Annual Report 2011

Van ‘t Hoff Institute for Molecular Sciences

University of Amsterdam

Preface

2011 was a very successful year for HIMS. The quality of our research was evaluated in 2010 (assessment published early 2011) and found to be of very good to excellent quality. In fact, the numerical scores were a bit above the national high level. Also the move from the downtown campus to the Science Park was finalized.
Evert-Jan Meijer was appointed professor of Molecular Simulations, finally bringing the computational chemistry groups up to full strength again.
Stefania Grecea and Jocelyne Vreede were appointed to assistant professor (UD) on a tenured position making the gender balance of the HIMS scientific staff a little less unfavourable.
The scientific output of the Institute remained at a very high level and 15 PhD-students successfully defended their thesis.
Also financially the year was successful, ending with a positive balance and with a number of new grants that is greater than ever before.
All of this makes us confident for the future that is as such far from clear. Budget reductions are discussed at the national level and special major research grants will be very much restricted. The government wants a much bigger participation by industry in research. The latter point is being addressed at HIMS at the moment and future public private partnerships are being developed. 2012 will be as exciting as 2011!

Prof. dr. Aart W. Kleijn

Prof. dr. Aart W. Kleijn

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Dr. Bas de Bruin (Homogeneous and Supramolecular Catalysis) and Dr. Jan van Maarseveen (Synthetic Organic Chemistry) presented NEMO lectures.

April 2011

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1 General considerations

The year 2011 was a very successful year for HIMS. A total of 8,70 M€[1] external funds (5,01 M€ in 2010) were acquired from subsidiaries such as NWO (1 Vici, 1 ERC, 1 Veni, 2 ECHO grants and special grants for Forensic - and Art Sciences projects), EU, NRSC-C, NanoNext (FES), Towards Biosolar (FES), COAST, etc. The output of HIMS was on a high level in 2011, although a little bit below the (top) level of 2010. HIMS published 1 paper (7 in 2010) in absolute top journals (impact factor > 15) and 8 papers (11 in 2010) in top journals (impact factor 10-15). The total number of refereed and other professional publications, patents and book(chapters) amounted to 195 (184 in 2010). HIMS filed 5 patents (3 in 2010), while 15 PhD dissertations (14 in 2010) were produced.

The work of the HIMS research groups raised national and international publicity, including publications in various newspapers and on various websites. HIMS highlights, awards and other measures of esteem with a high scientific and societal value, obtained in 2011, we are proud of are described below.

Institutional highlights

The quality of chemistry research at the University of Amsterdam (UvA) is of very good quality. These were the findings of an international review committee of twenty experts that examined the research achievements of seven Dutch universities in the field of chemistry. The assessment, published early 2011, was made on the basis of four criteria: quality, productivity, relevance (social, economic and cultural), and vitality & feasibility (the ability to adequately respond to significant changes in the environment and the future). Five HIMS research programmes were evaluated: Bio-Molecular Synthesis, Catalysis, Computational Chemistry, Macromolecular and Biosystems Analysis, and Molecular Photonics. The review committee adjudged the quality of the research groups of HIMS to be of very good to excellent quality, deeply rooted and respected in local and national networks, as well as being recognized internationally. It was also positively recognized that HIMS scientific results appear almost on a regular basis in high impact journals. The average rating for each criterion was 4.35 (4 = very good) and the citation score CPP/FCSm[2] was 1,81 (well above the international average).

The international review panel felt the interaction between different research groups of the Institute could be strengthened. However, the relocation of the HIMS to the Science Park Amsterdam, where all science disciplines have been located under one roof since last year, will help rectify this minor issue.

Following the recommendation by the international review panel, we strongly intend to strengthen our collaboration with the VU by focusing on 4 themes. As also recommended, we will enhance the visibility of molecular photonics by maintaining it as a separate programme. This leads to the following four themes and their embedding in the UvA-VU[3] and international landscape:

Sustainable chemistry, consisting of synthesis and catalysis. This is mainly an UvA activity, part of which may be transferred to a new research Institute at the UvA. A new chair on biocatalysis, funded by the Sectorplan, will be part of the theme.

Analytical Chemistry (including its applications in Forensic Science). This will be carried out in synergy with the VU and the national center COAST, which is established at HIMS. A new chair on supramolecular separations, funded by the Sectorplan, will be part of theme.

Molecular Photonics. This activity will be carried out together with the VU and AMC as part of Laser Lab Amsterdam.

Computational Chemistry. This activity will be carried out together with the VU and FOM-AMOLF as part of the Amsterdam Center for Multiscale Modelling (ACMM).

Besides these four themes there are small activities in themes 2 and 4 in the interdisciplinary areas of Forensic Sciences and Art Sciences, which are driven by activities at the UvA outside HIMS.

[1] Own matching budgets (3.82 M€ to be expected) excluded

[2] CPP/FCSm: impact of all articles, compared to the world citation average (CPP/FCSm=1.00) in the (sub) fields in which the institute is active.

[3] Our plan to join forces with the VU in the chemical area fits in the plans of the University of Amsterdam (UvA) and VU University Amsterdam to explore the benefits of a possible inter-institutional alliance. With both institutions sharing an ambition to further secure their international reputations as leading classic, comprehensive research universities, as well as an aim to make a quality leap in teaching and research so as to rank among the top universities in Europe and around world, such an alliance seems a logical step.

Dr Evert Jan Meijer has been appointed Professor of Molecular Simulations at the Faculty of Science of the University of Amsterdam (UvA). Evert Jan Meijer will focus on developing and applying computational methods that give insight into chemical, physical and biological processes on a molecular basis. A major research theme is the role of a complex fluctuating environment in (bio-) chemical processes. Research topics in this area of interest include the influence of a solvent in chemical processes, the mobility of electrical charges in liquids such as water, and (photo) chemically active proteins. A second major research theme focuses on the structure, stability and formation of materials, especially nanostructured materials such as carbon nanotubes and zeolites.

Dr Evert Jan Meijer

Dr. Stefania Grecea

In 2011 both Jocelyne Vreede (Computational Chemistry) and Stefania Grecea (Heterogeneous Catalysis and Sustainable Chemistry) were appointed Assistant Professor (UD). HIMS welcomes this increase in the number of female staff members.

Dr. Jocelyne Vreede

On 11 March a farewell symposium was held for Rob Zsom, marking his departure as director of the institute. The symposium was attended by current and former employees, friends and guests from the Dutch chemical research community. HIMS Institute's promising research portfolio in Chemistry, Chemical Analysis, Molecular intermezzi current and former HIMS performance as director of HIMS. The advice and management support to both

Dr. Rob Zsom

Group Leaders gave an overview of the the areas of Organic Synthesis, Computational Photonics and Catalysis. In more personal employees reflected on Rob Zsom's coming years Zsom will be engaged in policy HIMS and the Faculty of Science.

September was the official opening of the Institute Quantivision, a collaboration between the VUmc, AMC, NKI/AVL, VU, UvA and companies to develop medical imaging devices, software, and protocols to enhance the efficiency, efficacy and economy of healthcare. Molecular Photonics of HIMS is one of the participating teams, Wybren Jan Buma being one of the members of the Management Team.

The spin-off company, Yellow Diesel BV, of the group Rothenberg has finalised the lab development of a continuous process for manufacturing biodiesel by heterogeneous catalysis. The company is now seeking investment for scaling up the process to manufacturing scale.

InCatT B.V., which stands for Innovative Catalyst Technologies, a spin-off company of the homogeneous catalysis group Reek, has introduced new supramolecular strategies in transition metal catalysis. InCatT uses an evolutionary approach to find the best catalyst for industrial catalytic processes. Optimization of the best catalyst is done using a robot with 16 parallel reactors that records the gas-uptake curves providing the kinetic data that allows you to evaluate the catalyst performance and helps in the up-scaling of the reaction. InCatT also develops new technology and started to make new chemicals by using in-house developed technology.

Prizes and honors

Peter Schoenmakers (Analytical Chemistry; including its applications in Forensic Science) was awarded the 2011 Chromatographic Society Martin Medal. It is the highest honour the Society confers, awarded to scientists who have made outstanding contributions to the advancement of separation science. Schoenmakers received the Martin Medal during the HPLC2011 Symposium in Budapest (19-23 June).

Prof. Peter Schoenmakers

For research on a new biodegradable and recyclable synthetic resin professor Gadi Rothenberg was nominated for the Huibregtsenprijs 2011, awarded 7 november 2011 during the twelfth 'Avond van Wetenschap & Maatschappij' (Evening of Science&Society). Rothenberg was also interviewed on the radio program Wetenschap24.

Dr. Albert Alberts and Prof. Gadi Rothenberg at the Avond van Wetenschap & Maatschappij (photo credit: Frank van Driel)

Prof. Rothenberg was appointed to the Scientific Advisory Board of the new CNRS lab in Shanghai, funded jointly by Rhodia/Solvay, the CNRS, ENS-Lyon, and East China Normal University.

Hong Zhang of the Molecular Photonics group won the Amsterdam Science Park New Ideas Competition 2011 together with Maurice Aalders from the UvA university hospital AMC. The two researchers developed a catheter that is able to detect microbial infections at an early stage. Hong Zhang also presented his research in a short lecture *Luminescence upconversion nanoplatform* at the monthly faculty colloquium series (June 2011).

Jury president Louise Fresco presented the 'Nieuwe Ideeën Prijs 2011' to the winners Dr. Hong Zhang and Dr. Maurice Aalders

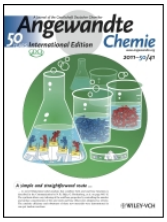
Jocelyne Vreede of the Computational Chemistry group was awarded the Best Publication Prize 2010 of the WiF (Women in the FNWI) Network. She received her award during the WiF Annual Meeting, held on March 17, 2011. Vreede received the prize for her 'breakthrough work published in a high-impact journal' on light-induced conformational changes in photoactive yellow protein.

Rosalba Bellini of the Homogenous and Supramolecular Catalysis group won a NRSC-C/NIOK award for best PhD lecture during the Twelfth Netherlands' Catalysis and Chemistry Conference.

The DPI first poster prize was granted to Nicole Franssen, also of the Homogenous and Supramolecular Catalysis group, for her poster of excellent quality.

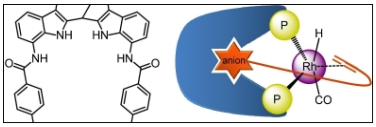
Sander Woutersen (Molecular Photonics) presented an invited lecture *"The operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy"* at Fysica 2011, a Symposium of the Nederlandse Natuurkundige Vereniging (NNV), celebrating the 90th anniversary of the NNV.

Noteworthy publications



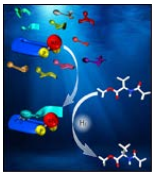
Raveendran Shiju and Gadi Rothenberg (Heterogeneous Catalysis and Sustainable Chemistry group) synthesized a robust solid catalyst that combines two antagonistic functions (acid and base) to catalyse one-pot tandem reactions. Their results, were published in the article *Silica with Site-Isolated Amine and Phosphotungstic Acid Groups: A Solid Catalyst with Tunable Antagonistic Functions for One-Pot Tandem Reactions* in Angewandte Chemie - International Edition.

Ana Célia Vila Verde and Peter Bolhuis (Computational Chemistry) contributed to a study published in Physical Review Letters *Ultrafast reorientation of dangling OH groups at the air-water interface using femtosecond vibrational spectroscopy,* which shows that molecules at the surface of a water mass rotate far faster than the water molecules within it.



The research of Pawel Dydio, a trainee research assistant in the Homogeneous and Supramolecular Catalysis group of Joost Reek, made it to the back cover of Angewandte Chemie International Edition. The publication *Remote Supramolecular Control of Catalyst Selectivity in the Hydroformylation of Alkenes* is also one of Angewandte's *hot papers* and was also highlighted in C2W.

Jos Oomens, who is professor at the Molecular Photonics group but also heads a research group at the FOM Institute for Plasma Physics Rijnhuizen, published the article *Spectroscopic Evidence for a Triplet Ground State in the Naphthyl Cation* in Angewandte Chemie International Edition on the structure and stability of the naphtyl carbocation.



The Homogeneous and Supramolecular Catalysis group of Joost Reek c.s. took a major step forward in the search for selective catalysts for the fine chemicals industry. The synthesis of a rhodium biphosphine complex with a carboxylate binding site was published in the article *Cofactor"-Controlled Enantioselective Catalysis* in the Journal of the American Chemical Society. The articles was also highlighted in C&E News and C2W.

The EurJOC microreview *CuI-Catalyzed Alkyne-Azide Cycloadditions from a Mechanistic and Synthetic Perspective* by Hiemstra and Van Maarseveen (Synthetic Organic Chemistry) has received 503 citations. This is by far the most-cited article of all articles published in 2006 in the subject category *'Chemistry, Organic'*, according to ISI Web of Science.

Hessel Castricum and Marjo Mittelmeijer-Hazeleger (Heterogeneous Catalysis and Sustainable Chemistry), in collaboration with colleagues from the University of Twente and the Energy Research Center of the Netherlands, developed a versatile membrane that is capable of separating gas and liquid mixtures in an energy-efficient manner. The research was published in the article *'Tailoring the Separation Behavior of Hybrid Membranes Organosilica by Adjusting the Structure of the Organic Bridging Group'* in Advanced Functional Materials.

Patents

A novel way to detect infections has been patented (patent 11166364.7-2204 "*Device and probe for detection of infection*" , Zhang/Molecular Photonics and Aalders/AMC).
Improvements on CLIPS-technology, P. Timmerman/Pepscan, L. E. M. Smeenk, N. Dailly, J. H. van Maarseveen/ Synthetic Organic Chemistry, EP 10188743.8, Filing date: 25 October 2011.
Functionalized Materials by Catalyzed Carbene Copolymerization; Jellema, E.; Jongerius, A.L.; Fransen, N.G.M.; de Bruin, B./Homogenous and Supramolecular Catalysis; WO 2011/157444 A1; PCT/EP2011/003016. International publication date: 22 December 2011.
Coordination Complex System Comprising a Second Building Block without Donor Moiety; Pawel Dydio, Joost NH Reek/Homogenous and Supramolecular Catalysis; EP11177920.3, Application date: 18 August 2011.
Calderone, V.R., Shiju, N.R., Rothenberg, G. & Curulla-Ferré, D. (). Core-shell particles with catalytic activity; EP11305657.6, Application date: 30 May 2011.
The ammoximation patent of Dr. Raveedran Shiju/Heterogeneous Catalysis and Sustainable Chemistry was sold to industry.

Public Outreach & Media Coverage

Dr. Bas de Bruin (Homogeneous and Supramolecular Catalysis) and Dr. Jan van Maarseveen (Synthetic Organic Chemistry) presented NEMO lectures with the titles *'Hoe maakt een spin een draad? (How does a spider make a thread?)'* and *'Waarom kunnen we niet zonder water? (Why do we need water?)'*, respectively, for audiences of young kids.

Dr. Bas de Bruin in NEMO

Dr. Jan van Maarseveen in NEMO

Professor Joost Reek (Homogeneous and Supramolecular Catalysis) was interviewed by the Dutch daily newspaper "De Pers" in an article *'De beste plant is nep'* on artificial leaves.

Prof. Joost Reek

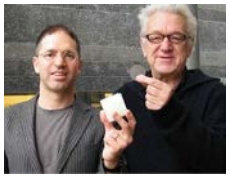
Joost Reek was interviewed (BNR-radio) on *'Bioinspired catalysis for green energy'*.

The article by Joost Reek and colleagues on *Cofactor-Controlled Enantioselective Catalysis* in the Journal of the American Chemical Society received media coverage both abroad (e.g. C&EN News, Chemistry World) and in the Netherlands (Chemisch2Weekblad/C2W).

David Dubbeldam of the Computational Chemistry group was portrayed in the 'Focus on Research' series, with which the University of Amsterdam brings its high profile research projects to the attention of the general public. David Dubbeldam performs computer calculations to decide what future metal-organic frameworks should look like. Metal-organic frameworks can be used to store gasses, such as carbon dioxide and hydrogen, but are also useful for purifying substances and catalysis.

Dr. David Dubbeldam

Gadi Rothenberg and Albert Alberts (Heterogeneous Catalysis and Sustainable Chemistry) received quite a lot of media coverage of their development of a new biodegradable and recyclable synthetic resin. It was featured in the national newspapers Trouw and Sp!ts. Rothenberg was a guest in the Hoe?Zo! popular science radio show.



Prof. Gadi Rothenberg and Dr. Albert Alberts

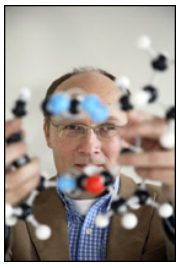
The Rothenberg group publication of an antagonistic catalyst in Angewandte Chemie was featured by the Dutch popular science website Kennislink and the chemistry biweekly C2W.

Cartoon representing the antagonistic characteristics of the new catalyst (Illustration: Itamar Daube)

HIMS scientific director professor Aart Kleijn and professor Gadi Rothenberg of the Heterogeneous Catalysis and Sustainable Chemistry group contributed to the 'State of Science' (Stand van de Wetenschap) series of the UvA Alumni Community. On 10 October 2011 they discussed for an interested - mostly non-expert audience - sustainable chemistry, catalysis, the relation between basic and applied research, knowledge transfer and innovation.

Teaching

The Chemistry Master teaching programme (many teachers come from HIMS) received the highest score according to the Guide of Higher Education (Keuzegids Hoger Onderwijs) 2011. This Guide is compiled annually by an independent editorial board of the Higher Education News Agency (Hoger Onderwijs Persbureau). The rankings of the Guide are based on the assessment of students and experts, contact hours with teachers and success rates. In the assessment were content, skills, pleasant staff, prepare for the career and good facilities major plus points.



Jan H. van Maarseveen (Synthetic Organic Chemistry) was awarded the Onderwijsbokaal of the ACD (best chemistry teacher 2010-2011). He was also the chairman of the UvA-VU committee that designed a new joint chemistry bachelor education program to begin in February 2012.

Dr. Jan van Maarseveen

Analytical Conference in Amsterdam

The SCM-5 (Separation and Characterization of Natural and Synthetic Macromolecules) conference took place in Amsterdam in early 2011, with Peter Schoenmakers (Chairman), Wim Kok (treasurer), and Petra Aarnoutse (secretary) carrying most of the organization. The conference attracted some 250 people.

Finances

Since 2006, the year of introduction of the new integral costs allocation model of the university board, the financial position of HIMS has much improved. HIMS finished the year 2011 with a positive financial result of +0.09 M€[4] (-0.15 M€ in 2010). This result is satisfactory, knowing that HIMS is confronted with a budget reduction of the structural university budgets (1e geldstroom) of 10% (1 M€) for the years 2009-2012.
Although the financial prospects of HIMS is influenced by the budget reductions to be realized in the years 2009-2012, increased revenues are expected from the realization of more PhD theses and the Sectorplan Natuurkunde & Scheikunde (SNS) in the coming years. Additional cost reductions were realized by some (early) retirements and by the discontinuation of the röntgen diffraction (RD) activities. Due to budgetary restrictions within the faculty, the RD activities of HIMS were ended at 31-12-2010 as a part of the HIMS cost reduction plan *Chemie Financieel Duurzaam.*

Grants

The year 2011 again turned out to be very successful in terms of external fund raising; a total of 8,70 M€ was acquired from important old and new subsidiaries. A selection of projects acquired in 2011.

Jarl Ivar van der Vlugt (Homogeneous and Supramolecular Catalysis) was awarded a (European Research Council) **ERC - Starting Grant**. He received 1.5 million euro for his research programme *'Smart Systems for Small Molecule Activation and Sustainable Homogeneous Catalysis'*

Dr. Jarl Ivar van der Vlugt

Dr. Bas de Bruin (Homogeneous and Supramolecular Catalysis) received a (1.5 M€) **NWO-CW VICI subsidy** for his research programme *'Investigation of new controlled (catalytic) radical-type transformations'*

Dr. Bas de Bruin

Prof. Jos Oomens

Jos Oomens of the FOM Institute Rijnhuizen, also endowed professor with the Molecular Photonics group of HIMS, also received a (1.5 M€) **NWO-CW VICI subsidy** for his research project on the *'Chemistry underlying novel peptide sequencing reactions'*

Aurora Cruz-Cabeza (Computational Chemistry) received a **NWO-VENI subsidy** for her research project *From Molecules to Crystals: Understanding the Key Factors that Govern the Observation of Crystal Structures.*

Dr. Aurora Cruz-Cabeza

Peter Schoenmakers (Macromolecular and Biosystems Analysis) was awarded a grant (270 k€) from the **NWO Forensic Science programme**, for his research project *COMFOR: The use of comprehensive two-dimensional chromatographic methods for chemical profiling of complex natural materials*.

Peter Schoenmakers and Gabriel Vivo (Macromolecular and Biosystems Analysis) received grants from **TA-COAST**[5] for their projects HYPERformance liquid chromatography (810 k€) and Chromametrics (530 k€), respectively.

[4] Including a partial restitution of a reservation made earlier and the budgets received for future appointments in the framework of the Sectorplan Natuurwetenschappen, the HIMS result 2011 amounts +0,7 M€.

[5] TA-COAST (TASC Comprehensive Analytical Science and Technology) is a nationwide research and education initiative directed by NWO-ACTS and the Topsector(Regiegroep) Chemie, which aims to generate breakthroughs and to cluster new techniques in analytical chemistry and spectroscopy by using information technology and nanotechnology. HIMS houses the headquarters of TA-COAST.

Within the framework of the **Science4Arts programme**, NWO has provided Piet Iedema c.s. funding (600 k€) for the project titled *'How paint changes: consequences for conservation, presentation and preservation of paintings from Van Eyck to Mondriaan'*. The project is a collaboration of HIMS with the Faculty of Humanities in the field of Conservation and Restoration of Works of Art. The PAinT project will be carried out by Dr Katrien Keune (HIMS), Dr Annelies van Loon (the Royal Picture Gallery Mauritshuis), and Maartje Stols-Witlox, lecturer in the Restoration Studies Master's programme. Two doctoral students will also be appointed. The main applicant, Prof. Piet Iedema, is responsible for the mathematical modelling of the aging of paint layers. Research will take place at the laboratories of HIMS, the Swammerdam Institute for Life Sciences (SILS) and Utrecht University.

Prof. Piet Iedema

Peter Bolhuis (Computational Chemistry) was awarded a **FOM 'Projectruimte' grant**. His proposal *'Controlling colloidal superstructures via critical Casimir attraction'* was written together with Peter Schall of the UvA Institute of Physics (IoP)

Prof. Peter Bolhuis

NWO stimulates international mobility of scientific talent via the **NWO_Rubicon grants**. Abraham Shultz, from Northwestern University, USA, came to HIMS with a Rubicon grant for his project *Embedding Photocatalysts for Artificial Photosynthesis*. He will study the embedding of existing and new catalysts into well-defined, crystalline materials and their immobilization on electrode surfaces. This will lead to new applications for scalable photocatalysis, whereby sunlight can be converted into chemical energy.

