolsadati Ouskoui (guest) T. Suhina (guest, IoP)	01-09-2011 01-02-2008 01-02-2011 01-02-2013 15-10-2008 01-10-2010 01-03-2009 01-08-2012 01-10-2010 15-10-2011 01-02-2009 01-04-2010 01-03-2010 01-11-2012 01-09-2012	31-08-2015 28-02-2013 31-01-2013 28-02-2015 14-10-2013 30-09-2014 14-03.2013 31-07-2016 30-09-2014 14-10-2016 30-09-2013 31-03-2014 31-10-2014 01-11-2013 01-09-2016
MSc + BSc students:	J. Bruijn H.J. Campbell D. den Uyl Z. Edelen E. Hakvoort P. Mazella F. Ruesink S.D. Tefera G. Torday	25-02-2013 01-10-2012 01-09-2013 01-09-2013 01-03-2013 25-06-2013 01-05-2012 01-09-2012 09-04-2013	25-02-2014 01-05-2013 01-06-2014 01-10-2013 10-06-2013 25-09-2013 25-03-2013 01-07-2013 31-05-2014

Mission of the group:
The Molecular Photonics group aims to advance the fundamental knowledge of the dynamics of excited states in molecules and nano-sized objects, and to contribute with its expertise to applications of the photosciences. Light-induced chemical conversions play a key role in many technological and biological processes - the most important of all being photosynthesis. Understanding the interaction of light and molecular matter is therefore highly significant. In particular we focus on the interaction of matter and light to design new molecules with pre-programmed properties. We like to understand how and why very specific light-active molecules perform specific functions.

Research results per sub project
Title: *An upconversion nanoparticle – zinc phthalocyanine based nano-photosensitizer for photodynamic therapy*
Researchers: aio K. Liu, L. Xia (CIOMP)
A efficient nanophotosensitizer was constructed for photodynamic therapy, which is based on near infrared (NIR) light upconversion nanoparticle (UCNP) and ZnPc photosensitizer (PS). The high 1O2 production led to a secure and efficient PDT treatment, as evidenced by the in vivo test where UCNPs-ZnPc of 50mg per kg body weight was locally injected into the liver tumor in mice, and a low 980 nm radiation dose of 351 J/cm2 (0.39 W） and short irradiation duration (15 min)caused the liver tumor inhibitory ratio of approximately 80.1%. Histological analysis revealed no pathological changes and inflammatory response in the heart, lung, kidney, liver or spleen. An article has been published.

Title: *Li^+ ions doping: An approach for improving the crystallinity and upconversion emissions of $NaYF_4$:Yb^{3+}, Tm^{3+} nanoparticles*
Researchers: aio F. Wu, X.M. Liu (CIOMP)
Upconversion luminescence efficiency of NaYF4:Yb^{3+},Tm^{3+} nanosystems has been improved via Li+ doping. Compared to lithium-free NaYF4:Yb^{3+},Tm^{3+} NPs, the UC emission centered at 452 nm and 479 nm of the NPs co-doped with 7 mol% Li^+ ions were enhanced by 8 and 5 times, respectively. The mechanism of the enhancement was explored, which led to the conclusion that the improvement of the nanoparticles' crystallinity and the distortion of the local symmetry around Tm^{3+} ions when introducing the Li^+ are responsible for the enhancement. An article has been published**.**

Title: Upconverison-C60 nanoplatform for NIR imagimg-guided photodynamic therapy of cancer cells
Researchers: X.M. Liu (CIOMP, visiting scholar), aio K. Liu
Upconversion-C60 nanoplatform was constructed for near infrared light (NIR) imaging-guided PDT of cancer in this project. Upon 980nm NIR continuous wave light excitation, the separately doping UCNPs NaYF4: Yb^{3+}, Er^{3+} / NaYF4: Yb^{3+}, Tm^{3+} emit strong upconverted multicolour light around 450 nm, 475 nm, 540 nm, 650 nm and 808 nm simultaneously. All of them, except the 808 nm band which is used for optical imaging, contribute to convert the excitation energy to C_{60} via FRET due to the broad absorption band of the latter, to trig PDT. The chemical and physical properties were also investigated in this work. In vitro experiments on cancer cells have confirmed its high photodynamic therapy efficiency. The results have been published in an article in Chem. Comm.

Title: Photocatalytic Water Splitting in Microfluidic Devices
Researcher: aio H.C. Chen
Hung-Cheng Chen has developed a series of new photosensitizers that are very useful for photochemical water oxidation. Publication of the results is delayed because we are investigating the options for patent applications. The next step of the project will be to implement the chemistry into a water splitting device.

Title: Fluorescence Monitoring of Organocatalytic Events
Researchers: aio T. Kumpulainen, guest aio M. Raeisolsadati Ouskoui
In the project of Tatu Kumpulainen organocatalytic reactions are investigated using fluorescence techniques. An important side line is the role of proton transfer modulating the fluorescence. A publication on proton transfer induced molecular motion is in preparation. Together with guest student Mina Raeisolsadati Ouskoui new fluorescent dyes of the BODIPY class are being investigated as labels and markers for organocatalytic reactions. The ultimate goal is to obtain insight into the reaction mechanisms of elementary organic reactions catalyzed by different organocatalysts using ultrasensitive fluorescence detection.

Title: Quantitative Probing of Friction in Multi-Asperity Contacts with Fluorescent Probes
Researchers: aio T. Suhina (Institute of Physics. Co-supervisor prof. Daniel Bonn)
Tomislav Suhina is employed as a FOM PhD student in the Institute of Physics, but mostly working under the supervision of prof. A.M. Brouwer in HIMS. He is developing molecular fluorescent probes for detecting contacts and forces in relation to friction. A rigidochromic fluorescent reporter previously studied by Chantal Carpentier in a different context turns out to be a very promising light-up probe for detecting contacts between objects on the nanoscale. A publication is in preparation. In parallel, deeper insight into the mechanism of operation is being obtained and the application to the analysis of the load dependence of frictional contacts is under investigation.

Title: The Primary Events in Organic Photovoltaics
Researcher: Hung-Cheng Chen, MSc.
We studied “Ultrafast charge and triplet generation in diketopyrrolo-pyrrole low bandgap polymer-PCBM blends: laser-fluence and morphology effects on hot singlet fission and geminate charge recombination to the triplet state in organic solar cell materials”. The primary photophysical events occurring in two types of thin film blends containing a low band gap polymer (PDPP) and PCBM as well as on the events occurring in the pristine polymer thin film were observed with femtosecond transient absorption spectroscopy (fs-TA) at three light intensity levels (with René Janssen, TUe Eindhoven). Manuscript in preparation. In due time a new organic photovoltaic materials will be selected for further spectroscopic studies.

Title: Photoactive Metal-Organic Frameworks
Researcher: Holly Campbell, MSc.
The incorporation of perylene bisimide (PDI) dyes into metal organic frameworks is a challenging task. Next to bis-pyridyl substituted naphtalenebisimide and tetraphenoxy bay-subtituted perylenebismide we focused on carboxyphenyl substituted tetrachloro bay-substituted perylenebismide. These ligands are now available. The latter compound enables MOF synthesis with just one organic component. It is clear that dimethylformamide as a solvent under hydrothermal conditions and tetra-chloro bay-substituted PDI are incompatible. Project can be continued by MSc or BSc student.

Title: Fullerene-C_{60}-Perylene-imide Light Harvesting Systems
Researcher: Zachary Edelen, BSc.
C_{60}–perylene-3,4-mono(dicarboximide) (C_{60}–PMI) dyads were studied in the search for new light-harvesting systems. These C_{60}–PMI dyads constitute good candidates for future photovoltaic applications with well-defined roles for both partners, i.e., PMI acting as a light-harvesting antenna and C_{60} playing the role of the acceptor in the photoactive layer. Nanosecond transient absorption spectroscopy in toluene has given clear evidence for PMI based triplet state formation, indicating singlet energy transfer followed by triplet energy transfer to the PMI unit. Furthermore, the ortho-substituted dyad shows substantially more PMI based fluorescence, as compared to the meta and para dyads. (with Pietrick Hudhomme, Angers, France). Manuscript in preparation.

Title: High-resolution UV/Vis and IR Spectroscopy of Isolated Photoactive Protein Chromophores
Researchers: aio Eric Tan, postdoc Saeed Amirjalayer
Experimental high-resolution spectroscopic studies have been performed in combination with advanced theoretical calculations that focus on the conformational heterogeneity and the excited-state dynamics of various forms of the chromophore of the Photoactive Yellow Protein (PYP), as well as the dependence of these dynamics on conformational and isosteric structure, and the biological environment. As it turns out, the results are not only important for understanding photoactive proteins but also put the phototoxicity of active ingredients of sunscreens in a completely new perspective. Two articles have been published, another two are being written.

Title: Fast Photodynamics Probed by Slow Spectroscopy
Researchers: aio Eric Tan, postdoc Saeed Amirjalayer, Paul Mazella, MSc.
Novel experimental approaches have been developed to study the excited-state dynamics of fast photoswitches such as azobenzene. These have enabled us to scan the potential energy surfaces of the $S_1(n\pi^*)$ and $S_2(\pi\pi^*)$ states, and obtain the first high-resolution absorption and excitation spectra of both states. An article will shortly be submitted. These results pave the way for detailed studies on other photochromic molecular systems that so far have not been accessible to isolated-molecule spectroscopy.

Title: Polycyclic Aromatic Hydrocarbon IR spectroscopy
Researcher: aio Elena Maltseva (in collaboration with Astrochemistry Network)
The IR absorption spectrum of a number of isolated polycyclic aromatic hydrocarbons (PAH) has been recorded in the CH stretch region. Astrochemists employ this spectral region as a powerful probe to analyse regions of star and planet formation throughout the universe using DFT calculations of harmonic force fields. The fact that the experimental spectra obtained now are dominated by effects of anharmonicity leads to the conclusion that a complete overhaul of analysis models is necessary. A manuscript is in preparation.

Title: Molecular Machines at Work in the Gas Phase
Researcher: aio Elena Maltseva, postdoc Saeed Amirjalayer
In collaboration with Prof. Feringa and Prof. Browne (RUG) high-resolution spectroscopy has been performed on molecular rotor systems based on chiral overcrowded alkenes and simplified versions of their chromophore. The initial results are encouraging but need to be followed up by more extensive double-resonance studies. At FELIX UV/Vis and IR studies have been performed on a new class of rotaxanes based on azodicarboximides (collaboration with Dr. Berna (Murcia, Spain) and Dr. Rijs (RU)). In combination with the results of quantum chemical calculations, these results have elucidated the conformational heterogeneity of the thread and the influence of the macrocycle on the spatial structure. A manuscript is in preparation.

