Annual Report 2012

Van 't Hoff Institute for Molecular Sciences

UNIVERSITY OF AMSTERDAM

Colophon

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(photos made for the new HIMS website)

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Preface

2012 was a year of consolidation for HIMS. The enormous amount of external funds raised in 2011 could not be sustained in 2012. HIMS had to start working on the novel projects introduced. Nevertheless, VICI grants from Dr Bas de Bruin and our extraordinary professor Jos Oomens, initiation of a research program in the field of Science4Art, significant novel NWO funding for Analytical Chemistry and a number of smaller grants demonstrate the viability of the HIMS researchers. Besides novel project budget also significant sums were obtained from the BAZIS funding of NWO for investments into new equipment.

The scientific output in 2012 was very significant and increased with respect to 2011. The Institute is doing very well in this respect. With the appointment of Dr Arian van Asten as extraordinary professor of Forensic Analytical Chemistry, the scientific staff of HIMS has been strengthened. Other extraordinary professors have been reappointed.

Highlights in education are the initiation with the VU of a joint program for the Bachelors in Chemistry. In addition, the chemistry education realized by HIMS staff members has been evaluated as excellent by a nationwide panel.

HIMS operates one national research school, the Holland Research School of Molecular Chemistry (HRSMC). This school has been re-accredited by the KNAW. In addition, NWO has given it a major grant.

The valorization and interaction with industry has also gone well, with as highlight the transfer of a very exciting patent to DSM. The development of sustainable plastics has been continued.

The launch of the new UvA website design has stimulated HIMS to strengthen its presence on the world wide web. HIMS researchers have been quite active in 2012 in outreach and contacts with media.

A new initiative really took off in 2012 for the entire faculty. The creation of the Amsterdam Faculty of Science will merge all science related research and education of the UvA and the VU. By the end of 2013 the groundwork done in 2012 should lead to a major new player in the international scientific arena. This alone already makes 2013 a very exciting year for HIMS.

Prof. Aart W. Kleijn
Director

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1. General considerations and highlights

1.1 Key figures of HIMS in 2012

The output of HIMS was on a higher level in 2012. HIMS published 5 papers (1 in 2011) in absolute top journals (impact factor > 15) and 7 papers (8 in 2011) in top journals (impact factor 10-15). The total number of refereed and other professional publications, patents and book(chapter)s amounted to 177 (195 in 2011; 184 in 2010). HIMS researchers had 2 patents granted in 2012 and filed 7 patents (5 in 2011; 3 in 2010), while 9 PhD dissertations (15 in 2011; 14 in 2010) were published.

With a total of 3,18 M€ in external funding (excluding the own matching budget of approximately 1.47 M€) the year 2012 was less successful than the top year 2011 (8,70 M€) and the year 2010 (5,01 M€). These funds were acquired from funding agencies such as NWO (HRSMC graduate program, 2 BAZIS, 1 ATHENA, 1 ECHO grants) and FOM, as well as from industry and other partners.

1.2 Personnel

The scientific staff numbers in 2012 (158,0 fte) were somewhat lower than in 2011 (163.2 fte)[1]. The reason can be mainly found in the decrease in the numbers of PhD students and postdocs in 2012 (104,9 fte combined). These were also a little bit lower than in 2010 (106,3 fte)[2].

Although the financial situation of the institute was (and still is) sound, in 2012 HIMS was not able to realize the envisaged appointments of two new full professors (Supramolecular Analysis and Biocatalysis) and a new assistant professor (UD/Supramolecular Analysis) in the framework of the Sectorplan Natuurkunde Scheikunde (SNS). These appointments will have to be realized in 2013.
Dr Arian C. van Asten of the Netherlands Forensic Institute was appointed (0,2 fte) as endowed Professor of Forensic Analytical Chemistry (with the Analytical Chemistry group) on 1 June 2012.

At the end of the year 2012 the number of vacancies at HIMS was 24 (including vacancies for various staff positions). Although this is half the number at the beginning of the year (47, which was exceptionally high), a small increase in scientific staff members is still to be expected in 2013.

1.3 Finances

HIMS finished the year 2012 with a positive financial result of +1.071K€ (+ 705 K€ in 2011). This result is satisfactory, knowing that HIMS has been confronted with a budget reduction of the structural university budgets (eerste geldstroom) of 10% (1 M€) in the years 2009-2012.

Although the financial results of HIMS were influenced by the budget reductions for the years 2009-2012, increased revenues were generated thanks to a rise in the number of PhD projects and funding through the new Sectorplan Natuur & Scheikunde (SNS).

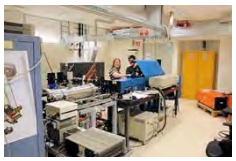
[1] Full time equivalents (fte), including all research, educational and general tasks.

[2] 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.

Additional cost reduction was realized by some (early) retirements and by the discontinuation of the röntgen diffraction (RD) activities. This was part of the HIMS cost reduction plan Chemie Financieel Duurzaam which was started in 2010 and completed in 2012.

1.4 Facilities

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 Analytical Chemistry, Computational Chemistry, Molecular Photonics and Bio-catalysis are in building D. For these groups 1566 m^2 lab space is available. Most offices and sitting rooms as well as the lecture halls are located in a separate central building, all on a very short distance from the lab spaces.

The two Catalysis research groups, the Synthetic Organic Chemistry group and the HIMS NMR-facilities are housed in a separate three floor building E, with 2052 m^2 available for the laboratories only. This building is on one side connected with the main building in which the other HIMS research groups are located, and on the other side with the bachelor student laboratories.

1.5 Highlights

In 2012 the work of the HIMS research groups gained attention inside the research community as well as outside. Here we present a selection of noteworthy HIMS highlights of 2012, illustrating the firm position of our institute both in a national and international perspective.

1.5.1 Institutional highlights

New appointment in the academic staff

Dr Arian C. van Asten (1968) of the Netherlands Forensic Institute (NFI) was appointed 0.2 fte as endowed Professor of Forensic Analytical Chemistry (with the Analytical Chemistry group) on June 1st 2012. His chair has been designated on behalf of *Stichting Leerstoel Criminalistiek* (Criminalistics Chair Foundation). As a professor by special appointment, Arian van Asten will focus on chemical profiling, analytical chemistry at the crime scene, chemical analysis for reconstruction purposes (including dating spores), chemical characterisation of microspores, databases and knowledge management, and measurement uncertainty in qualitative and quantitative forensic chemical analysis.

External professorships

Jos Oomens of the Molecular Photonics group was appointed 0,2 fte as endowed professor of *Molecular Structure and Dynamics* at the Radboud University Nijmegen. Hong Zhang of the same group was appointed as chair professor at the Northeast Normal University (China).

Valorisation

The Heterogeneous Catalysis and Sustainable Chemistry group of Gadi Rothenberg filed four patent applications, on new plastic composites and on a new Fischer Tropsch catalyst. Futhermore, the group came to an agreement with the German specialty chemicals company LANXESS to develop new catalytic routes to different olefins, key building blocks for synthetic rubber polymers. LANXESS will invest over a period of three years in this research project, with the aim of diversifying its sources for synthetic rubber raw materials.

The same Heterogeneous Catalysis and Sustainable Chemistry group transferred the patent and all related intellectual property rights on a new catalyst to DSM. The catalyst, discovered by Raveendran

Shiju, contributes to more sustainable processes for making fine chemicals and pharmaceutical intermediates and for polymer production. The transfer agreement includes a five year collaborative project to further develop the technology for application in DSM's operations.

Research school HRSMC reaccredited by the KNAW

The Holland Research School of Molecular Chemistry (HRSMC) was reaccredited for a period of six years by the Research School Accreditation Committee (ECOS) of the Royal Netherlands Academy of Arts and Sciences (KNAW). The HRSMC is a cooperation between research groups of the van 't Hoff Institute for Molecular Sciences (HIMS), the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Universiteit Leiden (UL), and the Institute for Electrons and Molecular Structure (EMS) of the department of chemistry of the Vrije Universiteit (VU). The University of Amsterdam legally represents the HRSMC and the HIMS bureau houses the supporting HRSMC staff and acts as secretary of the Research School. HIMS professor Wybren Jan Buma (Molecular Photonics group) is the Scientific Director.

Distinguished Chinese research delegation visits HIMS

Professor Cao Jinghua, deputy director general of the Chinese Academy of Sciences (CAS), visited the University of Amsterdam in december. Cao is responsible for the European collaboration of the Chinese Academy of Sciences and as such he was invited by the Royal Netherlands Academy of Arts and Sciences KNAW and the Netherlands Organisation for Scientific Research NWO. As a leading player in joint KNAW-CAS research, HIMS was asked to receive the distinguished Chinese delegation.

Front row, left to right: Mr. Bo Quan (officer from Chinese Embassy at Den Haag), Mr. Aart Kleijn (director of HIMS), Mr. Cao Jinhua (CAS), Mr. Wybren Jan Buma (HIMS), Mr. Hong Zhang (HIMS), Ms. Dongyao Wang (CAS)
Back row, left to right: Ms. Marianne van Driel (KNAW), Mr. Sander Woutersen (HIMS), Mr. Fred Brouwer (HIMS), Mr. Maurice Aalders (AMC), Mr. T. van Leeuwen (AMC)
Photograph: Suzanne Reitsma

'Combining disciplines in sustainability research' seminar

As member of the UvA Platform Sustainability HIMS director Aart Kleijn contributed to the seminar 'Combining disciplines in sustainability research' in november. Solving the issues of sustainability is one of the key areas of focus for the University of Amsterdam (UvA) and the city of Amsterdam. At the seminar young researchers (PhD, postdoc or Master's/Honours) presented their research contributing to sustainability.

New Amsterdam solar energy initiative

HIMS researchers Aart Kleijn (scientific director), Joost Reek (Homogeneous and Supramolecular Catalysis), Fred Brouwer and Wybren Jan Buma (Molecular Photonics) were among the thirty or so scientists who met on November 16th for a kickoff workshop to establish a new joint solar energy research initiative in Amsterdam. Called 'Solardam', the initiative is a cooperation between the University of Amsterdam (UvA), VU University and FOM-institute AMOLF.

1.5.2 Prizes, grants and honours

NWO Athena premium for Jocelyn Vreede

Jocelyne Vreede of the Computational Chemistry Group received an *Athena premium* worth 100,000 euro from the Netherlands Organisation for Scientific Research (NWO). With this premium NWO encourages the appointment of talented female researchers within chemistry. Vreede models the formation of protein-DNA bridges in bacteria

Vici grants (1,5 million euros) for Bas de Bruin and Jos Oomens

The Netherlands Netherlands Organisation for Scientific Research (NWO) awarded both Bas de Bruin (*picture*) and Jos Oomens a prestigious Vici grant as part of its Innovational Research Incentives Scheme. Vici is a 1.5 million euro grant for outstanding senior researchers who have successfully demonstrated the ability to develop their own innovative lines of research, and to act as coaches for young researchers. The research of Bas de Bruin (Homogenous and Supramolecular Catalysis group) is focused on understanding and developing (new) homogeneous catalytic reactions. Jos Oomens will research the chemistry underlying novel peptide sequencing methods. He heads the Molecular Dynamics group at FOM-Rijnhuizen and is also professor with the Molecular Photonics group of the Van 't Hoff Institute for Molecular Sciences.

Wybren Jan Buma Chairman of the *John van Geuns Fonds*

Wybren Jan Buma has been appointed as chairman of the *John van Geuns Fonds*, and as member and secretary of the board of the *Stichting Bèta Plus*. The John van Geuns Fonds is a foundation promoting the study of chemistry at the Universiteit van Amsterdam, in particular of chemical research concerned with the interaction of light and matter. In order to achieve this goal, the foundation supports staff and talented students with grants, facilitates guest lectures, and maintains a special chair in Molecular Spectroscopy.

FOM 'projectruimte' grant for proton research

The Foundation for Fundamental Research on Matter (FOM) awarded a 'Projectruimte' grant to Sander Woutersen (Molecular Photonics, *picture*) and Huib Bakker (affiliate professor and group leader at the FOM institute AMOLF). The grant consists of the cost for a PhD position and an investment budget of 195,000 euro. In their research project *The Protonic Hall Effect* Woutersen and Bakker will study the way in which protons move through water.

ECHO grant for molecular lassos

The Netherlands Organisation for Scientific Research (NWO) awarded Jan van Maarseveen of the Synthetic Organic Chemistry group an ECHO project grant. This is a 260,000 euro project grant for excellent chemical research, offering the opportunity to carry out a high quality science driven research project. Van Maarseveen will use the grant for the study of so-called lasso peptides.

BAZIS equipment grants for UvA/VU chemistry research

HIMS researchers together with colleagues of the Vrije Universiteit (VU) were awarded BAZIS-grants (Basic Equipment for Research Themes in Chemical Focus Areas) by the Netherlands Organisation for Scientific Research (NWO) and the Dutch Ministry of Education, Culture and Science. The BAZIS-grants enable a renewal of essential equipment. A total of nine HIMS researchers are involved in three BAZIS projects: *Structure elucidation; Photons for chemistry;* and *Amsterdam virtual chemistry*

Major NWO grant for researching paints used in fine arts

Within the framework of Science4Arts programme, The Netherlands Organisation for Scientific Research (NWO) awarded a total of € 3.6 million to six different projects. One of them is the project *Paint Alterations in Time.* This 'PAinT' project will be carried out by Katrien Keune (HIMS), Annelies

van Loon (HIMS and the Royal Picture Gallery Mauritshuis) and Maartje Stols-Witlox, lecturer in the Restoration Studies Master's programme. Piet Iedema (HIMS Computational Polymer Chemistry group) is responsible for the mathematical modelling of the aging of paint layers.

Strong role for HIMS in new Dutch research programme in Analytical Sciences
The HIMS Analytical Chemistry Group took the lead in two of nine research projects within the framework of the so-called Technology Area Comprehensive Analytical Sciences and Technology (TA-COAST). Peter Schoenmakers is in charge of the project on *Hyperformance liquid chromatography* taking (multi dimensional) liquid chromatography - mass spectrometry (LC-MS) methods to a higher level. Gabriel Vivó-Truyols heads the *Chromametrics* project for the development of state-of-the-art statistical en chemometrical methods for faster and more functional processing of the ever growing amount of data.

Joint Dutch-Chinese research on photonic nanomaterials financed by KNAW
A joint Dutch-Chinese research proposal on the medical application of novel photonic nanomaterials

was granted In the framework of the China Exchange Program between the Royal Netherlands Academy of Arts and Sciences (KNAW) and its Chinese counterpart, the Chinese Academy of Sciences (CAS). A total sum of 400,000 euro was awarded to a consortium of HIMS (Hong Zhang -*picture*- and Wybren Jan Buma) with the AMC (Maurice Aalders, Ton van Leeuwen) and the Chanchung Institute of Applied Chemistry (CIAC) (Hongjie Zhang).

STW Valorisation Grant
Ron Wever of the Biocatalysis Group and Bio-organic Chemistry Group was awarded a 25,000 euro Valorisation Grant by the Dutch Technology Foundation STW (together with the Delft BiAqua company). As a result of this a post doc researcher was able to perform three months of research at the Wever group to covalently link vanadium chloroperoxidase to membranes and study the effect of this immobilisation on the prevention of biofilm formation.

Morino Lectureship for Fred Brouwer

Fred Brouwer of the Molecular Photonics Group was honored with the Morino Lectureship of the Morino Foundation (Tokyo, Japan). He gave a series of lectures in eight major Japanese universities. He also was invited to Taiwan (Short-Term visiting Scholar, Chemistry Research Promotion Center, National Science Council, Taiwan), where he delivered lectures in four universities, including one at the Taiwan National Photochemistry meeting.

Rubicon Award for HIMS visitor
Rafael Gramage-Doria of the Université de Strasbourg was awarded a Rubicon grant by the Netherlands Organisation for Scientific Research (NWO). It will enable him to visit the HIMS research group for Homogeneous and Supramolecular Catalysis of Joost Reek to perform research on *bio-inspired supramolecular architectures for intra-cavit catalysis.*

Financial boost for Holland Research School of Molecular Chemistry
The Netherlands Organisation for Scientific Research (NWO) awarded the Holland Research School of Molecular Chemistry (HRSMC) 800,000 euro to train young researchers. HIMS acts as the lead organisation for HRSMC, a cooperation of HIMS research groups with chemistry groups from Leiden University and VU University Amsterdam.

Jan van Maarseveen best UvA teacher of 2012

Jan van Maarseveen of the Synthetic Organic Chemistry Group was elected as one of the final five candidates for the Best Teacher Award of the University of Amsterdam. Early 2013, he was indeed chosen as the Best Teacher of the entire UvA over the year 2012.

1.5.3 Noteworthy publications

Angewandte Chemie
A team of Dutch, German and Spanish scientists revealed the mechanism of rhodium catalyzed stereospecific 'carbene' polymerization reactions. These reactions allow the synthesis of new types of polymers. Annemarie Walters, Piluka Pilar del Río, Joost Reek and Bas de Bruin of the Homogeneous and Supramolecular Catalysis group made a major contribution to the research.

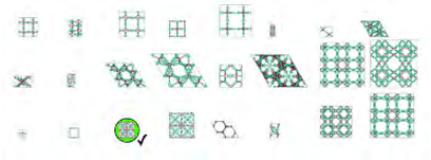
- J. C. Walters, O. Troeppner, I. Ivanović-Burmazović, C. Tejel, M. P. del Río, J. N. H. Reek, B. de Bruin, *Stereospecific Carbene Polymerization with Oxygenated Rh(diene) Species*, Angewandte Chemie, International Edition, 51(21), 5157-5161.