Prof. Wybren Jan Buma and Dr. Sander Woutersen (Molecular Photonics) each received a **NWO-Echo GRANT** of 0.26 mln €.

Personnel

The scientific staff numbers in 2011 (163.2 fte) were somewhat lower than in 2010 (170.8 fte). The reason can be found in the numbers of PhD students and Postdocs in 2011 (106,3 fte together), which were also a little bit lower than in 2010 (112.4 fte)[6]. Related with the sound financial situation of the institute, we could realize several new (full-time) appointments in the course of 2011, e.g. a new Professor in Complex Molecular Simulations (Dr. Evert Jan Meijer) and two new Assistant Professors/UD's (Dr. Jocelyne Vreede/Computational Chemistry and Dr. Stefania Grecea/Heterogeneous Catalysis and Sustainable Chemistry). The appointment of Sjoerd van der Wal as endowed Professor (Analytical Chemistry) was renewed for a final few years. Further appointments of two new Professors (Supramolecular Analysis and Biocatalysis) and a new Assistant Professor (UD/Supramolecular Analysis) are expected in 2012-2013 in the framework of the Sectorplan Natuurkunde Scheikunde (SNS).
Since the number of 47 vacancies at 01-01-2012 (37 at 01-01-2011) was exceptionally high (including vacancies for various staff positions), a small increase in scientific staff members is expected in 2011.

Strengthening of cooperation with industry

In 2011, the institute has made great efforts to bring cooperation with the industry to a higher level. In the area of sustainability and catalysis we look for strategic partners with the aim to start industrial partnerships with a few large companies to establish a new public-private research institute ISCA (institute for Sustainable Chemistry Amsterdam) with a total budget of around 15 million €. The plan was discussed with representatives of the Topsector Chemie, and found direct support since the initiative perfectly fits

[6] Main reason for the 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 because of restricted working places at HIMS and cost limitations.

with the internationalization plans of the Topsector Chemie. The formation of the ISCA shows slow but steady progress. Points of discussion are the financial share of the first large commercial partner, the participation of industrial partners in related *spin-offs* of HIMS and the appointment of the CEO.

Facilities

Since mid 2010 the Van 't Hoff Institute for Molecular Sciences is located in the new buildings of the Faculty of Science at the Science Park in the Watergraafsmeer. The laboratories for the research groups of Macromolecular and Biosystems Analysis, Computational Chemistry, Molecular Photonics and Bio-catalysis (group Wever) are placed in the new building D. For these groups 1566 m^2 lab space is available. Most offices and sitting rooms and the lecture halls are located in a separate building in the middle, all on a very short distance from the lab-space. The research groups for Catalysis and Organic Synthesis (group Hiemstra), including the NMR-facilities, are housed in a separate three floor building E with 2052 m^2 available for the laboratories only. This renovated building is attached on one side to the main building in which the other HIMS research groups are be located, and on the other side to the bachelor student laboratories.

Jacobus Henricus van 't Hoff

Faculty of Science building

HIMS facilities in the buildings of the Faculty of Science at the Science Park in the Watergraafsmeer

2 Research themes

2.1 Sustainable Chemistry

HIMS, uniquely in the Netherlands, covers all relevant catalysis sub-disciplines. In view of favourable expected funding opportunities and mostly excellent research ratings we plan[7] to establish a *Catalysis Centre of Excellence*, by combining our Catalysis and Bio-molecular Synthesis research in a theme/programme focussing on ***Sustainable Chemistry***. This combination is a good candidate for a future University research priority area ('onderzoekszwaartepunt') and has been proposed as such. In addition, we intend to create a separate research institute on this topic (see also chapter 3). The combined sustainable chemistry activities presently consist of five research groups, *Homogenous and Supramolecular catalysis* (Prof. Reek c.s.), *Heterogeneous Catalysis and Sustainable Chemistry* (Prof. Rothenberg c.s.), *Organometallic Chemistry and Catalysis* (Prof. Elsevier c.s.), *Synthetic Organic Chemistry* (Prof. Hiemstra c.s) and *Biocatalysis* (Prof. Wever c.s). The activities of the groups of the theme ***Sustainable Chemistry*** cover a great variety of catalysis sub-disciplines, while there are also (smaller) catalysis activities in the other HIMS themes ***Molecular Photonics, Analytical Chemistry*** and ***Computational Chemistry*** as well. Additionally the research in the Bio-Molecular Synthesis groups is directed at the development of efficient and selective, diversity-oriented synthetic methodology, in particular organocatalytic and biocatalytic procedures, and the target-oriented preparation of molecules of relevance in chemistry, biology and medicine.

2.1.1 Homogenous and Supramolecular Catalysis

Prof.dr. J.N. H. Reek, Dr. B. de Bruin, Dr. J.I van der Vlugt

Summary of research activities

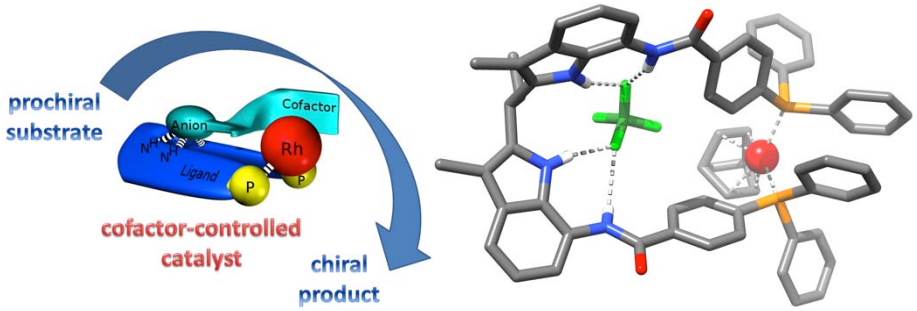
"Cofactor" Controls Metal Catalyst

Stereochemistry: Rhodium complex bearing an anion-binding pocket functions like an enzyme

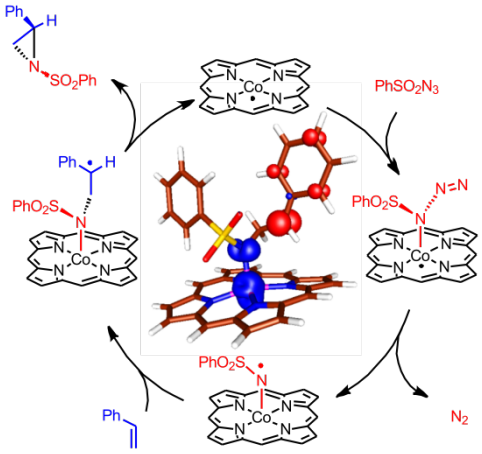
By equipping an achiral rhodium bisphosphine catalyst with a binding pocket for hosting chiral anion guest molecules, the HOMKAT group has created a system that mimics the way some enzymes employ cofactors––reactive small molecules—to modulate catalytic functions. The chemistry provides a means for generating chiral transition-metal complexes for asymmetric catalysis in which the catalytic activity and enantioselectivity of the metal complex are controlled independently, offering another tool for preparing biologically active compounds for pharmaceutical and agricultural applications. Drawing inspiration from nature and from transition-metal catalysis started with an achiral ligand made up of a pair of diphenylphosphine groups bridged by an amidoindolyl-based framework. When this supramolecular ligand attaches to rhodium, it creates a binding pocket next to the metal. The pocket has the chemical functionality and is just the right size to hold chiral α-hydroxy acids and α-amino acids. As the achiral rhodium complex noncovalently binds one of these chiral anions, its chirality effectively transfers to the rhodium complex. The cofactor-controlled system was evaluated by hydrogenating enamide compounds such as methyl 2-acetamidoacrylate. The highest enantioselectivity was obtained using a thiourea or a carbamate derivative as the cofactor. They observed in control experiments that both a bound cofactor and the bisphosphine ligand are necessary—the binding site must be an integrated part of the system near the metal center—else the catalyst has no enantioselectivity and racemic mixtures of products form. The researchers also carried out "natural selection" competition experiments in which they used mixtures of 12 cofactors that fight over the catalyst binding site. They discovered that the "winning" cofactor from a mixture is the one that binds

[7] Our initiative to establish a *Catalysis Centre of Excellence*, by combining our Catalysis and Bio-molecular Synthesis research in a theme/programme focussing on ***Sustainable Chemistry*** is in agreement with the recommendation of the international review committee that examined the research achievements the Dutch universities in the field of chemistry in 2010.

strongest to the rhodium complex and also induces the highest selectivity. The competition experiments are thus an efficient way to screen a large library of compounds and could be used to select the best cofactors for other biomimetic metal-ligand systems. The chemists have patented the strategy and plan to develop it alongside their other high-throughput ligand-screening strategies through a spin-off company, InCatT.



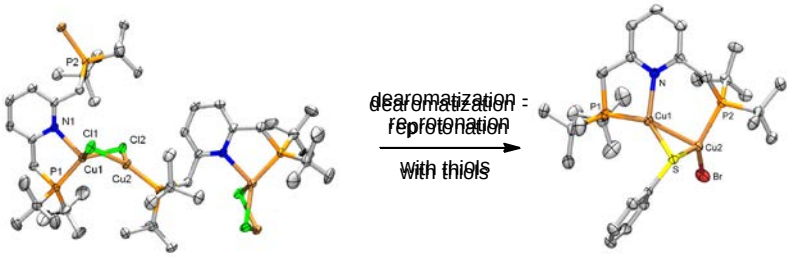
Controlled & Catalytic Radical-type Transformations



The HomKat group recently disclosed the unprecedented redox non-innocence of carbenes and nitrenes (*JACS* 2011 (2x), *Dalton Trans.* 2011). The discovery that carbene and nitrene precursors react with porphyrin-cobalt(II) complexes to form ligand radicals selectively, which are important reactive 'actor' ligand during catalysis, constitutes a fundamentally new approach to tune the catalytic reactivity of open-shell transition metal-substrate complexes and provides a new manner to control radical-type reactions in a catalytic manner.

The ligand centred radical-type reactivity allows selective C̄H, C̄C and C̄N bond making and breaking process, hydrogen-atom transfer reactions, and a variety of related ligand-centred transformations. These interesting intermediates play an important role in catalytic cyclopropanation, aziridination and hydro-carbon functionalization reactions mediated by these cobalt systems.

***Noninnocent, but not guilty*:** Research within the HomKat group has demonstrated that the versatile PNP^{tBu} scaffold can bind two Cu(I) centers, as a noninnocent pseudo-bridging ligand, resulting in a well-defined 1D-coordination chain. Ligand dearomatization using base and subsequent addition of thiols leads to unique asymmetrically substituted dinuclear Cu-species bearing a reactive halide co-ligand, whilst the versatile PNP^{tBu} ligand bridges the two Cu centers. Additional substitution of the halide-ligand proved feasible. The first DFT calculations (Atoms-in-Molecules) on any dinuclear Cu^{I} species have been presented (chem. Eur. J.).



Key publications 2011

Prof. J.N.H. Reek

P. Dydio, W.I. Dzik, M. Lutz, B. de Bruin, J.N.H. Reek* "Remote Supramolecular Control of Catalyst Selectivity in the Hydroformylation of Alkenes" *Angew. Chem. Int Ed.*,. **2011**,*50*, 396-400; **highlighted in C2W**

Cavarzan, A. Scarso*, P. Sgarbossa, G. Strukul, J.N.H. Reek*,"Supramolecular Control on Chemo- and

Regioselectivity via Encapsulation of (NHC)-Au Catalyst within a Hexameric Self-Assembled Host" *J. Am. Chem. Soc.* **2011**,*133*, 2848-2851.
P.Dydio, C. Rubay, T. Gadzikwa, M. Lutz, and J. N. H. Reek* "Cofactor"-Controlled Enantioselective Catalysis, *J. Am. Chem. Soc.* **2011**,*133*, 17176; **highlighted in C&E News and C2W**.
Dr. B. de Bruin
Tejel, C.; Asensio, L.; del Río, M. P.; de Bruin, B.; López, J. A.; Ciriano, M. A. *Angew. Chem. Int. Ed.* **2011**, *50*, 8839 – 8843.
Lyaskovskyy, V.; Olivos Suárez, A. I.; Lu, H.; Jiang, H.; Zhang, X. P.*; de Bruin, B.* *J. Am. Chem. Soc.* **2011**, *133*,12264 – 12273.
Lu, H.; Dzik, W.I.; Xu, X;. Wojtas, L.; de Bruin, B.*; Zhang, X.P.* *J. Am. Chem. Soc.* **2011**, *133*, 8518 – 8521.
Dr. J.I. van der Vlugt
W. I. Dzik, J. I. van der Vlugt, J. N. H. Reek, B. de Bruin,* *Angew. Chem. Int. Ed.* **2011**, *50*, 3356.
J. I. van der Vlugt,* E. A. Pidko, R. C. Bauer, Y. Gloaguen, M. K. Rong, M. Lutz, *Chem. Eur. J.* **2011**, *17*, 3850.

Grants
Dr. B. de Bruin
NWO-CW VICI Grant (Approved Dec. 2011; 5 PhD students, 1 PD , €1.500.000,-). Title: 'Investigation of new controlled (catalytic) radical-type transformations'.
NWO-CW ECHO Grant (Jan. 2011 - Jan. 2015; 1 PhD student, 4 yr, €260.000,-). Title: 'Cooperative and non-innocent ligands in hydrogenation, dehydrogenation and dehydrogenative coupling reactions'.

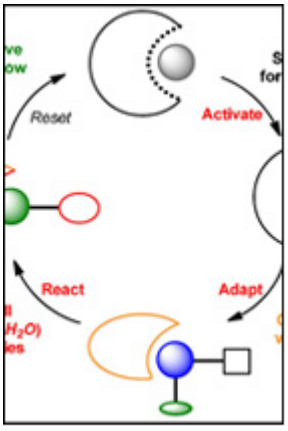

Dr. Bas de Bruin. Photo by Dirk Gillissen.

Prof. J.N.H. Reek/ Dr. B. de Bruin/ dr. J.I. van der Vlugt
NRSCC Grant (Nov 2011-Oct 2015; 2 PhD students, total €440.000,-). Title: 'Photocatalytic Dinitrogen Activation'.

Prof. J.N.H. Reek/ Dr. J.I. van der Vlugt
EVONIK (Nov 2011- Oct 2012; 1 PDF student, 1 yr, €125.000,-). Title: 'Robust Benchmark Photocatalysts for Water Oxidation'

Dr. J.I. van der Vlugt
ERC Starting Grant (Jan 2012-Dec 2017; 3 PhD., 3 PDF, €1.500.000,-). Title: '*EuReCat*: Small Molecule Activation with Cooperative First Row Transition Metal Complexes'


Dr. Jarl Ivar van der Vlugt



Proposed scheme for activation and functionalization of inherently unreactive substrates such as ammonia, carbon dioxide and water.

Outreach

Prof. J.N.H. Reek

BNR-radio on bioinspired catalysis for green energy applications **2011**

An artikel in the newspaper "de pers" (2 pages) on artificial photosynthesis. **2011**

Dr. B. de Bruin

NEMO Wakker-worden Kinderlezing "Hoe maakt een spin een draad, en kunnen we dat namaken?", 14 April **2011**.

Invited Lectures

Prof. J.N.H. Reek

Chinese academy of science Shanghai, China, march 2011, "New approaches to supramolecular transition metal catalysis"

Chinese academy of science Beijing, China, march 2011, "New approaches to supramolecular transition metal catalysis"

11th International Conference on Calixarenes, Taragona, Spain, June 2011, "Encapsulated transition metal complexes for catalysis"

Vth Euchem conference on N-Ligands (keynote lecture), Granada Spain, September 2011, "Template-ligand approach for the assembly of transition metal catalysts"

SCI National Conference, Lecce, Italy, September 2011 (plenary lecture), "Supramolecular strategies in Transition metal catalysis"

DoE workshop on CO2 reduction, Annapolis, USA, October, 2011, "Homogeneous catalysis using CO, in the context of CO2"

Zing conference on coordination chemistry, Mayan Riviera, Mexico, December 2011.

DoE workshop (US department of Energy) on CO_2 reduction. C-C bond forming reactions in relation to CO2 conversion.

Mini-symposium 'Advances & Challenges in Molecular Inorganic Chemistry & Homogeneous Catalysis; From (Electronic) Structure to Reactivity', UvA, Amsterdam, January 10, 2011. Title: 'supramolecular approaches to control selectivity in transition metal catalysis'.

Dr. B. de Bruin

Electrochemical Horizons 2011 Meeting, September 5-6, 2011, The University of Bath, UK. Title: 'Ligand Redox Non-innocence in Open-Shell Transition Metal Catalysis'

NRSC-C workshop, January 25, 2011. Title: 'Ligand Redox Non-innocence in Catalytic Carbene and Nitrene Transfer'.

University of Erlangen, January 17, 2011. Hosted by Prof. Karsten Meyer. Title: 'Ligand Redox Non-innocence in Catalytic Carbene and Nitrene Transfer'.

Mini-symposium 'Advances & Challenges in Molecular Inorganic Chemistry & Homogeneous Catalysis; From (Electronic) Structure to Reactivity', UvA, Amsterdam, January 10, 2011. Title: 'Ligand Redox Non-innocence in Catalytic Carbene and Nitrene Transfer'.

Dr. J.I. van der Vlugt

1st Conference 'Bioinspired Materials for Solar Energy Utilization', Crete (Sep 2011)

1st EuCheMS Inorganic Chemistry Conference (EICC), Manchester, UK (Apr 2011)

Patent Apllications

Functionalized Materials by Catalyzed Carbene Copolymerization; Jellema, E.; Jongerius, A.L.; Fransen, N.G.M.; de Bruin, B.; WO 2011/157444 A1; PCT/EP2011/003016. International publication date: 22 December 2011.

Coordination Complex System Comprising a Second Building Block without Donor Moiety; Pawel Dydio, Joost NH Reek; EP11177920.3, Application date: 18 August 2011.

2.1.2 Heterogeneous Catalysis and Sustainable Chemistry

Prof.dr. G Rothenberg, Dr. N.R. Shiju / Dr. S. Grecea

Summary of research activities

2011 was a good year for the Heterogeneous Catalysis and Sustainable Chemistry (HCSC) group, led by prof. dr. Gadi Rothenberg. The group published six papers in peer-reviewed journals, two of which were featured on issue covers. Group members published more than 10 additional peer-reviewed articles. Several international lectures were given by group members, patent applications were submitted, and one invention was even sold to industry.

Research at HCSC focused in 2011 on several key projects: Fischer-Tropsch catalysts (funded by Total Gaz & Power); Catalytic biomass conversion (projects funded by CatchBio and EOS/ Yellow Diesel); Predictive modelling in catalysis (funded by Avantium Technologies, NWO-Casimir and NRSC-C); Catalytic oxidative dehydrogenation (funded by NWO-ACTS) and design and synthesis of hybrid ceramic membranes (projects funded by the EU and STW). Alongside these, the group's inventions of the ammoximation catalyst and the sustainable resins have progressed into advanced research stages.

Key publications 2011

Novel and effective copper-aluminum propane dehydrogenation catayst. J. Schäferhans, S. Gómez-Quero, D.V. Andreeva and G. Rothenberg, *Chem. Eur. J.*, **2011**, 17, 12254.

A facile building-block syntesis of multifunctional lanthanide MOFs. S. Tanase, M.C. Mittelmeijer-Hazeleger, G. Rothenberg, C. Mathonière, V. Jubera, J.M.M. Smits and R. de Gelder, *J. Mater. Chem.*, **2011**, 21, 15544.

Mesoporous silica with site-isolated amine and phosphotungstic acid groups: A solid catalyst with tunable antagonistic functions for one-pot tandem reactions. N.R. Shiju, A.H. Alberts, S. Khalid, D.R. Brown and G. Rothenberg, *Angew. Chem. Int. Ed.*, **2011**, 50, 9615.

Cover image for Angewandte Chemie
(illustration credit: Itamar Daube, www.itamardaube.com)

Cover image for Green Chemistry
(illustration credit: Itamar Daube, www.itamardaube.com)

Invited Lectures

Rothenberg has given several plenary invited lectures, notably in Shanghai, Oslo, Jerusalem and Beer-Sheva. He also lectured at several UvA/HvA functions.

Shiju has given invited lectures at IIT-Mandi, EuropaCat (Glasgow) and the Euro Fed Lipid Congress in Rotterdam.

Castricum presented an invited lecture at the Gordon Research Conference on Nanoporous Materials & Their Applications in Holderness, NH, USA.

Grants

The group's STW project on hybrid silica membranes was renewed for its second term (total subsidy for the entire project €1M, together with U Twente; project will now continue till April 2013; 1PD at UvA plus funding for equipment, materials and technical support).

Rothenberg and Shiju successfully applied for an NRSC-C project in the area of thermocatalytic reactions/ high-temperature solar fuels (€220K, two-year PD will start March 2012).
Letters of agreement were signed with four industrial partners that will participate in cash in two large-scale STW projects, that are now being submitted in the 1st quarter of 2012.
The sale of the ammoximation patent to industry has credited the UvA and HIMS with an undisclosed sum.
The Faculty of Science has invested in the development of the sustainable plastics invention.

Patent application
Calderone, V.R., Shiju, N.R., Rothenberg, G. & Curulla-Ferré, D. (). Core-shell particles with catalytic activity; EP11305657.6, Application date: 30 May 2011.

Highlights
In September 2011, Dr. Stefania Grecea was appointed to a permanent position as assistant professor at HCSC. Her expertise in inorganic chemistry, inorganic spectroscopy and materials science will complement existing strengths in the group.

Also in September 2011, the group has set forth its strategy document for the period 2011–2015. This document outlines the group's strategy with regard to research directions, personnel, publications, patents, and outreach activities, and research funding, and equipment and lab management.

The ammoximation patent of Dr. Raveedran Shiju was sold to industry. This company will now invest also €0,25M in cash in a research project at HCSC aimed at developing this catalyst further.

The invention of the sustainable resin by Rothenberg and Alberts has raised much interest in the Netherlands and abroad. Rothenberg was interviewed on the radio program wetenschap24, and nominated for the prestigious Huibergstenprijs for this and his other achievements in research valorisation. Further development of the new materials is now is now in progress in collaboration with a international industrial player and with the help of the UvA's technology transfer office.

A new catalyst was discovered in HCSC in a project funded by a major multinational company. This catalyst is now being patented by the industrial partner.

Prof. Rothenberg was appointed to the Scientific Advisory Board of the new CNRS lab in Shanghai, funded jointly by Rhodia/Solvay, the CNRS, ENS-Lyon, and East China Normal University.