Title: Light on Molecular Machines
Researcher: postdoc Saaed Amirjalayer
Time-resolved IR absorption studies have been performed on the above mentioned molecular rotor and rotaxane systems. For the rotor the IR studies provide a detailed picture of the photochemical dynamics which in fact differs from the conclusions of previous studies. One of the noteworthy aspects is that direct evidence is obtained for the presence of sudden polarization. In collaboration with Prof. Meech (East-Anglia, UK) the photodynamics of the related 9,9'-bifluorenylidene - proposed as an alternative and flexible electron acceptor in organic photovoltaic cells –has been studied using transient absorption and time-resolved IR experiments. On the former studies an article has been submitted, on the former an article will be submitted shortly. For the rotaxane system the IR studies show that the mode of action is a bicycle-type of pedaling motion in the excited state. A manuscript is in preparation.

Title: Helium Nanodroplet Spectroscopy
Researcher: former aio Szymon Smolarek
Some years ago we have initiated in collaboration with Dr. Drabbels (EPFL, Switzzerland) a project on the critical Landau velocity in helium nanodroplets. This project has recently been closed with a publication on this subject in Physical Review Letters.

Title: Photophysics of Si nanocrystals
Researcher: aio Elinore de Jong (supervisor Prof. Tom Gregorkiewicz (IoP))
Optical carrier generation in silicon nanocrystals embedded in an SiO_2 matrix has been investigated. To this purpose carrier relaxation and recombination processes have been monitored by means of time-resolved induced absorption. A paper has been published in Physical Review B.

Title: The Physics and Chemistry of metallic Fe and FeS Nano Clusters
Researcher: aio Denis Kiawi (appointed at API, co-supervisor Prof. Rens Waters and prof. J. Oomens (RU))
A novel cluster source has been constructed and incorporated into the cluster spectrometer at the RU. Experimental IR spectra of neutral and ionic Fe clusters and of such clusters with astrochemically relevant species such as H_2O, CO, and H_2 have been obtained. These spectra have been used to elucidate the structure of the clusters and how these clusters affect the electronic structure of the absorbed species. A manuscript is being prepared.

Title: Dissociation reactions of protonated and deprotonated peptides in mass spectrometry
Reseracher: aio Josipa Grzetic (appointed at RU, supervisors Prof. Jos Oomens and Prof. W.J. Buma)
Low-energy collision-induced dissociation of mass-selected protonated peptides and mass analysis of the molecular fragments is widely used to determine the sequence of amino acid residues in peptides and proteins. However, the reaction mechanisms underlying peptide dissociation are only partly understood. It is believed that a better fundamental understanding of the dissociation chemistry can eventually improve the identification of peptides by mass spectrometry. To this purpose we have analysed the molecular structures of selected peptide fragments by IR photo-dissociation spectroscopy employing the widely tuneable radiation of the free electron laser FELIX in combination with a high-resolution tandem mass spectrometer. Two articles have been published.

Title: Amplified Vibrational Circular Dichroism
Researcher: aio Sergio Domingos
We have demonstrated that VCD signals can be amplified by up to three orders of magnitude by employing metal ions with low-lying electronically excited states. Studies on amino acids and peptides show that the local character of the amplification is an excellent probe for zooming in on local details of the spatial structure of large molecular systems. Using electrochemical switching the principle and application of a switchable VCD amplifier has been demonstrated. The latter amplifier enables us to suppress signals that are not related to the spatial region of interest. In 2013 one article has been published and one submitted. Another manuscript will shortly be submitted.

Title: Molecular movies of protein folding
Researchers: aio's Adriana Huerta Viga and Heleen Meuzelaar; postdocs Chris van Dijk and Matthijs Panman
(1) Guanidium is one of the most commonly used denaturants, but it is largely unknown how it denatures proteins. Using 2D-IR spectroscopy we discovered that guanidium specifically disrupts the H-bond network of the beta-sheets of a protein. (2) We have for the first time determined the orientation of a protein in a membrane using vibrational sum-frequency spectroscopy (cooperation with MPI Mainz); (3) We discovered that salt bridges can speed up protein folding. This result can explains the evolutionary origin of salt bridges that have no apparent (thermodynamic) function.

Title: How water lubricates molecular machines
Researcher: aio Steven Roeters
Using nuclear magnetic resonance, we have investigated how the rotational motion in a molecular wheel is influenced by different co-solvents. Preliminary analysis shows that acidic co-solvents speed up the motion even more than water does.

Title: Proton transport in nanoconfinement
Researcher: aio Tibert van der Loop
To investigate how confinement to nanometer-size volumes influences aqueous proton transport, we prepared nanometer-size droplets of acidic water, and observed the proton transport inside by measuring the frequency-dependent GHz dielectric response. Interestingly, whereas the GHz spectrum of protons in bulk water exhibits a 1/f frequency dependence (comparable to electrons in a metal), the protons in nano-confinement exhibit a resonance, showing that the protons "hit the wall". From the position of the resonance, the transport rate can be directly determined. These results are important for our understanding of proton transport in cell organelles and in the membranes of fuel cells.

Other activities
The Molecular Photonics group has hosted a number of external visitors that applied for use of our equipment via LaserLab Amsterdam. These projects concerned the following:
- Title: Lanthanide-doped $LaPO_4$ nanorods
  Applicant: Dr. Thierry Gacoin (Ecole Polytechnique, Palaiseau, France)
- Title: Probing the excited state development and subsequent photochemical reactions involved in visible light reduction of CO_2 using time-resolved IR
  Applicant: Dr. Mary Pryce (Dublin City University, Ireland)
- Title: Spectroscopic sensing of organic vapours on the surface of quantum dots
  Applicant: Dr. Paolo Prosposito (University of Rome Tor Vergata, Italy)

A collaboration with prof. Tomoki Ogoshi (Kanazawa, Japan), one of the inventors and leaders of the field of pillar-arenes has led to a joint publication in Chemical Communiations on a pillar-arene based fluorescent rotaxane. The collaboration with the Homogeneous Catalysis group in HIMS in the field of Solar Fuels has produced a highlight publication in ChemSusChem.

Key publications per academic staff member

- van den Bosch, B., Chen, H.-C., van der Vlugt, J. I., Brouwer, A. M. & Reek, J. N. H. A noble-metal-free system for photodriven catalytic proton reduction. *ChemSusChem* **6,** 790–793 (2013).
- Baggerman, J. *et al.* Induction of Motion in a Synthetic Molecular Machine: Effect of Tuning the Driving Force. *Chem. Eur. J.* **19,** 5566–5577 (2013).
- Ogoshi, T., Yamafuji, D., Yamagishi, T.-A. & Brouwer, A. M. Forster resonance energy transfer by formation of a mechanically interlocked [2]rotaxane. *Chem. Commun.* **49,** 5468–5470 (2013).

- van Walree, C. A.; van der Wiel B. C.; Williams, R. M.; “Photoinduced charge transport over branched conjugation pathways: donor-acceptor substituted 1,1-diphenylethene and 2,3-diphenylbutadiene”. *Physical Chemistry Chemical Physics.* **2013**, *15*, 15234 –15242.
- Williams R.M.; Van Anh, N.; van Stokkum, I. H. M.; “Triplet Formation by Charge Recombination in Thin Film Blends of Perylene Red and Pyrene: Developing a Target Model for the Photophysics of Organic Photovoltaic Materials”. *Journal of Physical Chemistry. B* **2013**, *117(38),* 11239-11248.
- Brauer, N.B.; Smolarek, S.; Loginov, E.; Mateo, D.; Hernando, A.; Pi, M.; Barranco, M.; W.J. Buma, W.J.; Drabbels, M. Critical Landau velocity in helium nanodroplets. *Phys. Rev. Letters* **2013** *111*, 153002.
- Tan, E.M.M., Amirjalayer, S., Smolarek, S., Vdovin, A., Rijs, A.M., Buma, W.J. Conformational heterogeneity of methyl 4-hydroxycinnamate: a gas-phase UV-IR spectroscopic study. *J. Phys. Chem. B* **2013**, *117(17)*, 4798-4805.

- Tan, E.M.M., Amirjalayer, S., Bakker, B.H., Buma, W.J. Excited state dynamics of Photoactive Yellow Protein chromophores elucidated by high-resolution spectroscopy and ab initio calculations. *Faraday Disc.* **2013**, *163*, 321-340.

- Xia L., Liu X.M.; Kong X.G.; Tu L.P.; Zhang Y.L.; Chang Y.L.;m Liu K.; Shen D.Z.; Zhao H.Y.; Zhang H. An upconversion nanoparticle – zinc phthalocyanine based nano-photosensitizer for photodynamic therapy. *Biomaterials* **2014**, *35,* 4146-4156
- Liu X.M.; Zheng M.; Kong X.G.; Zhang Y.L.; Zeng Q.H.; Sun Z.C.; Liu, K.; Buma W.J.; Zhang H. Separately Doping Upconverison-C60 Nanoplatform for NIR Image-Guided Photodynamic Therapy of Cancer Cells. *Chem. Commun.* **2013***, 49* , 3224-3226.
- Bian H.Y.; Liu Y.X.; Yan D.T.; Zhu H.C.; Liu C.G.; Xu C.S.; Wang X.J.; Zhang H. Spectral modulation through controlling anions in nanocaged phosphors. *J. Mater. Chem. C.* **2013***, 1*, 7896-7903

- Panman, M.R.; Bakker, B.H.; den Uyl, D.; Kay, E.R.; Leigh, D.A.; Buma, W.J.; Brouwer, A.M.; Geenevasen, J.A.J.; Woutersen, S. Water lubricates hydrogen-bonded molecular machines, *Nature Chemistry* **2013,** *5*, 929-934.
- Huerta-Viga, A.; Woutersen, S. Protein Denaturation with Guanidinium: A 2D-IR Study. *J. Phys. Chem. Lett.* **2013**, *4*, 3397-3401.H. Meuzelaar, H.; Marino, K.A.; Huerta-Viga, A.; Panman, M.R.; Smeenk, L.E.J; Kettelarij, A.J.; van Maarseveen, J.H.; Timmerman, P.; Bolhuis, P.G.; Woutersen, S.
- Folding Dynamics of the Trp-Cage Miniprotein: Evidence for a Native-Like Intermediate from Combined Time-Resolved Vibrational Spectroscopy and Molecular Dynamics Simulations, *J. Phys. Chem. B.* **2013**, *117*, 11490-11501.