The design and development of novel nonporous materials is of paramount importance in areas such as storage, separation, and catalysis. A targeted approach requires a proper quantitative description of these materials. David Dubbeldam and Rajamani Krishna of the Computational Chemistry group published an article on the identification of structures that are suitable for separating linear and mono-branched alkanes from di-branched alkanes.

- Dubbeldam, D., Krishna, R., Calero, S. & Yazaydin, A.Ö. (2012). *Computer-assisted screening of ordered crystalline nanoporous adsorbents for separation of alkane isomers.* Angewandte Chemie, International Edition, 51(47), 11867-11871.

Rajamani Krishna of the Computational Chemistry group contributed to research showing that the introduction of polyamines in porous polymer networks results in significant enhancement of CO_2-uptake capacities at low pressures. The best substituted network was found to exhibit high adsorption enthalpies for CO_2 and the largest selectivity of any porous material reported to date. It also had outstanding physicochemical stability and could be regenerated under mild conditions.

- Lu, W., Sculley, J.P., Yuan, D., Krishna, R., Wei, Z. & Zhou, H.-C. (2012). *Polyamine-tethered porous polymer networks for carbon dioxide capture from flue gas.* Angewandte Chemie, International Edition, 51(30), 7480-7484.



The attachment of gas-phase divalent metal ions that bind as strongly as Mg^{2+} and transition-metal ions to the dipeptide PhePhe has been shown to result in the displacement of the amide proton. More weakly coordinating ions bind in the known charge-solvation mode. This *iminol tautomerization rearrangement* has been characterized in research of HIMS professor Jos Oomens, by means of infrared multiple-photon dissociation spectroscopy using the FELIX Free Electron Laser. This clearly shows the tautomeric transition.

- Dunbar, R.C.; Steill, J.D.; Polfer, N.C.; Berden; Oomens, J. *Peptide bond tautomerization induced by divalent metal ions: characterization of the iminol configuration*, Angew. Chem. Int. Ed. 2012, 51, 4591-4593.

Dennis Hetterscheid and Joost Reek of the Homogeneous and Supramolecular Catalysis group reviewed various mononuclear water oxidation catalysts which have been reported in the last five years (a breakthrough considering the dogma that at least two metal sites were required to oxidize water efficiently). They also discussed their implementation in prototype devices that allow dioxygen formation to be coupled to dihydrogen production.

- Hetterscheid, D.G.H. & Reek, J.N.H. (2012). *Mononuclear water oxidation catalysts.* Angewandte Chemie, International Edition, 51(39), 9740-9747.

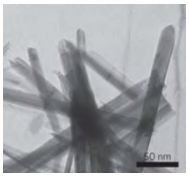
Nature Chemistry
Bas de Bruin of the Homogeneous and Supramolecular Catalysis group succesfully collaborated with German chemists from the University of Erlangen and the Max-Planck Institute for Bio-Inorganic Chemistry in Mülheim. Together they detected for the first time a transition metal complex containing an atomic 'nitridyl radical' ligand. Such atomic nitrogen ligands play an important role in - amongst others - catalytic activation of molecular nitrogen (Haber-Bosch ammonia synthesis).

- Markus G. Scheibel, Bjorn Askevold, Frank W. Heinemann, Edward J. Reijerse, Bas de Bruin, Sven Schneider *Closed-shell and open-shell square-planar iridium nitrido complexes* Nature Chemistry, 4(7), 552-558.

Nature Communications
HIMS professor Rajamani Krishna contributed to research on a porous metal-organic framework that can absorb large amounts of carbon dioxide (CO_2). Because of their low cost and non-toxic nature, metal-organic frameworks could become viable alternatives to the solvents that are presently used to chemically absorb CO_2 in industrial processes. In this publication a metal-organic framework is presented with high efficiencies at ambient temperatures and pressures.

- Shengchang Xiang, Yabing He, Zhangjing Zhang, Hui Wu, Wei Zhou, Rajamani Krishna & Banglin Chen. *Microporous metal-organic framework with potential for carbon dioxide capture at ambient conditions.* Nature Communications 3, 2012. Article number: 954

Nature Nanotechnology
Scientists at Johannes Gutenberg University in Mainz (Germany) and the Max Planck Institute for Chemistry in Mainz in collaboration with the Biocatalysis research group of the Van 't Hoff Institute for Molecular Sciences (University of Amsterdam) discovered that tiny vanadium pentoxide nanowires can inhibit the growth of bacteria and algae on surfaces in contact with seawater.



- Filipe Natalio, Rute André, Aloysius F. Hartog, Brigitte Stoll, Klaus Peter Jochum, Ron Wever & Wolfgang Tremel, *Vanadium pentoxide nanoparticles mimic vanadium haloperoxidases and thwart biofilm formation*, Nature Nanotechnology, *Nature Nanotechnology* **7,** 530–535 (2012)

Science
Computer simulations carried out by Rajamani Krishna of the Computational Chemistry group demonstrate the considerable potential of an iron-based 'metal organic framework' (MOF) for the separation of propene/propane and ethene/ethane mixtures. Krishna participated in international research published in Science magazine.

- Eric D. Bloch, Wendy L. Queen, Rajamani Krishna, Joseph M. Zadrozny, Craig M. Brown, Jeffrey R. Long: *Hydrocarbon Separations in a Metal-Organic Framework with Open Iron(II) Coordination Sites* Science, 30 March 2012, vol. 335 no.6076 pp. 1606-1610

ACS Nano
A team of scientists has developed a multifunctional nanoplatform for photodynamic therapy of cancer that can be activated by absorption of near-infrared light (NIR). It has now become possible to simultaneously perform photodynamic therapy *and* to image the therapeutic site. To obtain this breakthrough Hong Zhang (HIMS) closely collaborated with Maurice Aalders (AMC, UvA) and professor Xianggui Kong (CIOMP, Chinese Academy of Science). The work was published in ACS Nano.

- *Covalently Assembled NIR Nanoplatform for Simultaneous Fluorescence Imaging and Photodynamic Therapy of Cancer Cells*, Kai Liu, Xiaomin Liu, Qinghui Zeng, Youlin Zhang, Langping Tu, Tao Liu, Xianggui Kong, Yinghui Wang, Feng Cao, Saskia A.G. Lambrechts, Maurice C.G. Aalders, and Hong Zhang, ACS Nano *ACS Nano*, **2012**, *6* (5), pp 4054–4062

Chemical Society Reviews

The design and development of many separation and catalytic process technologies require a proper quantitative description of diffusion of mixtures of guest molecules within porous crystalline materials. Rajamani Krishna wrote a tutorial review presenting a unified, phenomenological description of diffusion inside meso- and micro-porous structures.

- Krishna, R. (2012). *Diffusion in porous crystalline materials.* Chemical Society reviews, 41(8), 3099-3118.

Front Covers

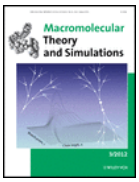
- Erik-Jan Ras, Manuel J. Louwerse and Gadi Rothenberg: *New tricks by very old dogs: predicting the catalytic hydrogenation of HMF derivatives using Slatertype orbitals.* Catal. Sci. Technol., 2012,2, 2456-2464.

- S.Y. de Boer, Y. Gloaguen, J.N.H. Reek, M. Lutz, J.I. van der Vlugt, *N-H bond activation by palladium(II) and copper(I) complexes featuring a cooperative bidentate PN-ligand* Dalton Trans. 2012, 41, 11276-11283.

- J.I. van der Vlugt, *First row transition metal cooperative catalysis* Eur. J. Inorg. Chem. 2012, 363-375. Invited micro-review *issue 'Cooperative & Redox Noninnocent Ligands'*

- Pablo Contreras Carballada et.al., *Variation of the Viologen Electron Relay in Cyclodextrin-Based Self-Assembled Systems for Photoinduced Hydrogen Evolution from Water* Eur. J. Org. Chem. 2012, 6729-6736

- Matthijs R. Panman et.al. Time-resolved vibrational spectroscopy of a molecular shuttle Phys. Chem. Chem. Phys., 2012, 14, 1865-1875



- Iedema, P.D. *Predicting MWD and Branching Distribution of Terminally Branched Polymers Undergoing Random Scission.* Macromol. Theory Simul. 2012, 21, 166–86.

1.5.4 Public outreach and media coverage

Gadi Rothenberg and Albert Alberts in National Geographic
The two researchers of the Heterogeneous Catalysis and Sustainable Chemistry Group were featured in the National Geographic edition for the Netherlands and Belgium with their development of biodegradable plastic.

Gadi Rothenberg and Albert Alberts on national television
In the 'EenVandaag' news show on Dutch national public television Gadi Rothenberg and Albert Alberts presented their research on biodegradable plastic.

Science meets Art

Researchers from the Heterogeneous Catalysis and Sustainable Chemistry group developed a process to use their newly developed, patented biodegradable material for construction plates. In addition to this they were tempted to turn such plates into pieces of art. One of these was presented to the president of the University of Amsterdam, Louise Gunning-Schepers and the dean of the Faculty of Science, Bart Noordam. *From left to right: Willem Fokkema, Gadi Rothenberg, Albert Alberts, Louise Gunning-Schepers, Aart Kleijn. Photo: V.R. Calderone*

Glass house lecture by Gadi Rothenberg
The year 2012 marked the 380th anniversary of the University of Amsterdam (UvA). In honour of this 76th 'lustrum' (anniversary occurring every five years), the UvA celebrated the opening of the academic year on a grand scale with the 'Glass House of Science and Scholarship'. Gadi Rothenberg was among a host of inspiring and renowned UvA professors holding lectures on the major questions arising in their fields of study.

HIMS researchers featured in 'Focus on research'

With the 'Focus on Research' series the University of Amsterdam brings its high profile projects to the attention of the general public. Both Arian van Asten and Jarl Ivar van der Vlugt (*picture*) were portrayed in this series. Jarl Ivar van der Vlugt (Homogeneous and Supramolecular Catalysis) was interviewed on his catalysis research. He foresees a dramatic change in the near future. Catalysis will become cleaner, cheaper, smarter, and more effective. Inspired by nature. Arian van Asten of the Analytical Chemistry group has been busy setting up the new Amsterdam Centre for Forensic Studies (ACFS) together with Maurice Aalders of the Amsterdam Medical Center.

HIMS at Doors Open Day Science Park
On Saturday, 6 October 2012, the Science Park was open to the public. Tours, demonstrations and more was offered to visitors who were curious about the scientific work carried out here. The institutes of the Faculty of Science contribute to this yearly event and also HIMS was represented. HIMS researchers could be found e.g. demonstrating chemical experiments.

Artificial Photosynthesis lecture
Joost Reek of the Homogeneous and Supramolecular Catalysis group presented a lecture for the Physics Society 'Wessel Knoops' on Artificial Photosynthesis.

Chemical Weekly C2W
HIMS research was featured regularly in the Dutch biweekly chemical magazine Chemisch2Weekblad (C2W). Most of the selected papers mentioned earlier received attention of the C2W news editors.

Albert Alberts at BNR
At the Dutch station Business News Radio Albert Alberts (Heterogeneous Catalysis and Sustainable Chemistry) was interviewed about his invention of biodegradable plastic.

Sander Woutersen on Greek and Latin
Sander Woutersen of the Molecular Photonics group gave a short talk on Dutch national radio about Greek and Latin in the natural sciences.

2. Research

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

All four themes share *molecular sciences* as a binding factor, as is reflected in the name of the institute. Within HIMS, we work on catalysis, human health, energy, devices, etc., from a molecular perspective, rather than from a process-engineering, pharmaceutical, or technological perspective.

HIMS participates in important national and international research programmes, such as NRSCC, CATCHBIO, COAST, NanoNext 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.

2.1 Research theme 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 to establish a strong focus on sustainable chemistry, with particular attention to catalysis. To this avail we combined all our Catalysis and Bio-molecular Synthesis research in the new research theme *Sustainable Chemistry* and proposed this theme as a future University Research Priority Area ('onderzoekszwaartepunt'). In July 2013 this was established as such.

The combined sustainable chemistry activities presently consist of five research groups, Homogeneous 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 (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. Homogeneous and supramolecular catalysis

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

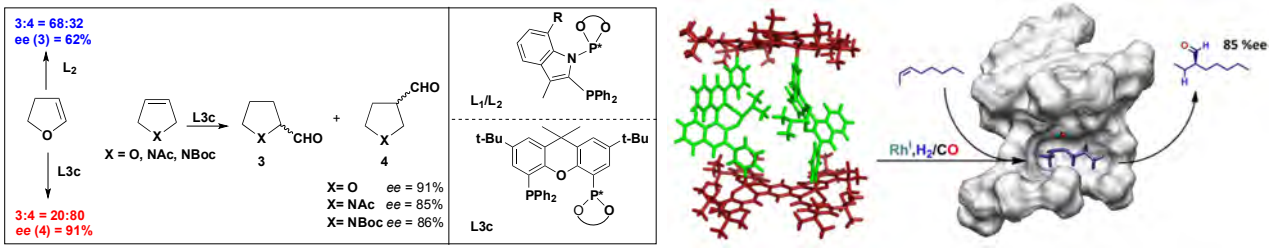
The general aim of the catalysis group is the development of new catalysts for known important conversions and catalysts for novel reactions that have no precedent. This challenge we approach in a multidisciplinary fashion. General important issues that are taken into account in these catalytic conversions are the atom-efficiency, the chemo-, region-, and stereo-selectivity, and of course the activity and the stability of the catalyst. We believe that catalysis plays a major role in the development of technology for the conversion of renewables into useful chemicals, and in the area of green energy applications; i.e. solar to fuel, CO_2 reduction, N_2 reduction, water oxidation

etc. As such, part of our research is focused on these challenges. We have developed a wide variety of tools and concepts and have experience in several reactions:

- Rational ligand design and ligand synthesis
- Kinetics, in situ spectroscopy and DFT calculations on reaction mechanisms
- Supramolecular approaches
- Bio-inspired approached, including catalyst encapsulation, bifunctional catalysis, catalyst selection
- Hydroformylation, hydrogenation, small molecule activation
- Metalloradicals and catalysis
- C1-carbene chemistry.

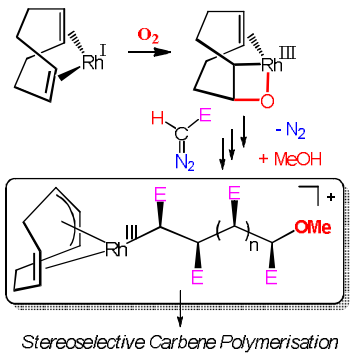
Research highlights

In the area of asymmetric hydroformylation the group has published a couple of break-troughs. A new ligand was designed of which the rhodium complex is able to hydroformylate challenging heterocyclic olefins such as dihydropyrrolidines and related dihydrofuran (*JACS*). These lead to a direct synthesis of important chiral building blocks such as beta-proline, derivatives intermediates that are difficult to access otherwise. In our on-going effort to address very challenging unfunctionalized internal alkenes as substrates, we reported a self-assembled chiral molecular box in which the active metal center was embedded in a chiral pocket (see figure).



This self-assembled catalyst showed for internal alkenes such as 2-octene the highest enantioselective conversion to the aldehyde (*JACS)*. Using the same ligand in combination with mono(Zn) templates such as porphyrins, resulted in unusual coordination chemistry and increased selectivity in asymmetric hydroformylation, but the ee of the product remained below 50% (*Chem. Eur. J*).

In the field of Rh-mediated carbene polymerization, which is a new method to prepare carbon-chain polymers from 'carbene'-monomers, significant advancements were made in understanding the mechanism behind this intriguing C-C bond forming reaction.

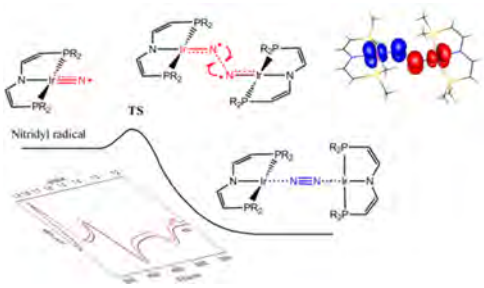


Stereoselective Carbene Polymerisation

Activation of the catalyst requires unusual transformation of the cyclooctadiene ligand of the pre-catalyst, which was unravelled in detail through high-resolution ESI-MS measurements (collaboration Erlangen), model studies, catalysis screening and supporting DFT calculations (*Angew. Chem.*).

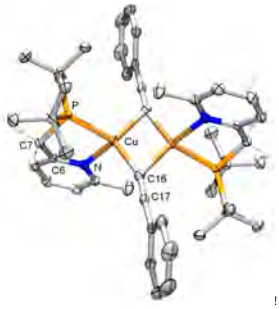
In the field of metallo-radical catalysis, we are moving along two important lines: (1) we try to enable a transition from the use of expensive noble transition metals in catalysis (reacting typically via two-electron pathways) to the use of first-row transition metals (reacting typically via one-electron radicaloid pathways). (2) we aim to get control over radical-type reactions, in which

substrate/ligand-centred radicals are generated on purpose and play an active role in catalysis. Significant progress has been booked in both directions and De Bruin further succeeded in getting a prestigious NWO-CW VICI grant in 2012 to expand on these efforts.



In collaboration with Schneider from Göttingen, we reported for the first time a transition metal nitridyl-radicals (*Nature Chemistry*). This species most likely plays an important role in several N_2-activation processes but had never been spectroscopically detected before.

We are currently expanding this chemistry, and explore other chemical routes for nitrogen activation. We reported on a new redox non-innocent ligand system which enables two-electron transformations directly from the ligand rather than the metal (*EurJIC*), and wrote a review article on the use of redox-active ligands in catalysis (*ACS. Catalysis*). Furthermore, the group investigated the electronic structure of a series of organometallic Fe-catalysts (collaboration Regensburg; *Inorg. Chem.*).