Photo (by Patrick Post), of Gadi Rothenberg and Albert Alberts, illustrating a Trouw article on Bioplastics (16 Feb 2011)

The Scientific Advisory Board members Can Li, Gadi Rothenberg, Avelino Corma, Michel Che with the French minister for Energy and Environment Nathalie Kosciusko-Morizet (second from right) on the opening day of E2P2L in Shanghai (photo credit: Rhodia-Solvay).

Relevance
The research topics at HCSC are highly relevant to today's society. This is reflected by the worldwide interest in the group's activities. For example, the invention of a sustainable resin plastic by Rothenberg and Alberts has been featured in more than 20 newspapers and magazines worldwide (including main news articles in the Dutch daily papers *Trouw* and *Spits!*). Similarly, the invention of a new ammoximation

catalyst by dr. Shiju has raised much attention.

The group's research is also highly relevant to the chemical industry, as proven by the fact that several large projects in the group are funded directly by key industrial players (most group members are paid either in part on in whole by industrial funding).

The group's spin-off company, Yellow Diesel BV, has finalised her lab development of the continuous process for manufacturing biodiesel by heterogeneous catalysis. The company is now seeking investment for scaling up the process to manufacturing scale.

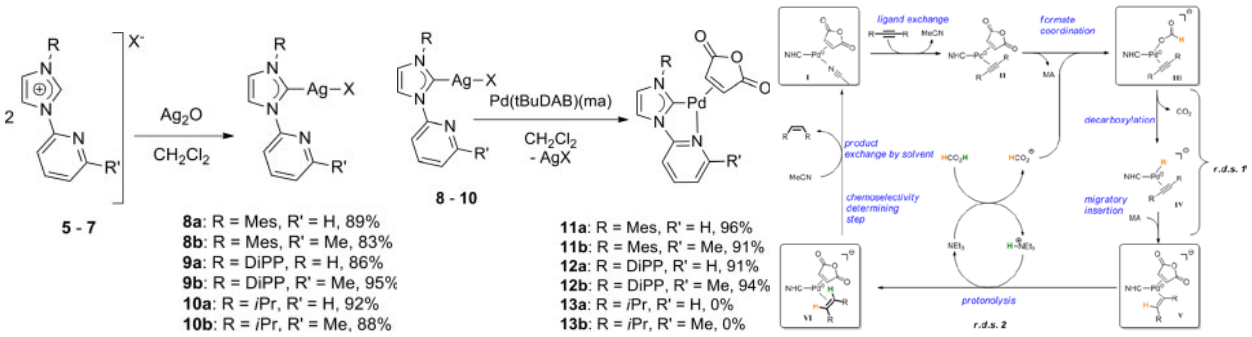
A new initiative started in the group following the HIMS discussion days in 2009 is the making of short films on research projects. The first such film, on the group in general, was released on YouTube in May 2011, and was viewed already more than 2,300 times worldwide. A Second film, made by the organisers of the *Avond Wetenschap & Maatschappij*, was also placed on the group's YouTube channel.

2.1.3 Organometallic Chemistry and Catalysis

Prof.dr. C. Elsevier

Summary of research activities

The group Molecular Inorganic Chemistry at the University of Amsterdam is involved in fundamental research in Coordination and Organometallic Chemistry, notably the synthesis, characterization and application of organometallic compounds and homogeneous catalysts. We try to approach catalysis in a rational way by studying single steps and constitute new catalytic cycles from these building blocks. We also engage in finding alternatives to existing reactions, for instance hydrogenations, by knowledge-driven choice and engineering of the metal-ligand combinations. The counterpart lies in careful analysis of the mechanism of homogeneous catalytic, metal-mediated reactions and to discover new solutions and improvement of processes, based on understanding of its details. Organometallic chemistry, which resides at the basis of all catalytic processes, is the main topic of the activities in the group. The reactions concerned are mainly bond-forming and bond-breaking reactions between carbon and the other elements, with emphasis on carbon, hydrogen, and late transition metals. Processes studied are, e.g., hydrogenation, hydrosilylation, C-C coupling reactions. Several of these have been studied under pressure and in neoteric solvents, e.g. supercritical fluids. Spectroscopic studies of reactions under pressure are carried out to evaluate the reaction and intermediates under conditions similar to those in the catalytic reactions studied. The research of the group has in the past partly aimed at the design and implementation of self-organizing amphiphilic metal-organic molecules, especially a novel class of metallo-amphiphiles that are characterized by the intrinsic presence of a metallic group as part of the amphiphile, that acts as the polar headgroup. These systems are particularly amenable to the formation of micelles and inverted micelles, or vesicles, with the aim to enhance catalysis and bond activation taking place at the interface of polar and apolar media (such as water/alkane). Other methodologies for heterogenization, immobilization and recycling of homogeneous catalysts receive ample attention.



The design and implementation of N-heterocyclic carbene (NHC) ligands as well as rigid bidentate N-ligands in late transition metal compounds aimed at catalytic carbon-element bond forming reactions continues to be an important research topic in the group. This year, studies revolved about palladium

compounds encompassing bidentate carbene-pyridyl ligands and similar materials. These studies concern a new niche as a part of the unique (base-free) transfer-hydrogenation reaction mediated by palladium-NHC species that we discovered and about which mechanism we have published recently (*J. Am. Chem. Soc.* ***2010****, 132,* 16900-16910). This methodology for the catalytic synthesis of *Z*-alkenes from alkynes *without* reduction to alkanes attracts a lot of interest. After obtaining insight in details of the mechanism, we have been able to provide a working catalyst that obviates the use of added base, which is based on bidentate C-N carbene-amine type ligands (see Appl. Organomet. Chem. **2011**, *25*, 276-282 and the schemes above).

An interesting range of new ruthenium compounds with bidentate carbene-amine and similar ligands have been synthesized and were applied in selective hydrogenations of ketones and esters (to be published).

Currently, one of the focal points of our research concerns the design and application of late transition metal complexes with heterotopic carbene and N-ligands for coordination chemistry and applications in homogeneous catalysis. This year we have synthesized a number of heterobidentate NHC ligands containing a secondary nitrogen-donor. Combining a strong donor with a more weakly coordinating donor, we intend to gain access to a class of catalysts which benefits from the hemilabile behaviour of the weaker donor N-ligand. Additionally, the basicity of the secondary nitrogen-donor is easily varied to obtain the desired functionality. Various electron-rich palladium complexes bearing an NHC-ligand functionalized with N-donors such as a pyridyl, pyrimidyl, and pyrazolyl donors have been studied. Varying their basicity, hence coordinative properties, leads to specific behaviour in e.g hydrogenation reactions.
Part of this project has been carried out in collaboration with Taiwanese colleagues (in a project financed by NWO and NSC): this lead to the synthesis of iridium-NHC complexes for catalytic indole synthesis and reductive amination (C-N bond formation), and palladium-NHC complexes for C-S bond formation. The palladium(NHC) systems with various tethers are unprecedented hydrogenation catalysts, since they catalyze *transfer* hydrogenation of alkynes to give *cis*-alkenes selectively. Usually transfer hydrogenation is restricted to ketones and imines. This collaboration has given rise to 14 papers, one of which appeared in 2011.

Key publications

- P. Hauwert, R. Boerleider, S. Warsink, J.J. Weigand, C.J. Elsevier. Mechanism of Pd(NHC)-catalyzed transfer hydrogenation of alkynes. *J. Am. Chem. Soc.*, **2010**, *132,* 16900-16910.
- S. Warsink, S. Bosman, J.J. Weigand, C.J. Elsevier. Rigid pyridyl-substituted NHC-ligands, their Pd(0) complexes and their application in selective transfer semi-hydrogenation of alkynes. Appl. Organomet. Chem. **2011**, *25*, 276-282.

Invited and keynote lectures 2011

- C.J. Elsevier; July 6, 2011;19th EuCheMS Conference on Organometallic Chemistry (EuCOMC), Toulouse, France, July 3-7, 2011. Contributed lecture. “Palladium-Carbene Species for Transfer Hydrogenation”

Highlights group

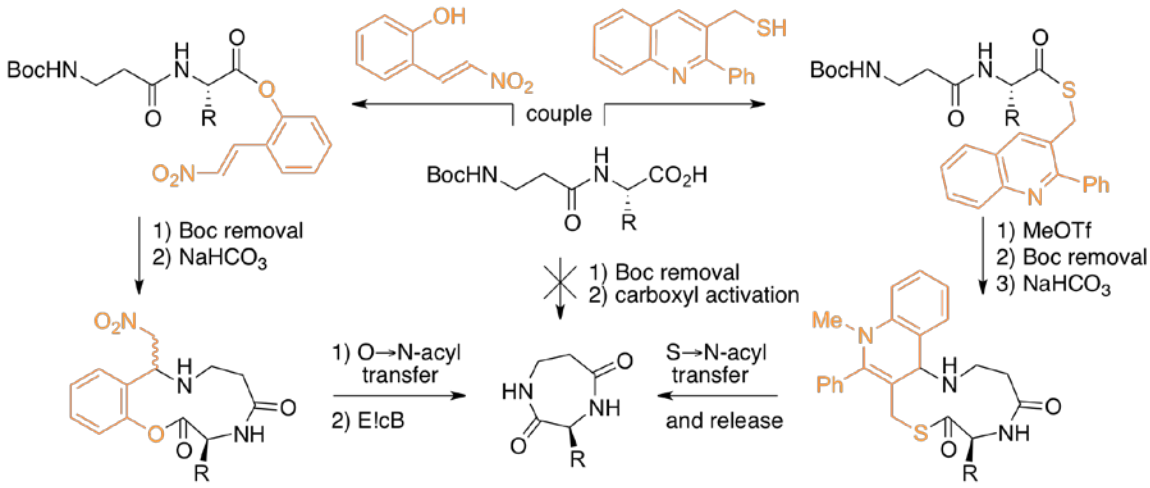
This year saw a growing interest and exciting results concerning catalyst immobilization. The progress has been good, although the number of papers was at a low (due to fast acceptance of papers there were many in 2010 and few in 2011). The officially finished NWO-NSC-project with the National Taiwan University at Taipei enjoyed new impetus in visits and the work by S. Warsink at Taipei and Bloemfontein. Soraya Sluijter joined the group as PhD student starting her work on late-transition-metal complexes of bis-carbenes in catalysis as main topic. She had a good start with synthesis of new ligands and complexes already during the first months of her studies.

2.1.4 Synthetic Organic Chemistry

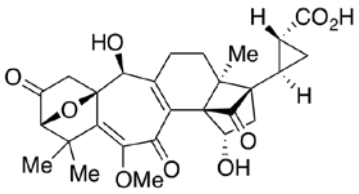
Prof. dr. H. Hiemstra, Prof. dr. P. Timmerman, Dr. J.H. van Maarseveen, Dr. S. Ingemann

Summary of research activities

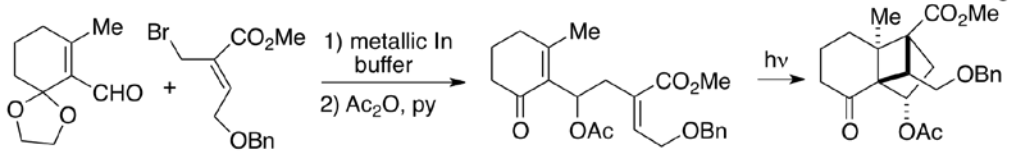
Synthetic methodology development*:* Due to their strained character, seven-membered bislactams are excellent targets for the development of novel and powerful lactamization methods. We have found that esterfication of *N*-terminal protected b-peptides with commercially available *o*-hydroxy-b-nitrostyrene, followed by liberation of the *N*-terminus gave the seven-membered strained bislactams in good yield. Mechanistis studies pointed to the intermediacy of an 11-membered macrocyclic intermediate, formed via an intramolecular aza-Michael reaction, which collapses to the seven-membered lactam via a ring-contractive O→N acyl-transfer reaction, followed by a retro-aza-Michael reaction liberating the lactam. In collaboration with the group of Prof. Levacher in Rouen (France) it was shown that also quinolines can be used as auxiliaries to facilitate lactamization using a similar mechanistic reaction pathway, although with less efficiency (*submitted*).



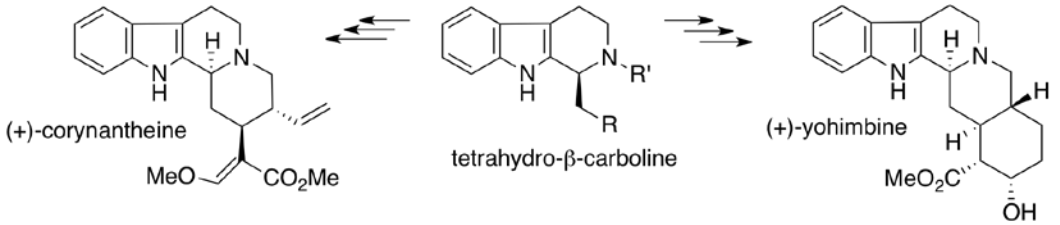
Target-oriented synthesis*:* In our research toward the total synthesis of the terpenoid hatching agent solanoeclepin A a very efficient and convergent synthesis of the tricyclic core was realized with all functionality in place to complete the total synthesis or simpler active analogues in order to combat potato cyst nematodes as parasites in potato production.



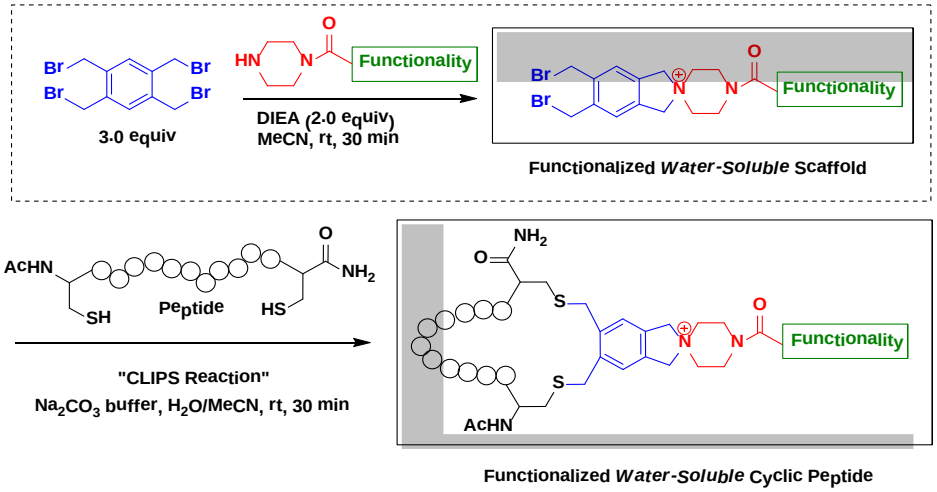
solanoeclepin A



Organocatalysis*:* Chiral biarylphosphoric acids were used to catalyse Pictet-Spengler reactions in order to prepare tetrahydro-b-carbolines in high ee's. Starting from these *N*-heterocycles we achieved the most efficient asymmetric total syntheses to date of indole alkaloids like (+)-corynantheine and (+)-yohimbine.



Chemical biology: Water-soluble scaffolds that are based on Pepscan 's (Lelystad, The Netherlands) CLIPS-technology have been prepared that conformationally constrain side chain unprotected linear peptides containing two cysteines. These scaffolds contain functionality with orthogonal reactivity to be used for labeling and ligation. This is illustrated by the chemical ligation of two dissimilar constrained peptides via oxime-ligation or strain-promoted azide-alkyne cycloaddition in aqueous media. Such functionalized scaffolds may be used for indirect labeling, i.e. by coupling of an appropriately functionalized FLAG, biotin, fluorescein, rhodamine or luciferin tag to a cyclized peptide carrying the compatible functional group at the scaffold. Also, these scaffolds provide a general and easy applicable route toward complex water-soluble double-loop mimics of discontinuous protein binding sites and can also be used to solubilize or label cyclic peptides. The method opens new perspectives in the field of protein mimicry.



Key publications 2011

Enantioselective copper-catalyzed propargylic substitution: synthetic scope study and application in formal total syntheses of (+)-anisomycin and (-)-cytoxazone, R.J. Detz, Z. Abiri, R. Le Griel, H. Hiemstra, J.H. van Maarseveen, *Chem. Eur. J.* **17**, 5921-5930 (2011).

Total synthesis of (+)-yohimbine via an enantioselective organocatalytic Pictet-Spengler reaction, B. Herlé, M.J. Wanner, J.H. van Maarseveen, H. Hiemstra, *J. Org. Chem.* **76**, 8907-8912 (2011).

Enantioselective syntheses of Corynanthe alkaloids by chiral Brønsted acid and palladium catalysis, M.J. Wanner, E. Claveau, J.H. van Maarseveen, H. Hiemstra, *Chem. Eur. J.* **17**, 13680-13683 (2011).

Invited and keynote lectures 2011

The staf was invited several times for lectures abroad:

H. Hiemstra

*Asymmetric Organocatalysis and Indole Alkaloid Total Synthesis,*Technische Universität Braunschweig, Germany, May 4, 2011.

Synthetic studies toward solanoeclepin A, the hatching agent of potato cyst nematodes, Universiteit Gent, Belgium, September 2nd, 2011.

Iminium ion chemistry and asymmetric organocatalysis, Novartis, Basel, Switzerland, October 19th 2011.

J.H. van Maarseveen

Towards Lactamization Organocatalysts, COST ORCA, Humboldt Universität, Berlin, Germany, March 4th, 2011.

*Tacking Small Peptide Cyclisations,*Durham University, Durham, England, UK, April 26th, 2011.

*Total Synthesis of Bioactive Compounds by Organocatalysis,*Utrecht University, Utrecht, May 20th, 2011.

Enantioselective Total Synthesis of Indole Alkaloids via Chiral Brønsted Acid-Catalysed Pictet-Spengler Reactions, Invited lecture at the 23rd International Conference on Heterocyclic Chemistry, Glasgow, Scotland, UK, August 20th, 2011.

P. Timmerman
Protein Surface Mimics via Chemical Fixation of Peptides, Invited lecture, TIDES-Symposium, IBC Life Sciences, Boston (MA), USA, May 22-25, 2011
A Synthetic Peptide that Mimics the Protein Surface of VEGF, Invited lecture, 22nd American Peptide Symposium, San Diego (CA), USA, June 25-30, 2011

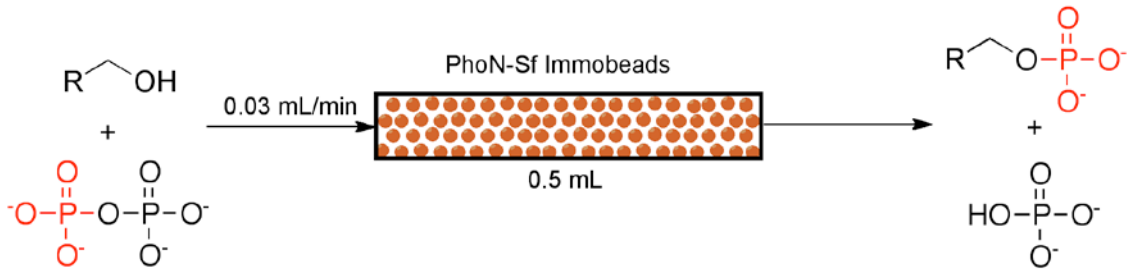
Highlights
The **research highlights** of 2011 were in the area of the application of enantioselective organocatalysis toward the total synthesis of biologically active indole alkaloids. The venerable alkaloid yohimbine, most well-known as a natural aphrodisiac, was prepared in a very short sequence of 9 steps and 16% overall yield, better than previous syntheses. Another indole alkaloid, (+)-corynantheine, was prepared for the first time in enantiopure form and in a very efficient manner.
Jan H. van Maarseveen was awarded the **Onderwijsbokaal** of the ACD (best chemistry teacher 2010-2011). He was also the chairman of the UvA-VU committee that designed a new joint chemistry bachelor education program to begin in February 2012.

Relevance
The most essential role of chemistry is making new molecules. Our group teaches and performs research in this key area of chemistry. Our work is directed both at the improvement of synthetic methodology and at the synthesis of biologically active molecules. Examples of the latter activities are our research toward the potato cyst hatching agent in collaboration with agricultural agencies and the synthesis of small (cyclic) peptides for medical applications.

Patent application
Improvements on CLIPS-technology, P. Timmerman, L. E. M. Smeenk, N. Dailly, J. H. van Maarseveen, EP 10188743.8, filing date 25-10-2011.

2.1.5 Biocatalysis
Prof.dr. R. Wever

Summary of research activities
We have developed a new method in which acid phosphatase is covalently immobilized on polymethacrylate beads with an epoxylinker. With the immobilized enzyme we were able to produce and prepare several phosphorylated compounds from the corresponding primary alcohol on gram scale using either a fed batch reactor or a continuous-flow packed-bed reactor.



Flow system in which an alcohol is phosphorylated by an enzyme (PhoN-Sf) with cheap pyrophosphate as phosphate donor

This method avoids the use of harsh chemicals that are normally used to phosphorylate compounds and in which also other functional groups have to be protected and deprotected. We have also immobilized an aldolase and using both this immoblized enzyme and the immobilized acid phosphatase in two consecutive packed-bed reactors we were able to produce several carbohydrates on gram scale as well. This was carried out in collaboration with the Department of Conservative and Preventive Dentistry, Academic Center for Dentistry, Amsterdam the antimicrobial effect of the vanadium chloroperoxidase toward in vitro *E. faecalis*

biofilms has been investigated and it is been concluded that the enzyme might provide an addition to current endodontic treatment, possibly as an antimicrobial dressing. In the cooperation with Prof. Dr. W. Tremel (Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg Universität, Mainz, Germany) the enzyme-like activities of the vanadium particles have been further investigated and in particular the brominating activity in the presence of hydrogen peroxide.

2.2 Computational Chemistry

Prof. P.G. Bolhuis, Prof. R. Krishna, Prof. Dr. E.J. Meijer, Dr. D. Dubbeldam, Dr. B. Ensing, Dr. C.P. Lowe, Dr. J. Vreede, Prof. A. Fasolino

Research topics

The research in the Computational Physics and Chemistry groups of Bolhuis, Krishna, and Meijer focuses on the study of materials, biological systems, and solution chemistry. Development and application of novel computational techniques are an essential part of the research. With many of the studied structures and processes intrinsically multiscale their computational approach focuses strongly on multiscale techniques. International collaboration with experimental and computational groups plays an important role.