Dissertations

- Lapoutre, V.J.F. (21 June 2013). *Infrared spectra of strongly bound clusters: Extending the limits of action spectroscopy.* Universiteit van Amsterdam (iv, 156 pag.). Prom./coprom.: prof.dr. J. Oomens & J.M. Bakker.
- Carpentier, C.E. (26 September 2013). *Three-dimensional visualization of contact networks in granular material.* Universiteit van Amsterdam (199 pag.). Prom./coprom.: prof.dr. D. Bonn, prof.dr. A.M. Brouwer & dr. P. Schall.
- Panman, M.R. (5 December 2013). *Observing invisible machines with invisible light: The mechanics of molecular machines.* Universiteit van Amsterdam (IX, 147 pag.). Prom./coprom.: prof.dr. W.J. Buma & dr. S. Woutersen.
- Rosa Domingos, S.M. (11 December 2013). *Amplified vibrational circular dichroism.* Universiteit van Amsterdam (viii, 152 pag.). Prom./coprom.: prof.dr. W.J. Buma & dr. S. Woutersen.

Grants and prizes

- Brouwer, A.M. (2013). Short Term Visiting Scholar, Lanzhou University, China.
- Buma, W.J. (2013). Bryan E. Kohler Distinguished Lectureship 2013.
- Buma, W.J. & Zhang, H. (2013). ZonMw grant for Institute Quantivision.
- Buma, W.J. & Woutersen, S. (2013). ECHO grant for a proposal concerning optically amplified vibrational circular dichroism.
- Zhang H. “NENU scholar” Chair Professor, Northeast Normal Unviersity
- Zhang H. 2013 Innovation project of National Key Laboratory of Luminescence and Application (China)

Invited lectures

- Brouwer, A.M. (2013, oktober 16). *Colorful Molecules.* Lanzhou, China, Lanzhou University, Short term visiting scholar program, student lecture.
- Brouwer, A.M., Carpentier, C.E., Suhina, T., Lorincz, K.A., Weber, B.A., Schall, P. & Bonn, D. (2013, October 17). *Fluorescence imaging of contacts and forces.* Shanghai, China, Novel Materials and Synthesis, invited lecture.

- Brouwer, A.M. *Fluorescence micro-spectroscopy in materials science.* Lanzhou, China, Lanzhou University, Short term visiting scholar program.
- Brouwer, A.M., Suhina, T., Carpentier, C.E., Schut, M.F.L., Weber, B.A., Bonn, D. & Schall, P. (2013, september 04). *FLUORESCENT MOLECULAR REPORTERS in SOFT MATTER.* Sinaia, Romania, Romanian International Conference on Chemistry and Chemical Engineering.
- Brouwer, A.M. (2013, oktober 16). *Measurement of luminescence spectra.* Lanzhou, China, Lanzhou University, Short term visiting scholar program, student lecture.
- Buma, W.J. (2013, april 15). *Excited state dynamics of Photoactive Yellow Protein chromophores elucidated by high-resolution spectroscopy and ab initio calculations*. Nottingham (UK), Faraday Discussion 163: Photo-initiated Quantum Molecular Dynamics.
- Buma, W.J. (2013, February 13). *Photons at work*. Riverside, USA, Kohler memorial lecture, University of California.
- *Buma, W.J. (2013, February 15). Taming* molecular complexity. Santa Barbara, USA, P-chem seminar, University of California.
- Buma, W.J. (2013, February 21). *Taming molecular complexity*. Bloomington, P-chem seminar, Indiana University at Bloomington.
- Buma, W.J. (2013, February 20). *Taming molecular complexity*. West-Lafayette, P-chem seminar, Purdue University.
- Buma, W.J. (2013, February 18). *Taming molecular complexity*. Urbana-Champaign, P-chem seminar, University of Illinois at Urbana-Champaign.
- Buma, W.J. (2013, February 14). *Taming molecular complexity*. Los Angeles, P-chem seminar, University of Southern California.
- Buma, W.J. (2013, May 01). *Taming molecular complexity*. Radboud University, Nijmegen, The Netherlands, FELIX kick-off meeting.
- Buma, W.J. (2013, February 19). *The difference between left and right*. West-Lafayette, Special seminar, Purdue University.
- Buma, W.J. (2013, February 11). *The difference between left and right*. Riverside, USA, P-chem seminar University of California.
- Ding, Y., Zou, P., Zhang, Y., Hong, X., Liu, Y., Buma, W.J. & Zhang, H. (2013, augustus 04). *Excitation Energy Migration in Upconversion Nanoplatforms: Role of the Shell*. 18th International Conference on Dynamical Processes in Excited States of Solids (DPC'13), Fuzhou, China.
- Huerta-Viga, A. *How Does Guanidinium Denature Proteins?* 6th European Conference on the Spectroscopy of Biological Molecules, Oxford (2013).
- Rosa Domingos, S.M. *Switchable amplified vibrational circular dichroism as a local probe of biomolecular structure,* 6th European Conference on the Spectroscopy of Biological Molecules, Oxford (2013).
- Zhang, H. (2013, August 23) *Ultrafast spectroscopy in nanosystems and biomedical application*, The 3rd National Meeting on Chemical Dynamics of China, Wuhu, China.
- Zhang H. (2013, August 03) *Photonic Nanoplatforms for Medical Application – Origin of Luminescence and Optimization,* The 4th National Meeting on the Luminescence Properties of Doped Nanomaterials, Hohhot, China.
- Williams, R.M. (2013, May 31). *The Primary Events in Organic Photovoltaics.* Tampere, Finland.
- Williams, R.M. (2013, January 28). *The Primary Events in Organic Photovoltaics.* Nijmegen, The Netherlands.
- Woutersen S. (August 2013), *The Effect of Salt Bridges on the Speed of Folding*, 6th European Conference on the Spectroscopy of Biological Molecules, Oxford (2013).

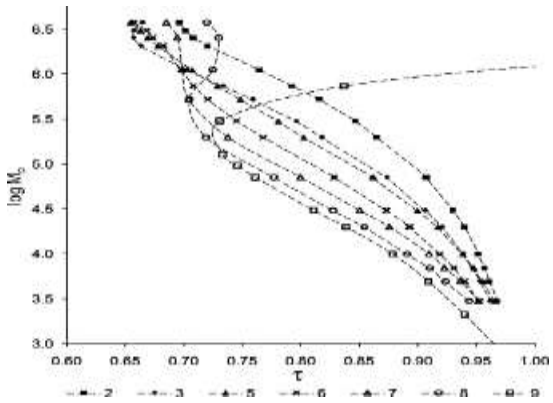
2.4 Analytical Chemistry

Theme:	Analytical Chemistry		
Group:	Analytical Chemistry (including its applications in Forensic Science)		
Group leader:	Prof. dr. P.J. Schoenmakers		
Academic staff:	Dr. W.Th. Kok Dr. G.I. Vivo Truyols Prof. dr. A.C. van Asten (BHGL) Prof. dr. J.G.M. Janssen (BHGL) Prof. dr. S. van der Wal (BHGL)		
Support staff:	T. Aalbers P. Aarnoutse P.G. Verschuren		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. M. Camenzuli Dr. A.F.G. Gargano	01-03-2013 09-09-2013	31-08-2014 31-08-2015
PhD students:	Drs. A.A. Baglai Drs. A. Barcaru Drs. G.M.H. Brust Drs. H. Cornelisson van de Ven Drs. E. Davydova Drs. J.Králová Drs. M. Marioli Dr. M. Pacheco B. Mourao Drs. A.D. Ngoc Drs. D. Peroni Drs. A.A.S. Sampat Drs. R.J. Vonk Drs. M. Woldegebriel	01-10-2012 01-04-2013 01-11-2009 01-10-2012 01-06-2011 01-08-2011 01-08-2011 01-09-2013 01-05-2011 01-09-2009 01-02-2012 01-04-2011 01-04-2013	30-09-2016 31-03-2017 31-10-2013 30-09-2016 31-05-2015 31-07-2015 31-07-2015 30-06-2016 29-04-2014 31-12-2013 31-01-2016 31-03-2015 31-03-2017
MSc students:	T. Angevaare H. Al Habobe M.Li M. Merkies D. Puszkar N. in ‘t Ven T. Zeng		

Mission of the group:
The Analytical- Chemistry Group focuses on the development of new or greatly improved techniques or methods for the analysis of complex mixtures. The technical focus is on one- and two-dimensional separation methods, on miniaturization (micro- and nano-fluidics), on hyphenation with detection (including MS), and on chemometric techniques for data handling and optimization. The application focus is on macromolecules (novel materials), forensic science and a variety of other fields.

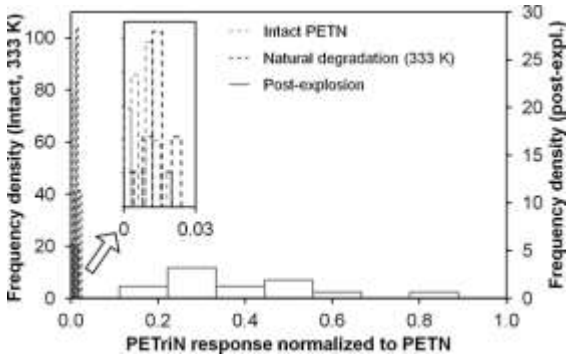
Research results per sub project
Multidimensional Separations
Researchers: Rudy Vonk and Katja Davidova (DiscoveRIE); Anna Baglai, Henrik van de Ven, Michelle Camenzuli, and Andrea Gargano (HyperLC). The DiscoveRIE project, sponsored by the EU, is carried out in collaboration with the Vrije Universiteit Brussel (S.Eeltink) and Thermo Scientific, an instrument company. It aims at the development of revolutionary spatial two- and threedimensional LC systems specifically targeting the complex challenges posed by biomarker discovery and clinical diagnostics. The first publications appeared in 2013.