Next to these efforts we are also expanding the activities in the emerging field of cooperative catalysis, especially focusing on the implementation of earth-abundant 1st row metal precursors. As an example, we reported on the cooperative N-H activation of amines with Pd- and Cu-species bearing reactive ligand scaffolds (*Dalton Trans.* front cover.)

In addition, the first example of cooperative C-H activation using a well-defined dinuclear Cu-complex with a reactive PNP-ligand is described. This leads to an all-in-one cooperative click reaction between organic azides and alkynes using this catalyst. A well-received review article on cooperative catalysis (one of the most accessed articles in 2012) was published in a dedicated issue of *EurJIC* (front cover).

Key Publications

Prof. J.N.H. Reek:

- S.H. Chikkali, R. Bellini, B. de Bruin, J.I van der Vlugt, and J. N. H. Reek* "Highly Selective Asymmetric Rh-Catalyzed Hydroformylation of Heterocyclic Olefins", *J. Am. Chem. Soc.* 2012, *134,* 6607.
- T. Gadzikwa, R. Bellini, H.L Dekker, and J. N. H. Reek* "Self-Assembly of a Confined Rhodium Catalyst for Asymmetric Hydroformylation of Unfunctionalized Internal Alkenes", *J. Am. Chem. Soc.* 2012, *134,* 2860
- R. Bellini, J. N. H. Reek*," Coordination Studies on Supramolecular Chiral Ligands and Application in Asymmetric Hydroformylation" *Chem. Eur. J.*, 2012, *18*, 7091.

Prof. B. de Bruin:

- Scheibel, M.G.; Askevold, B.; Heinemann, F.; Reijerse, E.J.; de Bruin, B.*; Schneider, S.*, Closed-Shell and Open-Shell Square-Planar Iridium Nitrido Complexes, *Nature Chemistry,* 2012, *4*, 552–558
- A.J.C. Walters, O. Troeppner, I. Ivanovic-Burmazovic, C. Tejel, M. Pilar, Del Rio, J. N. H. Reek, B. de Bruin" Stereospecific Carbene Polymerization with Oxygenated Rh(diene) Species" *Angew. Chem. Int Ed.*. 2012, *51*, 5157.

- Lyaskovskyy, V.; de Bruin, B.*, Redox Non-innocent Ligands – Versatile New Tools to Control Catalytic Reactions *, ACS Catalysis*, 2012, *2*, 270–279. Invited Review. Top 10 'most read' papers of the journal Q1 2012

Dr J.I. van der Vlugt:

- J.I. van der Vlugt*, First row transition metal cooperative catalysis *Eur. J. Inorg. Chem.* 2012, 363-375. invited micro-review *issue 'Cooperative & Redox Noninnocent Ligands'* (front cover)
- S.Y. de Boer, Y. Gloaguen, J.N.H. Reek, M. Lutz, J.I. van der Vlugt*, N-H bond activation by palladium(II) and copper(I) complexes featuring a cooperative bidentate PN-ligand *Dalton Trans*. 2012, *41*, 11276-11283. (front cover)

Dissertations

Bellini, R. (2012, September 18). *Chiral supramolecular ligands in transition metal catalysis.* University of Amsterdam (147 p). Prom./coprom.: Prof. Dr J.N.H. Reek.

Franssen, N.M.G. (2012, December 11). *Functional (co)polymers from carbenes: scope, mechanism & polymer properties.* University of Amsterdam (225 p). Prom./coprom.: Prof. Dr J.N.H. Reek & Prof. Dr B. de Bruin.

Grants & Prizes

NWO-CW VICI Grant B. de Bruin
(Aug. 2012 - Aug. 2017; 5 PhD students, 1 postdoc, 5 yr, €1.500.000).
Title: 'Radicals in Catalysis'.

Invited Lectures

Prof. J.N.H. Reek:

- Symposium on supramolecular chemistry Bejing, *Supramolecular approaches in transition metal catalysis.* China
- Symposium on supramolecular chemistry, *Supramolecular approaches in transition metal catalysis.* Chengdu, China
- ISHC-18 (International Symposium on Homogeneous Catalysis), *Supramolecular control in selective transition metal catalysis.* Toulouse, France.
- DOCDays, University Graz, *Supramolecular approaches in transition metal catalysis.* Graz, Austria.
- AMOLF institute, *Supramolecular approaches in transition metal catalysis.*
- University of Groningen *Supramolecular approaches in transition metal catalysis.*
- EASTMAN, *Supramolecular approaches in transition metal catalysis.* Texas USA

Prof. B. de Bruin:

- NWO studiegroep-bijeenkomst Ontwerp & Synthese, Structuur & Reactiviteit, Biomoleculaire Chemie en Farmacochemie, October 22-24, 2012. Lunteren, The Netherlands. *Bio-Inspired Catalytic Radical-type Transformations.* Plenary Lecture.

- International Conference on Bioinspired and Biobased Chemistry & Materials, Nice (France), October 3-5, 2012. *Bio-Inspired Catalytic Radical-type Transformations.* Keynote Lecture.
- Wöhler conference, Georg-August-Universität Göttingen, Sept. 26-28, 2012, chair Prof. F. Meyer. *Ligand Redox Non-innocence in Open-Shell Transition Metal Catalysis; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.* Plenary Lecture.
- GDCh lecture, Universität Regensburg, July 16, 2012, *Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.*
- International Conference on Porphyrins and Phthalocyanines (ICPP-7), Jeju (Korea), July 4-6, 2012. *Bio-Inspired Catalytic Radical-Type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.*
- International Symposium on Organic Free Radicals (ISOFR-11), Berne (Switserland), July 1-3, 2012. *Bio-Inspired Catalytic Radical-Type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.*
- Institute of Inorganic Chemistry & Max Planck Institute of Solid State Research, University of Stutgart (Germany), April 17, 2012. *Bio-Inspired Catalytic Radical-type Transformations.*
- Peking University of Beijing, Jan. 16, 2012, hosted by Prof. X. Fu. *Rhodium-Mediated Stereoselective Carbene Insertion Polymerisation.*
- Peking University of Beijing, Jan. 13, 2012, hosted by Prof. X. Fu. *Ligand Redox Non-innocence in Open-Shell Transition Metal Catalysis; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.*
- Chinese University of Hong Kong, Jan. 11, 2012, hosted by Prof. K.S. Chan. *Ligand Redox Non-innocence in Open-Shell Transition Metal Catalysis; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.*

Dr J.I. van der Vlugt:

- 25th International Conference on Organometallic Chemistry, Lisbon, Portugal (Sep 2012)
  Novel Avenues for Coordination Chemistry using Reactive (Metallo)Ligands

Outreach:

Prof. J.N.H. Reek:

- Wessel Knoops lecture, Volksuniversiteit Arnhem, Kunstmatige Fotosynthese

Prof. B. de Bruin:

- Highlight Nature Chemistry paper in C2W + UvA website
- Highlight Angewandte Chemie paper in C2W + UvA website
- Highlight VICI in C2W + UvA website

Dr J.I. van der Vlugt:

- Highlight ERC Research Grant UvA website

2.1.2 Heterogeneous Catalysis and Sustainable Chemistry

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

The year 2012 has been an excellent year for the research of the Heterogeneous Catalysis and Sustainable Chemistry group (HCSC). Several large research projects, funded by CatchBio, NWO-Aspect and Avantium Technologies have borne fruit, and the time and effort that all group members have invested in setting up the new labs at the Science Park has paid off handsomely. The group has reached its strategic targets on personnel and facilities and obtained high-quality research results. Moreover, the strong international reputation of the group leader has led to further industrial investment in two large-scale projects, one with Rhodia-Solvay and one with LANXESS. Finally, the patent, invented by Dr Shiju in 2010, was sold to the Dutch chemical company DSM.

Highlights

Co-invented by Dr Albert Alberts and Prof. Gadi Rothenberg, our new and patented biodegradable plastic made from plants has received much media attention in 2012, including newspapers, radio, and a prime-time feature in the programme *een vandaag*. The UvA has invested further in this project, and a total of six patents have been filed on it. Currently, Rothenberg and Alberts are in the process of scaling up the production and trying to bring the new plastic as a product into the construction and packaging markets.
HCSC has signed collaboration agreements with two major industrial players in 2012. The project with the German specialty chemicals company LANXESS centres on the search for a new catalytic route to 1,3-butadiene, the most important monomer for making rubber for car tires. LANXESS will invest over a period of three years in this research project, with the aim of diversifying its sources for synthetic rubber raw materials. In another project, multinational concern Solvay has signed a research agreement with Rothenberg's group, setting up a unique construction where the research group would try and help solving problems of Solvay business units that are related to the group's expertise in predictive modeling. This agreements cements over ten years of collaboration between Rothenberg's group and Rhodia (now Solvay).

Key publications:

- Understanding the redox behaviour of PbCrO4 and its application in selective hydrogen combustion. S. Gómez-Quero, C. Hernández-Mejía, R. Hendrikx and G. Rothenberg, *Dalton Trans.*, 2012, 41, 12289-12295.
- Transferable basis sets of numerical atomic orbitals. M.J. Louwerse and G. Rothenberg, *Phys. Rev. B,* 2012, 85, 035108.
- New tricks by very old dogs: Predicting the catalytic hydrogenation of HMF derivatives using Slater-type orbitals. E.J. Ras, M.J. Louwerse and G. Rothenberg, *Catal. Sci. Technol*., 2012, 2, 2456-2464 (front cover).

In 2012 the group published 6 papers in peer-reviewed journals.

Patents

HCSC submitted four patent applications (one on a new Fischer-Tropsch catalyst with TOTAL, and three on new plastic composites).

Lectures

Group members gave a total of 15 national and international lectures, including a special lecture of Prof. Rothenberg at the "glass house" (*het glazen huis)* during the opening day of the academic year at the invitation of the UvA board.

2.1.3 Molecular Inorganic Chemistry / Organometallic Chemistry

Prof.dr. C.J. Elsevier

Research objectives

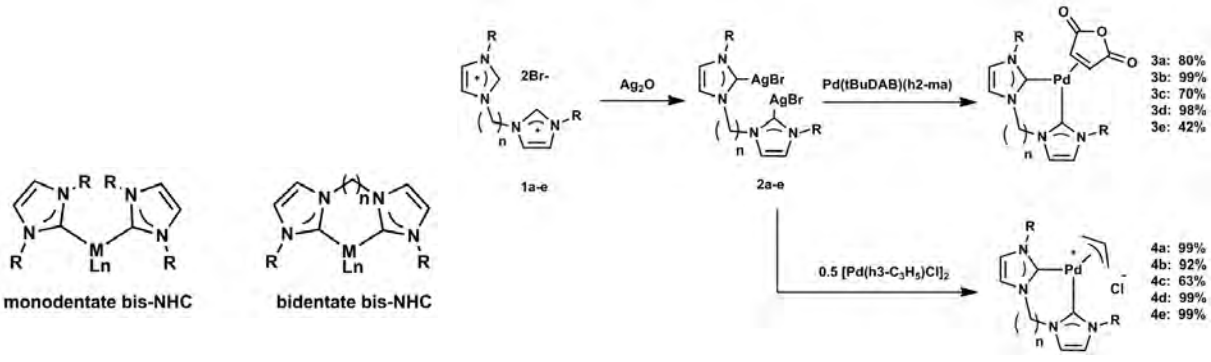
The Molecular Inorganic Chemistry group is involved in fundamental research in Coordination and Organometallic Chemistry, which resides at the basis of most catalytic processes, notably the synthesis, characterization and application of organometallic compounds in homogeneous catalysis.

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 to discover new solutions to problematic chemical transformations and improvement of processes. Processes studied are mainly hydrogenation and hydrosilylation reactions. 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 also aims at the design and implementation for heterogenization, immobilization and recycling of homogeneous catalysts.

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. Currently, a focal point of our research concerns the design and application of transition metal complexes with heteroditopic bis-carbene and carbene-N-ligands for organometallic chemistry and applications in homogeneous catalysis.

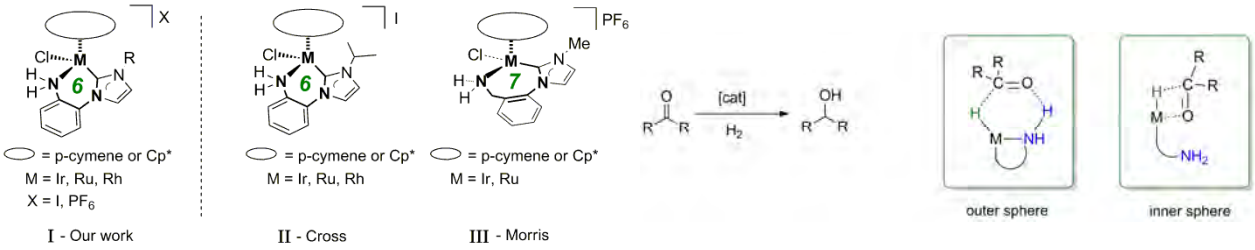
Highlights

We have studied base-free transfer-hydrogenation reactions mediated by palladium compounds encompassing bidentate carbene-triazolyl and bidentate bis-NHC ligands. These studies are part of our endeavor into a niche on which 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).



The research of this year further encompassed studies involving bidentate bis-NHC ligands (bidentate C,C-chelating ligands). The presence of two strong donor carbene functions will enforce high electron density on metal centers. In addition to the advantages concerning stability,

bis-NHCs are good candidates for fine-tuning of catalytic properties by altering the wingtips, backbone and linker, which having been explored in this year.



The design of new ligands for carbonyl-group hydrogenation reactions, based on N-heterocyclic carbene (NHC) with an amine functionality, was found to allow bifunctional substrate activation in the case of ketones and esters. These studies are part of a CatchBio project concerning environmental issues and depletion of fossil fuel reserves that entice us to develop renewable sources of energy and materials: sources that are either abundantly available or replaceable. The application of the ruthenium complex, which outperforms its reported analogues, was successfully extended to hydrogenation of more challenging biomass substrates.

We have developed several highly convenient and easy-to-use palladium(II) pre-catalysts for high selectivity in hydrogenations, resulting in a novel procedure that can easily be used, also by non-specialist chemists. The results will be published shortly in several papers (R.M. Drost et al).

Key publications

- D.S. Tromp, P. Hauwert, C.J. Elsevier. Synthesis of bis-N-alkyl-imidazolium salts and their palladium(0)(NHC)(2-MA)2 complexes. Appl. Organomet. Chem., **2012**, 26, 335-341.

Lectures

The group participated in several international conferences and the Dutch NCCC with lectures and posters.

2.1.4 Synthetic Organic Chemistry

Prof. H. Hiemstra, Prof. P. Timmerman (Pepscan), Dr J.H. van Maarseveen, Dr S. Ingemann

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.

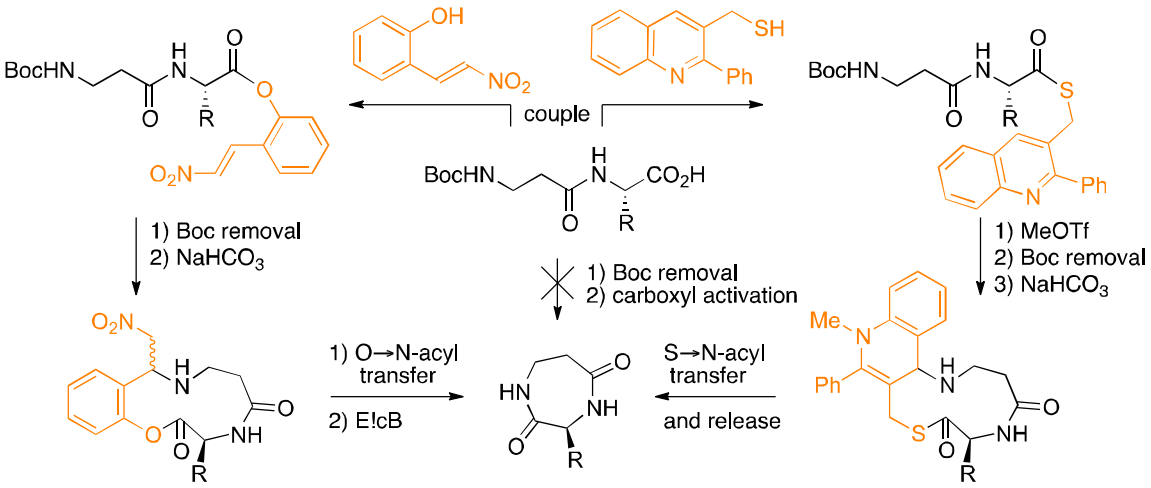
Research overview

A research highlight of 2012 was the total synthesis of mitragynine, a notorious indole alkaloid with various biological activities. Our synthesis makes use of an enantiopure organocatalyst and provides the natural product quite efficiently. Another highlight was the synthesis of several homo- and nor-analogues of quinidine in enantiopure form to be investigated as chiral organocatalysts.

Synthetic methodology development: Due to their strained character, seven-membered bislactams are excellent targets for the development of novel and powerful lactamization

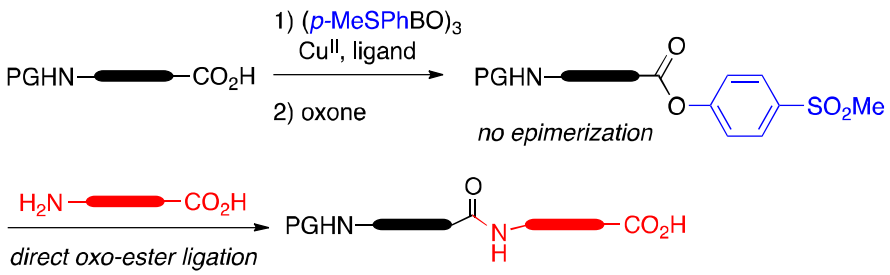
methods. We have found that esterification of *N*-terminal protected β-peptides with commercially available *o*-hydroxy-β-nitrostyrene, followed by liberation of the *N*-terminus gave the seven-membered strained bislactams in good yield.