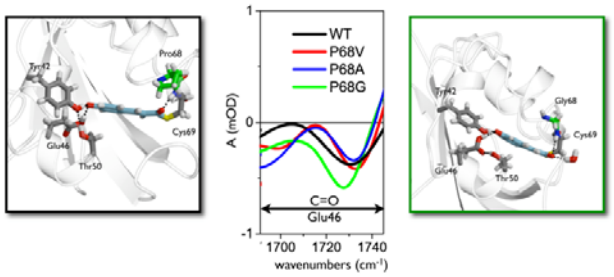
Research topics are:
Nanoporous materials
Stability and structure of carbon materials
Chemical reactivity in complex environment
Biomaterials
Protein conformational change and self assembly
Soft Matter
Development of computational techniques to model many-particle systems

Summary. of research activities

The group has kept a strong record in modelling complex phenomena in chemical, physical, and biological systems. Below highlights of the progress made in 2011 are listed.

Protein conformational changes (Bolhuis, Vreede, Ensing)

In proteins and enzymes, the local environment of an active cofactor plays an important role in controlling the outcome of a functional reaction. The Photoactive Yellow Protein (PYP) is a prime example of signaling protein, sensitive to light. We revealed key aspects of the signaling mechanism of PYP. **1**) In a combined experimental and simulation study we addressed the effect of substituting proline-68, positioned near, but not in direct contact with the chromophore, with other neutral amino acids. Our study revealed that the hydrogen bond interactions around the chromophore and the access of water molecules in the active site of the protein determine the efficiency of photoisomerization. The mutants provide additional hydrogen bonds to the chromophore, directly and by allowing more water molecules access to its binding pocket. (van Stokkum, Vreede and co-workers, J. Phys. Chem. B **115**, 6668, 2011).



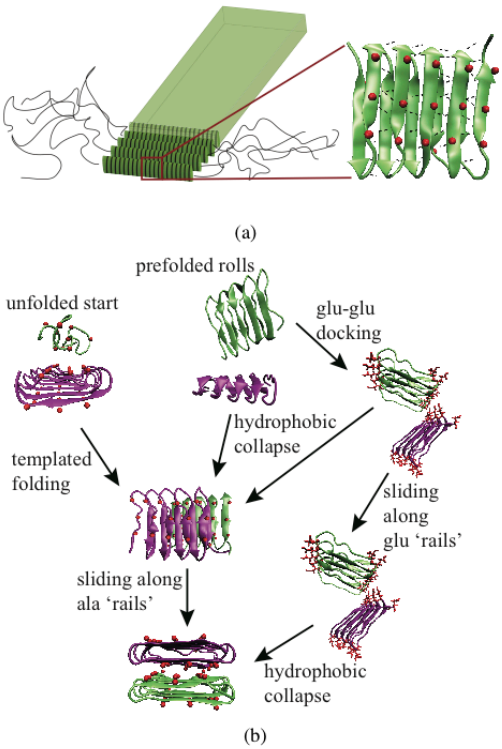
2) In separate studies we addressed the chemical and conformational changes in the PYP photocycle. The of the initial proton-transfer reaction in the chromophore binding pocket was revealed using transition path sampling simulations in combination with a hybrid quantum/force-field (QM/MM) level of theory. We discovered that the proton donation from Glu46 to the chromophore is concerted with a restructuring of the hydrogen-bond network involving various neighboring residues (Tyr42, Arg52 and Thr50) order to stabilize the negative charge on Glu46. The subsequent protein unfolding was addressed using the in-house developed path-metadynamics method. This provided the free energy profile along average transition pathway that involves a complex rearrangement of the chromophore binding pocket and its surrounding. (Vreede, Ensing, Meijer, Bolhuis, manuscripts in preparation).

Signal transduction upon binding of a ligand to a membrane protein can occur not only via allosteric conformational changes but also through fluctuations. We performed a numerical study on the influence of conformational fluctuations on the cooperativity of a binding reaction in a simple model of an integral membrane receptor consisting of transmembrane helices (Bolhuis and co-workers, Phys. Rev. Lett. **106**,

168103 (2011)). We found that small fluctuations lateral as well as perpendicular to the membrane can increase the cooperativity, with the former more dominant. Moreover, too much fluctuation induces negative cooperativity. Proteins with fewer than four helices do not show positive cooperativity under any circumstances. This behavior is rather robust, and independent of the receptor topology or ligand size. Fluctuations measured in all-atom molecular dynamics simulations of a G-protein coupled receptor fall within the predicted region of maximum cooperativity.

Biomaterials (Bolhuis)

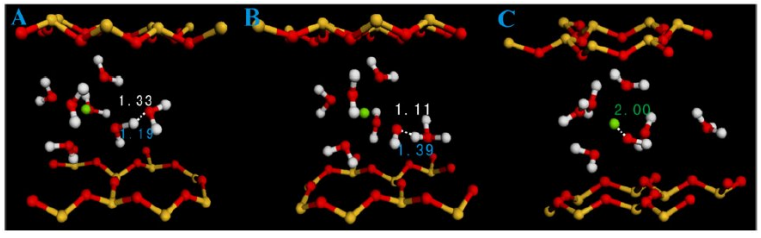
Self-assembly of polypeptides into fibrils promises the development of new functional supra-molecular biomaterials. Here, prediction of structure and kinetics is crucial to control the design of such novel biomaterials. We studied the self-assembling fiber formation of a triblock copolymer consisting of a middle silk-like block flanked by two hydrophilic end blocks. Previously, by extensive replica exchange molecular dynamics simulation we predicted the thermodynamically stable conformation of the middle block to be a ß-roll. Since the exact mechanism of the fibril formation remains unclear, we employed a multiscale modelling approach in combination with rare event simulations to elucidate key processes (Bolhuis and co-workers, Phys. Chem. Chem. Phys. **13**, 10457, 2011.). Atomistic scale simulations on the silk-based block suggest a mechanism in which a polypeptide prefolded into a beta-roll structure docks to the growing end of a fibril through the formation of Glu-Glu sidechain contacts. Subsequently it can slide to the optimal position before water is expelled to form a dry interface between the fibril end and the attaching block copolymer. In addition, we find that the folded state of the silk-based block is further stabilised through interactions with its neighboring block. Templated folding may also play a role in case a partially folded polypeptide attaches. The coarse-grained simulations indicate that the attachment and subsequent sliding is mediated by the hydrophilic flanks in a size dependent manner. The hydrophilic blocks prevent random aggregation and allow growth only at the end of the fibril. Our multiscale approach may be used for other fibril-forming peptides.



Whey proteins such as β-lactoglobulin are often used as thickening agents in the food industry. Cold-set gelation of whey proteins proceeds via heat-induced formation of small aggregates, followed by pH-induced gel-formation. In both steps thiol exchanges plays a crucial role. β-lactoglobulin contains buried two disulfide bridges, that need to be exposed during heating Using replica exchange molecular dynamics we found subtle exposure mechanism, in which the alpha-helical structure is not lost.

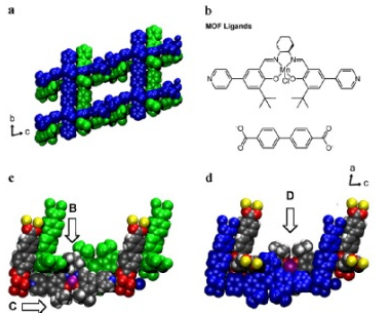
Chemical reactivity in complex environment (Ensing, Meijer)

Most (bio-)chemical processes occur in complex fluctuating environment, such as solvent, protein, or nanostructured cavities. We apply advanced ab intio molecular simulation techniques to address the role of the fluctuating environment. In a recent studies, we addressed the hydration of metal cations and their role in the acid chemistry of confined waters in interlayer space of smectites. In the latter study we also focussed owe also focused on the role of the smectite layer charge densities. Our study revealed that the layer charge enhances the water acidity enhancement in smectites, and that clear that clay frameworks can also enhance acidities of the cation-bound waters. As highly acidic cations (e.g. Mg2+, Ca2+, Al3+, Fe3+) occur as counterions in nature, their presence eventually makes the interlayer region a chemical



environment of high acid activity. (Meijer and co-workers, Geochimica et Cosmochimica Acta **75**, 4978, 2011).

Hard Materials (Dubbeldam, Fasolino, Krishna, Meijer) The design and development of novel nanoporous materials is of paramount importance in the areas as storage, separation, and catalysis. A targeted approach requires a proper quantitative description of the materials. We have focussed on zeolites, metal organic frameworks (MOFs) and carbon.

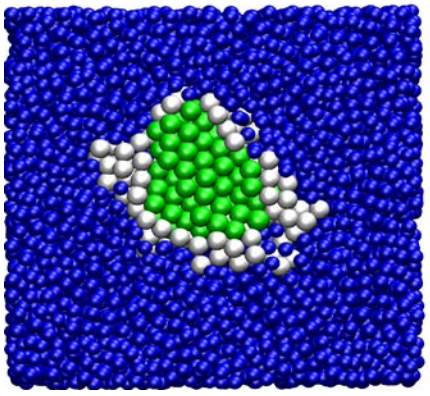


MOFs: Recent experiments showed that synthesized chiral MOFs with the catalyst incorporated into the framework yields enhanced stability and separation in chiral epoxidation. To elucidate this phenomena we performed hybrid quantum-force field (QM/MM) simulations where we focused on the role of steric effects of the MOF on the enantioselectivity of (salen)Mn (Dubbeldam and co-workers, J. Mol. Catal. A: Chem. **334**, 89, 2011). This study provided novel insight in 1) the most likely reaction pathway, 2) the difference between the pathway of the free molecular analogue and the one where the catalyst is incorporated into the framework and 3) the origin of the experimentally found improved stability and separation efficiency.

MOFs and zeolitic imidazolate frameworks (ZIFs) offer considerable potential for separating a variety of mixtures such as those relevant for CO(2) capture. In view of the vast number of MOFs, and ZIFs that have been synthesized there is a need for a systematic screening of potential candidates for any given separation task. A variety of metrics that quantify the separation performance, such as adsorption selectivity, working capacity, diffusion selectivity, and membrane permeability, are determined from a combination of Configurational-Bias Monte Carlo (CBMC) and Molecular Dynamics (MD) simulations. The practical utility of the suggested screening methodology is demonstrated by comparison with available experimental data. (Krishna and co-worker, PCCP, **13,** 10593, 2011).

Carbon: The thermodynamic properties of graphite under extreme conditions of temperature and pressure are of fundamental interest for different fields, from geology to crystal growth, but very difficult to access experimentally. We have shown determined equation of state and thermoelastic properties of graphite in the pressure-temperature range that has been unexplored by experiments. These results will be important in the design and understanding of graphite-based strong materials. (Meijer, Fasolino and co-workers, Carbon **49**, 364, 2011).

Soft Materials (Bolhuis)



We studied the mechanism of the homogeneous crystal nucleation from the supercooled liquid to the crystal phase in the soft-core colloid model for colloidal suspensions with the aim to identify optimal reaction coordinates (Bolhuis and co-workesr, Phys. Rev. Lett. **106**, 085701 2011, J. Chem.. Phys. **135**, 154110 2011).

We select optimal reaction coordinates from a set of novel order parameters based on the local structure within the nucleus, by employing transition path sampling techniques combined with a likelihood maximization of the committor function. We found that nucleation is governed by solid clusters that consist of an hcp core embedded within a cloud of surface particles that are highly correlated with their nearest neighbors but not ordered in a high-symmetry crystal structure. We found that the size of the cloud of prestructured particles surrounding the crystalline nucleus enhances the description of the transition.

The results shed new light on the interpretation of the surface and volume terms in classical nucleation theory. Further, we showed that the rearrangement of the inner core of the nucleus according to Ostwald's step rule is a separate process, independent of the growth of the nucleus.

Methods for Simulating Complex Systems

The transition path sampling method is potentially very powerful to investigate conformational changes in proteins. However, the proteins can adopt multiple states, whereas conventional path sampling focuses only on two states.

We implemented and applied the multiple state version of transition path (interface) sampling for a model biomolecular system: alanine dipeptide in explicit water (Bolhuis and co-workers, J. Chem.. Phys. **135**, 145102 2011). We extract the rate constant matrix for configurational changes between each pair of metastable states. The results are comparable with values from previous literature and show that the method is applicable to biomolecular systems.

In addition we elaborated on the properties of the reweighted path ensemble (Bolhuis and co-workers, J. Stat. Phys. **145**, 841, 2011)). In this paper we derive several distribution functions for the recently introduced reweighted path ensemble: the configurational and path densities, the reactive current, and the generalized committors for the different path types. We relate these distributions to the free energy and to the expressions for the rate constant in the transition state theory, the reactive flux method, the transition path (interface) sampling framework, and the Bayesian path statistics. In addition, we compute the transmission coefficient (distribution) from the reweighted path ensemble. Finally, we derive the path sampling shooting point distributions. For a simple two dimensional Langevin model we illustrate how these novel distributions can be used as analysis tools in rare event simulations.

Key publications 2011

L. Zhu, D. Frenkel, P.G. Bolhuis, *Role of Fluctuations in Ligand Binding Cooperativity of Membrane Receptors*, Phys. Rev. Lett. **106**, 168103, 2011.

W. Lechner, C. Dellago, P.G.Bolhuis, *Role of the Prestructured Surface Cloud in Crystal Nucleation*, Phys. Rev. Lett. 106, 085701, 2011.

G.A.E. Oxford, D. Dubbeldam, L.J. Broadbelt, R.Q. Snurr, *Elucidating steric effects on enantioselective epoxidation catalyzed by (salen)Mn in metal-organic frameworks* J. Mol. Catal. A: Chem. **334**, 89, 2011.

R. Krishna and J.M. van Baten, In silico screening of metal-organic frameworks in separation applications"", PCCP **13**, 10593 2011.

A.B. Rupenyan, J. Vreede, I.H.M. van Stokkum, M. Hospes, J.T.M. Kennis, K.J. Hellingwerf and M.L. Groot *Proline 68 tunes photochemistry yield in Photoactive Yellow Protein* J. Phys. Chem. B **115** 6668, 2011.

Z. Liu, B. Ensing, and P.B. Moore, *Quantitative assessment of force fields on both low-energy conformational basins and transition-state regions of the (φ, ψ) space* J. Chem. Theory. Comput. **7** 402, 2011.

X. Liu, X.C. Lu, R.C. Wang, E.J. Meijer, and H.Q. Zhou, Acidities of confined water in interlayer space of clay minerals, Geochimica et Cosmochimica Acta **75**, 4978, 2011.

Invited Lectures

Vreede – CECAM meeting on "Interactions between nucleic acids and proteins: Experiments and simulations", 2011 (Zurich, Switzerland); Chromating Meeting by the American Biophysical Societey, 2011 (Asilomar ,USA)

Ensing – CPMD2011 - Extending the limits of ab-initio Molecular Dynamics Simulations for Materials Science and Biophysics, September 5, 2011 (Barcelona, Spain).

Bolhuis - Mini Statistical Mechanics Meeting, Berkeley, Jan 2011; Multi-scale Simulations of Biological and Soft Materials, Kyoto, Japan, Sept 2011; ESF conference SimBioMa, Konstanz, Germany, Sept 2011; Conference on Computational Physics, Gatlinburg, TN, USA Oct 2011

Meijer – International meeting on Computational Geochemistry, August 2011 (Nanijng, China).

Outreach
Ensing was panel member and lecturer (title: NWO grant applications) at the CHAINS Talent Class, for the Dutch Science Foundation (NWO), Maarsen, The Netherlands (30-11-2011).

Grants
Ensing, Meijer, Dubbeldam – MolSim2011; ESF & CECAM grant
Bolhuis - FOM Projectruimte
Cruz-Cabeza, VENI grant
Meijer - Erasmus Mundus Master Course grant

Collaborations
Krishna – Karger (Leipzig), Smit (Berkeley)
Bolhuis – Kegel (Utrecht), Dellago (Vienna), Cohen Stuart(Wageningen), Tans (FOM-Amolf)
Meijer – van Santen (Eindhoven), Sprik (Cambridge), van Erp (Leuven), Bakker (AMOLF), Liu (Nanjing)
Lowe – Pagonabaragga (Barcelona)
Ensing - Nielsen (Texas), Moore (Philadelphia), Visscher (VU-Amsterdam), Woutersen (UvA/HIMS)
Dubbeldam – Snurr (Northwestern), T. van Erp (Leuven), Calero (Sevilla), Vlugt (Delft University)
Vreede – Hellingwerf (UvA), Dame (Leiden), Wassenaar (Groningen), Shimizu and Rezus (FOM-Amolf), Groot (VU-Amsterdam), Joyeux (Grenoble, France), Hoff (Oklahama, USA)

Organized conferences/schools
Ensing – Winterschool Theoretical Chemistry and Spectroscopy (Han-sur-Lesse)
Meijer, Ensing, Dubbeldam – Winterschool MolSim 2011 (Amsterdam)
Bolhuis – ACMM Spring and Fall symposia (Amsterdam)
Bolhuis – FOM Biophysics meeting 3-4 October 2011 (Veldhoven)
Lowe – Write it Right, International workshops on writing scientific papers (multiple editions)

Membership committees
R. Krishna
Fellow of the Indian Academy of Sciences.
Fellow of the Indian Academy of Engineering.
Fellow of the Indian Institution of Chemical Engineers.
P.G. Bolhuis
Member NWO TOP/Echo committee 2010
Member FOM BRM program committee
E.J. Meijer
UvA representative Scientific Council CECAM.
Member Scientific Committee International Erasmus Mundus program ATOSIM

B. Ensing
Member NWO/CW Study group "Spectroscopy and Theoretical Chemistry"
Member of educational board of the Holland Research School of Molecular Chemistry (HRSMC)
Member of NWO/CW Veni grant committee.

Highlights
Jocelyne Vreede was appointed in 2011 as Assistant Professor (UD) in the Computational Chemistry theme. Vreede also received the WiF Best Publication Prize 2010 (awarded 2011). Ensing was awarded by the Servizio Relazioni Internazionali of the University of Padova, Padua, Italy, as Bando Visiting Professor 2011–2012. David Dubbeldam of the Computational Chemistry group was portrayed in the 'Focus on Research' series, with which the University of Amsterdam brings its high profile research projects to the attention of the general public. David Dubbeldam performs computer calculations to decide what future metal-organic frameworks should look like. Metal-organic frameworks can be used to store gasses, such as carbon dioxide and hydrogen, but are also useful for purifying substances and catalysis.

2.3 Analytical Chemistry (including its applications in Forensic Science)

Prof.dr. P. Schoenmakers, Prof.dr. H.G. Janssen, Prof.dr. S. van der Wal, Dr. W.Th.Kok, Dr. G. Vivo Truyols

Summary of research activities

2011 was a year of transition in the analytical-chemistry / forensic-science group. Most of the temporary scientists in the group left or arrived in 2011. There is a gradual shift in the activities of the group, with increasing emphasis on generic analytical science and technology and applications in forensic science. The analysis of (synthetic) polymers is receiving less attention.

The group is part of a strong focus on analytical chemistry that was assigned to Amsterdam in the Sectorplan Natuurwetenschappen (SNS). It is a host to COAST, the public-private partnership on analytical sciences, and together with the Free University runs the only MSc program in the field that was recognized in the SNS.

A strength of the group is the good embedding of several part-time professors, particularly Hans-Gerd Janssen and Sjoerd van der Wal. The appointment of the latter was renewed for a final few years. A successor would be very welcome.

Prof. Sjoerd van der Wal

Key publications 2011

Ghaffar, A., Draaisma, G. J. J., Mihov, G., Dias, A. A., Schoenmakers, P. J., van der Wal, S. "Monitoring the in Vitro Enzyme-Mediated Degradation of Degradable Poly(ester amide) for Controlled Drug Delivery by LC-ToF-MS", Biomacromolecules, 12 (2011) 3243-3251.

Uliyanchenko, E., van der Wal, S., Schoenmakers, P. J., "Deformation and degradation of polymers in ultra-high-pressure liquid chromatography", J. Chromatogr. A 1218 (2011) 6930-6942.

Qureshi, R. N., Kaal, E., Janssen, H. G., Schoenmakers, P. J., Kok, W. T. "Determination of cholesterol and triglycerides in serum lipoproteins using flow field-flow fractionation coupled to gas chromatography-mass spectrometry" Anal. Chim. Acta 706 (2011) 361-366.

Highlights

Peter Schoenmakers was awarded the 2011 Chromatographic Society Martin Medal. It is the highest honour the Society confers, awarded to scientists who have made outstanding contributions to the advancement of separation science. Schoenmakers received the Martin Medal during the HPLC2011 Symposium in Budapest (19-23 June).

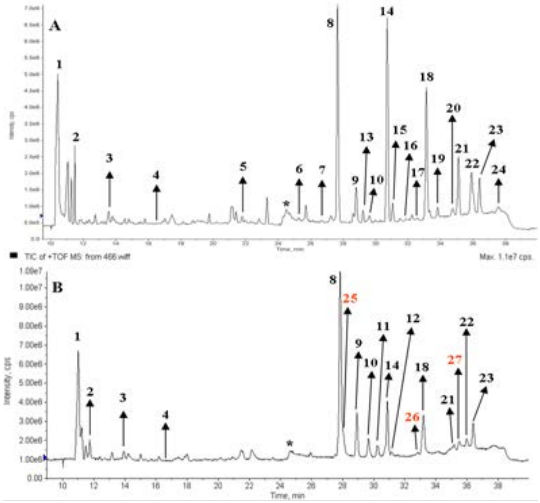
Arian van Asten (NFI) started his secondment as a visiting scientist for 0.2 fte in the analytical-chemistry / forensic-science group, pending formal establishment of his position.

Prof. Xulin Jiang (Wuhan University, China) spent six month in the group as a visiting professor.

The Eureka-DiscoveRIE project (2 AIOs), two NanoNext projects (2 AIOs), and an STW Smartsep (1 AIO) were started.

The SCM-5 (Separation and Characterization of Natural and Synthetic Macromolecules) conference took place in Amsterdam in early 2011, with Peter Schoenmakers (Chairman), Wim Kok (treasurer), and Petra Aarnoutse (secretary) carrying most of the organization. The conference attracted some 250 people.

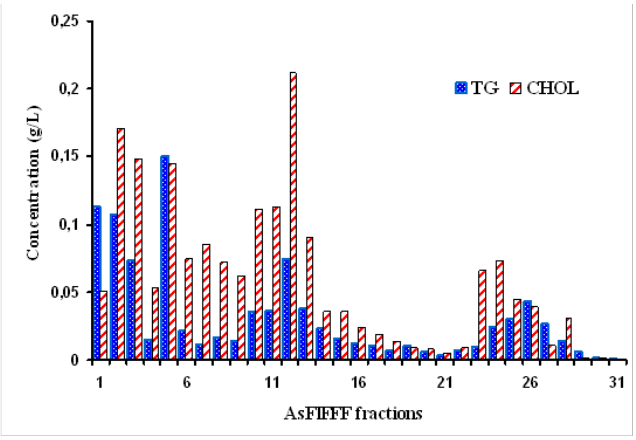
Two PhD thesis were successfully defended (Rashid Qureshi, “Asymmetric FFF of Macromolecules of Biological Interest”and Abdul Ghaffar, “Degradation and Analysis of Synthetic Polymeric Materials for Biomedical Applications”.