Related research on multdimensional separations is carried out in the COAST-sponsored project HyperLC. In this project a variety of industrial partners is involved. Part of the research work is being carried out by the PhD students and postdocs involved at the premises of these partners. The project is now in full swing and the first publications are in preparation.
Rob Edam defended his PhD thesis on “Comprehensive Characterization of Branched Polymers”, a DPI project, in Februari 2013.



Effect of macropore size of monolithic columns on HDC selectivity for polymers (R.Edam)

Forensic Research
Researchers: Hanneke Brust, Andjoe Sampat, Martin Lopatka.
Hanneke Brust has finished the experimental work for her project on forensic analysis. She worked mostly on methods for the analysis of explosives and residues, together with prof Arian van Asten (NFI). She is expected to defend her thesis in 2014.



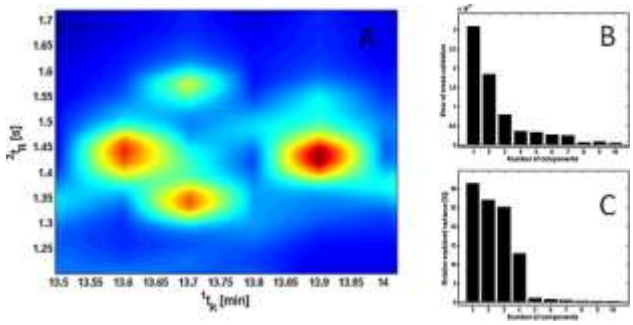
Distribution of PETriN/PETN peak-area ratios obtained post-explosion, intact PETN and after natural degradation (H.Brust).

The COAST-sponsored project COMFOR is a collaboration between Gabriel Vivo and prof M.Sjerps (NFI, KdV). The aim of the project is to develop 2-dimensional separation methods for forensic applications. Andjoe Sampat focuses on the instrumental aspects, while Martin Lopatka develops chemometric tools for data processing and interpretation.

NanoNext projects
Researchers: Ngoc A Dang, Marta Mourao, Arend Kolk (TB biomarkers); Jana Kralova (Nanofluidics).
Ngoc A Dang finished her experimental work on GC methods for biomarker discovery for tuberculosis. She is expected to defend her thesis in 2014. Marta Mourao started as a PhD student in this project in 2013; she will continue the work initiated by Ngoc A Dang. The project is carried out under the supervision of dr Arend Kolk and prof H.-G. Janssen, and various other institutes are involved.
In another NanoNext project (Nano-LoC) Jana Kralova works together with researchers of the Vrije Universiteit Brussels on the development of nano-scale separations for point-of-care devices. Prototypes of micro-fluidic devices for field-flow fractionation were developed and are now being tested. One of the possible applications is for plasma cholesterol monitoring.

Chemometric Research
Researchers: Andrei Barcaru and Michael Woldegebriel
The COAST-project Chromametrics started in 2013. The project aims at the development of statistical and chemometric methods for the analysis of the large datasets that are obtained by, e.g. , 2D chromatography or LC-MS, with applications in forensic, and industrial analysis and in food safety. In this project under the supervision of Gabriel Vivo-Truyols a collaboration with RIKILT and DSM is established.

Other projects
Researchers: Maria Marioli; Daniela Peroni; Sonja Kaal-Peters.
Maria Marioli works in an STW program (SmartSep) on the development of methods and devices for the purification of biopharmaceuticals, where scaling-up of the methods is an important issue. This work is carried out in collaboration with researchers from the University of Twente.
Daniela Peroni finished her industry-financed project on the extention of the possibilities of GC-methods. She defended het PhD in November 2013 (promotor: prof H.-G. Janssen).
Sonja Kaal-Peters was an external PhD student, employed by Unilever. She defended her PhD, on her work on chromatographic profiling in metabolomics under the supervision of prof Janssen, in November 2013.



Algorithms for peak detection in GCxGC (S.Peters)

Key publications
- "Study on the performance of different types of three-dimensional chromatographic systems" Davydova, E; Schoenmakers, PJ; Vivo-Truyols, G; J. Chromatogr. A, 1271 (2013) 137-143.
- "Visualization procedures for proteins and peptides on flat-bed monoliths and their effects on matrix-assisted laser-desorption/ionization time-of-flight mass spectrometric detection";
- Wouters, B; Vanhoutte, DJD; Aarnoutse, P; Visser, A; Stassen, C; Devreese, B; Kok, WT; Schoenmakers, PJ; Eeltink, S; J. Chromatogr. A, 1286 (2013)222-228.
- "A new method for the automated selection of the number of components for deconvolving overlapping chromatographic peaks"; Peters, S; Janssen, HG; Vivo-Truyols, G; Anal. Chim. Acta, 799 (2013) 29-35.
- "Pentaerythritol tetranitrate (PETN) profiling in post-explosion residues to constitute evidence of crime-scene presence"; Brust, H; van Asten, A; Koeberg, M; van der Heijden, A; Kuijpers, CJ; Schoenmakers, PJ; Forensic Sci. Int., 230 (2013) 37-45.
- Comprehensive two-dimensional gas chromatography with a multi-capillary second dimension: A new column-set format for simultaneous optimum linear velocity operation Peroni, D; Sampat, AAS; van Egmond, W; de Koning, S; Cochran, J; Lautamo, R; Janssen, HG; J. Chromatogr. A, 1317 (2013) 3-11.
- The identification of biomarkers differentiating Mycobacterium tuberculosis and non-tuberculous mycobacteria via thermally assisted hydrolysis and methylation gas chromatography-mass spectrometry and chemometrics, Dang, NA; Kolk, AHJ; Kuijper, S; Janssen, HG; Vivo-Truyols, G; METABOLOMICS, 9 (2013) 1274-1285.

Dissertations

- Edam, R. (21 Februari 2013). *Comprehensive characterization of branched polymers.* Universiteit van Amsterdam (176 pag.). Prom./coprom.: prof.dr.ir. P.J. Schoenmakers.
- Peroni, D. (29 November 2013). *Advancing GC×GC through integrated sample preparation methods and optimized column formats.* Universiteit van Amsterdam (172 pag.). Prom./coprom.: prof.dr.ir. J.G.M. Janssen & prof.dr.ir. P.J. Schoenmakers.
- Peters, S. (12 November 2013,). *Chromatographic profiling: From samples to information.* Universiteit van Amsterdam (202 pag.). Prom./coprom.: prof.dr.ir. J.G.M. Janssen, prof.dr.ir. P.J. Schoenmakers & dr. G. Vivó-Truyols.

Invited lectures

- Asten, A.C. van (2013, april 20). *CSI Innovations, revolutionizing crime scene investigation.* London, United Kingdom, Forensic ExpoLondon, invited lecture.
- Asten, A.C. van (2013, juni 20). *Forensic Challenges for LC and LC-MS.* Amsterdam, The Netherlands, HPLC 2013, invited lecture.
- Janssen, J.G.M. (2013, juni 16). *Food Analysis: A challenging area for liquid chromatography and mass spectrometry.* Amsterdam, the Netherlands, HPLC 2013.
- Janssen, J.G.M. (2013, juni 21). *Novel comprehensive chromatographic techniques for detailed analysis of the minor and major components of edible oils and fats.* Ghent, Belgium, Compositional analysis of lipids.
- Janssen, J.G.M. & Peroni, D. (2013, mei 12). *Optimization of Column Formats and Flow Conditions in GCxGC.* Palm Springs, CA, USA, 10th symposium on comprehensive GCxGC.
- Kok, W.Th., (2013, October 6). *Combining TDA and CE to study asphaltenes.* ITP2013, Tenerife, ES, , invited lecture.
- Schoenmakers, P.J., *HyperFormance polymer separations*, SCM-6, Dresden, plenary lecture.
- Schoenmakers, P.J., *Towards HyperFormance 2D-LC*, HPLC2013 Hobart, Australia, plenary lecture.
- Vivo-Truyols, G., *Methods for data handling for 2D-chromatography*, IFPAC2013, Baltimore, Feb 2013. Invited lecture.

3. Evaluation

Based on a self-evaluation report and a site visit on 18 October 2013, the Scientific Advisory Board (WAR) of HIMS assessed the research conducted within HIMS. The WAR gave a general advice to HIMS and specifically addressed the research within the four research themes: Sustainable Chemistry, Analytical Chemistry, Molecular Photonics and Computational Chemistry. A summary of the extensive WAR-report is given below.

> *The research institute HIMS has a clear focus with four groups operating in relevant research areas that are recognized nationally and internationally. The scientific director of HIMS, Prof. Kleijn, has been succeeded by Prof. Reek shortly after the site visit by the WAR. The WAR strongly supports the choice for Prof. Reek as scientific director in view of his excellent scientific profile and management capacities. Adequate support by a managing director is important. The position of HIMS within the University of Amsterdam (UvA) benefits from the recent recognition of the Sustainable Chemistry theme as UvA 'zwaartepunt'. Analytical Chemistry (UvA/VU) is an important field (also for industry) and has disappeared as a separate research theme at other Dutch universities which gives the HIMS group a unique position. Computational Chemistry at HIMS is historically strong and it continues to be a leading group worldwide. The Molecular Photonics group also continues with a strong profile, in line with the recommendations in the QANU report of 2010 which criticized earlier restructuring plans which would have reduced the visibility of Molecular Photonics.*
>
> *The research at HIMS is of high scientific quality with an increasing number of high impact publications. The research receives sufficient funding from external sources. There is a number of developments and changes which require an adequate strategy, especially the merger of the science faculties of the UvA and VU (Free University of Amsterdam) and the 'Sectorplan' Chemistry and Physics. The vision and strategy of HIMS concerning the merger of the Science Faculties of the UvA and the VU, forming the Amsterdam Faculty of Science (AFS) is aimed at strengthening the existing research themes. The concentration of sustainability related chemistry research ('green') around the present location of HIMS (Science Park) and bio-chemical/medical research related to health ('red') at the 'Zuid-As' close to the VU Medical center is a valid strategy. The merger will give opportunities to strengthen the HIMS research, especially in the areas of Computational/Theoretical chemistry and Molecular Photonics where strong research activities at the VU can merge with the HIMS groups. In the area of Sustainability it is important to continue the chair of Organic Chemistry at the VU within the Sustainability research in the Science Park. The chair has a strong track record in sustainable chemistry and is an extremely valuable complementary addition to the Sustainability research within HIMS. The implications and opportunities related to the merger for specific groups will be discussed in more detail below. In addition to a positive overall evaluation there are several more general concerns and recommendations for the institute.*

Composition of the WAR

Prof. dr. Andries Meijerink (chair), Universiteit Utrecht
Dr. Tom van Aken, Avantium
Prof. dr. Wim Briels, Universiteit Twente
Prof. dr. David Reinhoudt, Universiteit Twente
Prof. dr. Floris Rutjes, Radboud Universiteit
Prof. dr. Michel Nielen, Wageningen Universiteit
Dr. Louis Vertegaal, NWO

4. Valorisation

HIMS researchers explore a range from pure basic scientific inspired quests to application inspired fundamental research projects. Out of the thirteen granted research proposals (see section 1.4.4) ten projects were inspired by future utilisation of the project. Some projects have already companies participating and co-financing them.