Mechanistic 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 quinolines are also useful as auxiliaries to facilitate lactamization using a similar mechanistic reaction pathway, although with less efficiency.

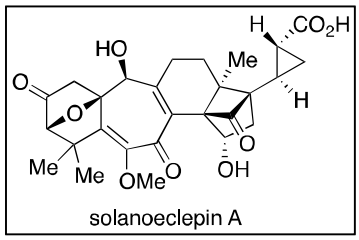


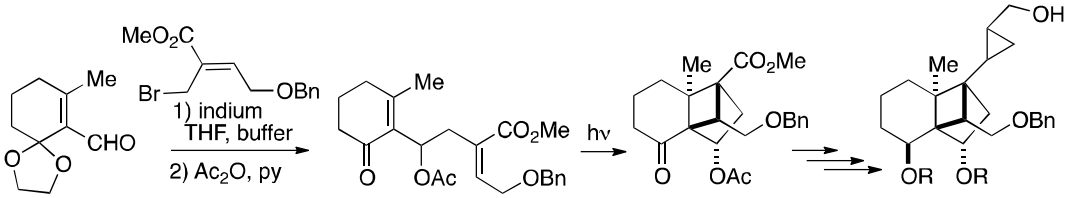
Although generally accepted as "text book chemistry", the preparation of esters, but especially amides from acids can be problematic. This is most profound in the peptide series. To avoid racemization peptides are generally elongated at the *N*-terminus, because activation of the terminal carboxyl moiety of a peptide inevitably leads to epimerization.

On the other hand, methods that allow racemization-free *C*-terminal elongation of peptides are greatly desired. Very recently we achieved epimerization-free *C*-terminal activation of peptides via aryl esterification using the so-called Chan-Lam reaction between carboxylic acids and arylboronic acids. The new methodology will be devoted to novel peptide ligation strategies, peptide cyclization, and, ultimately, protective group free reverse peptide synthesis.

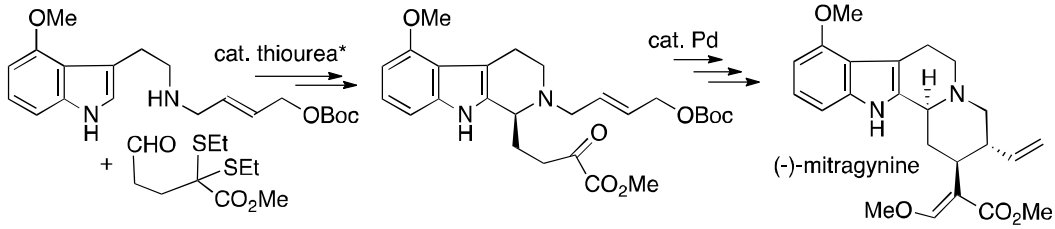


Target-oriented synthesis: In our research toward the total synthesis of the terpenoid hatching agent solanoeclepin A an efficient and convergent synthesis of the tricyclic right hand core was realized. This work should lead to the synthesis of simpler and biologically active analogues in order to combat potato cyst nematodes as parasites in potato production. The two key steps, namely the indium-induced aldehyde addition and the photochemistry were greatly optimised. The photochemical [2+2]-cycloaddition was studied in collaboration with the Rutjes group in Nijmegen in order to conduct this process in a flow system suitable for scale-up.

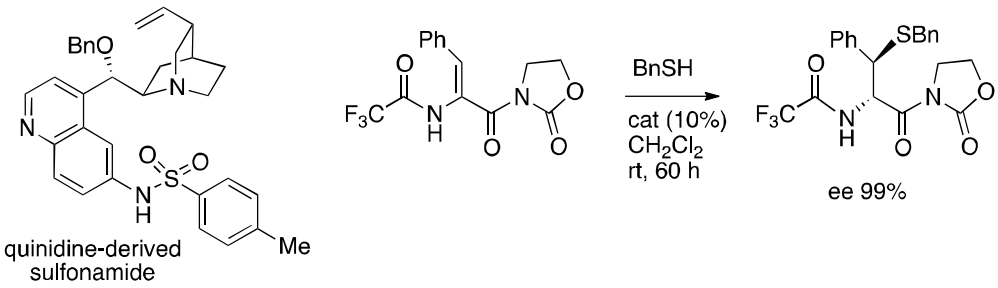




Organocatalysis: Chiral biarylphosphoric acids and thiourea were used to catalyse Pictet-Spengler reactions in high ee's. By using a chiral thiourea we achieved the particular Pictet-Spengler reaction indicated below in 89% ee. This transformation and a palladium-catalysed allylic substitution were the key steps in the most efficient asymmetric total synthesis to date of the renowned indole alkaloid mitragynine.

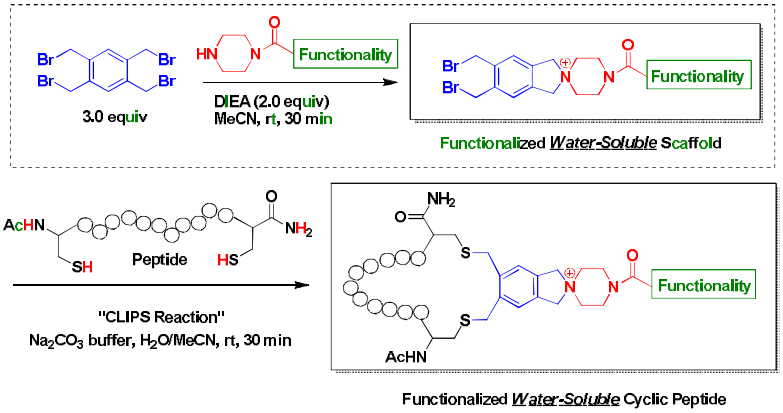


Other enantioselective organocatalysis research is based on the cinchona alkaloid skeleton. The sulfonamide derived from quinidine catalyses the conjugate addition of benzylmercaptan to the electronpoor alkene providing the two addition products in quantitative yield in an 84:16 anti/syn ratio and 99% ee for the major diastereomer. This reaction is useful for the synthesis of enantiopure cysteine analogues.



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 easily 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

- L.E.J. Smeenk, N. Dailly, H. Hiemstra, J.H. van Maarseveen, P. Timmerman, *Synthesis of water-soluble scaffolds for peptide cyclization, labeling and ligation,* Org. Lett. 14, 1194-1197 (2012).
- J.P.A. Rutters, Y. Verdonk, R. de Vries, S. Ingemann, H. Hiemstra, V. Levacher, J.H. van Maarseveen, *Synthesis of strained cyclic peptides via an aza-Michael-acyl-transfer reaction cascade,* Chem. Commun. 48, 8084-8086 (2012).
- I.P. Kerschgens, E. Claveau, M.J. Wanner, S. Ingemann, J.H. van Maarseveen, H. Hiemstra, *Total syntheses of mitragynine, paynantheine and speciogynine via an enantioselective thiourea-catalysed Pictet-Spengler reaction,* Chem. Commun. 48, 12243-12245 (2012).

Prizes and grants

- A CW/NWO Echo grant was acquired for research toward the total synthesis of (simple analogues of) the lasso peptide microcin J25.
- Dr Jan van Maarseveen was one of the final five candidates for the Best Teacher Award of the University of Amsterdam. Early 2013, he was indeed chosen as the Best Teacher of the entire UvA, 2012, which is a great honour.
- At the PAC symposium 2012 in Leiden advanced master students presented our results on the synthesis of several homo- and nor-analogues of quinidine in enantiopure form to be investigated as chiral organocatalysts. They won three poster prizes.

Invited lectures

Prof. H. Hiemstra

- *Solanoeclepin A, a hatching agent of potato cyst nematodes*, HLB, Wijster, the Netherlands, January 30th 2012.
- *Toward the synthesis of solanoeclepin A, a hatching agent of potato cyst nematodes*, Bayer Crop Science AG, Monheim am Rhein, July 3rd 2012.

Dr J.H. van Maarseveen

- *An Enantioselective Organocatalytic Approach towards the Mitragynine Series,* COST ORCA, Université de Provence, Marseille, France, April 1st, 2012.
- *Organocatalysis and transition metal-based catalysis, a powerful combination towards biologically active indole alkaloids*. Chalmers University, Gothenburg, Sweden, January 12th 2012.

Prof. P. Timmerman

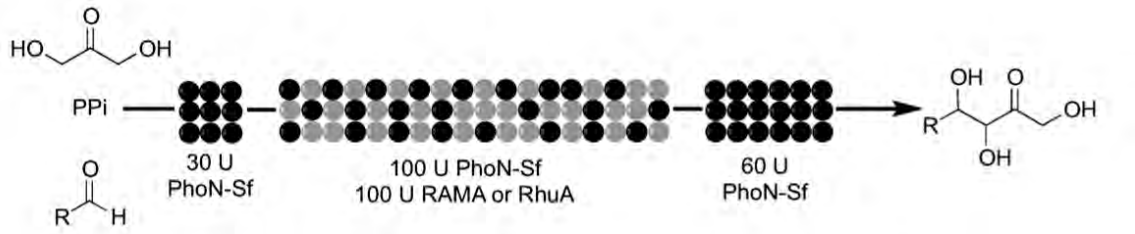
- *Next Generation HIV-fusion Inhibitors, Lead Finding & Optimization using PEPSCAN technologies*, TIDES-Symposium, IBC Life Sciences, San Diego (CA), USA, May 2012.
- *Shaping Peptides to Drugs: Discovery & Optimization of CLIPS-constrained Peptides*, EuroPeptides-symposium, IBC Life Sciences, Berlin, November 2012.
- *CLIPS Epitope Mapping,* EuroPeptides Workshop, Berlin, November 2012.

2.1.5 Biocatalysis

Prof. R. Wever

The research topics studied in the Biocatalysis group are highly relevant for society. The aim of the group to replace existing chemical procedures by more sustainable biocatalytic procedures has been successful. Four papers have been published in which enzymatic procedures are reported that may replace classical organic synthetic procedures and that offer green alternatives. Our cooperation with the group of Prof. W. Tremel (Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg Universität, Mainz, Germany) on V_2O_5 nanoparticles has resulted in a publication in to Nature Nanotechnology which aroused quite some interest worldwide.

Research overview



Packed bed reactor consisting of three reactors containing immobilized acid phosphatase (PhoN-Sf), immobilized aldolases and acid phosphatase.

We have developed a new flow process to synthesize complex chiral carbohydrates analogues from achiral inexpensive building blocks in a three-step catalytic cascade reaction. The first reactor contained immobilized acid phosphatase which phosphorylated dihydroxyacetone to dihydroxyaceton phosphate using pyrophosphate as the phosphate donor. The second flow reactor contained fructose-1,6 -diphosphate aldolase (rabbit muscle aldolase) or rhamnulose-1-phosphate aldolase and acid phosphatase. The immobilized aldolases coupled the formed dihydroxyacetone phosphate to aldehydes resulting in phosphorylated carbohydrates. A third reactor containing acid phosphatase dephosporylated the phosphorylated product and yielded the final product. Different aldehydes were used to synthesize carbohydrates on a gram scale.

The system allows the continuous synthesis of various aldol products in good yields and further optimization of this labour free method is possible. This work was carried out in collaboration with Prof. F.P.J.T. Rutjes and Dr L.J.C van Hemert (Radboud University, Nijmegen).

Our cooperation with Prof. J. Sanders (Valorisation of Plant Production Chains Group, Department of Agrotechnology and Food Sciences, Wageningen University) on the conversion of amino acids from protein-rich biomass waste into valuable nitriles by the vanadium chloroperoxidase was very successful. For the first time the conversion of glutamic acid to 3-cyanopropionic acid in high yield and selectivity was reported using vanadium chloroperoxidase and hydrogen peroxide. The reaction proceeds with a catalytic amount of sodium bromide and constitutes a general and sustainable route to industrial nitriles from biomass.

Sulfated compounds are in general synthesized by the pharmaceutical/chemical industry using complexes of sulfur trioxide (SO_3) with tertiary amines or amides. However, use of this reactive reagent suffers from numerous disadvantages such as harsh reaction conditions and lack of reaction selectivity. Additionally, in order to prevent side reactions of labile functionalities and to enhance the chemo- or regioselectivity of the overall reaction, these functionalities have to be protected. We have developed an enzymatic method for sulfation of compounds under mild conditions using a bacterial recombinant arylsulfotransferase. This enzyme, in great contrast to all other known bacterial arylsulfotransferases, is able to use a variety of non-phenolic alcohols as sulfate acceptor. Because of these properties, this unique enzyme is a promising tool for biotransformation processes providing a green and simple method to specifically sulfate compounds without need for functional group protection.

In the cooperation with Prof. W. Tremel (Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg Universität, Mainz, Germany) the enzyme-like activities of vanadium nanowires have been further investigated. It is shown that vanadium pentoxide nanowires act like naturally occurring vanadium haloperoxidases to prevent marine biofouling. In the presence of bromide ions and hydrogen peroxide, the nanowires catalyse the oxidation of bromide ions to hypobromous acid (HOBr). Singlet molecular oxygen ($^1O_2$) is formed and this exerts strong antibacterial activity, which prevents marine biofouling without being toxic to marine biota. Vanadium pentoxide nanowires may have the potential to be an alternative approach to conventional anti-biofouling agents.

In cooperation with the Department of conservative and preventive dentistry, Academic Centre for Dentistry, Amsterdam the effect of the vanadium chloroperoxidase on in vitro *E. faecalis* biofilms has been investigated. It has been concluded that the enzyme might provide an addition to current endodontic treatment, possibly as an antimicrobial dressing.

Key publications

- M. A. Van der Horst, J. F. T. Van Lieshout, A. Bury, A. F. Hartog, R. Wever. Sulfation of various alcoholic groups by an arylsulfate sulfotransferase from *Desulfitobacterium hafniense* and synthesis of estradiol sulfate. *Adv. Synth. Catal.* 2012, *354*, 3501-3508

- L. Babich, A. F. Hartog, M.A. Van der Horst and R. Wever. Continuous-flow reactor-based enzymatic synthesis of phosphorylated compounds on a large scale. *Chem. Europ. J.*, 2012*, 18*, 6604-6609.

- L. Babich, A. F. Hartog, L. J. C. Van Hemert, F. P. J. T. Rutjes and R. Wever. Synthesis of carbohydrates in a continuous flow reactor by immobilized phosphatase and aldolase. *ChemSusChem*, 2012, *5*, 2348-2353

- But, J. Le Notre, E.L. Scott, R. Wever and J. P. M. Sanders. Selective oxidative decarboxylation of amino acids to produce industrially relevant nitriles by vanadium chloroperoxidase. *ChemSusChem*, 2012**,** *5*, 1199-1202.

- F. Natalio, R. Andre, A. F. Hartog, B. Stoll, K. P. Jochum, R. Wever, and W. Tremel. Vanadium pentoxide nanoparticles mimic vanadium haloperoxidases and thwart biofilm formation. *Nature Nanotechnology*, 2012, *7*, 530-535. *Highlighted in C2W*

- F. Persoon, M. A. Hoogenkamp, A. Bury, P. R. Wesselink, A. F. Hartog, R. Wever, and W. Crielaard. Effect of vanadium chloroperoxidase on *Enterococcus faecalis* biofilms. *J. Endod.*, 2012, *38,* 72-74.

Grant

STW Valorisation Grant. Applicants R. Wever and M. Paravidino (Biaqua, Delft) Total 25,000 euro. Post doc for 3 months (November 2012- January 2013). The small STW Valorisation Grant has been used in a project to covalently link the vanadium chloroperoxidase to membranes and the effect of this immobilisation on preventing biofilm formation has been studied. Unfortunately due to lack of time a conclusive experiment could not be carried out.

Lectures and presentations

- R. Wever, J. C. Hemert, L. Babich, A. Bury, A.F. Hartog and F. P. J. T. Rutjes (July 2012). *Pyrophosphate as the driving force in the synthesis of non-natural carbohydrates by enzymatic cascade reactions*. Rotterdam, The Netherlands, 19th International Conference on Phosphorus.

- R. Wever, J. C. Hemert, L. Babich, A. Bury, A.F. Hartog and F. P. J. T. Rutjes, (April 10, 2012). *Pyrophosphate as the driving force in the synthesis of non-natural carbohydrates by enzymatic cascade reactions.* Graz, Austria, Multistep enzyme-catalyzed processes.

- R. Wever (August 2012). *Vanadium chloroperoxidase and some applications.* The 8th International Vanadium Symposium Chemistry, Biological Chemistry, & Toxicology (V8). Arlington, USA

2.2 Research theme Computational Chemistry

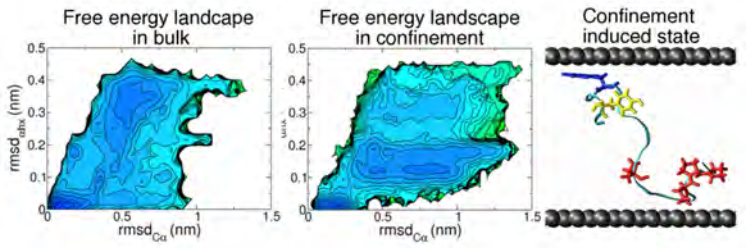
Prof. P.G. Bolhuis, Prof. R. Krishna, Prof. E.J. Meijer, Dr D. Dubbeldam, Dr B. Ensing, Dr C.P. Lowe, Dr J. Vreede, Prof. A. Fasolino, Dr A.J. Cruz-Cabeza (VENI-fellow)

Research in the Computational 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.
Our 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; and Development of computational techniques to model many-particle systems

Research highlights

The group has kept a strong record in modelling complex phenomena in chemical, physical, and biological systems. Below some highlights of the progress made in 2012 are listed.