*TIC chromatograms of samples of degradation products of (A) di-block PEA and (B) tri-block PEA coatings in pulse feed-in mode analysis at 20 µL injection volumes of α-Chymotrypsin (5 U/mL in PBS) and 100 µL/min flow rate. The peak numbers correspond to structural assignments based on m/z values. Peak with * represents the α-CT peak in each chromatogram (thesis of Abdul Ghaffar).*

Invited Lectures

Peter Schoenmakers presented plenary lectures at SCM-5 (Amsterdam), HPLC2011 Budapest and HPLC2011 Dalian (China), and a State-of-the-Art lecture during SCM-5 (Amsterdam).
Hans-Gerd Janssen presented an invited tutorial lecture during SCM-5, a keynote presentation at the Beijing Conference and Exhibition on Instrumental Analysis, and lectures at the 8th GCxGC Symposium (San Diego) and HPLC2011 Dalian (China).
Gabriel Vivó-Truyols presented an invited tutorial lecture at SCM-5. He was also invited to present a key-note lecture at the Predictive-Analytics summit in Amsterdam.



"Lipoprotein profiling in human serum by Field-Flow Fractionation and pyrolysis-GC-MS"

Grants

The group has been very successful in the first call of TA-COAST organized by NWO-ACTS. Gabriel Vivó Truyols obtained funding for his project on Chromametrics (2 positions at UvA), in which RIKILT, the NFI and DSM Resolve participate. Peter Schoenmakers was successful in creating the HYPERformance LC project (4 positions in Amsterdam, 1 in Groningen), with ThermoFisher Scientific, DSM Resolve, AkzoNobel, RIKILT, Shell, Syngenta, TNO Q&S, and Avantor Performance Materials as private partners and the RU Groningen, the Vrije Universiteit Brussel en de Hogeschool Arnhem Nijmegen as knowledge institutes.

Peter Schoenmakers was also awarded a grant (270 k€) from the NWO Forensic Science programme, for his research project COMFOR: The use of comprehensive two-dimensional chromatographic methods for chemical profiling of complex natural materials.

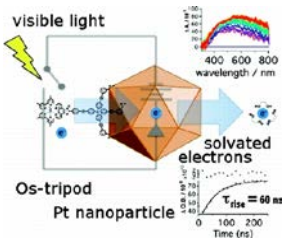
2.4 Molecular Photonics

Prof.dr. W.J.Buma, Prof.dr. A.M. Brouwer, Prof.dr. H.J. Bakker, Prof.dr. J. Oomens, Dr. H. Zhang, Dr. R.M. Williams, Dr. S. Woutersen

Summary of research activities

Light-induced chemical conversions play a key role in many technological and biological processes. The research of the Molecular Photonics group addresses the key areas of *Dynamics of supramolecular and biomolecular systems*, *Photoprocesses in nanostructures*, and *Photochemical processes*. Highlights of our research activities in 2011 include the following.

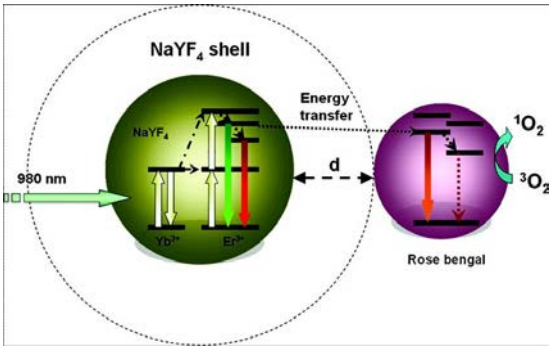
***Luminescent silicon*.** A study on the photophysical properties of small silicon nanoparticles in collaboration with Zuilhof (WUR) was completed. In addition to luminescence, a long-lived transient absorption signal was observed, which until now was never reported for silicon nanoparticles. Somewhat to our disappointment, the photochemical stability was insufficient for single particle luminescence observation, and the two-photon absorption cross section was small. Some of the results were quite different from those of other workers in the field with superficially similar materials. It is clear that improvement of the synthesis and purification methods is necessary for this field. Only when robust protocols are available that are reproducible in different laboratories, consistent results can be expected to emerge (*J. Phys. Chem. C* **2011**, *115*, 20888-20895).



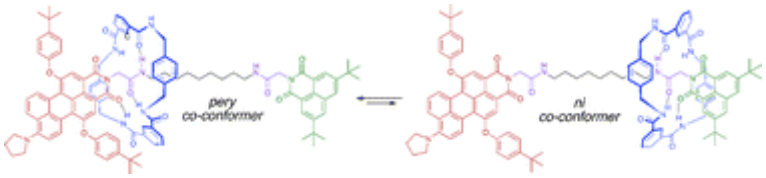
***Tripodal osmium polypyridyl complexes for self-assembly on platinum nanoparticles*.** The combination of platinum nanoparticles with a tripodal osmium complex that anchors to the metal surface leads, under visible light irradiation, to the formation of solvated electrons. The formation kinetics is limited by the detachment of the electron from the platinum surface into the solution, the particle showing a type of capacitor behavior (*J. Phys. Chem. Letters.* **2011**, *2*, 1460–1463).

***Breakthrough in concentration quenching threshold of upconversion lumin*escence.** Aiming at improving the upconversion luminescence efficiency of rare earth (RE) ions doped nanoparticles for medical application, a novel strategy of spatially separating the doping area has been adopted leading to an impressive increase of the quenching threshold from 2% to 8% (*Chem. Commun*. **2011**, *47*, 11957-11959).

***Critical shell thickness for singlet oxygen generation in upconversion core/shell nanoplatform*.** The influence of the structure of upconversion nanoparticles on their Förster resonant energy transfer (FRET) applications has been studied using nano-conjugates constructed by core/shell upconversion $NaYF_4$:Yb^{3+},Er^{3+}@$NaYF_4$ nanoparticles and photosensitizers. The optimal shell thickness for the most efficient FRET has been determined from the photophysics and singlet oxygen generation. It has been found that this optimal shell thickness is a trade-off between the opposing optimal conditions for upconversion and FRET efficiency (*J. Phys. Chem. Letters* **2011**, *2*, 2083-2088).



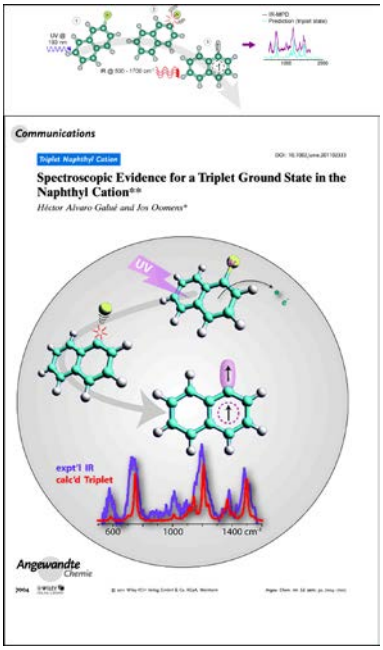
***Cyclodextrin-based systems for photoinduced hydrogen evolution*.** Light-driven catalytic three component systems for the reduction of protons, consisting of a cyclodextrin-appended iridium complex as photosensitizer, a viologen-based electron relay, and cyclodextrin-modified platinum nanoparticles as the catalyst, were found to be capable of producing molecular hydrogen effectively in water, using a sacrificial electron donor. By investigating different photocatalytic systems, it was found that the amount of hydrogen produced was directly proportional to the emission quantum yield of the photosensitizer (*Phys. Chem. Chem. Phys.* **2011**, *13*, 7903-7909).



Solvatochromic rotaxanes. Fluorescent molecules of which absorption and emission colors depend on the medium have been a longstanding research topic in our laboratory. We now combined this functionality with molecular shuttles, leading to a strongly fluorescent bistable rotaxane in which the relative position of the macrocyclic ring with respect to the fluorophore gives a strong response in the spectral domain (*Chem. Commun.* **2011**, *47*, 4977-4979).

Ultrafast dynamics of a nanoscopic wheel probed by vibrational photon echoes. The dynamics of the hydrogen bonds connecting the axle and rim of a rotaxane-based nanometer-size wheel in solution have been investigated using femtosecond infrared photon echoes. We find that the hydrogen-bond dynamics is liquid-like on a time scale 1 ps and less, but structurally frozen on longer (up to at least 200 ps) time scales (*J. Chem. Phys.* **2011**, *134*, 134504/1-134504/7).

Switchable rotaxanes in the gas phase. The structural and dynamical properties of isolated, jet-cooled [2]rotaxanes that feature two binding stations incorporated into the thread have been studied using IR spectroscopy and *ab initio* calculations. Considering the size and structural as well as conformational complexity of such systems, this is quite a remarkable accomplishment. This analysis has elucidated the conformational structure of each component and has provided vibrational markers that enable one to map interactions between the various components. Equally important, the experiments form the basis for subsequent studies of shuttling in the gas phase (*J. Phys. Chem. A* **2011**, *115*, 9669-9675).



Electronic spectroscopy of ions in helium nanodroplets. Recently, we developed in collaboration with Drabbels (EPFL) a new experimental method to record IR spectra of molecular cations in helium droplets that has now been adopted to record electronic spectra of molecular ions. These experiments constitute the first application of helium nanodroplets to obtain electronic spectra of molecular ions. Since helium droplets can be readily doped directly with a variety of ions from different sources, the method is extremely versatile (*J. Phys. Chem. Letters.* **2011**, *2*, 1563–1566).

The electronic ground state of the naphthyl cation. Infrared spectroscopy of the isolated naphthyl carbocation provides evidence for a triplet electronic ground state, in which a π electron is promoted to the vacant σ orbital. Previous computational studies have been ambiguous as to the relative stabilities of the singlet and triplet states; DFT calculations predict both states to be practically isoenergetic (*Angew. Chem. Int. Ed.* **2011**, *50*, 7004-7007).

Key publications 2011

Wang, Y.; Liu, K.; Liu, X.; Dohnalova, K.; Gregorkiewicz, T.; Kong, X.; Aalders, M.C.G.; Buma, W.J.; Zhang, H.. Critical shell thickness of core/shell upconversion luminescence nanoplatform for FRET application. *J. Phys. Chem. Letters* **2011**, *2*, 2083-2088.

Günbaş, D.D.; Zalewski, L.; Brouwer, A.M. (2011). Solvatochromic rotaxane molecular shuttles. *Chem. Commun.* **2011**, *47*, 4977-4979.

Galue, H.A.; Oomens, J.; Spectroscopic evidence for a triplet ground state in the naphthyl cation. *Angew. Chem. Int. Ed.* **2011**, *50*, 7004-7007.

Invited Lectures
Molecular Photonics staff members have given invited lectures at the following prestigious conferences:
Oomens presented the lecture "*CID product structures of protonated and deprotonated peptides by IRMPD spectroscopy*" at the Gordon Research Conference on Gaseous Ions.
Buma has given the plenary invited lecture "*Photoactive proteins: sense and simplicity by high-resolution spectroscopy*" at the Gordon Research Conference on Biological molecules in the gas phase, and in solution.
Zhang presented the invited lecture "*NIR to visible upconversion nanoparticles and biofunctionalization*", on the 6th European Molecular Imaging Meeting.
Woutersen presented the invited lecture "*Slippery when wet: lubricating a molecular machine with water*" at the Time-Resolved Vibrational Spectroscopy XV conference.

Grants
Brouwer participates in the FOM program '*Towards BioSolar Cells'* with Reek and Gardeniers on photochemical water splitting in microfluidic devices (1 PhD student in Molecular Photonics).
Brouwer also participates in a large FOM program on '*Fundamental aspects of friction'*, led by Frenken (Leiden), in which Brouwer collaborates with Bonn (IoP) on the fluorescence visualization of mechanical effects. A PhD student will be appointed in 2012.
A NRSCC proposal of Brouwer with Reek on light-induced dinitrogen activation was approved (440 k€).
Woutersen received in May 2011 NWO-CW ECHO grant (260 k€) for the project "*How water lubricates molecular machines*".
Buma received a NWO-CW ECHO grant (260 k€) for the project "*Molecular motors at work in the gas phase*".
Together with Löwik (LUMC) and Aalders (AMC), Zhang is one of the program leaders of IMPACT ("*Image-guided and/or targeted photodynamic therapy using a combination of a new photosensitiser with upconverting nanoparticles*") that has been granted 1.55 M€ in the framework of the IOP Photonic Devices program (1 PhD student, 1 PD, and 80 k€ consumables for Molecular Photonics)

Highlights


In May 2011 Hong Zhang won the Science Park New Ideas Competition 2011 together with Maurice Aalders from the UvA university hospital AMC. The two researchers developed a catheter that is able to detect microbial infections at an early stage.

UvA scientists Dr. Hong Zhang (HIMS) and Dr. Maurice Aalders (AMC) receive the Science Park New Ideas Competition prize 2011.

September 21 marked the official opening of Institute Quantivision, a collaboration between the VUmc, AMC, NKI/AVL, VU, UvA and companies to develop medical imaging devices, software, and protocols to enhance the efficiency, efficacy and economy of healthcare. Molecular Photonics is one of the participating teams, Buma being one of the members of the Management Team. This Institute has originated from the ZONmw initiative *Innovative Medical Devices Initiative* to establish regional Centers of Research Excellence, where healthcare, business and science collaborate on the development of new medical devices that enable future health care at high standards, in an aging population with decreasing numbers of working forces.

Relevance
S. Woutersen has been invited to give a lecture at *Fysica 2011* ("*The operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy*").

A novel way to detect infections has been patented (patent 11166364.7-2204 "*Device and probe for detection of infection*" , Zhang and Aalders).

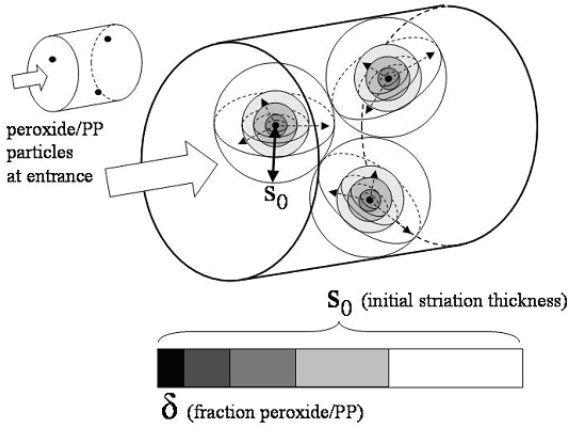
2.5 Other activities (Polymer Systems and Art Sciences)

Prof.dr. P. Iedema

Summary of research activities

The year 2011 was the first full year of the PhD students Nazila Yaghini, MSc and Ivan Kryven, MSc, bot working on grants from the Marie Curie project "Nanopoly" and the Dutch Polymer Institute. Nazila is developing computational tools to predict branching architectures of low-density Polyethylene. Ivan works on numerical recipies to efficiently solve convolution problems in population balances describing reactive polymer systems.

The cooperation with industry (Sabic) has resulted in a few publications in the area of polymer processing and branched polymers. The article recent in *Chemical Engineering Science* (Figure below) treats the impact of micromixing on the distributive properties of Polypropylene undergoing controlled peroxide-shift in a twin-screw extruder.



Micromixing model of peroxide-shift of Polypropylene.

Several mathematical issues concerning random chain scission have been addressed in an article publiced in *Polymer*. The Monte Carlo sampling approach has been generalized to yield analytical expressions for distributive properties.

Key publications 2011

Iedema, P.D., Remerie, K., Ham, M., Biemond, E. & Tacx, J. (2011). *Controlled peroxide-induced degradation of polypropylene in a twin-screw extruder: Change of molecular weight distribution un conditions controlled by micromixing.* Chemical Engineering Science, 66(22), 5474-5486.

Iedema, P.D. (2011). *Mathematical modeling of distributive properties of linear homo- and copolyn subjected to scission.* Polymer, 52(16), 3537-3549.

Schalkx, H., Iedema, P.D., Reissland, B., van Velzen, B. (2011). *Aqueous Treatment of Water-sensi Paper Objects.* Journal of Paper Conservation, 12 (1),11-20.

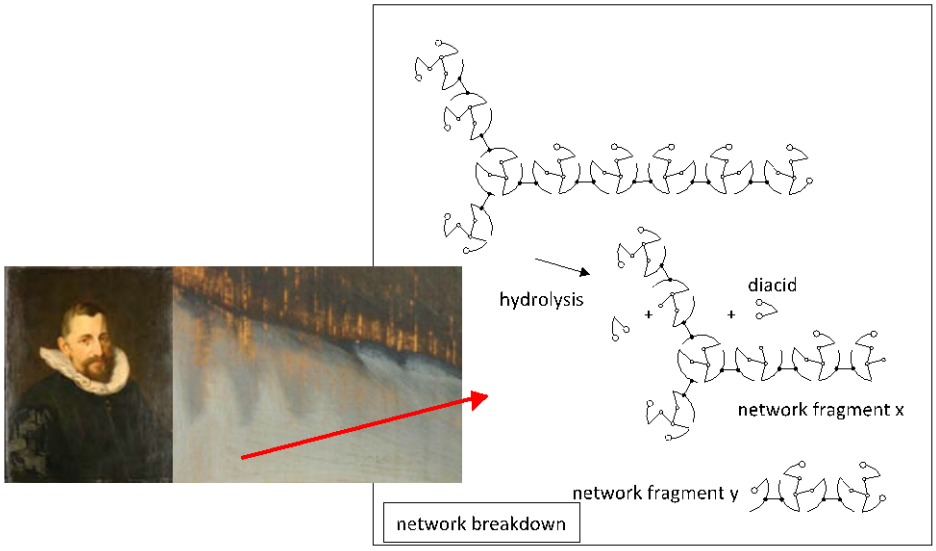
Grants

A network grant (600 k€) has been obtained from the NWO-Programme "Science4Arts" under the title: *Below the Surface of Oil Paintings - the effects of conservation treatments, display and storage conditions on the chemical reactivity and mobility in oil paints*

Highlights

The involvement in research activities in the area of Conservation and Restoration of Art Objects (CR) has further intensified. This has resulted in a paper in the *Journal of Paper Conservation* addressing some interesting transport phenomena occurring in equipment ('capillary unit') for the cleaning of gouache paintings. Furthermore, a network grant has been obtained from the NWO-Programme "Science4Arts" under the title: *Below the Surface of Oil Paintings - the effects of conservation treatments, display and*

storage conditions on the chemical reactivity and mobility in oil paints. This has started the cooperation with experts in the CR-field: Dr. Annelies van Loon (Mauritshuis), Dr. Katrien Keune and Drs. Maartje Stols-Witlox (Teacher CR-Master at Humanities Faculty). Some preliminary experiments concerning the migration of metal soaps in a paint layer have been carried out. This was used as input for writing and submitting a full proposal in the Science4Arts Programme that further involved the extension of the research network with museums, other research institutes and industries (DSM, Shell). Besides acting as the main applicant for the full proposal under the name *PAinT* (acronym for *PA*int *in T*ransition) Prof. Iedema has set up an outline for the mathematical treatment of degrading linseed oil based paint networks. It is the first in its kind in the Arts area, as shown in the Figure below.



Mathematical model of linseed oil based paint layer degradation

3 Strategy, activities and results

HIMS is performing scientific and applied research of importance for a sustainable society, energy supply, health, forensic applications, and is active in valorisation of know-how. HIMS participates in important national and international research programmes, such as NRSCC, CATCHBIO, COAST, and also in the FES programmes *Towards Biosolar Cells* and *Towards a Sustainable Open Innovation Ecosystem (NanoNext.NL*). HIMS is also partner in the programme quantitative multidimensional imaging for individualized treatment (QUANTIVISION); part of the countrywide initiative NWO-Theme *New Instruments for Healthcare* (NIG). Most of these programmes are performed together with researchers from the AMC, VU, FOM institutes and the chemical industry. In addition, HIMS is active in several EU programmes. HIMS recently started research activities in forensic sciences. HIMS will also expand their teaching efforts and in art sciences research activities will be started soon. Finally, HIMS will increase the number of PhD diplomas and the efficiency of their doctoral research path, in line with the 100+ programme of the faculty.
An overview of the HIMS activities, objectives and results for 2011, as defined in the FNWI-UvA/CvB agreement (convenant) 2010-2012, are given in the following table.

	Activities	***Objectives and results***
2011	a. recruitment of outside and guest PhD students b. improve the efficiency of the doctoral research path through better control and guidance c. develop policies for appointing of 3-5 endowed (part-time) professors d. discussions with education- and teaching directors, from within and outside the faculty, about a greater HIMS share in teaching tasks e. agree with the colleagues of the VU for the three HIMS key-areas on the creation of Centers of Expertise (according ACMM) f. new research initiatives with the VU, including in the new field of renewable energy (including Physics UvA and VU) g. New research initiatives in the field of forensic- and - art sciences with various partners, based on such new NWO (early 2010) and EU programs h. Strengthening of cooperation with industry i. Submission of individual grants (e.g. NWO-Vernieuwingsimpuls or ERC) j. Submission of equipment grants (e.g. NWO-Groot) k. Increase of the number of doctorate degrees as compared to the average level of the last years (15/year)	Ad a. 1-2 additional PhD Ad b. develop and formulate policies; increased efficiency when compared with past period Ad c. preparation and appointment of 1-2 new (preferably endowed) part-time professors Ad d. HIMS share in the curricula will be increased in relation with the new Ba-Chemistry and with the Ma-Sustainability (all with the VU) Ad e. start CoE *Synthesis & Catalysis* and start joint activities for *Analysis* (in COAST) *and Spectroscopy* (in LaserLab Amsterdam) Ad f. prepare and submit 1-2 new research projects; first are submitted at FOM and STW Ad g. prepare and submit 1-2 projects together with various relevant partners Ad h. establishment of a company in the Science Park; stimulate new spin-off activities Ad i. submission of 2 individual grants Ad j. submission of NWO Groot proposal for mass spectrometry equipment Ad k. realisation of 20 doctorate degrees

Realisation of activities
Recruitment of outside and guest PhD students (activity a)
The institute has succeeded to appoint in 2011 three outside PhD students (research will be performed externally, but doctorate degrees will be obtained at HIMS) as well as three guest PhD students (externally employed, but research performed internally/at HIMS) (point a). All guest (external) PhD students are from abroad (France, Malaysia and China) and will perform their PhD studies at HIMS using a grant from their own country or from an international exchange programme. Doctorate degree defences for the new outside and guest PhD students are planned for 2015 and 2016. In 2011 four guest PhD candidates, from Pakistan (2x), China and Vietnam, obtained their doctorate degree at HIMS.

The target for the number of doctorate degree defences at HIMS (point k) is not achieved in 2011: instead of the 20 foreseen only 15 were realized. At least three of the five missed defences were delayed and will take place in 2012.