In case results of HIMS research may have future commercial value, HIMS follows an active approach to find industrial partners to collaborate with. The Technology Transfer Office supports HIMS scientists with contracts, IP affairs and advises on funding (grants). Where appropriate HIMS protects its intellectual property. Usually industrial partners, that are the potential users of the knowledge, will be involved in an early stage. Therefor the institute often does not allways apply for patents itself.

In 2013 one new patent was filed, in collaboration with the French IFP Energies nouvelles: Reek, J.N.H. (2013) *Nouveau complexe à base de nickel et son utilisation dans un procédé d'oligomérisation des oléfines*.

Four patent applications submitted in 2011 entered the national registration phase.

- Core-shell particles with catalytic activity. V.R. Calderone, N.R. Shiju, G. Rothenberg and D. Curulla-Ferre, WO 2012/163969 (May 30, 2011). (Application by Total Raffinage)
- Composite material comprising synthetic filler and specific polymer. A.H. Alberts and G. Rothenberg, EP 2511326; WO 2012/140239 (April 14, 2011).
- Laminate comprising carrier and coating polymer. A.H. Alberts and G. Rothenberg, WO 2012/140238 (April 14, 2011).
- Composite material comprising bio-filler and specific polymer. A.H. Alberts and G. Rothenberg, WO 2012/140237 (April 14, 2011).

The bioplastic project has made much progress in 2013 towards valorisation, and we foresee that it will be spun out as an independent company in 2014. Other activities on valorisation intiatives like Towards Biosolar Cells, Quantivision and spin-off company InCatT expanded.

In 2013 the organizations ASML, FOM, NWO, UvA and VU launched the Advanced Research Centre for Nano-Lithography (ARCNL). Prof. Fred Brouwer of HIMS was involved in the scientific bid book that the academic partners prepared for ASML, whereupon ASML choose for Amsterdam as location of the centre. The centre is a prime example of a public-private research collaboration.
The ARCNL will eventually start in 2014, with Prof. Fred Brouwer as one of its group leaders.

On 21 June, the kick off meeting of the Innovation Lab Chemistry Amsterdam (ILCA) took place.
ILCA is the product of cooperation between Top ChemieΔ , Topteam Chemie, TI-COAST and the Amsterdam Universities, and is situated in the Matrix VI building at Science Park Amsterdam. Apart from housing, ILCA provides networks and valorization, and supervises enterprises and financing.
The kickoff meeting on 21 June was an opportunity to get to know the Innovation Lab. Part of the program was meant to bring companies, starting entrepreneurs, scientists and some talented students together with the intention to enhance the network of chemistry in the metropole region of Amsterdam. It featured some inspiring presentations and a brainstorm session dealing with cases, which involved short pitches of challenges which a company might have to deal with, and how they could be handled successfully by cooperation. The initial steering committee of ILCA was chaired by HIMS director Prof. Aart Kleijn.

5. Organisation and finances

The HIMS organisation is being managed by a director and supported by a bedrijfsbureau. The director Prof. Aart Kleijn was succeeded by Prof. Joost Reek per 1 November 2013. Ultimo 2013 the support organisation of HIMS was staffed as follows:

Operations management (bedrijfsvoering)
G.J.J. Zonneveld - de Boer, Drs. H.E. Zwaan - van der Plas (HRSMC)[2]

Supporting team
P.J.E. Hagen, R. Weijer, R.B. Hippert, M.P.C. Sabandar - Mumu

Special tasks
Dr. R.L.J. Zsom (Strategy), Prof. dr. A. Oskam (Facilities), E. Duin-Berteling BA (Safety).
P.F. Collignon (ICT)

HIMS is home to the headquarters of the following three research organizations that have overlapping interests in research topics with HIMS.

5.1.1. HRSMC

The Holland Research School of Molecular Chemistry (HRSMC) was founded in 1994 and has been re-accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW) in 1999 and 2005. Importantly, in 2012 the Accreditation Committee (ECOS) of the KNAW decided to re-accredit the HRSMC for the period 2012-2018.

The HRSMC comprises research groups of 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); and the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Leiden University (UL). The Universiteit van Amsterdam legally represents the HRSMC. Currently Prof. dr. W.J. Buma (HIMS) is the scientific director. The main targets of the HRSMC are:

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

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

[2] HRSMC – Holland Research School of Molecular Chemistry. The UvA/HIMS is coordinator (penvoerder) of the HRSMC. Prof. dr. W.J. Buma chairs the HRSMC.

Apart from organizing and providing high-level PhD education -which is also accessible for (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 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. Presently, six MSc students have been admitted to this Excellence Program.

Major activities 2013

1. Annual HRSMC symposium (November 21, 2013), organized at the national Biodiversity Center, 'Naturalis' in Leiden. The annual HRSMC symposium, which was attended by ca. 150 scientists, also included poster sessions with 42 posters mainly presented by PhD students.
2. The HRSMC educational activities of 2013 consisted of:
   - The two weeks Course *'Molecular Simulation'*, organized under the auspices of CECAM (January 7-18, 2013, UvA)
   - The Course *'Physical Methods in Inorganic Chemistry'* (January 30 – February 7, 2013, UL/UvA)
   - HRSMC Course *'Molecular Modeling'* (May 13 - 24, 2013, VU)
   - The Summer School *'New Vistas for Organic Synthesis'* (July 1-4, 2013, Maastricht)
   - The KNCV/HRSMC Career Advice Activity for PhD students and postdocs (November 28 2013, UvA, the KNCV is the Royal Dutch Chemistry Association).

   Furthermore, the HRSMC has participated in the organization of the Winter School '*Theoretical Chemistry and Spectroscopy*' (9-13 December, Han-sur-Lesse)

   The Molecular Simulation course as well as the two Schools have by now become rather well known with the majority of the participants actually coming from abroad. The Schools receive considerable funding from European programs.

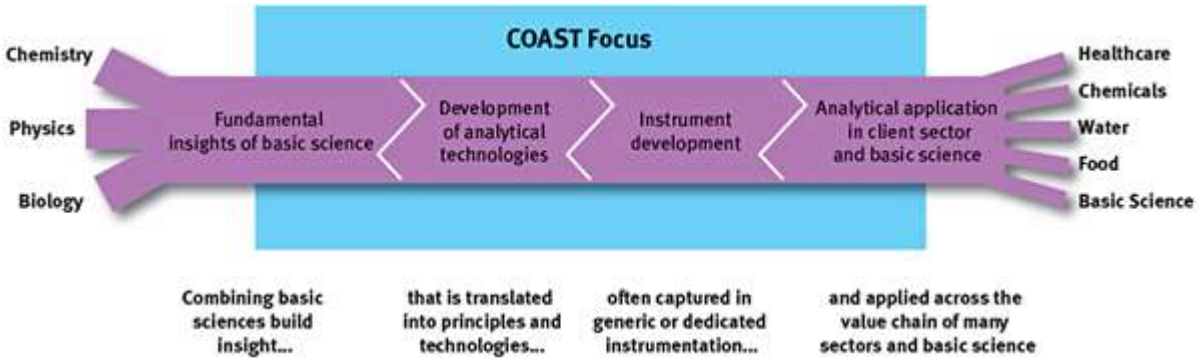
5.1.2. TI-COAST

HIMS houses the headquarters of TI-COAST, the Dutch public-private partnership in Comprehensive Analytical Science and Technology (hence the abbreviation).

COAST aims to advance Dutch excellence in its TOPsectoren by providing pivotal analytical knowledge and instruments based on fundamental science and by ensuring transfer of analytical expertise between application areas. COAST plans to achieve this by securing and improving Dutch expertise in analytical science and technologies.

COAST's mission is to strengthen analytical science in the Netherlands by uniting R&D, human capital and infrastructure:

- To advance R&D and innovation in analytical technologies and encourage cross-fertilization between analytical technologies and application areas (see also position photo with COAST focus);
- To improve education in analytical science and to increase the number of graduates;
- To provide access to research facilities and knowledge for players within and across application areas.



By putting these pieces together, COAST aims to promote analytical science as a valuable economic activity in its own right and as a catalyst for innovation and economic value in its application areas. COAST has tailored its Strategic Agenda to meet these challenges.

5.1.3. Co van Ledden Hulsebosch Center

On September 13th, 2013, the Co van Ledden Hulsebosch Center (CLHC), Amsterdam Center for Forensic Science and Medicine was officially opened. The CLHC is the result of a collaboration of the Faculty of Science, the Academic Medical Center (AMC) and the Netherlands Forensic Institute (NFI) in an effort to create a substantial forensic scientific program in Amsterdam and the Netherlands.

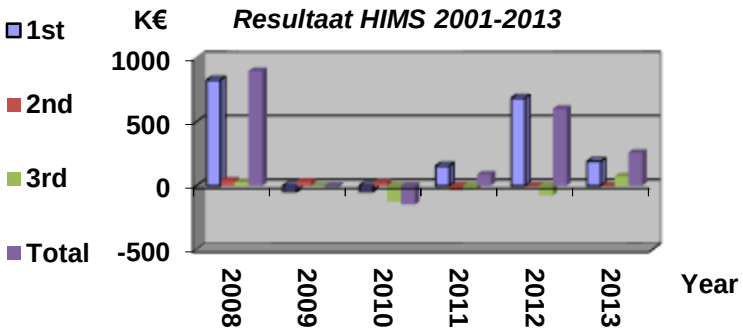
The CLHC is a virtual organization, the motto "*Big in Forensic Science, small in everything else*" is indicative of the aim to develop forensic science in the associated institutes through an organization that has almost no overhead or expenses. This is achieved by a very active in-kind participation from the institutes. The forensic expertise and focal point sits ideally with two CLHC coordinators that have been appointed by the director of the institute. The coordinators usually directly participate in forensic research and education in their field of expertise. All special chairs in forensic science at the UvA for instance also fulfill a CLHC coordinator role.