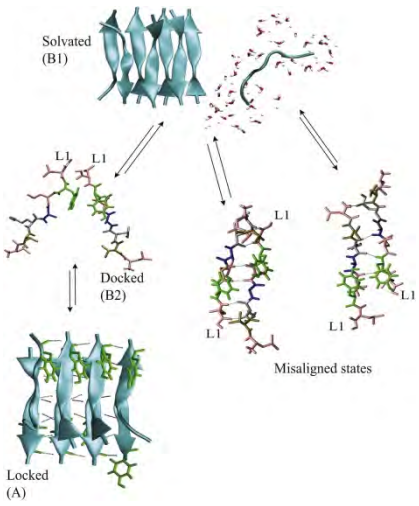
Protein conformational changes (Bolhuis, Vreede) Although protein folding is typically studied in dilute solution, folding in a living cell will be affected by interactions with other biomolecules and excluded volume effects. Marino and Bolhuis (J. Phys. Chem. B, 116, 11872, 2012) examine the effect of hydrophobic confinement on folding of the Trp-cage miniprotein, by using replica exchange molecular dynamics simulations to probe the differences between folding in the bulk, on a hydrophobic surface, and confined between two hydrophobic walls.



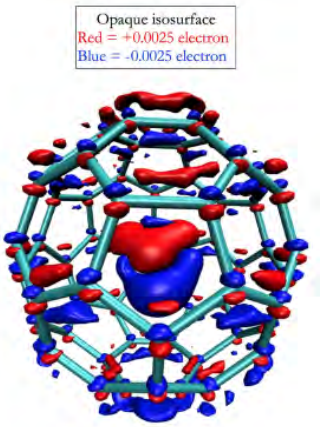
In addition to promotion of helix formation due to reduced conformational entropy of the unfolded state upon confinement, adsorption of Trp-cage to a hydrophobic surface stabilizes intermediate structures not present in the bulk. These new intermediate structures may alter the folding mechanism and kinetics and show the importance of including environmental effects when studying protein folding.

The histone-like nucleoid structuring protein (H-NS) is a DNA-organizing protein in bacteria. It contains a DNA-binding domain and a dimerization domain, connected by a flexible linker region. We determined in a molecular-dynamics study of the H-NS dimerization domain how the parallel complex is sensitive to changes in salt conditions (Vreede et al., Biophys. J. 103, 89. 2012). It is unstable in absence of NaCl, but stable at physiological salt concentrations. In contrast, the stability of the antiparallel complex is not salt-dependent. The stability of the parallel complex also appears to be affected by mutation of the critical but nonconserved cysteine residue at position 21, whereas the antiparallel complex is not. Together, our simulations suggest that osmoregulation could be mediated by changes in the ratio of parallel- and antiparallel-oriented H-NS dimers.

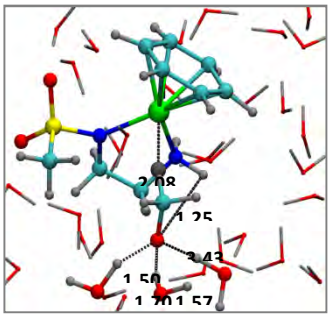
Biomaterials (Bolhuis, Vreede) We investigated the molecular mechanism of monomer addition to a growing amyloid fibril composed of the main amyloidogenic region from the insulin peptide hormone, the LVEALYL heptapeptide (Schor, Vreede, Bolhuis (Biophys. J. 103, 1296, 2012). Application of transition path sampling in combination with reaction coordinate analysis reveals that the transition from a docked peptide to a locked, fully incorporated peptide can occur in two ways.
Both routes involve the formation of backbone hydrogen bonds between the three central amino acids of the attaching peptide and the fibril, as well as a reorientation of the central Glu side chain of the locking peptide toward the interface between two beta-sheets forming the fibril. The mechanisms differ in the sequence of events. A major conclusion is that proper docking is important for correct alignment of the peptide with the fibril, as alternative pathways result in misfolding.



Chemical processes in complex environment (Meijer, Ensing) Most (bio)chemical processes occur in a complex, often fluctuating, environment, such as solvent, protein, or nanostructured cavities. We apply advanced ab intio molecular simulation techniques to address accurately the chemical rearrangements and the role of the environment.

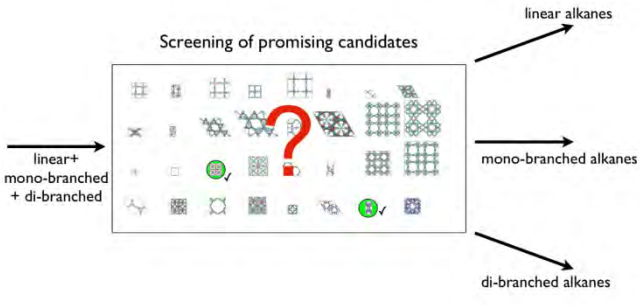


We studied the effect of confinement by C60 on the properties of a water molecule (Ensing et al, J. Phys. Chem. A 116, 12184, 2012). We found that H2O@C60 complex (that was only recently synthesized) has a relatively small dipole moment, deviating significantly from earlier estimates.
Our analysis showed that the induced dipole of the C60 takes a large value in the direction opposite to the water, yielding an overall complex value much smaller than that of an isolated water molecule, strongly reducing the overall dipole moment. Remarkably, the rather strong interaction between the C60-cage and the water molecule is mainly due to dispersion interaction and contains only a small contribution due electrostatic interaction.



We studied the role of an aqueous solvent on ruthenium-catalyzed transfer hydrogenation of formaldehyde using an explicit water model (Chem. Phys. Chem. 13, 3492, 2012). Our results suggest that the reaction mechanism in aqueous solution is significantly different from that predicted in the gas phase (concerted hydride and proton transfer) or in methanol solution (subsequent hydride and solvent mediated proton transfer).
We found that in an aqueous solvent the transition state is associated with the hydride transfer, converting the formaldehyde in a transient methoxide. The proton is transferred in a subsequent stage, being donated to the a solvent molecule. The catalyst remains protonated, in contrast to what was observed in simulations for the reaction in a methanol solvent.

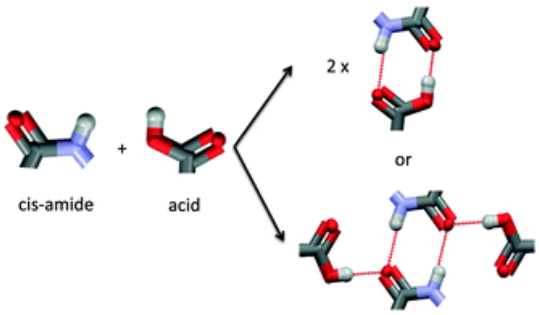
Hard Materials (Dubbeldam, Krishna, Lowe, Cruz-Cabeza) The design and development of novel nonporous materials is of paramount importance in the areas as storage, separation, and catalysis. A targeted approach requires a proper quantitative description of the materials. One focus concerned the identification of structures that are suitable for separating linear and mono-branched alkanes from di-branched alkanes (Dubbeldam, Krishna et al., Angew. Chem. Intl. Ed. 51, 11867, 2012).



By screening >100 nonporous materials for their hexane separation efficiency we identified the ZIF-77 structure as an important candidate yielding a selectivity two orders of magnitude better than current technology.

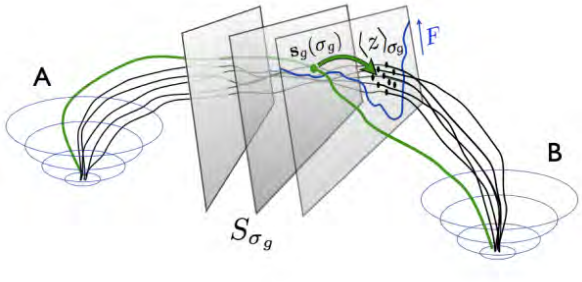
The results of the 100+ structures we examined in full detail lead to a clear molecular picture of alkane adsorption. The study has led to a patent application for ZIF-77 as an octane-number-enhancer for gasoline and as an alkane separation device. A second focus constituted a study into the feasibility of zeolitic imidazolate framework (ZIFS) as possible efficient candidates for the separation of gas molecules in the quest for clean energy from fossil fuels (Dubbeldam et al., Energy & Environmental Science 5, 7637, 2012).

In our focus area of molecular crystal structures we have studied synthon preferences in cocrystals of *cis*-carboxamides with carboxylic acids using a combination of database analyses, cocrystallisation experiments and theoretical calculations. We classify the *cis*-carboxamides into three families: primary amides, cyclic amides (lactams) and cyclic imides.



Using crystal structure prediction calculations, we sample the phase space of the cocrystals and generate observed as well as non-observed cocrystal structures and synthons in order to compare their relative stability as calculated with the PIXEL method. We conclude our study with a set of rules of synthon preferences derived from our observations and theoretical calculations. Whilst primary amides almost always form heterosynthons with carboxylic acids, cyclic imides seldom crystallize with them and cyclic amides represent a difficult prediction challenge. The study highlights the role played by the side interactions in the stability of the studied synthons.

Methods for Simulating Complex Systems (Ensing) We have developed a new advanced sampling method for the simulation of complex activated molecular transitions. Several existing techniques focus on computing the free energy profile as a function of a geometric reaction coordinate. However, often these approaches fail as the proper reaction coordinate is not known a priory, especially in the case of more complex transitions such as reactions in solution, or coupled in a bimolecular environment.



Our new method, named "path-metadynamics" (Ensing et al., Phys. Rev. Lett. 109 (2012), 020601) simultaneously determines the reaction mechanism and the associated free energy profile in a single simulation. The mechanism is expressed as a path in the free energy landscape that is spanned by a set of intuitive collective variables, for example the distances between the atoms that are involved in bond breaking and making. We demonstrated that the method is very efficient and robust, and implemented it in various widely used molecular dynamics packages.

Key publications

- G. Díaz Leines and B. Ensing, *Path Finding on High-Dimensional Free Energy Landscapes*, Phys. Rev. Lett. 109 (2012).
- K. A. Marino and P.G. Bolhuis, *Confinement-Induced States in the Folding Landscape of the Trp-cage Miniprotein*, J. Phys. Chem. B, 116, 11872 (2012)
- M. Schor, J. Vreede, and P.G. Bolhuis, *Elucidating the Locking Mechanism of Peptides onto Growing Amyloid Fibrils through Transition Path Sampling*, Biophys. J. 103, 1296 (2012)
- D. Dubbeldam, R. Krishna, S. Calero and O. Yazaydin, *Computer-assisted screening of ordered crystalline nanoporous adsorbents for separation of alkane isomers*, *Angew. Chem. Int. Ed.* 51, 11867-71 (2012)
- J. Vreede and R. Th. Dame, *Predicting the effect of ions on the conformation of the H-NS dimerization domain*, Biophys. J. 103, 89 (2012)
- A.M. Moragues-Bartolome, W. Jones and A.J. Cruz-Cabeza, *Synthon Preferences in Cocrystals of cis-Carboxamides:Carboxylic Acids*, CrystEngComm, 14, 2552, 2012.

- Pavlova and E.J. Meijer, *Understanding the role of water in aqueous ruthenium catalyzed transfer hydrogenation of ketones* , Chem. Phys. Chem. 13, 3492, 2012
- Lu, W., Sculley, J.P., Yuan, D., Krishna, R., Wei, Z. & Zhou, H.-C. (2012). *Polyamine-tethered porous polymer networks for carbon dioxide capture from flue gas.* Angewandte Chemie, International Edition, 51(30), 7480-7484.
- Krishna, R. (2012). Diffusion in porous crystalline materials. *Chemical Society reviews, 41*(8), 3099-3118.

Grants and Prizes

- Ensing - Bando Visiting Professor 2011–2012 awarded by the Servizio Relazioni Internazionali of the University of Padova, Padua, Italy.
- Ensing, Meijer, Dubbeldam – MolSim2012; CECAM grant
- Bolhuis & Meijer – NWO Bazis grant

Patent application

D. Dubbeldam and R. Krishna, *Process for separating mixtures containing straight-chain and branched alkanes*, *European Patent Office, Application No./12165907.2-2103* (April, 2012).

Organized conferences/schools

- Ensing – Winterschool Theoretical Chemistry and Spectroscopy, December 2012 (Han-sur-Lesse)
- Meijer, Ensing, Dubbeldam – Winterschool MolSim 2012 (Amsterdam)
- Bolhuis – ACMM Spring and Fall symposia (Amsterdam)
- Lowe – Write it Right, International workshops on writing scientific papers (multiple editions)
- Bolhuis, Ensing et al. – Lorentz Center extended workshop, Modelling the Dynamics of Complex Molecular Systems, August 13 - September 7, 2012 (Leiden)
- Meijer et al. – 14th International Conference on Theoretical Aspects of Catalysis (ICTAC-14), June 26-30, 2012 (Vlissingen)
- Ensing et al. – “Multiscale modeling of biomolecular systems" symposium at (MMM2012) October 15-19, 2012 (Singapore)

2.3 Research theme Analytical Chemistry (including its applications in Forensic Science)

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

In 2012 the shift in emphasis of the analytical-chemistry group from polymer analysis to more general analytical (separation) science became more visible, although some of the new projects were slow to get started. The job market for analytical scientists is such that temporary researchers leave early and that post-doctoral researchers are very hard to find.

Traditionally, the group has had strong ties with industry and this was reflected in many “bi-lateral” and “multi-lateral” research projects. With the advent of COAST the ties with industry are getting even stronger. This is reflected in the research of the group, but – remarkably – also in education. The MSc^{+} honours program is an initiative through COAST in which industry

contributes to education both in kind (transferring knowledge) and in cash (student grants). This will strengthen the position of the analytical-science program in Amsterdam.

The strong position that the Sectorplan Natuurwetenschappen (SNS) assigns to Amsterdam as a unique national centre for analytical chemistry is slow to materialize, despite the support of COAST, the public-private partnership on analytical sciences, which has its office in Amsterdam Science Park.

Arian van Asten (NFI), previously a visiting scientist in the group, was officially appointed professor in forensic chemistry.

Research overview

The *forensic-research* program is developing well, inspired by the energetic Arian van Asten. The collaboration with the Korteweg-de-Vries institute for mathematics is excellent and stimulating. The first in-house promotion in forensic science is to take place in late 2013 or early 2014. There are many initiatives to maintain a strong research effort.

The *chemometrics* efforts in the group (Gabriel Vivó Truyols) are in part focused on forensic science, but there are also strong links with food science and the chemical industry. Ironically, the upward trend in forensic research appears to be accompanied by a downward trend in forensic teaching, as the UvA forensic-science master appears to be heading in a different direction.

In the core area of the group, *analytical separation science*, there is strong focus on multi-dimensional separations. This includes comprehensive two-dimensional gas chromatography (GC×GC, Hans-Gerd Janssen) and comprehensive two-dimensional liquid chromatography (LC×LC, Peter Schoenmakers). Several new researchers started within the framework of the HYPERformance LC project (NWO / TA-COAST). This area also benefits from collaboration with the University of Valencia (Prof. M.C. García-Álvarez-Coque) and with several major instrument manufacturers.

Projects on *nanotechnology* (Wim Kok), *biomaterials* (Sjoerd van der Wal) and *gas chromatography for diagnosis of tuberculosis* (Arend Kolk) complete a very broad research program. On the latter subject the group collaborates with the AMC (Prof. Peter Sterk).

Key publications

- Peroni, D., Egmond, W. van, Kok, W.T. & Janssen, J.G.M. (2012). *Advancing liquid/liquid extraction through a novel microfluidic device: Theory, instrumentation and applications in gas chromatography.* Journal of Chromatography A, 1226, 77-86.
- Uliyanchenko, E., Cools, P.J.C.H., Wal, S. van der & Schoenmakers, P.J. (2012). *Comprehensive two-dimensional ultrahigh-pressure liquid chromatography for separations of polymers.* Analytical Chemistry, 84(18), 7802-7809.
- Vivó-Truyols, G. (2012). *Bayesian approach for peak detection in two-dimensional chromatography*. Analytical Chemistry, 84(6), 2622-2630.

Dissertations

Bedani, F. (2012, June 08). *Modes of operation and parameter selection in on-line comprehensive two-dimensional liquid chromatography.* University of Amsterdam (viii, 124 p.). Prom./coprom.: Prof. Dr Ir J.G.M. Janssen & Dr W.Th. Kok.

Uliyanchenko, E.V. (2012, July 03). *Ultra-performance polymer separations.* University of Amsterdam (218 p.). Prom./coprom.: Prof. Dr. Ir P.J. Schoenmakers & Prof. Dr S. van der Wal.

Pruim, W.P. (2012, December 18). *Towards fast multidimensional separations in microfluidic devices.* University of Amsterdam (107 p.). Prom./coprom.: Prof. Dr Ir P.J. Schoenmakers & Dr. W.T. Kok.

Grants

The NWO-funded *COMFOR* project on forensic profiling was started together with the Korteweg-de-Vries institute for mathematics (Prof. Marjan Sjerps), with two PhD students with vastly different backgrounds working side to side.

Contracts were signed for two *NWO/TA-COAST* projects:

Gabriel Vivó Truyols reached agreement with RIKILT, the NFI and DSM Resolve for the *Chromametrics* project (2 positions at UvA), but the actual research could not yet be started in 2012.

Peter Schoenmakers finalized 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. The first two researchers (PhD students) started on this project in the final quarter of 2012.

Conference

Professor Arian van Asten chaired the scientific committee of a very successful conference of the European Academy of Forensic Science (EAFS 2012; 1200 participants) in The Hague.