Improve the efficiency of the doctoral research path through better control and guidance (activity b)
The policy of the Institute to improve the efficiency of PhD programs (point b) comprises three activities. HIMS started a biweekly PhD colloquium, in which a starting PhD student and a PhD student in the final phase of the doctoral research project will respectively give a presentation on research plans and results achieved. The organization of the colloquium cycle is responsibility of dr. Bernd Ensing. New policies to promote the efficiency of the doctoral research path, are subject of structural discussions within the HIMS advisory board (BAR; Beleidsadviesraad). Finally the institute has successfully introduced a financial arrangement for PhD candidates to facilitate the promotion efficiency (2000 € for a finalized and approved thesis within four years and two months).

Develop policies for appointing of 1-6 endowed (part-time) professors (activity c)
The plan to establish or continue three to five endowed chairs (period 201-2012) in the field of chemistry in collaboration with the chemical industry (point c) has been only partly realized. In November 2011, The University Board authorized the Foundation Criminalistics to establishment the new endowed chair Forensic Analytical Chemistry. Meanwhile, the curatorium of the chair has nominated a candidate chairholder in the person of the head of the research department of the Dutch Forensic Institute (Nederlands Forensisch Instituut/NFI). In addition possibilities to connect to the institute a forensic medical specialist of the AMC as an endowed professor were explored. Furthermore, we are still actively seeking suitable candidates for reoccupation of the endowed chairs in the field of Industrial Fine Chemicals (Stichting Beta Plus), Molecular Spectroscopy (John van Geuns Fonds) and Action Spectroscopy (Stichting Physica).
A greater HIMS share in teaching tasks (activity d)
The institute is looking for ways to increase service education in chemistry (point d). Next year, the teaching load of HIMS will be decreased, with a corresponding decrease in income, as a direct consequence of the shared Bachelor of Chemistry with the VU. As part of the faculty's research cluster Sustainable Chemistry, which is part of the new research profile of the UvA, we are working on a curriculum for a minor Sustainability. The intention is that this minor can be followed by students of all UvA courses and without much knowledge of chemistry. The curriculum for the joint Master of Sustainability of UvA and VU is determined. The Master will start in 2012. One disappointment is that HIMS staff members were not selected in 2011 for teaching at the Amsterdam University College (AUC). The impression is that the VU has the role of preferred supplier of the AUC. An inventory will determine whether the establishment of the teaching portfolio of the AUC was correctly performed in 2011.
The creation of Centers of Expertise (according ACMM) (activity e)
Important progress has been made regarding the establishment of three Centers of Expertise (point e) in areas where UvA and VU have complementary expertise and that are important for the Dutch chemical industry.
Since 2010 the Molecular Photonics Group is a full partner in *LaserLab Amsterdam*, a partnership of VU and UvA. Buma of HIMS acts as the Program Manager of the programme *Analytical Chemistry and Spectroscopy*. Under the umbrella of LaserLab Europe, where LaserLab Amsterdam is part of, the Molecular Photonics group of HIMS offered various European research groups access to its specialized instrumentation and infrastructure. Another activity directly related with the participation in Laser Lab Amsterdam, is the participation of Molecular Photonics in IQ (Institute *QuantiVision*), one of the eight major research centers of excellence of the Innovative Medical Devices initiative in the Netherlands.
The Center of Excellence COAST is the nationwide research and education initiative - directed by NWO and the Topsector Chemie - in the field of Analytical Chemistry in the Netherlands, which now has more than the 60 industries, institutes and academic groups participating. Headquarter of COAST is located at HIMS in the Science Park Amsterdam, where an important part of the research and (academic) education COAST also takes place. Researchers of HIMS are project managers of two of the nine projects approved by COAST in 2011.
The catalytic groups of Reek and Rothenberg are actively working to set up CoE in the field of catalysis and sustainable chemistry, preferably in the form of an institute to be established together with the industry

(ISCA, see also point h). In collaboration with the VU we are exploring an initiative in the field of sustainable energy and sustainable chemistry (point f). This is a broader initiative, where ISCA could be part of.

New research initiatives with the VU (activity f)

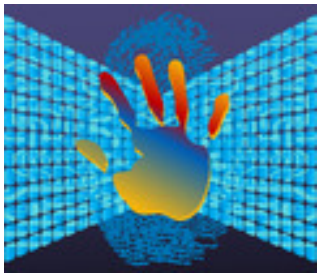
In 2011 a promising start was made with the acquisition of research grants from NWO and STW based on the UvA-VU collaboration (point f). In 2010 FOM decided to reconstruct the present Institute for Plasma Physics Rijnhuizen - the Netherlands institute for nuclear fusion, to the new FOM institute for fundamental energy research. The intention is, in consultation with other disciplines, to explore the opportunities for a broader institute, including the initiative to set up some so-called focus groups at universities in the Netherlands. In relation with this initiative the UvA and VU in 2011 submitted together a revised application for *solar fuels* to FOM. In cooperation with the groups of Van Grondelle and Croce (both VU) and Hellingwerf (SILS), Reek has prepared a FOM programme proposal. The research proposed is in the field of Photosynthetic Efficiency of biological and bio-inspired systems to prepare fuels from atmospheric CO2. Kleijn actively contributed to the succession of Prof. Griessen (VU) in the field of materials for solar fuels. Collaboration with the University of Amsterdam in this area seems easily possible.

New research initiatives in the field of forensic- and art sciences with various partners (activity g)

The past year was a successful year for the two interdisciplinary areas of HIMS: Forensic Science and Art Science (point g). On the 14th of December the Amsterdam Center for Forensic Studies (ACFS) opened with a symposium. In the center the knowledge of scientists of the Dutch Forensic Institute (NFI), the Amsterdam Medical Center (AMC) and the faculty are virtually brought together. Within this framework, NFI, AMC and faculty agreed through a *memorandum of understanding* on important issues as confidentiality, and sharing information and databases. The investments of HIMS in this area also led to results in 2011 by acquisition of research budgets (2e geldstroom). Peter Schoenmakers received a grant from NWO for his research project COMFOR: *The use of comprehensive two-dimensional chromatographic methods for chemical profiling or complex natural materials*. Gabriel Vivo (HIMS) and Marian Sjerps (KdVI) also received a NWO project grant for a proposal to develop forensic applications for detection of substances based on chromatography and mass spectrometry techniques. Peter Iedema received a large grant from the NWO Science4Arts programme for the research project *Below the Surface of Oil Paintings*.

NWO
Nederlandse Organisatie voor Wetenschappelijk Onderzoek

Forensic Sciences



Science4Arts

Strengthening of cooperation with industry (activity h)

In 2011, the institute has made great efforts to bring cooperation with the industry to a higher level (point h). In the area of sustainability and catalysis we look for strategic partners. The institute aims to start industrial partnerships with a few large companies to establish a new public-private research institute with a total budget of around 15 million €. The plan was discussed with representatives of the Topsector Chemie, and found direct support since the initiative perfectly fits with the internationalization plans of the Topsector

Institute for Sustainable Chemistry Amsterdam (ISCA)

Chemie. The formation of the ISCA shows slow but steady progress. Points of discussion are the financial share of the first large commercial partner, the participation of industrial partners in related *spin-offs* of HIMS and the appointment of the CEO.

The institute also discussed with two industrial parties - DSM Resolve and Eastman – the possible establishment of a *" dependence "* of these companies at the Science Park. These discussions are not yet finalized.

Submission of individual grants (activity i)
In the past year, many employees of HIMS tried to acquire a large individual research grant from NWO (Vernieuwingsimpuls) or the European Union (ERC grant) (point i). Bas de Bruin received late 2011 a VICI grant of 1.5 million € for his research *Radical in Catalysis: Selective Metal-Mediated Radical-Type Transformations*. Jos Oomens of the FOM Institute Rijnhuizen as well as professor at HIMS, also received a VICI grant. Four HIMS staff members submitted a VIDI proposal in 2011 (Vreede, Grecea, Shiju and Van der Vlugt). The result of this competition is not yet known. From HIMS also several applicants submitted for ERC starting grants. Some applications have penetrated to the second evaluation round and one project is approved already. Jarl Ivar van der Vlugt (Supramolecular and Homogeneous Catalysis) received 1.5 million € for his program *Smart Systems for Small Molecule Activation and Sustainable Homogeneous Catalysis*. Aurora Cruz-Cabeza (Computational Chemistry) received a VENI grant for her project *How do molecules crystallise?*

Submission of equipment grants (activity j)
The renewal of major equipment is always an issue (point j). Three groups have filed a request within the BAZIS program - related with the Sectorplan Natuurwetenschappen - (equipment for 200-400 K€), a fourth group has an application pending for the NWO Middelgroot programme, (800 K€). Maurice Janssen, VICI laureate with a position at the VU, has received a grants of 80K€ for a BAZIS application which was submitted jointly with Buma.

Research program of the Director

DIFFER
Dutch Institute for Fundamental Energy Research
Formerly FOM Institute for Plasma Physics Rijnhuizen

When the new director, Aart Kleijn, came to HIMS it was agreed that he would not take his research activities with him to HIMS. The move would be too costly and time consuming for a relatively short period. Therefore, his research program on the dynamics on molecular interactions at solid surfaces is carried out at the FOM Institute DIFFER, formerly the FOM Institute for Plasma Physics Rijnhuizen. The research program is part of the activities of FOM and not of the HIMS. Kleijn remains a part-time FOM employee to carry out this work. The work is concerned with four specific research programs:

1. Gas dynamics of the large simulator of plasma surface interaction in a fusion reactor such as ITER.
2. The influence of neutron bombardment on the hydrogen retention properties of metals.
3. The interaction of N-atoms with various surfaces.
4. The interaction of simple molecules and stepped nickel surfaces.

The items 1 and 2 are part of the FOM fusion program. 3 is funded by M2i in a collaborative project with ASML. 4 is an NWO-CW project that is carried out at Leiden University. The 3 PhD students and 1 postdoc have a daily supervisor at the institution concerned. When communicating about this work Kleijn always uses the UvA affiliation in addition to FOM and/or Leiden.

Holland Research School of Molecular Chemistry (HRSMC)
Accreditations in 1994, 1999, 2006 & (expected for) 2011

The Holland Research School of Molecular Chemistry (HRSMC) was founded in 1994 and has been twice re-accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW). The HRSMC is now in the third period 2005-2012. Formally, the third period was from 2005-2011. However, in 2009 the HRSMC received a one year extension from the KNAW (because of the Research Quality Assessment 2001-2009 that took place in 2010 at the institutes). In 2011, the HRSMC was visited by a Peer Review Committee in order to apply for re-accreditation for the fourth 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.

Activities 2011

1. Annual HRSMC symposium (November 4, 2011). The Annual HRSMC symposium, which was attended by ca. 140 scientists, also included poster sessions with 45 posters, mainly presented by PhD students.
2. The HRSMC educational activities of 2011 consisted of:
   - The two weeks Course 'Molecular Simulation', organised under the auspices of CECAM (January 3-14 2011, UvA)
   - The HRSMC Course 'Physical Methods in Inorganic Chemistry' (Jan. 24, 28, 31 and Feb. 1, 2011, UvA/UL)
3. In addition the following special activities were organized:
   - The research groups of Prof. dr. H. Hiemstra (UvA), Prof. dr. R.V.A. Orru (VU) and Prof. dr. H.S. Overkleeft/Prof. dr. G. van der Marel organized two 'Synthetic Chemistry problem solving sessions'.
   - Following the advice of the Education Committee, the first HRSMC lab visit within Research Theme 2 (Photochemistry and (Laser) Spectroscopy) was organized at the UL on January 25, 2011. Four HRSMC research groups were visited by PhD students, postdocs and staff members from other UL, VU and UvA HRSMC groups. As within research theme 2 a lot of specialized equipment is used, this lab visits were organized to share expertise and knowledge, and to stimulate collaboration.
   - Following the advice of the PhD platform, an Introduction Event for first-year PhD students as well as a Social Event for all HRSMC members was organized on June 9, 2011. At the Introduction Event several Board members and members of the Education Committee gave an overview of the research and educational activities within the HRSMC. The Social Event, a soccer tournament and some games, was organized by PhD students and the HRSMC, as a networking activity between UvA, UL and VU PhD students.

4 Dissemination of knowledge, valorisation, promotional activities

Valorisation of know-how is of increasing importance, as evidenced by the two HIMS spin-off companies, *InCatT* (Prof. Reek c.s.) established in 2009 and *YellowDiesel* (Prof Rothenberg c.s.) established in 2008. Both companies were realized under the umbrella of the UvA Holding. In order to protect our intellectual property, HIMS follows an active patenting policy, on most occasions directly with our industrial partners. The institute has applied for several patents, while some new projects are promising. Patent Apllications of HIMS in 2011:
A novel way to detect infections has been patented (patent 11166364.7-2204 "*Device and probe for detection of infection*" , Zhang/Molecular Photonics and Aalders/AMC).
Improvements on CLIPS-technology, P. Timmerman/Pepscan, L. E. M. Smeenk, N. Dailly, J. H. van Maarseveen/ Synthetic Organic Chemistry, EP 10188743.8, filing date: 25-10-2011.
Functionalized Materials by Catalyzed Carbene Copolymerization; Jellema, E.; Jongerius, A.L.; Fransen, N.G.M.; de Bruin, B./Homogenous and Supramolecular Catalysis; WO 2011/157444 A1; PCT/EP2011/003016. International publication date: 22 December 2011.
Coordination Complex System Comprising a Second Building Block without Donor Moiety; Pawel Dydio, Joost NH Reek/Homogenous and Supramolecular Catalysis; EP11177920.3, Application date: 18 August 2011.
Calderone, V.R., Shiju, N.R., Rothenberg, G. & Curulla-Ferré, D. (Heterogeneous Catalysis and Sustainable Chemistry). Core-shell particles with catalytic activity; EP11305657.6, Application date: 30 May 2011.
The ammoximation patent of Dr. Raveedran Shiju/Heterogeneous Catalysis and Sustainable Chemistry (filed in 2010) was sold to industry. Our industrial partner will invest also €0,25M in cash in a research project at HCSC aimed at developing this catalyst further.
In the future out-licensed patents could be important for HIMS as source of income.

The work of the HIMS research groups raised national and international publicity, including publications in various newspapers and on various websites. HIMS research highlights, awards and other measures of esteem with a high scientific and societal value we are proud of are:

General
HIMS scientific director professor Aart Kleijn and professor Gadi Rothenberg of the Heterogeneous Catalysis and Sustainable Chemistry group contributed to the 'State of Science' (Stand van de Wetenschap) series of the UvA Alumni Community. On 10 October 2011 they discussed for an interested - mostly non-expert audience - sustainable chemistry, catalysis, the relation between basic and applied research, knowledge transfer and innovation.
The Chemistry Master teaching programme (many teachers come from HIMS) received the highest score according to the Guide of Higher Education (Keuzegids Hoger Onderwijs) 2011.

Sustainable Chemistry
Jan van Maarseveen presented a NEMO lectures with the title *'Waarom kunnen we niet zonder water? (Why do we need water?)'* for an audiences of young kids.
Jan van Maarseveen was elected again by the ACD as best chemistry teacher 2010-2011 (as he was in 2009-2010).
A patent application *"Improvements on CLIPS-technology"* was filed by P. Timmerman, L. E. M. Smeenk, N. Dailly and J. H. van Maarseveen (EP 10188743.8, filing date 25-10-2011)
Prof. Rothenberg was appointed to the Scientific Advisory Board of the new CNRS lab in Shanghai, funded jointly by Rhodia/Solvay, the CNRS, ENS-Lyon, and East China Normal University.
For research on a new biodegradable and recyclable synthetic resin professor Gadi Rothenberg was nominated for the Huibregtsenprijs 2011, awarded 7 november 2011 during the twelfth 'Avond van Wetenschap & Maatschappij' (Evening of Science&Society).
Several key publications of the Catalysis theme have attracted the attention of the popular press, leading to radio interviews and articles and commentaries in popular journals and on the web. To mention are:

Joost Reek was interviewed by the Dutch daily newspaper "De Pers" in an article *'De beste plant is nep'* on artificial leaves. Joost Reek was also interviewed (BNR-radio) on *'Bioinspired catalysis for green energy'*.
Gadi Rothenberg was interviewed on his valorization activities in the radio program Wetenschap24
The Angewandte Chemie International Edition publication *Remote Supramolecular Control of Catalyst Selectivity in the Hydroformylation of Alkenes* of Joost Reek c.s. was highlighted in C2W
The article by Joost Reek and colleagues on *Cofactor-Controlled Enantioselective Catalysis* in the Journal of the American Chemical Society received media coverage both abroad (e.g. C&EN News, Chemistry World) and in the Netherlands (Chemisch2Weekblad/C2W).
Gadi Rothenberg and Albert Alberts (Heterogeneous Catalysis and Sustainable Chemistry) received quite a lot of media coverage of their development of a new biodegradable and recyclable synthetic resin. It was featured in the national newspapers Trouw and Sp!ts. Rothenberg was a guest in the Hoe?Zo! popular science radio show.
The Rothenberg group publication of an antagonistic catalyst in Angewandte Chemie was featured by the Dutch popular science website Kennislink and the chemistry biweekly C2W
The spin-off company, Yellow Diesel BV, of the group Rothenberg has finalised the lab development of a continuous process for manufacturing biodiesel by heterogeneous catalysis. The company is now seeking investment for scaling up the process to manufacturing scale (more details below).
The spin-off company, InCatT, of the group Reek, develops new technology in the field of homogeneous catalysis and supramolecular catalysis and started to make new chemicals by using in-house developed technology (more details below).
Dr. Bas de Bruin presented a NEMO lecture with the title *'Hoe maakt een spin een draad? (How does a spider make a thread?)'* for an audience of young kids.
A patent application on *Coordination Complex System Comprising a Second Building Block without Donor Moiety* was filed by Joost Reek c.s. (EP11177920.3).
A patent application on *Functionalized Materials by Catalyzed Carbene Copolymerization* by Bas de Bruin c.s. was published (WO 2011/157444 A1; PCT/EP2011/003016).
A patent application on *Core-shell particles with catalytic activity* was filed by Shiju and Rothenberg c.s. (EP11305657.6)
The ammoximation patent of Dr. Raveedran Shiju was sold to industry.
More details, see chapter 2.1.

Computational Chemistry
Jocelyne Vreede (Veni laureate) of the Computational Chemistry group was awarded the Best Publication Prize 2010 of the WiF (Women in the FNWI) Network. She received her award during the WiF Annual Meeting, held on March 17, 2011. Vreede received the prize for her 'breakthrough work published in a high-impact journal' on light-induced conformational changes in photoactive yellow protein.
David Dubbeldam was portrayed in the 'Focus on Research' series, with which the University of Amsterdam brings its high profile research projects to the attention of the general public. David Dubbeldam performs computer calculations to decide what future metal-organic frameworks should look like. Metal-organic frameworks can be used to store gasses, such as carbon dioxide and hydrogen, but are also useful for purifying substances and catalysis.
The Computational groups organized several conferences/schools. To mention are the Winterschool Theoretical Chemistry and Spectroscopy in Han-sur-Lesse (Ensing), the Winterschool MolSim 2011 in Amsterdam (Meijer, Ensing, Dubbeldam), the ACMM Spring and Fall symposia in Amsterdam (Bolhuis), the FOM Biophysics meeting 3-4 October 2011 in Veldhoven (Bolhuis) and the Write it Right, International workshops (multiple editions) on writing scientific papers (Lowe).
More details, see chapter 2.2.

Macromolecular and Biosystems Analysis
Peter Schoenmakers was awarded the 2011 Chromatographic Society Martin Medal. It is the highest honour the Society confers, awarded to scientists who have made outstanding contributions to the advancement of separation science. Schoenmakers received the Martin Medal during the HPLC2011 Symposium in Budapest (19-23 June).
TA COAST (TASC Comprehensive Analytical Science and Technology) was officially launched on November 1st, 2010. This national initiative on strengthening the foundations of analytical science took

many years of preparation by a number of people, including Peter Schoenmakers and Hans-Gerd Janssen. COAST has elected Science Park Amsterdam as its headquarters and Peter Schoenmakers is its Education Director. Peter Schoenmakers and Gabriel Vivo (Macromolecular and Biosystems Analysis) received grants in 2011 from TA-COAST .
The SCM-5 (Separation and Characterization of Natural and Synthetic Macromolecules) conference took place in Amsterdam in early 2011, with Peter Schoenmakers (Chairman), Wim Kok (treasurer), and Petra Aarnoutse (secretary) carrying most of the organization. The conference attracted some 250 people.
More details, see chapter 2.3.

Molecular Photonics
Hong Zhang of the Molecular Photonics group won the Amsterdam Science Park New Ideas Competition 2011, together with Maurice Aalders from the UvA university hospital AMC. The two researchers developed a catheter that is able to detect microbial infections at an early stage. A patent application *"Device and probe for detection of infection"* was also filed (patent 11166364.7-2204).
Hong Zhang presented his research in a short lecture *Luminescence upconversion nanoplatform* at the monthly faculty colloquium series (June 2011).
Sander Woutersen (Molecular Photonics) presented an invited lecture *"The operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy"* at Fysica 2011, the special Symposium of the Nederlandse Natuurkundige Vereniging (NNV), celebrating the 90th anniversary of the NNV.
Molecular Photonics of HIMS is one of the participating teams in the Institute Quantivision, a collaboration between the VUmc, AMC,NKI/AVL, VU, UvA and companies to develop medical imaging devices, software, and protocols to enhance the efficiency, efficacy and economy of healthcare. Wybren Jan Buma being one of the members of the Management Team.
More details, see chapter 2.4.

Forensic Sciences
Peter Schoenmakers and Gabriel Vivo received both, as one of the first applicants, grants from the NWO Forensic Science programme. The project is a collaboration of HIMS with Netherlands Forensic Institute (NFI).
More details, see chapter 2.3.

Conservation and Restoration of Art objects
NWO has provided Piet Iedema c.s. funding (600 k€) for the project titled '*How paint changes: consequences for conservation, presentation and preservation of paintings from Van Eyck to Mondriaan'*. The project is a collaboration of HIMS with the Faculty of Humanities in the field of Conservation and Restoration of Works of Art. More details, see chapter 2.5.

Valorization

For valorization of know-how the year 2011 was a very successful year for HIMS. Gadi Rothenberg and Albert Alberts (Heterogeneous Catalysis and Sustainable Chemistry) received much media attention for their synthesis of a biodegradable resin, with potentially a wide range of applications. Their invention is protected with a patent. It is important that this form of plastic does not contain chlorine, and is excellently injection mouldable. The invention has raised a lot of interest in the Netherlands and abroad. There are several contacts with companies interested in the patent.