The main aim of the CLHC is to establish a broad and successful forensic science program in Amsterdam, a program that will gain international recognition and attract other academic partners in the Netherlands and abroad. This program is accomplished through a matrix approach in which the center acts as an incubator and communicator. The center organizes brain storm sessions to bring forensic experts and scientists together, tries to create external funding opportunities for forensic scientific research and provides an overview of all forensic activities. The matrix approach allows the University of Amsterdam to develop a very broad and substantial forensic science program that is based on the scientific expertise in the various institutes including medical, biological, physical and chemical sciences, mathematics, statistics, informatics and data science. By expanding the connections within the UvA to include the social and legal sciences the research portfolio could even be expanded further. The overall forensic science program and its results are actively communicated by the CLHC both internally and externally to build the forensic network and provide an overview of the overall effort. Hence this year report contains a detailed overview of all achievements in forensic science from the various associated institutes and research teams.

5.2 HIMS finances

In 2013 the financial position of HIMS has stabilized. In 2013 the structural university budgets (1st moneystream/ 1e geldstroom) for HIMS were reduced with 6% (366k€). Though the result remains positive.

HIMS results 2007 – 2013 (all funding sources; k€)[1]



Funding sources
1st: University (direct) funding and NRSCC Catalysis
2nd: NWO, ERC, FOM and STW
3rd: EU, EL&I and Industrial

The total budget for 2013 was 14.949 k€ (165k€ higher than in 2012) and the total costs were 14.691 k€ (see table below). The integral result obtained in 2013 (+258 k€, all funding sources) is substantial lower (-813 k€) than obtained in 2012. Actual financial numbers of 2013 (and 2012 for comparison) are given in the tables below[2].

HIMS resources and results 2013

2013	1st	1st other	1st total	2nd	3rd	total
Total benefits/budget	**4.361**	**1.234**	**5.595**	**4.734**	**4.620**	**14.949**
Personnel costs	-2.594	-894	-3.488	-1.662	-1.496	**-6.646**
Other costs	-1.711	-206	-1.917	-3.075	-3.053	**-8.045**
Total costs	**-4.305**	**-1.100**	**-5.405**	**-4.737**	**-4.549**	**-14.691**
Result 2013	**56**	**134**	**190**	**-3**	**71**	**258**
Reservation Sector Plan		466	466			**466**
Result excluding reservation	**56**	**-332**	**-276**	**-3**	**71**	**-208**

HIMS resources and results 2012

2012	1st	1st other	1st total	2nd	3rd	total
Total benefits/budget	**4.876**	**1.085**	**5.961**	**4.769**	**4.054**	**14.784**
Personnel costs	-2.791	-440	-3.231	-1.567	-1.554	**-6.352**
Other costs	-1.311	-262	-1.573	-3.210	-2.576	**-7.361**
Total costs	**-4.103**	**-703**	**-4.804**	**-4.777**	**-4.130**	**-13.713**
Result 2012	**773**	**382**	**1.157**	**-8**	**-76**	**1.071**
Reservation Sector Plan		470	470			**470**
Result including reservations	**773**	**-88**	**685**	**-8**	**-76**	**601**

[1] Results excluding (restitution of) reservations
[2] For more details see section 6.3

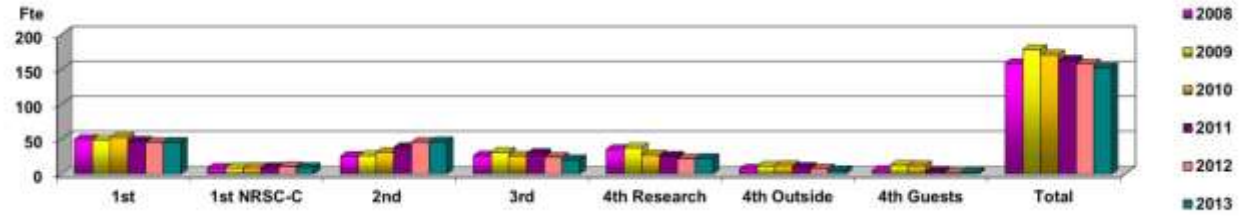
In comparison to 2012 the university budget (1st moneystream without others) for 2013 was 515 k€ lower. The 2nd moneystream reduced 35 k€ while the 3rd moneystream increased with 566 k€.

The costs in the 1st moneystream increased with 202k€, when compared to 2012. The total personal costs were reduced with 197 k€. In 2013 664 k€ of the personal costs could be transferred from the 1st to the 2nd and 3rd moneystream (to projects), since 4,7 fte of the HIMS co-workers in fixed positions (3,6 fte staff, 1,1 fte technicians) were financed by external projects. There was also a vacancy for a technician. The other costs increased with a 400k€ . There were unexpected costs for use of server facilities (60k€) , for financing of Sustainable Plastics (75k€) and for financing on investments for NMR-equipment (Zwaartepunt Sustainable Chemistry).

The budgets for projects in the 2nd moneystream and also the costs in the 2nd moneystream stayed on an equal level. The budgets for projects in the 3rd moneystream increased with 566 k€.

With a total of 6,45 M€ in external funding (excluding the own matching budget of approximately 2,6 M€) the year 2013 was more successful than the year 2012 (3,18 M€). With a total of 6.45 M€ in external funding (excluding the own matching budget of approximately 2.6 M€) the year 2013 was very successful (average 2010-2012: 5.8 M€). These funds were acquired from funding agencies such as NWO (Chemical Sciences, *Vernieuwingsimpuls*, FOM, ZonMW), SmartMix CatchBio and ERC (one Advanced Grant), as well as from industry and other partners.

The graph below shows the **personnel development of HIMS** for the years 2007-2012 per funding source.



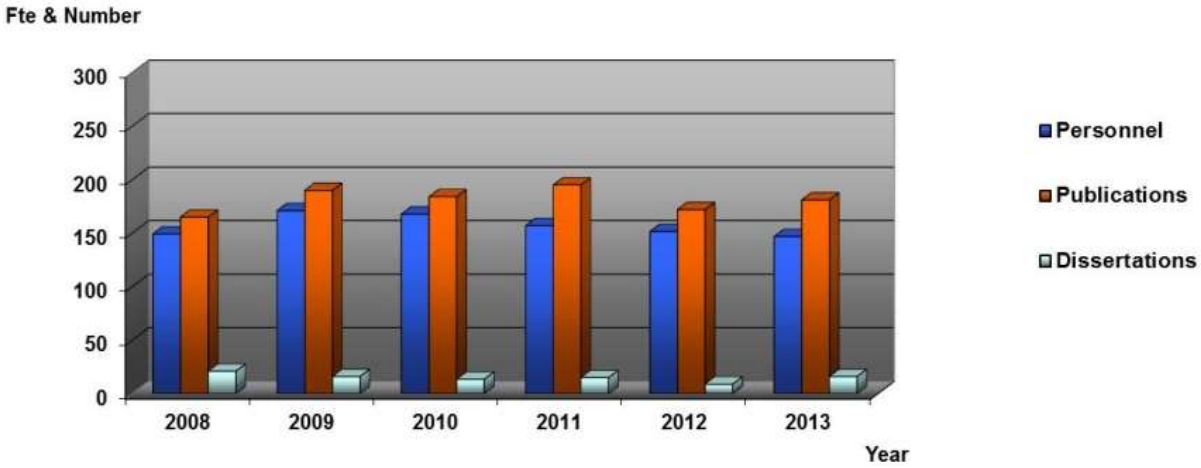
The personnel numbers in the graph are based on full-fte input

1st Direct funding (eerstegeldstroom; university/direct funding)
1st NRSC-C (Top Research School Catalysis)
2nd Research grants (tweedegeldstroom; NWO-CW, ERC, FOM, STW, KNAW)
3rd Contract research (derdegeldstroom; EU, DPI, AGENTSCHAP.NL, FES/NanoNed, NFI, Industrial)
4th Other (vierdegeldstroom; guest PhD students & guest researchers employed elsewhere, PhD students with finished contracts/not yet graduated)

Externally financed projects (inclusive NRSCC) count for ~63% of our personnel costs in 2013 (in 2012: ~70%).

HIMS personnel input data for 2011-2013 are ~15 fte lower than for 2008-2010, mainly caused by a reduced amount of projects in the last years. Additionally in the years 2011-2013 a negative influence on fte's (small decrease in research staff numbers) can be found in the change in guest administration of our guest PhD students (PhD students with projects finished, but PhD defences still to come). In former years the PhD guest students were full-time appointed for the duration of their guest appointment after finishing their contracts. Presently they are administrated part-time when still present at HIMS (mostly 0.1 fte) or even 0.0 fte, when finishing their thesis elsewhere. This is because of restricted working places at HIMS and cost limitations.

Research input [1] (fte) and output (number of publications and dissertations) 2008-2013



[1] Professors, Associate Professors (UHD's), Assistant Professors (UD's), Post-docs, PhD researchers and Research Technicians; management and supporting staff not included. The personnel numbers shown in the graph are based on full-fte input

In the year 2012 there were less publications and dissertations than the years before. In 2013 the number of dissertations and publications slightly increased.

6. Facts and figures

6.1 Personnel

In the following table the research input of the HIMS staff members is presented as full time equivalents (fte) per employment type. Since these numbers exclude education activities the total does not amount to the total amount of HIMS employees.