Lectures

Peter Schoenmakers presented plenary lectures at

- HPLC2012, Anaheim (CA, USA), June 16-21: *Ultra-High-Performance Separations of Macromolecular Samples* (invited)
- ISC2012, Torun (Poland), September 9-13: *Comprehensive two-dimensional HYPERformance LC* (invited)
- Int. Symposium on Polymer Analysis and Characterization (ISPAC) in Kerkrade (NL).
- ACS Fall Meeting (Philadelphia, PA, USA).
- NIST (Gaithersburg, MD, USA).

Hans-Gerd Janssen presented an invited lecture:

- 36th International Symposium on Capillary Chromatography, Riva del Garda (Italy), May 27- June 1): *Improving the balance between first and second dimension separation speeds in cryogenically modulated comprehensive GC×GC*

Gabriel Vivó Truyols presented lectures at

- the Massart-Award Symposium of the Belgian Chemometrics Society in Ghent (invited)
- Chemometrics in Analytical Chemistry (CAC) conference in Budapest (HU).

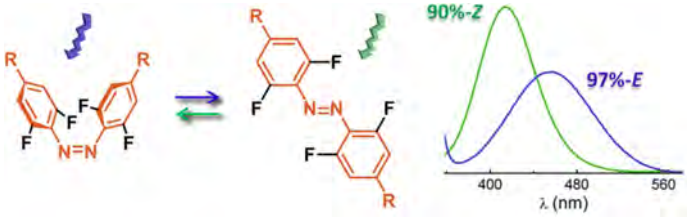
2.4 Research theme Molecular Photonics

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

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*.

Research highlights

Azobenzene at work. Two different international collaborations involving azobenzene led to high-impact papers. Together with prof. Eléna Ishow (Cachan/Nantes, France) we investigated azobenzene derivatives that are used for moving matter in order to create patterned surfaces using light. In this particular case, the azo units were connected to fluorescent groups, and our studies demonstrated that it is possible to create fluorescent patterns in amorphous films of low-molecular weight compounds, provided that the fluorescent unit and the azo chromophore were separated by a sufficiently large spacer (*Chem. Eur. J.* 2012, *18*, 3706–3720).



A small project with prof. Stefan Hecht and Dr David Bléger (Humboldt University, Berlin) demonstrated the power of qualitative Molecular Orbital theory in spectroscopy. We designed fluorinated azobenzenes with the purpose of spectrally separating the low-energy absorption bands of the E and Z isomers, and the Berlin group synthesized and characterized the compounds. In agreement with the predictions, a separation of 50 nm between the absorption maxima was found.

As a result it is now possible to excite the isomers selectively and switch acyclic azobenzenes with visible light with higher conversion than before to the E (97 %) and Z (90 %) isomers. The thermal conversion from the Z isomer to the E form is remarkably slow, which is advantageous for some applications. Finally, the carboxylic linker groups, which enhance the photophysical properties also enable straightforward incorporation of these improved photoswitches in many systems of interest in biological and materials chemistry (*J. Am. Chem. Soc.* 2012, *134*, 20597-20600).

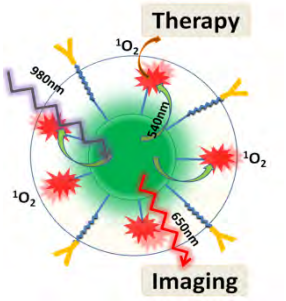
Photoinduced proton coupled electron transfer in aviram's hemiquinones. The structure and reactivity of a covalently linked catechol-ortho-benzoquinone (hemiquinone) is studied by UV-Vis and IR absorption spectroscopy. Nanosecond transient absorption spectroscopy of the hemiquinone reveals the formation of bi-radical state consisting of two semiquinone units. It is a long-lived state resulting from proton coupled electron transfer (PCET). (*Photochem. Photobiol. Sci.* 2012, *11*, 957-961).

Photoinduced hydrogen evolution from water. Multi-component systems for the light-driven reduction of protons, comprising of an iridium complex of general formula $[Ir(ppy)_2(pytl\text{-}R)]Cl$ as photosensitizer, platinum nanoparticles as the catalyst, and a sacrificial donor like EDTA depend on electron relays such as substituted viologens for the production of molecular hydrogen. Guest-appended viologens were

designed to assemble the components of the photocatalytic system in a supramolecular manner in order to promote the electron transfer between the cyclodextrin-appended photosensitizer [Ir(ppy)2(pytl-βCD)]Cl and cyclodextrin-modified Pt nanoparticles. The presence of adamantane or bile acid groups on the viologen induced stabilization and aggregation of the radical cations which is disadvantageous for hydrogen formation (*Eur. J. Org. Chem.* 2012, 6729-6736).

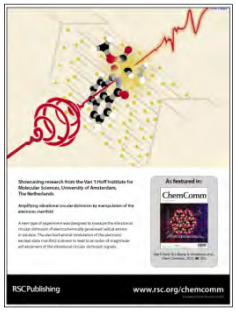
Immunoassays based on quantum dots and gold nanorods. Multi-sized quantum dots (QDs) donors and tailor-made gold nanorods (GNRs) have been employed to form a FRET nanoplatform for homogeneous immunoassays developed for analysis of multiple virus antigens. The single GNRs/multiple QDs nanocomposite based nanosensor offers a simple and sensitive approach for multiple analytes detection in a homogeneous format and have the potential to be applied in wide areas, such as medical-immune detection, point-of-care testing, high-throughput screening, and clinical diagnostics (*Chem. Commun.* 2012, *48*, 1781-1783).

Aptamer optical biosensors. An luminescence resonance transfer based optical biosensor of an aptamer-upconversion conjugate has been constructed. It has been demonstrated that photosensitized breakage and damage of aptamers are eliminated by employing upconversion nanoparticles (UCNPs) as donors. The aptamers-UCNPs strategy holds promising potential for future applications, such as liquid biochip and homogeneous immunoassay with high sensitivity and excellent specificity (*Chem. Commun.* 2012, *48*, 1156-1158).



Simultaneous fluorescence imaging and photodynamic therapy of cancer cells. A highly efficient multifunctional nanoplatform for simultaneous upconversion luminescence (UCL) imaging and photodynamic therapy (PDT) has been developed based on selective energy transfer from multicolor luminescent $NaYF_4$:Yb^{3+},Er^{3+} upconversion nanoparticles (UCNPs) to photosensitizers (PS). Different from popular approaches based on electrostatic or hydrophobic interactions, over 100 photosensitizing molecules were covalently bonded to every 20 nm UCNP, which significantly strengthened the UCNP-PS linkage and reduced the probability of leakage/desorption of the PS. Tests performed on JAR choriocarcinoma and NIH 3T3 fibroblast cells verified the efficient endocytosis and photodynamic effect of the nanoplatform with 980 nm irradiation specific to JAR cancer cells. (*ACS Nano* 2012, *6*, 4054-4062)

Amplified chirality. Vibrational circular dichroism, the circular dichroism associated with vibrational transitions, is a powerful spectroscopic method that makes it possible to probe molecular chirality at the level of specific chemical bonds. In general, VCD is difficult to measure because of the extremely small signal magnitudes. We have discovered that VCD can be amplified dramatically by changing the charge of a chiral molecule using electrochemistry. In this way, we "create" low-lying electronic states that lead to VCD enhancement through vibronic coupling. The method is simple, non-invasive, and widely applicable. (*Chem. Commun.* 2012*, 48,* 353-355).



Water in nanoconfinement. It is generally believed that confinement into nanometer-size volumes changes the properties of liquid water. Such nanometer-size volumes can be easily prepared in reverse micelles. However, up to now dynamical studies have mostly employed ionic surfactants, which compromises the results because of the high concentration of counter ions in the water. We have investigated water in inside nonionic reverse micelles, where this problem does not occur. Using a combination of x-ray scattering and time-resolved spectroscopy we investigate the structure and dynamics of the nanoconfined water as a function of temperature and micelle size.

We find that even small micelles contain a surprisingly large fraction of water that behaves exactly like bulk water, and that the confinement affects the reorientation dynamics of only the first outer layer. We find that the activation energy for the reorientation of the surface water molecules is close to that of water molecules in ice (*J. Chem. Phys.* **2012**, *137*, 044503).

Mapping out the operation cycle of a molecular machine. Time-resolved vibrational spectroscopy has been used to investigate the inter-component motion of an optically triggered molecular shuttle. The operation cycle of this molecular shuttle involves several intermediate species, which are separately observable in the amide I and amide II regions of the IR spectrum. From the time- and frequency-resolved data we have obtained a detailed picture of each stage in the operation cycle of the molecular shuttle (*Phys. Chem. Chem. Phys.* **2012**, *14*, 1865–1875).

Photoactive proteins in the gas phase. Chromophores of two different photoactive proteins have been studied in the gas phase in their biologically active form using the FELIX Free Electron Laser. For the fluorescent chromophore of the Green Fluorescent Protein (GFP), p-hydroxy-benzylidene-2,3-dimethylimidazolidinone (HBDI), we obtained the first IR spectrum of the anionic chromophore. Unlike the spectrum of the anion recorded in solution, the gas-phase experimental spectrum is convincingly reproduced by DFT calculations. In this study we moreover obtained an IR spectrum for the m/z 200 radical anion fragment of the chromophore that allowed for an unambiguous determination of its structure and in particular the radical site (*Int. J. Mass. Spec.* **2012**, *330-332*, 118–123).

The Photoactive Yellow Protein (PYP) has become a model system for studying biological light-induced signal transduction because of its small size and excellent stability. In our studies we have addressed the isomeric structures of the anion of its chromophore (*p*-coumaric acid (*p*CA)) by IR spectroscopy and have shown that the higher-energy isomer (carboxylate, +60 kJ/mol) is predominantly formed. Electrospray ionization has become common practice in mass spectrometry. The conclusion that that kinetic trapping can be a determining factor in the isomer distribution that is generated is therefore important, as evidenced by the observation that this behavior has led to considerable ambiguity in previous studies on the gas-phase photochemical properties of anionic *p*CA (*J. Phys. Chem. Lett.* **2012**, *3*, 2259-2263).

*Peptide bond tautomerization induced by divalent metal ions***.** The attachment of gas-phase divalent metal ions that bind as strongly as Mg^{2+} and transition-metal ions to the dipeptide PhePhe has been shown to result in the displacement of the amide proton. More weakly coordinating ions bind in the known charge-solvation mode. This iminol tautomerization rearrangement has been characterized by infrared multiple-photon dissociation spectroscopy using the FELIX Free Electron Laser which clearly shows the tautomeric transition. (*Angew. Chem. Int. Ed.* **2012**, *51*, 4591-4593).

Key publications:

- Bléger, D.; Schwarz, J.; Brouwer, A.M.; Hecht, S.; o-Fluoroazobenzenes as readily synthesized photoswitches offering nearly quantitative two-way isomerization with visible light, *J. Am. Chem. Soc.* 2012, *134*, 20597-20600.
- Liu, K.; Liu, X.M.; Zeng, Q.H.; Zhang, Y.L.; Tu, L.P.; Liu, T.; Kong, X.G.; Wang, Y.H.; Cao, F.; Lambrechts, S.A.G.; Aalders, M.C.G.; Zhang, H.; Covalently assembled NIR nanoplatform for simultaneous fluorescence imaging and photodynamic therapy of cancer cells, *ACS Nano* 2012, *6*, 4054-4062.

- Domingos, S.R.; Panman, M.R.; Bakker, B.H.; Hartl, F.; Buma, W.J.; Woutersen, S.; Amplifying vibrational circular dichroism by manipulation of the electronic manifold, *Chem. Commun.* 2012*, 48,* 353-355.
- Dunbar, R.C.; Steill, J.D.; Polfer, N.C.; Berden; Oomens, J.; Peptide bond tautomerization induced by divalent metal ions: characterization of the iminol configuration, *Angew. Chem. Int. Ed.* 2012, *51*, 4591-4593.

Dissertations

Piatkowski, L. (2012, January 27). *Water interacting with interfaces, ions and itself.* University of Amsterdam (174 p.). Prom./coprom.: Prof. Dr H.J. Bakker.

Plugge, M. (2012, February 16). *On the fluorescence properties of chromophores near metallic nanostructures.* University of Amsterdam (159 p.) (Wöhrmann Print Service). Prom./coprom.: Prof. Dr A.M. Brouwer.

Alvaro Galué, H. (2012, June 15*). Infrared spectroscopy of mass-selected aromatic and diamondoid molecular ions: a laboratory quest for the organic inventory in space.* University of Amsterdam (174 pag.). Prom./coprom.: Prof Dr J. Oomens.

Grants

Professors Buma and Brouwer received together with professor Janssen (VU) a 400,000 euro NWO-BAZIS grant for the project "*Photons for Chemistry*".

Dr Woutersen received a FOM Projectruimte grant of 400,000 euro (1 aio + 195 k€) for the project "*The protonic Hall effect*".

Dr Zhang received in collaboration with professors Aalders and van Leeuwen (both AMC) and the Changchun Institute of Applied Chemistry of the Chinese Academy of Sciences a 250,000 euro KNAW-China grant for the project "*Sensitive in-situ detection of circulating cancer cells using a multifunctional fiber modified with photonic nanoconjugates*".

Conferences

Professor Brouwer organized the HRSMC/EPA summer school on *Photochemistry* (Wijk aan Zee, September 15-19).

Professor Buma was the co-chairman of the HRSMC and ESF SILMI Programme Graduate School on *Modern developments in spectroscopy* (Noordwijk, April 2012).

Lectures

Professor Brouwer was honored with the Morino Lectureship (Morino Foundation, Tokyo, Japan) and gave a series of lectures in eight major Japanese universities. He also was invited to Taiwan (Short-Term visiting Scholar, Chemistry Research Promotion Center, National Science Council, Taiwan), where he delivered lectures in four universities, including one at the Taiwan National Photochemistry meeting.

Molecular Photonics staff members have given invited lectures at various prestigious conferences. Examples include

- IUPAC 8th International Conference on Novel Materials and Synthesis (NMS VIII) & 22nd International Conference on Fine Chemistry and Functional Polymers (Brouwer: "*Imaging Force Networks in Granular Matter*"),
- Gordon Research Conference on Electronic spectroscopy and dynamics (Buma: "*The difference between left and right*")
- CECAM Workshop 2012 on Vibrational Optical Activity: interplay of theory and experiment (Buma: "*Boosting up the difference between left and right*")
- NMLP2012 conference (Zhang: "*Photonic nanoplatforms for medical applications – origin of luminescence and optimization*")
- 60th Annual meeting on mass spectrometry and allied topics, (Oomens: *Spectroscopic identification of non-oxazolone b2 peptide fragments*)
- Workshop Exploiting Free Electron Lasers in Chemistry (Oomens: *Molecular structure determination in mass spectrometry by FEL-based ion spectroscopy*)
- 6th International Conference on Coherent Multidimensional Spectroscopy (Woutersen: "*Time-resolved two-dimensional infrared spectroscopy of an operating molecular machine*").

Other highlights

Professor Buma has been appointed as chairman of the *John van Geuns Fonds* foundation, and as member and secretary of the board of the *Stichting Bèta Plus*.

Dr Zhang has been appointed in 2012 as a chair professor at the Northeast Normal University (China).

Professor Oomens has been appointed as professor *Molecular structure and dynamics* at the Radboud University Nijmegen

Professor Cao Jinghua, deputy director general of the Chinese Academy of Sciences (CAS), visited the University of Amsterdam on Wednesday in December 2012. He met with researchers of the Van 't Hoff Institute for Molecular Sciences (HIMS), and in particular of the Molecular Photonics group, one of the major research partners of CAS in the Netherlands. Professor Cao visited the Netherlands by invitation of the Royal Netherlands Academy of Arts and Sciences (KNAW) and the Netherlands Organisation for Scientific Research (NWO). Since recently he has been appointed responsible for the European collaboration of the Chinese Academy of Sciences.

From left to right: Front row: Mr. Bo Quan (officer from Chinese Embassy at Den Haag), Prof. Aart Kleijn (director of HIMS), Mr. Cao Jinhua (CAS), Prof. Wybren Jan Buma (HIMS), Dr Hong Zhang (HIMS), Ms. Dongyao Wang (CAS) Back row: Ms. Marianne van Driel (KNAW), Dr Sander Woutersen (HIMS), Prof. Fred Brouwer (HIMS), Prof. Maurice Aalders (AMC), Prof. T. van Leeuwen (AMC).

Outreach

Dr Woutersen gave a short talk on Radio 1 on December 16, 2012 regarding Greek and Latin in the natural sciences.

2.5 Other research activities

2.5.1. Science for Arts and Computational Polymer Chemistry

Prof. P. Iedema, Dr A. van Loon, Dr K. Keune

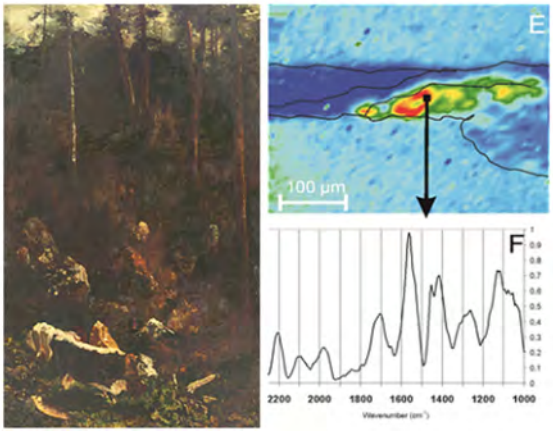
Research Highlights

Paint Alterations in Time – PAinT.

The Science for Arts department of the group was successful in the acquirement of this 600,000 euro project in the NWO Science4Arts Programme. The aim of the project is to discover the chemical driving forces behind the reactions and migration processes of organometallic compounds in oil paint layers.