The invention of a catalyst for ammoximation reactions by Shiju also received a much attention. The ammoximation patent was sold to a chemical company. This company will now invest also €0,25M in cash in a research project at HCSC aimed at developing this catalyst further. The Rothenberg group proved to be increasingly relevant to the chemical industry, as evidenced by several large projects directly funded by industrial partners.

Rothenberg and coworkers also invented a new catalyst, within a project funded by a multinational company. The patent is taken over by our industrial partner.

Spin-off companies of HIMS

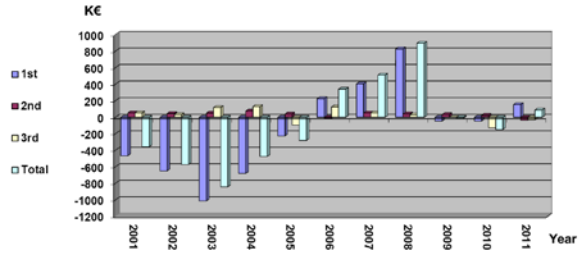
The spin-off company *Yellow Diesel BV* , started by the Heterogeneous Catalysis and Sustainable Chemistry group of Gadi Rothenberg, under the umbrella of the UvA Holding BV in 2008, has completed the experimental phase of the process of manufacturing biodiesel using heterogeneous catalysis. The company is now looking for investors that can help in the development of the process at production level. Furthermore, Rothenberg c.s are working on the development of second generation biofuels through heterogeneous catalysis. The development project is a collaboration between Yellow Diesel BV, Solarix BV and the University of Amsterdam and is funded by AgentschapNL. The current oil prices, which amounts ~ 110 - 112 dollars per barrel of crude Brent oil are too low to make the production of biodiesel profitable without government interference, but investors are still interested in Yellow Diesel project because the crude oil prices are expected to increase further in 2012.

Another spin-off company of HIMS, InCatT BV, focuses on marketing a technological invention in the field of homogeneous catalysis. InCatT was initiated in 2009 by HIMS chemist Joost Reek under the umbrella of the UvA Holding BV. The technology of InCatT is based on the concept of supramolecular catalysis developed and patented by research in the Supramolecular and Homogeneous Catalysis group of Reek. InCatT produces and tests homogeneous libraries of catalysts for its customers. The testing of the libraries of catalysts takes place in an unique evolutionary way to find the best catalyst for a particular catalytic process. Optimization of the best catalyst is done using a robot with 16 parallel reactors that records the gas-uptake curves providing the kinetic data that allows you to evaluate the catalyst performance and helps in the up-scaling of the reaction. InCatT also develops new technology and started to make new chemicals by using in-house developed technology. The InCatT laboratories are located in the building of the university (within HIMS), which makes possible to use the latest research results in the field of homogeneous catalysis.

5 Management and finances

Since 2006, the year of introduction of the new (integral costs) allocation model of the university board, the financial position of HIMS has much improved, reflecting the foreseen effect of the reorganization of the chemistry department that took place in the years 2002-2004 (see the graph below, showing the financial results - benefits minus costs - in the current decade). The effect of the more recent budget reduction of the structural university budgets (1st moneystream/ 1e geldstroom) of 10% (1 M€) for the years 2009-2012 is also clearly illustrated by the graph below.

HIMS result 2001 – 2011 (all funding sources; k€)



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

The total budget for 2011 was 14.596 k€ (213 k€ less budget available than in 2010; received budgets for future Sectorplan appointments excluded); the total costs were 14.508 k€ (see Table below). The integral result obtained in 2011 (+88 k€, all funding sources) is higher than obtained in 2009 (-12 k€) and 2010 (-147 k€). This result is very satisfactory, knowing that HIMS is confronted with a budget reduction of the structural university budgets (1st moneystream/ 1e geldstroom) of 10% (1 M€) for the years 2009-2012. This reduction forced the institute in the years 2009-2010 to spend less on salary costs and concomitantly a few vacancies for fixed positions could not be fulfilled in that years. Fortunately, following the better financial position in 2011, we could welcome two new (female) staff members in HIMS.

Actual financial numbers of 2011 (and 2010 for comparison) are given in the subsequent tables.

HIMS resources and results 2011 (k€)

2011	1st	1st others	1st total	2nd	3rd	total
Total benefits / budget	**4.346**	**1.005**	**5.351**	**4.290**	**4.955**	**14.596**
Personnel costs	-3.437	-354	-3.791	-1.582	-1.533	-6.906
Other costs	-1.194	-212	-1.406	-2.743	-3.453	-7.602
Total costs	**-4.631**	**-566**	**-5.197**	**-4.325**	**-4.986**	**-14.508**
Result 2011	**-285**	**439**	**154**	**-35**	**-31**	**88**

Including the partial restitution (+147 k€) in 2011 - from the reservation made in 2010 for discontinuation of the röntgen diffraction (RD) activities and budgets received for appointments in the framework of the Sectorplan Natuurwetenschappen (+470 k€; reservation for costs to be made in the coming years) - the HIMS result 2011 amounts +705 k€.
For more details, see chapter 7,3

HIMS resources and results 2010 (k€)

2010	1st	1st others	1st total	2nd	3rd	total
Total benefits / budget	**5.926**	**471**	**6.397**	**3.482**	**4.929**	**14.809**
Personnel costs	-3.512	-293	-3.805	-1.470	-1.475	-6.750
Other costs	-2.435	-203	-2.638	-1.988	-3.580	-8.206
Total costs	**-5.947**	**-496**	**-6.443**	**-3.458**	**-5.055**	**-14.956**
Result 2010	**-21**	**-25**	**-46**	**24**	**-126**	**-147**

Including the one-time reservation (-490 k€) made in 2010 - for discontinuation of the RD activities - the HIMS result 2010 amounts -637 k€.

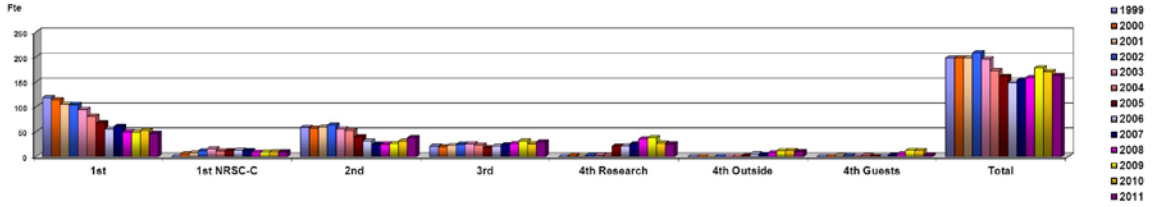
When compared with 2010, the university budget 2011 (1st moneystream) was reduced with 576k€ (the partial restitution of 147 k€ from an earlier reservation for discontinuation of the RD activities excluded). The 2nd moneystream budget increased with 807 k€, while the 3rd moneystream budget showed a slight growth of 26 k€.

The costs in the 1st moneystream were reduced with 1.246 k€, when compared to 2010. One of the reasons was that the position of work in progress was corrected in 2011. Also there were more personnel costs that could be transferred from the 1st to the 2nd and 3rd moneystream (to projects). In 2011 9.0 fte of the HIMS coworkers in fixed positions (7.1 fte staff, 1.9 fte technicians) were financed by external projects (~730 k€ costs could be charged to external parties).
Because of the increasing budgets for projects in the 2nd moneystream, also the costs in the 2nd moneystream increased (with 867 k€).

The result of 2011 is +558 k€ (the partial restitution of 147 k€ from an earlier reservation for discontinuation of the RD activities excluded), which is 705 k€ better than the result of 2010. This increase is mainly due to the correction of the position of work in progress with 538k€ .

Again, HIMS was also very successful in 2011 with acquisition of external funds for new projects: A total of 8,70 M€ external funds (5,01 M€ in 2010) were acquired from subsidiaries such as NWO (1 Vici, 1 ERC, 1 Veni, 2 ECHO grants and special grants for Forensic - and Art Sciences projects), EU, NRSC-C, NanoNext (FES), Towards Biosolar (FES), COAST, etc.

The graph below shows the personnel development of HIMS 2001-2011 per funding source.



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

1st Direct funding (eerstegeldstroom; university/direct funding)

1st NRSC-C (Top Research School Catalysis)

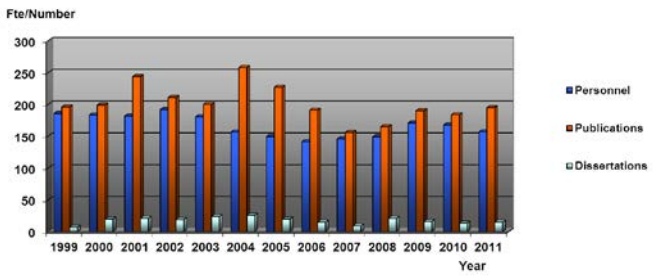
2nd Research grants (tweedegeldstroom; NWO-CW, ERC, FOM, STW, KNAW)

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 count for ~70% of our personnel costs in 2010 (in 2001 that was much less, ~40%). HIMS personnel input data for 2009-2011 was ~15-20 Fte higher than for 2006-2008, mainly related to an increase in projects in the last years.

Research input [1)] (Fte) and output (Number of publications and dissertations)



[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

The increase in projects in the latter years is reflected by an increase in output in the last years (number of publications in 2009-2011) and is in the coming years also to be expected in relation with the expected increase in the number of dissertations.

6 External evaluation

An international review committee of twenty experts examined in 2010, under the guidance of the QANU (Quality Assurance Netherlands Universities), the research achievements of seven Dutch universities, including the UvA (only HIMS) in the field of chemistry. Five HIMS research programmes were evaluated: *Bio-Molecular Synthesis, Catalysis, Computational Chemistry, Macromolecular and Biosystems Analysis, and Molecular Photonics*. The assessment, published early 2011, was made on the basis of four criteria: quality, productivity, relevance (social, economic and cultural), and vitality & feasibility (the ability to adequately respond to significant changes in the environment and the future). The review committee concluded that chemistry research at the University of Amsterdam (HIMS only) is of very good quality, as is shown in the table below.

QUANU quality scores of the HIMS research themes

HIMS themes	**Research group**	**Q**	**P**	**R**	**V**	***Average***
Biomolecular Synthesis	Hiemstra	***4***	***4***	***4***	***4***	***4,0***
	Wever					
Catalysis	Reek	***4***	***5***	***5***	***5***	***4,8***
	Elsevier					
	Rothenberg					
Computational Chemistry	Krishna	***5***	***5***	***5***	***3***	***4,5***
	Bolhuis/Smit					
Molecular Photonics	Buma	***4***	***5***	***4***	***5***	***4,5***
	Brouwer					
Macromolecular and Biosystems Analysis	Schoenmakers	***4***	***4***	***5***	***3***	***4,0***
HIMS	***Q = Quality*** ***R = Relevance*** ***P = Productivity*** ***V = Viability***	***4,2***	***4,6***	***4,6***	***4,0***	***4,4***
Netherlands		***4,2***	***4,1***	***4,6***	***4,2***	***4,3***

Source: Research Review Chemistry (Quuality Assurance Netherlands Universities (QANU), Utrecht, April 2011)

The review committee adjudged the quality of the research groups of HIMS to be of very good to excellent quality, deeply rooted and respected in local and national networks, as well as being recognized internationally. It was also positively recognized that HIMS scientific results appear almost on a regular basis in high impact journals. The average rating for each criterion was 4.35 (4 = very good) and the average HIMS citation score CPP/FCSm[8] was 1,81, also well above the international average (see the following table). The Committee supports the stronger collaboration and revision of the chemistry programmes at UVA and VU as they expect this will lead to a better critical mass and in view of already existing synergies to substantial added value. The committee supports the programmed implementation of the UvA-VU collaboration and revision of the chemistry programmes described in the Sectorplan Natuurkunde Scheikunde (SNS), which will lead to a substantial restructuring of the Institute - reducing the present five themes in future to less with a strong emphasis on sustainability and energy. The Committee sees a balanced effort, which includes a strengthened computational chemistry programme at UvA, as the only really promising way in the context of the Amsterdam Center for Multiscale Modelling (ACMM). The Committee regrets that a promising programme such as Molecular Photonics is not profiled more strongly in the foreseen restructuring. The Committee strongly supports the Biocatalysis initiative (new chair) within the Sector Plan as this will strengthen further the already highly successful catalysis group but it cannot judge the impact of the planned new chair for Supramolecular Separations as the direction there is less clear.

[8] CPP/FCSm: impact of all articles, compared to the world citation average (CPP/FCSm=1.00) in the (sub) fields in which the institute is active.

Following the recommendation of the international review panel the HIMS strategy for the coming years is as follows for the institute as a whole as well as for and the individual programmes.

The Institute

The international review panel felt the interaction between different research groups of the Institute could be strengthened. The relocation of the HIMS to the Science Park Amsterdam, where all science disciplines have been located under one roof since 2010, will help rectify this minor issue. We strongly intend to strengthen even further our collaboration with the VU. This will be implemented by focusing on 4 themes in HIMS. Following the recommendation by the committee we will enhance the visibility of Molecular Photonics by maintaining it as a separate programme. This leads to the following four themes and their embedding in the UvA-VU and national landscape:

Sustainable Chemistry, consisting of Synthesis and Catalysis. This is mainly an UvA activity, part of which may be transferred to a new research Institute at the UvA (Institute for Sustainable Chemistry/ISCA, see chapter 3). A new chair on Biocatalysis, funded by the SNS, will be part of the theme.

Analytical Chemistry. This will be carried out in synergy with the VU and the national center TA COAST, which is established at HIMS. A new chair on Supramolecular Separations, funded by the SNS, will be part of the theme.

Molecular Photonics. This activity will be carried out together with the VU and AMC as part of Laser Lab Amsterdam.

Computational chemistry. This activity will be carried out together with the VU as part of the Amsterdam Center for Multiscale Modelling (ACMM).

Besides these four themes there are small activities in themes 2 and 4 in the interdisciplinary areas of Forensic Sciences and Art Sciences, which are driven by activities outside HIMS. These activities have not been reviewed by the panel.

Quality and academic reputation

The citation analysis (see below in more detail) has shown that the Institute is performing very well and that the younger staff is building up considerable strength. We expect very good to excellent research in the future. The interactions between the groups will be strengthened where possible. We do emphasize that our present four themes have strong interactions with outside partners listed above.

Resources

The university funding will not show dramatic growth. The Institute has to maintain and will try to increase its share of external funding. Filling of vacancies will be done as much as possible, but with the perspective that regular university funding will not increase.

Productivity

The output in publications is very good and this level needs to be maintained. Attempts will be made to boost the interaction with industry. We aim to increase the output in terms of patents and valorisation. Sustainability will be the focus of theme 1 and will be studied in theme 2, 3 and 4 as well.

Strategy for the future

Most of the strategy has been outlined above and in chapter 3. Quality of research will be closely monitored. In 2012 Prof. Ron Wever will retire. The activities in the field of Biocatalysis will be continued, also with support from SNS funding. Forensic Sciences and Art Sciences will be carried out at a modest scale in line with other research activities in HIMS and at the University of Amsterdam. The Institute will not take a leading role in these fields, but supports such interdisciplinary research at a modest level.

PhD training

PhD training will be examined regularly, both at the HIMS level and also through research schools, notably HRSMC, which is managed by prof. W.J. Buma at HIMS. A new system for PhD student monitoring will be created with the aim to better assess and tutor the students. Special PhD-student seminars were established in 2011 within HIMS.

Programme level

Bio-molecular synthesis (theme 1)

It is vital for a successful continuation of the biocatalysis research programme that the plan for the succession of Prof. R. Wever will be realized in 2012, using the available SNS funding. The group intends to seek additional external funding to expand its size and replace some of the aging equipment. This theme will merge with theme 2.

Catalysis (theme 2)

The catalysis groups are planning to create a Center of Excellence in Catalysis & Chemistry (Institute for Sustainable Chemistry/ISCA; see also chapter 3), after accommodating HIMS theme 1. The quality of the scientific output is expected to increase in this way. The theme will strive to maintain its excellence in all aspects.

Computational chemistry (theme 3)

The review committee acknowledges the excellent quality and relevance of the main focus of the theme. In addition, the productivity and quality of the research was viewed to be excellent throughout the whole review period. As far as viability is concerned, the University of Amsterdam appointed a new professor in 2011 (Dr. Evert Jan Meijer), which will guarantee an excellent viability of the theme for the future.

Macromolecular and Biosystems Analysis (theme 4)

The review committee recognizes the high relevance of the main focus of the theme. The committee is surprised that mass spectrometry is positioned in SILS rather than HIMS. We believe that this will not at all limit the quality of mass spectrometry at the UvA. The group will expand and diversify by the appointment of a SNS funded professor in the field of Supramolecular Separations. We expect that this will contribute to an increase the number of publications from the theme. The interaction between the theme and TA COAST will remain very close and strong. The continued interaction with the VU will be pursued.

Molecular photonics (theme 5)

Following the recommendation by the committee we will enhance the visibility of molecular photonics by maintaining it as a separate programme. The theme certainly aims to further increase its scientific quality and publish even more in top quality journals. The theme is actively working on developing new photo sciences methods to further improve the standing of the group.

On the occasion of the 2010 evaluation, the CWTS conducted a bibliometric analysis over the period 1999-2008. The results of the bibliometric analysis for the HIMS themes & groups are shown in the table below.

Latest CWTS scores of the HIMS research themes and groups

HIMS themes & Other activities	**Research group**	**CPP/FCSm 1999-2008**	
		group	**theme**
Bio-Molecular Synthesis	Hiemstra	2.01	1.86
	Wever	0.99	
Catalysis	Reek / Van Leeuwen	2.07	1.87
	Elsevier	1.37	
	Rothenberg	1.51	
Computational Chemistry	Krishna	1.82	2.14
	Bolhuis/Smit	2.34	
Macromolecular and Biosystems Analysis	Schoenmakers	1.26	1.26
Molecular Photonics	Buma	1.89	1.81
	Brouwer	1.50	
Röntgen Diffraction	Peschar / Schenk[1]	0.80	1.02
Polymer & Process Systems	Iedema	0.98	
Reactor Dynamics	Van den Heuvel[2]	1.50	
Total HIMS		**1.81**	

PP/FCSm: Impact of an institute/group's articles, compared to the world citation average in the (sub)fields in which the institute/group is active.
Source: Bibliometric analysis performed by the Center for Science and Technology Studies (CWTS), 2010

[1]discontinued 01-01-2011

[2]retired and discontinued 01-10-2010

In the period 1999-2008 HIMS published 1602 papers used in the present CWTS analysis. These publications had an average of 37.5 references per paper and were cited in total 30,767 times, incl. self-citations (on average 19.2 citations per paper, identical to the average of all Dutch universities). References to papers published before 1980 and to non-published papers were not used in the analysis.

CPP/FCSm, the ratio of the average number of citations per publication (corrected for self-citations) CCP and the world mean field citation score FCSm is an important indicator of a publication's impact compared to the international average. It should be noted that the registration in the present 2010 CWTS analysis (future perspective; publications of staff members per theme present at January 01, 2008) is quite different from the registration in the older analyses (past performance; publications of all staff members per theme present in that period).

Compared to the journal and field average impact levels, HIMS performs very well. With CPP/JCSm and CPP/FCSm values of 1.21 and 1.81 respectively, the HIMS researchers score higher than the average of all Dutch chemistry researchers combined (see table above).
The output is stable over the years (see also the table below), while the impact shows a fluctuating pattern, with high impact scores at both the initial and final blocks of the trend analysis. Since this is due to high impact papers in the early years and some high impact publications in 2007 and 2008, it shows that the younger staff has reached the high quality level of their predecessors and re-established the international position of the individual research groups. All five HIMS themes have individual scores well above 1.0.

An important observation of the present CWTS analysis is that in all seven fields representing >5% of the output, HIMS groups achieve high impact scores. In three of these seven fields impact levels amount to twice the worldwide average (see table above). It was noted that the present Biocatalysis group of HIMS has a lower impact; their output represents only a small portion of HIMS.

Another observation of the CWTS analysis is that for the UvA the single institute output (41%, CPP/FCSm 1.87) covers the largest share of the output, although the difference with international output (36%, CPP/FCSm 1.80) is small. The remaining output (23%, CPP/FCSm 1.74) is national output. For HIMS very high impact scores were reached in the period 1999-2008 . In the coming years the senior staff of HIMS will be increasingly involved in international programs and projects (e.g. REVCAT/CAT, Erasmus Mundus/COMP, with the Chinese Academy of Science/MOLP). In relation with such programmes we expect that the HIMS international output will increase accordingly in the coming years.

Finally, an increase of the visibility is evidenced by the CWTS analysis for UvA/HIMS: the institute is more visible as might be expected from the output volume. In conclusion, the overall results of the 2010 bibliometric analysis are more than satisfactory for HIMS.

A comparison of the latest CWTS scores (future perspective) in relation with earlier analyses (past performance) is shown in the table below.

CWTS scores of HIMS compared with the average scores of all Dutch universities [3]

Report	Period	CPP/JCSm	CPP/FCSm	JCSm/FCSm
HIMS 2002 [1)]	**1991-2001**	**1.13**	**1.51**	**1.33**
HIMS 2008 [2)]	**2001-2007**	**1.08**	**1.58**	**1.43**
HIMS 2010 [3)]	**1999-2008**	**1.21**	**1.81**	**1.47**
All universities 2010 [3)]	**1999-2008**	**1.20**	**1.67**	**1.39**

[1)] Source: Chemistry, Past Performance and Future Perspective, Association of Universities in The Netherlands (VSNU), 2002

[2)] Source: Bibliometric analysis performed by the Center for Science and Technology Studies, 2008

[3)] Source: Bibliometric analysis performed by the Center for Science and Technology Studies, 2010

CPP/FCSm: Impact of an institute/group's articles, compared to the world citation average in the (sub)fields in which the institute/group is active.

CPP/JCSm: Impact of an institute/group's articles, compared to the average citation rate of the institute/group's journals.

JCSm/FCSm: Impact of the journals in which an institute/group has published, compared to the world citation average in the fields covered by these journals.

7 Facts and figures

7.1 Personnel

7.1.1 Research input

In the following table the research input of the HIMS staff members is presented as full time equivalents (fte) per employment type.