Research- and supporting staff 2013 of the HIMS themes, per employment type (fte)[a]

	SC	COMP	ACF	MOLP	Other	**Total**
Tenured staff	5,0	3,0	1,5	2,5	0,5	12,5
Non-tenured staff	13,4	3,5	2,4	3,3	1,8	24,4
PhD candidates	20,6	9,8	9,8	14,0	2,3	56,4
Total research staff	**38,9**	**16,3**	**13,7**	**19,7**	**4,6**	**93,3**
Technicians [b]	13,1	0,0	2,5	3,3	0,0	18,9
Visiting fellows [c]	0,1	0,0	0,2	0,1	0,0	0,4
Total research	**52,1**	**16,3**	**16,4**	**23,1**	**4,6**	**112,5**
Supporting staff					5,5	5,5
Total staff	**52,1**	**16,3**	**16,4**	**23,1**	**10,1**	**118,0**

Research themes: SC = Sustainable Chemistry; COMP = Computational Chemistry; ACF = Analytical Chemistry (including its application in Forensic Science); MOLP = Molecular Photonics; Other includes: PS = Polymer Systems and RD = Röntgen Diffraction (discontinued 2011)

Research- and supporting staff 2013 of HIMS and the HIMS groups, per employment type (fte)[a]

	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	Other	**Total**
Tenured staff	1,5	0,0	1,5	0,5	1,5	2,0	1,0	1,5	1,5	1,0	0,5	12,5
Non-tenured staff	0,0	0,9	7,3	0,0	5,2	2,7	0,8	2,4	3,1	0,2	1,8	23,6
PhD candidates	2,4	0,1	14,6	2,1	1,5	6,8	3,0	9,8	10,4	3,6	2,3	59,0
Total research staff	**3,9**	**1,0**	**23,4**	**2,6**	**8,2**	**11,5**	**4,9**	**13,7**	**14,9**	**4,8**	**4,6**	**95,8**
Technicians [b]	3,2	0,8	4,8	2,0	2,4	0,0	0,0	2,5	2,2	1,1	0,0	19,4
Visiting fellows [c]	0,1	0,0	0,0	0,0	0,0	0,0	0,0	0,2	0,1	0,0	0,0	0,4
Total research	**7,2**	**1,7**	**28,1**	**4,6**	**10,5**	**11,5**	**4,9**	**16,4**	**17,2**	**5,9**	**4,6**	**115,6**
Supporting staff											5,5	5,5
Total staff	**7,2**	**1,7**	**28,1**	**4,6**	**10,5**	**11,5**	**4,9**	**16,4**	**17,2**	**5,9**	**10,1**	**118,0**

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Other: groups Iedema and Peschar (discontinued 2011)

[a] Note that the table shows the net time available for research only. The numbers are based on an input of 0.5 fte (full-time equivalent) per fte tenured staff and visiting fellows[c], 0.9 fte per fte non-tenured staff (visiting researchers, postdocs) and 0.75 fte per fte PhD student and 1.0 fte for technicians, supporting staff; not all appointments are full-time.

[b] Various technicians contribute to teaching, however their research input is represented as 1.0 fte..

[c] Endowed and visiting professors.

6.2 Research

6.2.1. Research input of the HIMS themes

Research- and supporting staff 2013 of HIMS per funding type (fte)[a]

HIMS themes	SC	COMP	ACF	MOLP	Other	**Total research**	***%***	Supp. staff	**Total staff**	***%***
Direct funding[1a]	16,9	3,0	3,2	6,4	0,5	**30,0**	***27***	4,1	34,1	***29***
Indirect funding [1b]	7,6	0,0	0,0	0,0	0,0	**7,6**	***7***	0,0	7,6	***6***
Direct[1a] + indirect[1b]	**24,5**	**3,0**	**3,2**	**6,4**	**0,5**	**37,6**	**34**	**4,1**	**41,7**	***35***
Research grants[2]	13,2	9,6	4,9	5,3	2,6	**35,6**	***32***	0,0	35,6	***30***
Contract research[3]	7,1	0,9	4,4	1,2	1,5	**15,1**	***13***	1,5	16,6	***14***
Other[4]	7,3	2,9	3,9	10,2	0,0	**24,3**	***21***	0,0	24,3	***21***
Total	**52,1**	**16,4**	**16,4**	**23,1**	**4,6**	**112,6**	***100***	**5,6**	**118,2**	***100***

SC = Sustainable Chemistry; COMP = Computational Chemistry; ACF = Analytical Chemistry (including its application in Forensic Science);
MOLP = Molecular Photonics; Other includes: PS = Polymer Systems

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	**Other**	**Total research**	Supp staff	**Total staff**	**%**
Direct funding[1a]	3,8	0,8	6,9	2,5	2,9	1,6	1,4	3,2	4,3	2,2	0,5	**30,1**	4,1	**34,1**	***29***
Indirect funding[1b]	1,4	0,1	3,7	1,5	0,9	0,0	0,0	0,0	0,0	0,0	0,0	**7,6**	0,0	**7,6**	***6***
Direct[1a] + indirect[1b]	**5,2**	**0,9**	**10,6**	**4,0**	**3,8**	**1,6**	**1,4**	**3,2**	**4,3**	**2,2**	**0,5**	**37,7**	**4,1**	**41,7**	***35***
Research grants[2]	0,8	0,0	12,2	0,0	0,2	8,2	1,4	4,9	3,0	2,3	2,6	**35,6**	0,0	**35,6**	***30***
Contract research[3]	0,0	0,0	3,0	0,6	3,6	0,8	0,1	4,4	1,2	0,0	1,5	**15,2**	1,4	**16,6**	***14***
Other[4]	1,2	0,9	2,3	0,0	2,9	0,9	2,0	3,9	8,7	1,4	0,0	**24,2**	0,0	**24,2**	***21***
Total	**7,2**	**1,8**	**28,1**	**4,6**	**10,5**	**11,5**	**4,9**	**16,4**	**17,2**	**5,9**	**4,6**	**112,7**	**5,5**	**118,2**	***100***

HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; PB = group Bolhuis;
PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Other: group Iedema

[1a] Direct funding (eerstegeldstroom; university/direct funding)
[1b] Indirect funding (eerstegeldstroom; university/indirect funding, NRSC-C/Top Research School Catalysis)
[2] Research grants (tweedegeldstroom; NWO-CW, FOM, STW, KNAW, ERC)
[3] Contract research (derdegeldstroom; EU, DPI, AGENTSCHAP.NL, EL&I/NanoNext, NFI, Industrial)
[4] Other (vierdegeldstroom; guest PhD students & guest researchers employed elsewhere, PhD students with finished contracts/not yet graduated, etc.)
[a] Note that the table shows the net time available for research (source METIS). The numbers are based on an input of 0.5 fte (full-time equivalent) per fte tenured staff and visiting fellows, 0.9 fte per fte non-tenured staff (visiting researchers, postdocs) and 0.75 fte per fte PhD student and 1.0 fte for technicians; not all appointments are full-time.

Externally financed projects acquired in 2013 (mln €) per funding type[1]

HIMS themes	SC	COMP	MB	MOLP	Other	**Total[6]**
1st - NRSC-C [2]	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [3]	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [4]	0.81	0.10	0.46	1.26	0.05	**2.68**
3rd [5]	3.73	0.00	0.05	0.00	0.00	**3.78**
Total	**4.54**	**0.10**	**0.51**	**1.26**	**0.05**	**6.45**

SC = Sustainable Chemistry; COMP = Computational Chemistry; MBA= Macromolecular and Bio-systems Analysis;
MOLP = Molecular Photonics; Other includes: PS = Polymer Systems

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	PI	Total[6]
1st - NRSC-C [2]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [3]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [4]	0.48	0.03	0.30	0.00	0.00	0.10	0.00	0.46	1.26	0.00	0.05	**2.68**
3rd [5]	0.00	0.00	3.26	0.19	0.28	0.00	0.00	0.05	0.00	0.00	0.00	**3.78**
Total	**0.48**	**0.03**	**3.56**	**0.19**	**0.28**	**0.10**	**0.00**	**0.51**	**1.26**	**0.00**	**0.05**	**6.45**

HH = group Hiemstra; RW = group Wever; JR = group Reek(including De Bruin); CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; PI: group Iedema

[1] Matching contributions UvA/FNWI (total 2,6 mln € foreseen) excluded; own contributions HIMS (in kind and cash/from reserves) included
[2] NRSC-C (TOP Research School Catalysis);
[3] COF, CvB (Funds from University Board);
[4] NWO-CW, FOM, STW, KNAW, ERC
[5] EU, DPI, AGENTSCHAP.NL, NanoNext, NFI, Industry
[6] Rounding difference 0,01.

6.2.2. Research output of the HIMS themes

Research output 2013 per type of publication

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint[1]	Total
Refereed articles	64	34	15	46	6	-8	**168**
Non-refereed articles	0	0	0	0	0		**0**
Books	0	0	0	0	0		**0**
Book chapters	5	0	1	0	0		**6**
PhD-theses	6	3	3	4	0		**16**
Conference papers	2	2	0	0	0		**4**
Patents	3	0	0	0	0		**3**
Professional publications	4	0	3	1	0		**8**
Publications general public	0	0	0	0	0		**0**
Other research output	0	0	0	0	0		**0**
Total	**84**	**39**	**22**	**51**	**6**	**-8**	**205**

SC = Sustainable Chemistry; COMP = Computational Chemistry; ACF = Analytical Chemistry (including its application in Forensic Science); MOLP = Molecular Photonics; Other includes: PS = Polymer Systems

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	PI	Joint[1]	Total
Refereed articles	3	4	39	4	12	5	13	12	9	15	41	5	6	-8	168
Non-ref. articles	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Books	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Book chapters	1	2	0	0	0	2	0	0	0	1	0	0	0		**6**
PhD-theses	1	1	3	0	1	0	1	2	0	3	3	1	0		**16**
Conference papers	0	0	0	0	2	0	1	1	0	0	0	0	0		**4**
Patents	0	0	3	0	0	0	0	0	0	0	0	0	0		**3**
Prof. publications	0	0	3	0	1	0	0	0	0	3	1	0	0		**8**
Publ. general public	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Other output	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Total	**5**	**7**	**48**	**4**	**16**	**7**	**15**	**15**	**9**	**22**	**45**	**6**	**6**	**-8**	**205**

HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; AK = group Kleijn; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; PI: group Iedema

[1] Number of joint results obtained from collaborations between different research groups

Number of refereed articles 2013, in ranges of different impact factor

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint[1]	**Total**
>15	2	1	0	1	0		**4**
10-15	8	1	0	0	0		**9**
5-10	18	6	0	3	1	-3	**28**
<5	35	27	16	39	10	-5	**127**
Total	**63**	**35**	**16**	**43**	**11**	-8	**168**

SC = Sustainable Chemistry; COMP = Computational Chemistry; ACF = Analytical Chemistry (including its application in Forensic Science); MOLP = Molecular Photonics; Other includes: PS = Polymer Systems: PS = Polymer Systems/Art Sciences

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	PI	Joint[1]	**Total**
>15	0	0	2	0	0	0	0	0	1	0	1	0	0		**4**
10-15	0	0	6	0	2	0	0	1	0	0	0	0	0		**9**
5-10	1	0	12	1	4	1	2	2	2	0	3	0	0	-3	**28**
<5	2	4	19	3	7	4	12	9	6	16	34	5	6	-5	**127**
Total	**3**	**4**	**39**	**4**	**13**	**5**	**14**	**12**	**9**	**16**	**38**	**5**	**6**	**-8**	**168**

HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; AK = group Kleijn; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB=group Brouwer; PI= group Iedema

[1] Number of joint results obtained from collaborations between different research groups

6.2.3. Efficiency of the doctoral research path

The following tables show the efficiency of the doctoral research path (period of appointment 2005-2009; planned PhD defense 2009-2013).