Dr Annelies van Loon and Dr Katrien Keune have been appointed as the staff members leading the group and drs. Joen Hermans has joined the team as a PhD student. The project is carried out in collaboration with the Humanities Faculty, from where drs. Maartje Stols-Witlox is delegated in the core team. All main Dutch museums are involved in the project, among which the Maurithuis acts a co-applicant.

Several research activities preliminary to the project have already borne fruit in the form of papers and presentations on occasions like the meeting in Brussels, September 2012, on "New Findings on The Three Marys at the Tomb by Van Eyck in Museum Boijmans Van Beuningen". A special website for the PAinT-projects has been constructed: s4a-paint.uva.nl.



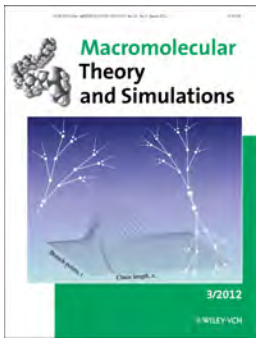
Degradation of Emerald green in oil paint and its contribution to the rapid change in colour of the Descente des vaches (1834–1835) painted by Théodore Rousseau (left)

E: part of the FTIR spectrum corresponding to pixel in the FTIR image at 1572 cm−1, showing characteristic vibrations of Emerald green at 1572 and 1427 cm−1

F: backscatter electron image detail

Branching and scission modeling in the context of polymer modification

Ongoing research regarding this subject has been reported in a number of papers in *Macromolecular Theory and Simulations*, among which one made it to a cover story (image). One of the interesting results was that it turned out to be possible to construct an analytical equation describing the rather complex branching topology resulting from 'end-to-end' branching.



As a result from a collaboration with BASF (Ludwigshafen) a paper has been written on the melt-mixing process of linear (CD) and hyperbranched (AB_2) polycondensates. A simplified scheme could be solved by solving the population balances in a deterministic manner. The full problem could only be dealt with using Monte Carlo simulations. A typical and unexpected phenomenon observed, from the modelling results, is the difference in time between the change of the molar mass distribution and the change of the copolymer composition. The former takes place in a few seconds, the latter – the real 'mix-melting' – takes a few hours.

Key publications

Science for Arts

- Noble, P., Van Loon, A., Alfeld, M., Dik, J., and Janssens, K. (2012). *'Rembrandt and/or studio,* Saul and David*,* c.*1655: revealing the curtain using cross-section analyses and X-ray fluorescence imaging',* In: Technè*,* No. 35, Special Issue Rembrandt, Scientific Approaches and Restorations: 36-45.
- Keune, K., Boon, J., Boitelle, R. and Shimazu, Y. (2012). *'Degradation of Emerald green in oil paint and its contribution to the rapid change in colour of the* Descente des Vaches *(1834-35) painted by Théodore Rousseau',* In: Studies in Conservation*.* In print.
- Wallert, A., Keune, K., Van Iperen, J. and Pedrosa, J. (2012). *'Early Northern Netherlandish Paintings and Gilding Techniques and Cologne; some Parallels',* In: Zeitschrift für Kunsttechnologie und Konservierung, 26, Heft 1: 230-240.

Computational Polymer Chemistry

- Iedema, P.D., Dreischor, M., Hungenberg, K.-D.,Orlov, Y. (2012). *Predicting the change of MWD caused by interchange reactions during melt-mixing of linear and branched polycondensates (AB2),* Macromol. Theory Simul., 21, 629–647.
- Iedema, P.D. *Predicting MWD and Branching Distribution of Terminally Branched Polymers Undergoing Random Scission.* Macromol. Theory Simul. 2012, 21, 166–86.
- Iedema, P.D. *Investigating the Architecture of Segmented and Branched Polymers under Random Scission by Mathematical Modeling.* Macromol. Theory Simul. 2012, 21, 187-208.

2.5.2 Research program of the Director

Prof. A.Kleijn

When Aart Kleijn joined HIMS as director 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.

DIFFER
Dutch Institute for
Fundamental Energy Research

Summary of research activities

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.

Activity 1-3 are ongoing. Activity 1 will be terminated with the PhD-thesis of Hans van Eck at the technical University Eindhoven. Activity 2 is ongoing and will lead to the PhD examination of Rianne ‘t Hoen at the UvA. Activity 3 is ongoing in collaboration with M2i and ASML. Activity 4 has been ended with the PhD-thesis of Christine Hahn at Leiden University. Some papers still need to be published.

3 Strategy, activities and results

3.1 The Institute

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.

A formal overview of the HIMS activities, objectives and results for 2012 is defined in the FNWI-UvA/CvB agreement between Institute, Faculty of Science and Board of the University (2010-2012). An overview is given in the following table. The results, indicated very briefly in the last column of the table, are discussed below.

	Activities	***Objectives***	***Results***
2012	a. Positioning of research field of Sustainable Chemistry	Creation of the Institute for Sustainable Chemistry Amsterdam (ISCA) with industrial partners	Creation of ISCA failed due to financial crisis.
		Expansion of bilateral collaboration with industry.	Bilateral collaborations have been expanded little. Sustainable chemistry has been pushed as a research focus of the UvA.
	b. Better control and guidance of PhD-students	Increase of promotion yield, less than 20% drop outs after 15 month test.	Following system in place through PhD-students seminars and careful tracking of progress.
	c. development of hiring policy for 3-5 ordinary professors	From 5 to 7 professors in 2012.	On track.
	d. raising the share of HIMS staff in internal and external chemistry education.	2-3 additional courses in education by FNWI, FGW and AUC.	So far not possible.
	e. filling all open positions in the SNS program (analytical chemistry, biocatalysis).	All positions are filled.	Hiring failed to lacking financial support for new chairs.
	f. For all HIMS themes try to collaborate with colleagues of the VU in supra-university collaborations.	HIMS activities are carried out as part of ACMM, Laserlab Amsterdam, TI-COAST.	Has been realized.
	g. New research initiatives with the VU in the area of sustainable energy (with physics). Explore mass spectrometry.	Two novel research activities.	Joint creation of solardam initiative. Mass spectrometry exploration carried out through hiring policy SNS positions.
	h. New research projects in forensic sciences and science for arts/	2-4 new research projects in 2011-2012.	Realised.
	i. Consolidate SOFT matter cluster. ERC synergy grant proposal with IoP recruitment of outside and guest PhD students	Create Soft matter research focus of FNWI. Exploration private-public partnerships with a.o. Shell.	Research focus of FNWI has been established. Successful interaction created.

	k. Finishing pending PhD programs. improve the efficiency of the doctoral research path through better control and guidance	15 PhD exams in 2012. Appointment of 1-2 new (preferably endowed) part-time professors	9 PhD exams in 2012 due to contract extensions and illness.
	l. About 10 proposal submissions with NWO, STW, ERC, both investments and exploitation.	Granting of 5 proposals.	Realised.
	m. Increase number of yearly evaluations of personnel.	75% of staff has been evaluated.	Significant improvement has been realized. FNWI cannot deliver correct numbers.

a. Positioning of research field of Sustainable Chemistry

To collaborate with industry on topics from sustainable chemistry (notably catalysis) HIMS has tried to create the new *Institute for Sustainable Chemistry Amsterdam (ISCA).* The idea was to perform research in areas of long term interest of the industries involved.

Several meetings with relevant and interested industries have been arranged and contacts with potential new staff members have been made. The idea was that with an industrial contribution of about 25% of the total ISCA budget long term research relevant to industry would be carried out. Industry, through the board of ISCA, would have a strong voice in the determination of the research goals of ISCA. The other sources of income for ISCA would be the second money stream (NWO, EU) and the UvA. The FOM Institute AMOLF could serve as a model for ISCA.

Unfortunately, due to the economic crisis and shrinking budgets for research in industry the project could not be continued. As a follow up to ISCA now Sustainable Chemistry has been proposed as a research focus of the University of Amsterdam. A consortium of HIMS professors headed by Joost Reek has prepared a proposal for such a 'UvA zwaartepunt'. In addition, several bilateral collaborations with industry have been pursued, which is detailed in chapter 4.

b. Better control and guidance of PhD-students

In 2012 a total of 9 PhD diplomas were obtained by HIMS students. This is low in comparison with the preceding years (2011: 15; 2010: 14; 2009: 16) and also in relation to the total number of PhD-students (59). This is mainly due to the delays students encountered because of the moving of the HIMS laboratories in 2010. In some cases delays added up to many months before full operation was resumed. In addition there were a number of cases of prolonged illness.

HIMS is now putting a progress monitoring system in place. The aim is to make sure that students passing the evaluation after 15 months can within reason obtain their PhD within 4 years. The dropout rate should be decreased and the commitment of students and staff to a successful PhD track increased. The director monitors progress of the students twice a year and discusses this with the staff.

The year 2013 will be an important test. In this year HIMS expects to increase the number of PhD diplomas and the efficiency of their doctoral research path, in line with the 100+ programme of the faculty.

The PhD-student seminars are an important instrument in this respect. They are held every other week with most of the PhD-students and the staff present. All PhD-students have to give lectures at the beginning (<1 year) and the end (>2 years) of their research period.

c. Development of hiring policy for 3-5 ordinary professors

This is a multiyear effort and preparations have been made for several appointments in 2013. Dr Arian van Asten has been appointed as extraordinary professor in 2012.

d. Raising the share of HIMS staff in internal and external chemistry education.

Most of the HIMS teaching takes place in the chemistry curriculum. This has been joined with the VU in 2012. As a result the teaching load on HIMS has decreased a little because of joint courses. It is attempted at all possible occasions to involve HIMS staff more in teaching in other curricula, in and outside of our faculty. The number of opportunities is most unfortunately limited. The further merging of UvA and VU will have a large impact on this point.

e. Filling all open positions in the SNS program (analytical chemistry, biocatalysis).

In the light of the possible creation of ISCA (see a) hiring was put on hold to allow integration of the new professors in ISCA. After the decision to stop development of ISCA hiring has started for both positions. In biocatalysis an excellent candidate rejected the offer - his home University made him an offer that HIMS could not possibly match because of a lack of resources. In analytical chemistry an excellent candidate was identified (who rejected our offer in April 2013). For both chairs hiring is powerfully continued.

f. For all HIMS themes try to collaborate with colleagues of the VU (supra-university collaboration).

The themes Analytical Chemistry, Computational Chemistry and Molecular Photonics have strong interactions with VU colleagues through respectively COAST, ACMM and LaserLab Amsterdam. The theme Sustainable Chemistry is mainly concentrated in HIMS. For this theme the aspiration is to become a UvA Research Focus.

g. New research initiatives with the VU in the area of sustainable energy (with physics). Explore mass spectrometry.

Together with VU and AMOLF colleagues the Solardam consortium has been created. This consortium will investigate conversion of solar energy in electricity, and also into liquid fuels (solar fuels). The consortium is now establishing itself, also in the framework of the coming AFS.
It was attempted to hire a new professor of mass spectrometry. The latter is nationally seen by COAST as having a center of gravity in Amsterdam. The appointment of the new professor should strengthen the ties with the analytical chemists at the VU.

h. New research projects in forensic sciences and science for arts.

In 2012 several projects have been realised in these areas providing them with a solid base for excellent research, see 2.3 and 2.5.1.

i. Consolidate SOFT matter cluster. ERC synergy grant proposal with IoP.

The SOFT matter cluster has been created with the FNWI. From HIMS professors Bolhuis and Brouwer are participating. The cluster is headed by professor Bonn (IoP). Bolhuis and Bonn have also submitted a synergy grant to ERC, but most unfortunately without success.

j. Recruitment of outside and guest PhD students.

Outside students can be students working in other, non-UvA laboratories, who will get their PhD at the UvA and in this way financially support HIMS without significant cost for the institute. HIMS has a few of these students. Their number might be going down because the external Institutes are demanding part of the financial reward.
In addition we have bursary students from other countries such as China. Their recruitment is going on, also thanks to the successful visit of a delegation of the Chinese Academy of Sciences (see 2.4). Furthermore, HIMS was involved in the creation of a FOM-Shell program on computational sciences in collaboration with India. The students involved will be regular FOM students.

k. Finishing pending PhD programs. Improve the efficiency of the doctoral research path through better control and guidance.

This point has already been discussed under item b above.

l. About 10 proposal submissions with NWO, STW, ERC, both investments and exploitation.

In 2012 a number of new proposals has been granted involving about 8 M€. Proposals are listed under all research groups.

m. Increase the number of yearly evaluations of personnel.

The number of yearly evaluations has increased very much. Quantitative data have not been provided yet.

3.2 Other activities operated by HIMS

3.2.1 Holland Research School of Molecular Chemistry (HRSMC)

Accreditations in 1994, 1999, 2005 and 2012

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

The HRSMC comprises of research groups of the van ‘t Hoff Institute of Molecular Chemistry (HIMS, University of Amsterdam); the Institute for Electrons and Molecular Structure (EMS, VU University); and the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION), all of Leiden University. The University of 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
    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 HRSMC approach 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.

In 2012 the HRSMC has been elected as one of the thirteen Graduate Schools to receive substantial funding from the Netherlands Organisation for Scientific Research (NWO). With this funding the HRSMC can offer young PhD students the opportunity to develop their research ideas within the framework of the programme "*Sustainability, the Molecular Approach*". The funding is part of NWO's Graduate Programme and aims to develop Dutch PhD Educational Programmes.

Major HRSMC activities 2012

1. Annual HRSMC symposium (November 22, 2012). 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 2012 consisted of:
   - Synthetic Chemistry problem solving sessions,
   - the two weeks Course *Molecular Simulation*, organised under the auspices of CECAM (9-20 January 2012, UvA),
   - the Tulip School on *Modern Developments in Spectroscopy* (April 10-13, Noordwijk)
   - the EPA *Summerschool on Photochemistry* (September 15-19, Wijk aan Zee).
   - the KNCV/HRSMC Career Advice Activity for PhD students and postdocs (March 2). The KNCV is the Royal Dutch Chemistry Association.

   Furthermore, the HRSMC has participated in the organization of the Winter School Theoretical Chemistry and Spectroscopy (December 10-14, Han-sur-Lesse)

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

3.2.2. Comprehensive Analytical Science and Technology (TI-COAST)

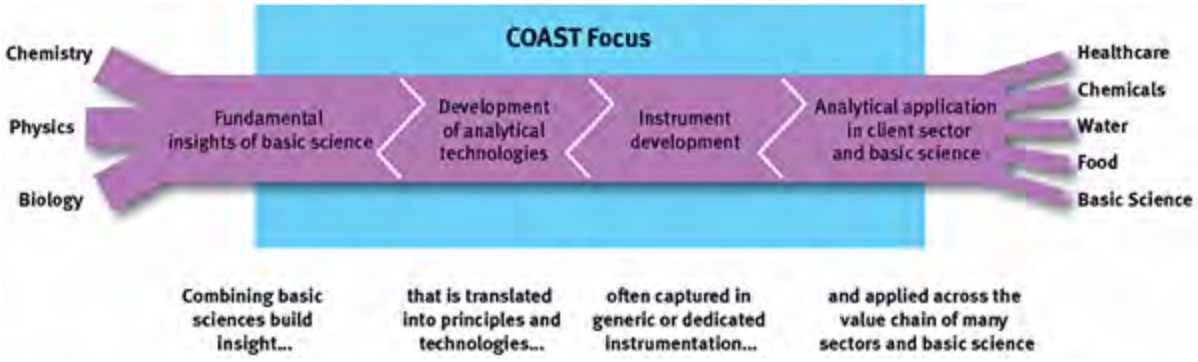
HIMS houses the headquarters of TI-COAST, the Dutch public-private partnership in Comprehensive Analytical Science and Technology (hence the abbreviation).

COAST aims to advance Dutch excellence in its *TOPsectoren* by providing pivotal analytical knowledge and instruments based on fundamental science and by ensuring transfer of analytical expertise

between application areas. COAST plans to achieve this by securing and improving Dutch expertise in analytical science and technologies.

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

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



'COAST' has developed and now executes an integrated plan for Research, Education and Technological Infrastructure.

To accomplish this it runs a number of programs. TA-COAST for example is part of the R&D program cluster of COAST and aims to generate breakthroughs in analytical science with application in multiple economic sectors. TA-COAST is subsidized by NWO and the Ministry of Economic Affairs.

Another example is the MSc+ (grant) program for talented MSc students in Analytical Sciences.

4 Valorisation

4.1 Patents

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 in the last years, while some new projects are promising.

The following patents were granted in 2012:

- Smeenk, L.E.J., Maarseveen, J.H. van, Dailly, N. & Timmerman, P.: *Preparation of novel bicyclic peptide mimetics via CLIPS technology, their antibody binding affinity and their use for structural mimicry of protein surfaces,* WO 2012057624.
- Reek, J.N.H. & Coppens, M.O.: *Mesoporous diphosphine-transition metal complex catalyst for hydroformylation,* WO 2012004352.

The following patents were filed in 2012.

- Dubbeldam, J D. and Krishna, R.: *Process for separating mixtures containing straight-chain and branched alkanes* (European Patent Office, Application No./12165907.2-2103.
- Dimian, A.C., Rothenberg, G. & Schut, R.: *Production and separation of fatty acid alkyl esters*, WO 2012072557.
- Dimian, A.C., Rothenberg, G. & Schut, R.: *Production of fatty acid alkyl esters for biodiesel fuels,* WO 2012072574.
- Calderone, V.R., Shiju, N.R., Rothenberg, G. and Curulla-Ferre, D.: *Core-shell particles with catalytic activity,* WO 2012/163969.
- Alberts, A.H. and Rothenberg, G.: *Composite material comprising synthetic filler and specific polymer,* WO 2012/140239.
- Alberts, A.H. and Rothenberg, G.: *Laminate comprising carrier and coating polymer,* WO 2012/140238.
- Alberts, A.H. and Rothenberg, G.: *Composite material comprising bio-filler and specific polymer,* WO 2012/140237.