Research - and supporting staff 2011 of the HIMS themes, per employment type (fte)[a] **source: METIS**

	BMS	CAT	COMP	MBA	MOLP	Others	**Total**
Tenured staff	2,1	3,2	3,0	1,6	2,6	1,0	13,4
Non-tenured staff	2,1	19,1	3,9	3,9	1,4	0,1	30,5
PhD candidates	4,6	14,9	8,9	9,1	15,3	1,5	54,3
Total research staff	**8,8**	**37,2**	**15,8**	**14,6**	**19,2**	**2,6**	**98,2**
Technicians [b]	5,1	10,5	0,0	2,5	3,2	2,0	23,3
Visiting fellows [c]	0,1	0,0	0,0	0,2	0,1	0,0	0,4
Supporting staff						6,2	6,2
Total staff	**13,9**	**47,7**	**15,8**	**17,3**	**22,5**	**10,8**	**128,0**

Research - and supporting staff 2011 of HIMS and the HIMS groups, per employement type (fte)[a] **source: METIS**

	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	Others	**Total**
Tenured staff	1,6	0,5	1,5	0,6	1,1	1,6	1,0	0,4	1,6	1,6	1,0	1,0	13,4
Non-tenured staff	1,2	0,9	13,2	0,0	5,9	3,5	0,0	0,5	3,9	1,2	0,2	0,1	30,5
PhD candidates	3,1	1,5	10,3	2,3	2,4	5,0	3,9	0,0	9,1	12,7	2,6	1,5	54,3
Total research staff	**5,9**	**2,9**	**25,0**	**2,8**	**9,4**	**10,1**	**4,9**	**0,8**	**14,6**	**15,5**	**3,7**	**2,6**	**98,2**
Technicians [b]	4,3	0,8	4,9	2,0	3,6	0,0	0,0	0,0	2,5	2,2	1,0	2,0	23,3
Visiting fellows [c]	0,1	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,2	0,1	0,0	0,0	0,4
Supporting staff												6,2	6,2
Total staff	**10,2**	**3,7**	**29,9**	**4,8**	**13,0**	**10,1**	**4,9**	**0,8**	**17,3**	**17,8**	**4,7**	**10,8**	**128,0**

[a] Note that the table shows the net time available for research. 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.

Research themes: BMS = Bio-Molecular Synthesis; CAT = Catalysis; COMP = Computational Chemistry; MBA = Macromolecular and Bio-systems Analysis; MOLP = Molecular Photonics; Others includes: PS = Polymer Systems and RD = Röntgen Diffraction (discontinued 01-01-2011)

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna (retired 13-09-2011); PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema and Peschar (discontinued 01-01-2011)

7.1.2. Scientific staff

Sustainable Chemistry
5 research groups

Prof.dr. J.N.H. Reek, Vici Laureate (rg-1.1)
Supra-Moleculaire Katalyse

Prof.dr. C.J. Elsevier (rg-1.2)
Coördinatie- en Organometaalchemie

Prof.dr. G. Rothenberg, Vidi Laureate (rg-1.3)
Heterogene Katalyse en Duurzame Chemie

Prof.dr. H. Hiemstra (rg[9]-1.4)
Synthetische Organische Chemie

Prof.dr. R. Wever (rg-1.5)
Biokatalysatoren en Bio-Anorganische Chemie

Vacancy (rg-1.4)
Industriële Fijnchemie (0.2 Fte)
(bijzonder hoogleraar Stichting Betaplus)

Prof.dr. P. Timmerman (rg-1.4)
Protein-mimetic Chemistry (0.2 Fte)
(bijzonder hoogleraar Genootschap ter bevordering van Natuur-, Genees- en Heelkunde)

Dr. B. de Bruin (rg-1.1), uhd, Vidi, Vici & ERC Laureate
Dr. J.H. van Maarseveen (rg-1.4), uhd
Dr. J.I. Van der Vlugt (rg-1.1), ud, Veni & ERC Laureate
Dr. E. Eiser (rg-1.2), ud (0.1 Fte)
Dr. S. Grecea (rg-1.3), ud, Veni lauriate
Dr. N.R. Shiju (rg-1.3), ud
Dr. S. Ingemann Jørgensen (rg-1.4), ud
Dr. D.G.H. Hetterscheid (rg-1.1), Veni lauriate, pd

Computational Chemistry
3 research groups

Prof. dr. E.J. Meijer (rg-2.1), KNAW fellow
Moleculaire Simulaties

Prof. dr. R. Krishna (rg-2.2; retired 13-09-2011)
Chemische Reaktorkunde

Prof.dr. P.G. Bolhuis (rg-2.3), Vici, Vidi & FOM Springplank Laureate
Simulaties van bio-moleculaire systemen

Prof. dr. A. Fasolino/KUN (rg-2.1)
Computationele Fysica van de Gecondenseerde Materie (0.0 Fte)

[9] rg = research group

Dr. C.P. Lowe (rg-2.3), uhd, KNAW fellow
Dr. B. Ensing (rg-2.1), ud, Vidi laureate
Dr. D. Dubbeldam (rg-2.3), ud, Vidi laureate
Dr. J. Vreede (rg-2.3), ud, Veni laureate
Dr. A. Cruz-Cabeza (rg-2.3), Veni lauriate, pd

Analytical Chemistry / Forensic Analytical Chemistry
1 research group [10]

Prof.dr.ir. P.J. Schoenmakers (rg-3)
Analytical Chemistry including its applications in Forensic Science

Prof.dr.ir. J.G.M. Janssen/Unilever
Analytische Scheidingen van Biomacromoleculen (0.2 Fte)
(bijzonder hoogleraar Stichting Betaplus)

Prof.dr. S. van der Wal /DSM
Bioterials Analysis (0.2 Fte)
(bijzonder hoogleraar Stichting Betaplus)

Dr. W.Th. Kok, uhd
Dr. G. Vivó Truyols, ud

Molecular Photonics
1 research group

Prof.dr. W.J. Buma (rg-4)
Molecuulspectroscopie

Prof.dr. A.M. Brouwer, uhd (rg-4)
Molecuulspectroscopie (0.2 Fte)
(bijzonder hoogleraar John van Geunsfonds)

Prof.dr. H.J. Bakker/FOM-Amolf
Ultrasnelle Spectroscopie van Moleculen in de Gecondenseerde Fase (0.0 Fte)

Prof.dr. J. Oomens/FOM-Rijnhuizen, Vici Laureate
Action Spectroscopy (0.2 Fte)
(bijzonder hoogleraar Stichting Fysica)

Dr. H. Zhang, ud
Dr. R.M. Williams, ud
Dr. S. Woutersen, Vidi & ERC Laureate, uhd

Art sciences/Polymer and Process Systems

Prof.dr. P. Iedema
Fysische Technologie

Prof.dr. N. Tennent/GW (0.0 Fte)
Art sciences

[10] Collaboration with De Koster and Smilde from SILS

7.1.3. Management of HIMS

Scientific Director
Prof. dr. A Kleyn

Management team (bedrijfsvoering)
G.J.J. Zonneveld - De Boer, Drs. H.E. Zwaan - Van der Plas (HRSMC[11])

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. Ad Oskam (Facilities), M. Mittelmeijer (Safety), P.F. Collignon (ICT)

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

7.2 Research

7.2.1 Research input of the HIMS themes

Research - and supporting staff 2011 of HIMS per funding type (fte)[a] **source: METIS**

HIMS themes	BMS	CAT	COMP	MBA	MOLP	Others	**Total**	***%***
Direct funding[1a]	5,3	10,6	2,6	4,1	5,1	7,8	**35,4**	***28***
Indirect funding [1b]	2,4	5,3	0,0	0,0	0,0	0,0	**7,7**	***6***
Research grants[2]	2,4	10,4	10,9	0,9	5,0	0,0	**29,5**	***23***
Contract research[3]	0,2	12,8	1,3	5,4	1,4	2,9	**23,9**	***19***
Other[4]	3,7	8,5	1,0	7,0	11,2	0,1	**31,5**	***25***
Total	**13,9**	**47,7**	**15,8**	**17,3**	**22,5**	**10,8**	**128,0**	***100***

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	Others	**Total**	***%***
Direct funding[1a]	4,0	1,3	4,9	2,5	3,3	1,3	0,5	0,8	4,1	3,1	1,9	7,8	35,4	***28***
Indirect funding[1b]	1,5	0,9	3,1	1,3	0,9	0,0	0,0	0,0	0,0	0,0	0,0	0,0	7,7	***6***
Research grants[2]	1,6	0,8	8,7	0,0	1,7	7,4	3,5	0,0	0,9	3,4	1,6	0,0	29,5	***23***
Contract research[3]	0,2	0,0	7,0	0,9	5,0	0,5	0,8	0,0	5,4	1,4	0,0	2,9	23,9	***19***
Other[4]	3,0	0,8	6,2	0,3	2,1	0,9	0,2	0,0	7,0	9,9	1,2	0,1	31,5	***25***
Total	**10,2**	**3,7**	**29,9**	**4,8**	**13,0**	**10,1**	**4,9**	**0,8**	**17,3**	**17,8**	**4,7**	**10,8**	**128,0**	***100***

[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/NanoNed, 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.

Research themes: BMS = Bio-Molecular Synthesis; CAT = Catalysis; COMP = Computational Chemistry; MBA = Macromolecular and Bio-systems Analysis; MOLP = Molecular Photonics; Others includes: PS = Polymer Systems and RD = Röntgen Diffraction (discontinued 01-01-2011)

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna (retired 13-09-2011); PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema and Peschar (discontinued 01-01-2011)

Externally financed projects acquired in 2011 (mln €) per funding type[1]

HIMS themes	BMS	CAT	COMP	MBA	MOLP	Others	**Total**
1st - NRSC-C [2]	-	0.66	-	-	-	-	**0.66**
1st - Others [3]	-	0.20	-	-	-	-	**0.20**
2nd [4]	-	3.12	0.36	1.90	0.54	0.61	**6.52**
3rd [5]	0.01	0.51	-	0.78	0.02	-	**1.32**
Total	**0,01**	**4.49**	**0.36**	**2.68**	**0.56**	**0.61**	**8.70[6]**

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	PI	**Total**
1st - NRSC-C [2]	-	-	0.44	-	0.22	-	-	-	-	-	-	-	**0.66**
1st - Others [3]	-	-	-	-	0,20	-	-	-	-	-	-	-	**0.20**
2nd [4]	-	-	3.12	-	-	0.30	0.06	-	1.90	0.54	-	0.61	**6.52**
3rd [5]	-	0.01	0.11	-	0.40	-	-	-	0.78	0.02	-	-	**1.32**
Total	**-**	**0.01**	**3.67**	**-**	**0.82**	**0.30**	**0.06**	**-**	**2.68**	**0.56**	**-**	**0.61**	**8.70[6]**

[1] Matching contributions UvA/FNWI (total 3.8 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, NanoNed, Industry

[6] Budgets were obtained for 15 PhD's and 6 postdocs in 2010

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna (retired 13-09-2011); PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; PI: group Iedema

7.2.2 Research output of the HIMS themes

Research output 2011 of HIMS per type of publication **source: METIS**

HIMS themes	BMS	CAT	COMP	MBA	MOLP	Others	Joint[1]	**Total**
Refereed articles	**16**	**48**	**38**	**19**	**58**	**3**	**-2**	**180**
Non-refereed articles	2	3	0	0	0	1		6
Books	0	0	0	0	0	0		0
Book chapters	0	1	0	0	2	0		3
PhD-theses	2	5	2	2	4	0		15
Patents	1	3	0	0	1	0		5
Professional publications	0	0	0	0	1	0		1
Total	**21**	**60**	**40**	**21**	**66**	**4**	**-2**	**210**

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	PI	RP	Joint[1]	**Total**
Refereed articles	**11**	**5**	**29**	**1**	**10**	**8**	**12**	**6**	**20**	**19**	**51**	**7**	**2**	**1**	**-2**	**180**
Non-refereed articles	2	0	1	0	2	0	0	0	0	0	0	0	1	0		6
Books	0	0	0	0	0	0	0	0	0	0	0	0	0	0		0
Book chapters	0	0	1	0	0	0	0	0	0	0	1	1	0	0		3
PhD-theses	1	1	3	2	0	0	1	1	0	2	2	2	0	0		15
Patents	1	0	2	0	1	0	0	0	0	0	1	0	0	0		5
Prof. publications	0	0	0	0	0	0	0	0	0	0	0	1	0	0		1
Total	**15**	**6**	**36**	**3**	**13**	**8**	**13**	**7**	**20**	**21**	**55**	**11**	**3**	**1**	**-2**	**210**

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

Research themes: BMS = Bio-Molecular Synthesis; CAT = Catalysis; COMP = Computational Chemistry; MBA = Macromolecular and Bio-systems Analysis; MOLP = Molecular Photonics; Others includes: PS = Polymer Systems and RD = Röntgen Diffraction (discontinued 01-01-2011), and some other discontinued activities

Research groups: 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; RP group Peschar (discontinued 01-01-2011)

***Number of citations 2011 of HIMS, in ranges of different impact factor S*ource: METIS**

HIMS themes	BMS	CAT	COMP	MBA	MOLP	Others	Joint[1]	**Total**
>15	0	0	0	0	1	0		**1**
10-15	1	6	0	0	1	0		**8**
5-10	6	11	10	2	11	0		**40**
<5	9	31	28	17	45	3	-2	**131**
Total	**16**	**48**	**38**	**19**	**58**	**3**	**-2**	**180**

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	Others	Joint[1]	**Total**
>15	0	0	0	0	0	0	0	0	0	0	1	0	0		**1**
10-15	1	0	4	0	1	1	0	0	0	0	1	0	0		**8**
5-10	2	4	7	0	4	0	4	2	4	2	8	3	0		**40**
<5	8	1	18	1	5	7	8	4	16	17	41	4	3	-2	**131**
Total	**11**	**5**	**29**	**1**	**10**	**8**	**12**	**6**	**20**	**19**	**51**	**7**	**3**	**-2**	**180**

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

Research themes: BMS = Bio-Molecular Synthesis; CAT = Catalysis; COMP = Computational Chemistry; MBA = Macromolecular and Bio-systems Analysis; MOLP = Molecular Photonics; Others includes: PS = Polymer Systems and RD = Röntgen Diffraction (discontinued 01-01-2011), and some other discontinued activities

Research groups: 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; Others: groups Iedema and Peschar (discontinued 01-01-2011)

7.2.3 Efficiency of the doctoral research path

The following tables show the efficiency of the doctoral research path (period of appointment 2003-2007; planned PhD defense 2007-2011).

Employed PhD-candidates of HIMS

Enrolment (-)				Success rates of graduation							
Starting Year	Enrolment		Total	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F	(M+F)								
2003	9	5	**14**	1	4	1	2	0	2	3	1
2004	12	2	**14**	0	8	2	0	1	1	2	0
2005	7	3	**10**	1	3	1	1	0	0	1	3
2006	12	4	**16**	1	7	4	0	0	0	4	0
2007	2	6	**8**	0	2	0	0	0	0	6	0
Total	**42**	**20**	**62**	**3**	**24**	**8**	**3**	**1**	**3**	**16**	**4**
Cumulative 2003-2007											
BMS	4	2	**6**	0	4	1	0	0	0	1	0
CAT	17	3	**20**	2	9	3	3	0	0	2	1
COMP	6	5	**11**	1	5	1	0	0	1	3	0
MBA	5	6	**11**	0	0	1	0	1	0	7	2
MOLP	8	4	**12**	0	6	2	0	0	2	1	1
Others	2	0	**2**	0	0	0	0	0	0	2	0
Total	**42**	**20**	**62**	**3**	**24**	**8**	**3**	**1**	**3**	**16**	**4**
%	***68***	***32***	***100***	***5***	***39***	***13***	***5***	***2***	***5***	***26***	***6***

Non-employed PhD-candidates of HIMS

Enrolment (-)				Success rates of graduation							
Starting Year	Enrolment		Total	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F	(M+F)								
2003	3	1	**4**	0	2	1	1	0	0	0	0
2004	1	1	**2**	0	1	0	0	1	0	0	0
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	0	0	0	0	1	3	0
Total	**17**	**5**	**22**	**6**	**9**	**1**	**1**	**1**	**1**	**3**	**0**
Cumulative 2003-2007											
BMS	2	0	**2**	0	0	1	0	1	0	0	0
CAT	0	0	**0**	0	0	0	0	0	0	0	0
COMP	2	3	**5**	0	4	0	1	0	0	0	0
MBA	6	2	**8**	4	2	0	0	0	0	2	0
MOLP	7	0	**7**	2	3	0	0	0	1	1	0
Others	0	0	**0**	0	0	0	0	0	0	0	0
Total	**17**	**5**	**22**	**6**	**9**	**1**	**1**	**1**	**1**	**3**	**0**
%	***77***	***23***	***100***	***27***	***41***	***5***	***5***	***5***	***5***	***14***	***0***

M = male; F = Female Research themes: BMS = Bio-Molecular Synthesis; CAT = Catalysis; COMP = Computational Chemistry; MBA = Macromolecular and Bio-systems Analysis; MOLP = Molecular Photonics; Others = 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. Other delays are related to personal circumstances, often a job and/or a family with children 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

Bio-Molecular Synthesis (BMS)

Enrolment (-)				Success rates of graduation							
Starting year	Enrollment M	Enrollment F	Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
2003	3	0	**3**	0	2	1	0	0	0	0	0
2004	2	0	**2**	0	1	0	0	1	0	0	0
2005	0	0	**0**	0	0	0	0	0	0	0	0
2006	1	1	**2**	0	1	1	0	0	0	0	0
2007	0	1	**1**	0	0	0	0	0	0	1	0
Total	**6**	**2**	**8**	**0**	**4**	**2**	**0**	**1**	**0**	**1**	**0**
%	***75***	***25***	***100***	***0***	***50***	***25***	***0***	***13***	***0***	***13***	***0***

Catalysis (CAT)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment M	Enrolment F	Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
2003	1	2	**3**	0	1	0	2	0	0	0	0
2004	3	0	**3**	0	2	1	0	0	0	0	0
2005	7	1	**8**	1	3	1	1	0	0	1	1
2006	6	0	**6**	1	3	1	0	0	0	1	0
2007	0	0	**0**	0	0	0	0	0	0	0	0
Total	**17**	**3**	**20**	**2**	**9**	**3**	**3**	**0**	**0**	**2**	**1**
%	***85***	***15***	***100***	***10***	***45***	***15***	***15***	***0***	***0***	***10***	***5***

Computational Chemistry (COMP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment M	Enrolment F	Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
2003	3	3	6	1	2	0	1	0	1	1	0
2004	2	2	4	0	4	0	0	0	0	0	0
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	0	1	0
Total	**8**	**8**	**16**	**1**	**9**	**1**	**1**	**0**	**1**	**3**	**0**
%	***50***	***50***	***100***	***6***	***56***	***6***	***6***	***0***	***6***	***19***	***0***

Macromolecular and Bio-systems Analysis (MBA)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F	(M+F)								
2003	2	0	**2**	0	0	1	0	0	0	1	0
2004	2	0	**2**	0	0	0	0	1	0	1	0
2005	2	2	**4**	0	2	0	0	0	0	0	2
2006	2	1	**3**	2	0	0	0	0	0	1	0
2007	3	5	**8**	2	0	0	0	0	0	6	0
Total	**11**	**8**	**19**	**4**	**2**	**1**	**0**	**1**	**0**	**9**	**2**
%	***58***	***42***	***100***	***21***	***11***	***5***	***0***	***5***	***0***	***47***	***11***

Molecular Photonics (MOLP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F	(M+F)								
2003	2	1	**3**	0	1	0	0	0	1	0	1
2004	4	1	**5**	0	2	1	0	0	1	1	0
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	1	0	0	0	1	1	0
Total	**15**	**4**	**19**	**2**	**9**	**2**	**0**	**0**	**3**	**2**	**1**
%	***79***	***21***	***100***	***11***	***47***	***11***	***0***	***0***	***16***	***11***	***5***

Others

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F	(M+F)								
2003	1	0	**1**	0	0	0	0	0	0	1	0
2004	0	0	**0**	0	0	0	0	0	0	0	0
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	0
Total	**2**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**
%	***100***	***0***	***100***	***0***	***0***	***0***	***0***	***0***	***0***	***100***	***0***

Total HIMS

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F	(M+F)								
2003	12	6	**18**	1	6	2	3	0	2	3	1
2004	13	3	**16**	0	9	2	0	2	1	2	0
2005	11	4	**15**	1	8	1	1	0	0	1	3
2006	14	5	**19**	3	8	4	0	0	0	4	0
2007	9	7	**16**	4	2	0	0	0	1	9	0
Total	**59**	**25**	**84**	**9**	**33**	**9**	**4**	**2**	**4**	**19**	**4**
%	***70***	***30***	***100***	***11***	***39***	***11***	***5***	***2***	***5***	***23***	***5***

M = male; F = Female Research themes: BMS = Bio-Molecular Synthesis; CAT = Catalysis; COMP = Computational Chemistry; MBA = Macromolecular and Bio-systems Analysis; MOLP = Molecular Photonics; Others = group Iedema

7.3 Finance 2011

The table below shows the HIMS financial result 2011, excluding the teaching activities of the HIMS staff (1020 k€).

HIMS result 2011 (k€)

	1st	1st others	1st total	2nd	3rd	Total
HIMS						
Budget (fixed)	4.211		4.211			**4.211**
Budget (variable[1])	3.708	814	4.522	2.091	2.649	**9.262**
Other income	61	191	252	15	205	**472**
Matching contract research	-3.634		-3.634	2.184	2.101	**651**
Budget total	**4.346**	**1.005**	**5.351**	**4.290**	**4.955**	**14.596**
percentage	***30***	***7***	***37***	***29***	***34***	***100***
Personal costs	-3.437	-354	-3.791	-1.582	-1.533	**-6.906**
Other costs (projects)	-740	-295	-1.035	-490	-1.683	**-3.208**
Overhead (central)	692		692	-354	-338	**0**
Overhead (faculty)	-884	-127	-1.011	-891	-616	**-2.518**
Overhead (institute)	1.540	210	1.750	-971	-779	**0**
Various costs	-18		-18	-2	-1	**-21**
Other (secundary) costs	-1.784		-1.784	-35	-36	**-1.855**
Costs total	**-4.631**	**-566**	**-5.197**	**-4.325**	**-4.986**	**-14.508**
percentage	***32***	***4***	***36***	***30***	***34***	***100***
Result	**-285**	**439**	**154**	**-35**	**-31**	**88**
Restitution from reservation RD	147		147			**147**
Reservation Sectorplan appoinments		470	470			**470**
Result including reservations	**-138**	**909**	**771**	**-35**	**-31**	**705**

1st - Direct funding (eerstegeldstroom; university/direct funding)

1st - others - CvB, NRSC-C/Top Research School Catalysis

2nd - Research grants (tweedegeldstroom; NWO-CW, FOM, STW, KNAW, ERC)

3rd - Contract research derdegeldstroom; EU, DPI, AGENTSCHAP.NL,TA-COAST, EL&I/NanoNed, NanoNext, Industrial)

[1] 1e gs part assigned via allocation model

Including the partial restitution (+147 k€) in 2011 - from the reservation made in 2010 for discontinuation of the röntgen diffraction (RD) activities and budgets received for appointments in the framework of the Sectorplan Natuurwetenschappen (+470 k€; reservation for costs to be made in the coming years) - the HIMS result 2011 amounts +705 k€.