Employed PhD-candidates

Enrolment (-)				**Success rates of graduation**							
Starting Year	**Enrolment**		**Total (M+F)**	**< 4 years**	**4 - 5 years**	**5 - 6 years**	**6 -7 years**	**>7 years**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
	M	**F**									
2005	7	3	**10**	1	3	1	1	0	0	1	3
2006	12	4	**16**	1	7	4	1	0	0	3	0
2007	2	6	**8**	0	2	1	0	-	0	5	1
2008	4	9	**13**	0	6	3	-	-	0	3	2
2009	4	7	**11**	0	3	-	-	-	0	7	1
Total	**29**	**29**	**58**	**2**	**21**	**9**	**2**	0	0	**19**	**7**
Cumulative 2005-2009											
SC	20	11	**31**	2	14	3	1	0	0	7	4
COMP	3	6	**9**	0	2	2	0	0	0	5	0
ACF	1	8	**9**	0	1	1	1	-	0	5	3
MOLP	4	4	**8**	0	4	3	-	-	0	1	0
Other	1	0	**1**	0	0	-	-	-	0	1	0
Total	**29**	**29**	**58**	**2**	**21**	**9**	**2**	**0**	**0**	**19**	**7**
%	***50***	***50***	***100***	***3***	***36***	***16***	***3***	***0***	***0***	***33***	***12***

Non-employed PhD-candidates

Enrolment (-)				Success rates of graduation							
Starting Year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	4	1	**5**	0	5	0	0	0	0	0	0
2006	2	1	**3**	2	1	0	0	0	0	0	0
2007	7	1	**8**	4	1	0	1	-	1	1	0
2008	5	1	**6**	0	2	0	-	-	1	3	0
2009	5	0	**5**	0	1	-	-	-	0	3	1
Total	**23**	**4**	**27**	**6**	**10**	**0**	**1**	**0**	**2**	**7**	**1**
Cumulative 2005-2009											
SC	2	0	**2**	0	0	0	0	0	0	2	0
COMP	1	1	**2**	0	2	0	0	0	0	0	0
ACF	8	2	**10**	4	2	0	1	-	0	2	1
MOLP	12	1	**13**	2	6	0	-	-	2	3	0
Other	0	0	**0**	0	0	-	-	-	0	0	0
Total	**23**	**4**	**27**	**6**	**10**	**0**	**1**	**0**	**2**	**7**	**1**
%	***85***	***22***	***100***	***22***	***37***	***0***	***4***	***0***	***7***	***26***	***4***

M = male; F = Female Research themes: SC = Sustainable Chemistry; COMP = Computational Chemistry;
ACF = Analytical Chemistry (including its application in Forensic Science); MOLP = Molecular Photonics; Other = group Iedema

As can be seen from the tables, a number of PhD students have not received their doctor title within 6 years. Several delays are directly related to the reorganization of the chemistry department in 2002-2004 and the subsequent leave of PhD supervisors. Several PhD students completed their PhD for the same reason outside the UvA. In 2013 3 PhD's with starting years 2001 (2) and 2003 (1) completed their PhD. Other delays are related to personal circumstances, often a job and/or a family with children, health problems were reasons.
Most PhD students who discontinued their doctoral research did so in their first year and changed their career on their own initiative. In a few cases the 4-year PhD project was completed but the PhD student decided not to defend a PhD thesis. Again, reasons were a combination of a job and/or a family with children.

Employed and Non-employed PhD-candidates

Sustainable Chemistry (SC)

Enrolment (-)				Success rates of graduation							
Starting year	Enrollment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	7	1	**8**	1	3	1	1	1	0	1	1
2006	7	1	**8**	1	4	2	0	0	0	1	0
2007	0	1	**1**	0	0	0	0	-	0	1	0
2008	3	4	**7**	0	4	0	-	-	0	1	2
2009	5	4	**9**	0	3	-	-	-	0	5	1
Total	**22**	**11**	**33**	**2**	**14**	**3**	**1**	0	**0**	**9**	**4**
%	***67***	***33***	***100***	***6***	***42***	***9***	***3***	***0***	***0***	***27***	***12***

Computational Chemistry (COMP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	1	1	**2**	0	2	0	0	0	0	0	0
2006	1	1	**2**	0	0	1	0	0	0	1	0
2007	1	1	**2**	0	1	0	0	-	0	1	0
2008	1	2	**3**	0	1	1	-	-	0	1	0
2009	0	2	**3**	0	0	-	-	-	0	2	0
Total	**4**	**7**	**11**	**0**	**4**	**2**	**0**	**0**	**0**	**5**	**0**
%	***36***	***64***	***100***	***0***	***36***	***18***	***0***	***0***	***0***	***45***	***0***

Macromolecular and Bio-systems Analysis (including its application in Forensic Science) (MBA)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	2	2	**4**	0	2	0	0	0	0	0	2
2006	2	1	**3**	2	0	0	1	0	0	0	0
2007	3	5	**8**	2	0	1	1	-	0	4	1
2008	1	1	**2**	0	1	0	-	-	0	2	0
2009	1	1	**2**	0	0	-	-	-	0	1	1
Total	**9**	**10**	**19**	**4**	**3**	**1**	**2**	**0**	**0**	**7**	**4**
%	***47***	***53***	***100***	***21***	***16***	***5***	***11***	***0***	***0***	***37***	***21***

Molecular Photonics (MOLP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	1	0	**1**	0	1	0	0	0	0	0	0
2006	3	2	**5**	0	4	1	0	0	0	0	0
2007	5	0	**5**	2	2	0	0	-	1	0	0
2008	4	3	**7**	20	2	2	-	-	1	2	0
2009	3	0	**3**	0	1	-	-	-	0	2	0
Total	**16**	**5**	**21**	**2**	**10**	**3**	**0**	**0**	**2**	**4**	**0**
%	***76***	***24***	***100***	***10***	***48***	***14***	***0***	***0***	***10***	***19***	***0***

Others (group Iedema)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	0	0	**0**	0	0	0	0	0	0	0	0
2006	1	0	**1**	0	0	0	0	0	0	1	0
2007	0	0	**0**	0	0	0	0	-	0	0	0
2008	0	0	**0**	0	0	0	-	-	0	0	0
2009	0	0	**0**	0	0	-	-	-	0	0	0
Total	**1**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**
%	***100***	***0***	***100***	***0***	***0***	***0***	***0***	***0***	***0***	***100***	***0***

Total HIMS

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2005	11	4	**15**	1	8	1	1	0	0	1	3
2006	14	5	**19**	3	8	4	1	0	0	3	0
2007	9	7	**16**	4	3	1	1	-	1	6	1
2008	9	10	**19**	0	8	3	-	-	1	6	2
2009	9	7	**16**	0	4	-	-	-	0	10	2
Total	**52**	**33**	**85**	**8**	**31**	**9**	**3**	**0**	**2**	**26**	**8**
%	61	39	**100**	9	35	11	4	0	2	30	9
Cumulative 2005-2009											
SC	22	11	**33**	2	14	3	1	0	0	9	4
COMP	4	7	**11**	0	4	2	0	0	0	5	0
ACF	9	10	**19**	4	3	1	2	0	0	7	4
MOLP	16	5	**21**	2	10	3	0	0	2	4	0
Other	1	0	**1**	0	0	0	0	0	0	1	0
Total	**52**	**33**	**85**	**8**	**31**	**9**	**3**	**0**	**2**	**26**	**8**
%	***61***	***39***	***100***	***9***	***36***	***11***	***4***	***0***	***2***	***31***	***9***

M = male; F = Female

6.3 Finance 2013

The table below shows the HIMS financial result 2013.

HIMS result 2013 (k€)

	1st (1 structural	1st (2 Other	1st total	2nd (3	3rd (4	Total
HIMS						
Budget (fixed)	4.033		4.033			**4.033**
Budget (variable[5])	4.240	1.234	5.474	2.314	3.128	**10.916**
Other income			0			**0**
Matching contract research	-3.912		-3.912	2.418	1.494	**0**
Budget total	**4.361**	**1.234**	**5.595**	**4.732**	**4.622**	**14.949**
Percentage	**29**	**8**	**37**	***32***	**31**	***100***
Personal costs	-2.594	-894	-3.488	-1.662	-1.496	**-6.646**
Other costs (projects)	-1.389	-206	-1.595	-3.075	-3.053	**-7.723**
Overhead (central)			0	-72	-86	**-158**
Overhead (faculty)	-310	-89	-399	-602	-413	**-1.414**
Overhead (institute)	797	139	936	942	655	**2.533**
Various costs			0			**0**
Other (secundary) costs	-809	-50	-859	-268	-156	**-1.283**
Costs total	**-4.305**	**-1.100**	**-5.405**	**-4.737**	**-4.549**	**-14.691**
Percentage	***29***	**7**	***37***	***32***	***31***	***100***
Result 2013	**56**	**134**	**190**	**-5**	**-73**	**258**
Reservation Sectorplan appointments			466			466
Result excluding reservation	**56**	**134**	**-276**	**-5**	**-73**	**-208**

[1] Direct funding (1st, eerstegeldstroom; university/direct funding,
[2] NRSC-C/Top Research School Catalysis)
[3] Research grants (2nd, tweedegeldstroom; NWO-CW, FOM, STW, KNAW, ERC)
[4] Contract research (3rd, derdegeldstroom; EU, DPI, AGENTSCHAP.NL, FES/NanoNed, Industrial)
[5] 1e gs assigned via allocation model

The HIMS result for 2013 amounts to + 258 k€. This result includes a reservation of 466 k€ budget for appointments in the framework of the Sectorplan Natuur- en Scheikunde. It is a reservation for costs to be made in the coming years.