4.2 Cooperation with industry

HIMS has transferred the patent and all related Intellectual Property rights on a new catalyst to DSM. The catalyst was discovered by Dr Raveendran Shiju of the Heterogeneous Catalysis and Sustainable Chemistry group (Prof. Gadi Rothenberg). It contributes to more sustainable processes for making fine chemicals and pharmaceutical intermediates and for polymer production.

The same Heterogeneous Catalysis and Sustainable Chemistry group signed an agreement with the German specialty chemicals company LANXESS. It centres on the search for a new catalytic route to 1,3-butadiene, the most important monomer for making rubber for car tires. LANXESS will invest over a period of three years in this research project.

In another project, multinational concern Solvay has signed a research agreement with Rothenberg's group, setting up a unique construction where the research group would try and help solving problems of Solvay business units that are related to the group's expertise in predictive modeling.

4.3 Spin off companies

Valorisation of know-how is of increasing importance, as evidenced by two HIMS spin-off companies, both realized under the umbrella of the UvA Holding.

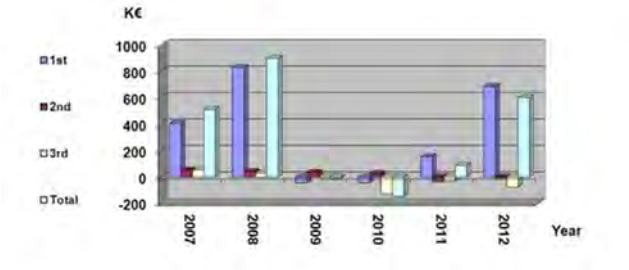
The spin-off company *Yellow Diesel BV* was started by the Heterogeneous Catalysis and Sustainable Chemistry group of Gadi Rothenberg in 2008. It pursues the development of second generation biofuels through heterogeneous catalysis. YellowDiesel has finalised the lab development of a continuous process for manufacturing biodiesel and is now seeking investment for scaling up to manufacturing scale.

The spin-off company *InCatT BV* focuses on marketing a technological invention in the field of homogeneous catalysis. InCatT was initiated in 2009 by HIMS chemist Joost Reek. 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.

5. Management and finances

In 2012 the financial position of HIMS has further improved. The institute has restored its sound financial position of the years before 2009. In that year the structural university budgets (1st moneystream/ 1e geldstroom) for HIMS were reduced with 10% (1 M€). This resulted in a dramatic decrease of the HIMS financial results in 2009 and 2010, of which HIMS now clearly has recovered.

HIMS results 2007 – 2012 (all funding sources; k€)[1]



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

The total budget for 2012 was 14.784 k€ (429k€ less budget available than in 2011) and the total costs were 13.713 k€ (see Table below). The integral result obtained in 2012 (+1.071 k€, all funding sources) is appreciably higher than obtained in 2011 (+705 k€) and 2010 (-637 k€). Actual financial numbers of 2012 (and 2011 for comparison) are given in the tables below[2].

HIMS resources and results 2012

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

HIMS resources and results 2011[3]

2011	1st	1st other	1st total	2nd	3rd	total
Total benefits/budget	**4.493**	**1.475**	**5.968**	**4.290**	**4.955**	**15.213**
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	**-138**	**909**	**771**	**-35**	**-31**	**705**
Restitution from reservation RD	147		147			**147**
Reservation Sector Plan		470	470			**470**
Result including reservations	**-285**	**439**	**154**	**-35**	**-31**	**88**

[1] Results excluding (restitution of) reservations
[2] For more details see chapter 7.3
[3] Including the partial restitution (+147 k€) from the reservation made in 2010 for discontinuation of the X-ray diffraction activities the 2011 HIMS result amounts to +705 k€.

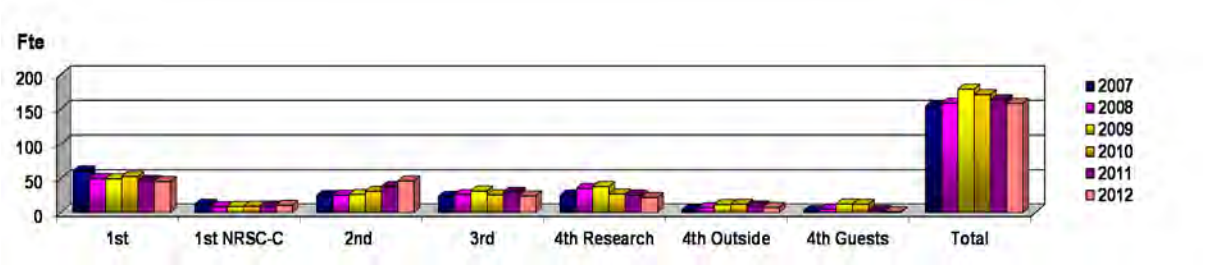
In comparison to 2011 the university budget (1st moneystream) for 2012 was almost indentical. The 2nd moneystream increased with 479 k€ while the 3rd moneystream was reduced with 901 k€.

The costs in the 1st moneystream were reduced with 393k€, when compared to 2011. There were some corrections on the work in progress related to the years before. The total personal costs were reduced with 554 k€. In 2012 882 K€ of the personal costs could be transferred from the 1st to the 2nd and 3rd moneystream (to projects), since 7.3 fte of the HIMS co-workers in fixed positions (5.6 fte staff, 1.7 fte technicians) were financed by external projects.

Because of the increasing budgets for projects in the 2nd moneystream (with 479 k€), also the costs in the 2nd moneystream increased (with 454k€). In the 3rd moneystream it was the opposite.

With a total of 3,18 M€ in external funding (excluding the own matching budget of approximately 1.47 M€) the year 2012 was less successful than the top year 2011 (8,70 M€) and the year 2010 (5,01 M€). These funds were acquired from funding agencies such as NWO (HRSMC graduate program, 2 BAZIS, 1 ATHENA, 1 ECHO grants) and FOM, as well as from industry and other partners.

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



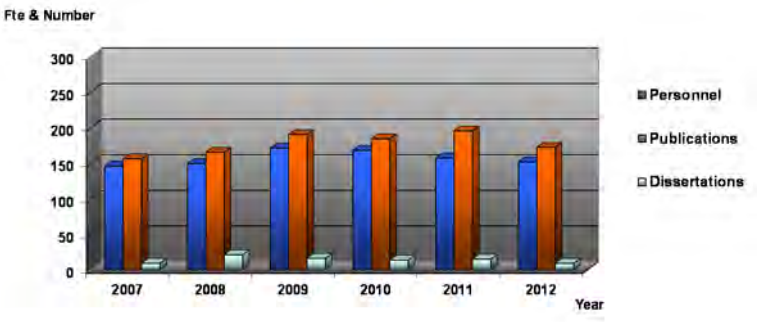
The personnel numbers in the graph are based on full-fte input

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

Externally financed projects count for ~70% of our personnel costs in 2012 (much less in 2011: ~40%).

HIMS personnel input data for 2010-2012 are ~15 fte higher than for 2007-2009, mainly caused by an increase in projects in the last years. Additionally in the years 2010-2012 a negative influence on fte's (small decrease in research staff numbers) can be found in the change in guest administration of our guest PhD students (PhD students with projects finished, but PhD defences still to come). In former years the PhD guest students were full-time appointed for the duration of their guest appointment after finishing their contracts. Presently they are administrated part-time when still present at HIMS (mostly 0.1 fte) or even 0.0 fte, when finishing their thesis elsewhere. This is because of restricted working places at HIMS and cost limitations.

Research input [1)] (fte) and output (number of publications and dissertations) 2007-2012



[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

In 2010 the research achievements in the field of chemistry of seven Dutch universities were reviewed (covering the period 2001-2009). Regarding the University of Amsterdam the international review committee of twenty experts evaluated five HIMS research programmes: *Bio-Molecular Synthesis, Catalysis, Computational Chemistry, Macromolecular and Biosystems Analysis,* and *Molecular Photonics*.

In the HIMS 2011 Annual Report we reported on this evaluation in detail, as well as on a preceding bibliometric analysis published in 2010 (performed by the Center for Science and Technology Studies CWTS).

In 2012 a new Scientific Advisory Committee (SAC) of HIMS is being formed. The new SAC will gather in the course of 2012 for the three yearly (internal) review of HIMS (covering the period 2010 - 2012).

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 2012 of the HIMS themes, per employment type (fte)[a]

source: METIS

	SC	COMP	ACF	MOLP	Other	**Total**
Tenured staff	5,4	3,0	1,5	2,5	0,8	13,2
Non-tenured staff	17,1	2,7	0,7	2,8	0,3	23,6
PhD candidates	22,1	10,8	11,0	13,5	1,6	59,0
Total research staff	**44,6**	**16,5**	**13,2**	**18,8**	**2,7**	**95,8**
Technicians [b]	13,3	0,0	2,5	3,4	0,2	19,4
Visiting fellows [c]	0,0	0,0	0,3	0,1	0,0	0,4
Total research	**57,9**	**16,5**	**16,0**	**22,3**	**2,9**	**115,6**
Supporting staff					6,5	6,5
Total staff	**57,9**	**16,5**	**16,0**	**22,3**	**9,4**	**122,1**

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

Research- and supporting staff 2012 of HIMS and the HIMS groups, per employment type (fte)[a]

source: METIS

	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	Other	**Total**
Tenured staff	1,5	0,3	1,5	0,6	1,5	2,0	1,0	1,5	1,5	1,0	0,8	13,2
Non-tenured staff	0,0	0,9	10,6	0,0	5,6	2,1	0,6	0,7	2,5	0,3	0,3	23,6
PhD candidates	2,6	1,0	15,0	2,3	1,2	6,8	4,0	11,0	11,2	2,3	1,6	59,0
Total research staff	**4,1**	**2,2**	**27,2**	**2,8**	**8,3**	**10,9**	**5,6**	**13,2**	**15,2**	**3,7**	**2,7**	**95,8**
Technicians [b]	3,3	0,8	4,9	2,0	2,4	0,0	0,0	2,5	2,2	1,2	0,2	19,4
Visiting fellows [c]	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,3	0,1	0,0	0,0	0,4
Total research	**7,4**	**3,0**	**32,1**	**4,8**	**10,7**	**10,9**	**5,6**	**16,0**	**17,5**	**4,9**	**2,9**	**115,6**
Supporting staff											6,5	6,5
Total staff	**7,4**	**3,0**	**32,1**	**4,8**	**10,7**	**10,9**	**5,6**	**16,0**	**17,5**	**4,9**	**9,4**	**122,1**

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

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

7.1.2 Scientific Staff

Research theme Sustainable Chemistry (1)
5 research groups

Prof. dr. J.N.H. Reek, Vici Laureate (rg[1]-1.1)
Homogeneous and Supramolecular Catalysis

Prof. dr. C.J. Elsevier (rg-1.2)
Molecular Inorganic Chemistry

Prof. dr. G. Rothenberg, Vidi Laureate (rg-1.3)
Heterogeneous Catalysis and Sustainable Chemistry

Prof. dr. H. Hiemstra (rg-1.4)
Synthetic Organic Chemistry

Prof. dr. R. Wever (rg-1.; retired 01-09-2012)
Biocatalysis and Bio-organic Chemistry

Vacancy (rg-1.4)
Industral Fine Chemistry (0.2 Fte)
(bijzonder hoogleraar Stichting Betaplus)

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

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

Research theme Computational Chemistry (2)
3 research groups

Prof. dr. E.J. Meijer (rg-2.1), KNAW fellow
Molecular Simulations

Prof. dr. P.G. Bolhuis, Vici, Vidi and FOM Springplank Laureate (rg-2.3)
Simulation of Bio-molecular Systems

Prof. dr. R. Krishna (rg-2.2;retired 13-09-2011)
Chemical Engineering

[1] rg = research group

Prof. dr. A. Fasolino/KUN (rg-2.1)
Computational Physics of Condensed Matter(0.0 Fte)

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

Research theme Analytical Chemistry (including its applications in Forensic Science) (3)
1 research group [2]

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

Prof. dr. ir. J.G.M. Janssen / Unilever
Analytical Separation of Biomacromolecules(0.0 Fte)
(bijzonder hoogleraar Stichting Betaplus)

Prof. dr. S. van der Wal / DSM
Bioterials Analysis (0.0 Fte)
(bijzonder hoogleraar Stichting Betaplus)

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

Research theme Molecular Photonics (4)
1 research group

Prof. dr. W.J. Buma (rg-4)
Molecular Spectroscopy

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

Prof. dr. H.J. Bakker/FOM-Amolf
Ultrafast Spectroscopy of Molecules in the Condensed Phase (0.0 Fte)

Prof. dr. J. Oomens/FOM-Rijnhuizen
Action Spectroscopy (0.0 Fte)
(bijzonder hoogleraar Stichting Physica)

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

[2] Collaboration with De Koster and Smilde from SILS

Computational Polymer Chemistry and Science for Arts

Prof. dr. P. Iedema
Physical Technology

Prof. dr. N. Tennent / FGW (0,0 Fte)
Art Sciences

7.1.3. Management of HIMS

Scientific Director
Prof. dr. A.W. Kleijn

Management team (bedrijfsvoering)
G.J.J. Zonneveld - de Boer, Drs. H.E. Zwaan - van der Plas(HRSMC)[3]

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

Special tasks
Dr. R.L.J. Zsom (Strategy), Prof. dr. A. Oskam (Facilities), dr. M. Mittelmeijer (Safety). P.F. Collignon (ICT)

[3] 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 2012 of HIMS per funding type (fte)[a] source: METIS

HIMS themes	SC	COMP	ACF	MOLP	Other	**Total research**	*%*	Supp. staff	**Total staff**	*%*
Direct funding[1a]	16,9	2,2	3,6	5,4	0,8	**28,8**	***25***	5,3	34,1	***28***
Indirect funding [1b]	8,6	0,0	0,0	0,0	0,0	**8,6**	***7***	0,0	8,6	***7***
Direct[1a] + indirect[1b]	**25,5**	**2,2**	**3,6**	**5,4**	**0,8**	**37,4**	**32**	**5,3**	**42,7**	***35***
Research grants[2]	14,6	11,9	2,6	5,8	0,3	**35,1**	***30***	0,0	35,1	***29***
Contract research[3]	9,1	1,0	5,3	1,1	1,5	**18,1**	***16***	1,2	19,3	***16***
Other[4]	8,8	1,4	4,6	10,0	0,3	**25,0**	***22***	0,0	25,0	***20***
Total	**57,9**	**16,5**	**16,0**	**22,3**	**2,9**	**115,6**	***100***	**6,5**	**122,1**	***100***

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

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	**Other**	**Total research**	Supp staff	**Total staff**	**%**
Direct funding[1a]	3,7	1,1	5,7	2,6	3,8	1,3	0,9	3,6	3,1	2,3	0,8	**28,8**	5,3	**34,1**	***28***
Indirect funding[1b]	1,5	0,9	3,3	1,5	1,4	0,0	0,0	0,0	0,0	0,0	0,0	**8,6**	0,0	**8,6**	***7***
Direct[1a] + indirect[1b]	**5,2**	**2,0**	**9,0**	**4,1**	**5,3**	**1,3**	**0,9**	**3,6**	**3,1**	**2,3**	**0,8**	**37,4**	**5,3**	**42,7**	***35***
Research grants[2]	1,1	0,4	12,2	0,0	0,9	8,8	3,1	2,6	3,9	1,9	0,3	**35,1**	0,0	**35,1**	***29***
Contract research[3]	0,1	0,0	4,8	0,8	3,4	0,3	0,8	5,3	1,1	0,0	1,5	**18,1**	1,2	**19,3**	***16***
Other[4]	1,0	0,5	6,1	0,0	1,1	0,5	0,9	4,6	9,3	0,7	0,3	**25,0**	0,0	**25,0**	***20***
Total	**7,4**	**3,0**	**32,1**	**4,8**	**10,7**	**10,9**	**5,6**	**16,0**	**17,5**	**4,9**	**2,9**	**115,6**	**6,5**	**122,1**	***100***

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

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

Externally financed projects acquired in 2012 (mln €) per funding type[1]

HIMS themes	SC	COMP	ACF	MOLP	Other	**Total[6]**
1st - NRSC-C [2]	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [3]	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [4]	0.81	0.12	0.00	1.36	0.00	**2.28**
3rd [5]	0.89	0.00	0.00	0.00	0.00	**0.89**
Total	**1.70**	**0.12**	**0.00**	**1.36**	**0.00**	**3.18**

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

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	PI	**Total**[6]
1st - NRSC-C [2]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [3]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [4]	0.62	0.03	0.16	0.00	0.00	0.10	0.02	0.00	1.08	0.28	0.00	**2.28**
3rd [5]	0.00	0.00	0.00	0.00	0.89	0.00	0.00	0.00	0.00	0.00	0.00	**0.89**
Total	**0.62**	**0.03**	**0.16**	**0.00**	**0.89**	**0.10**	**0.02**	**0.00**	**1.08**	**0.28**	**0.00**	**3.18**

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

[1] Matching contributions UvA/FNWI (total 1.5 mln € foreseen) excluded; own contributions HIMS (in kind and cash/from reserves) included
[2] NRSC-C (TOP Research School Catalysis);
[3] COF, CvB (Funds from University Board);
[4] NWO-CW, FOM, STW, KNAW, ERC
[5] EU, DPI, AGENTSCHAP.NL, NanoNext, NFI, Industry
[6] Budgets were obtained for 2 PhD's and 6 postdocs in 2012

7.2.2 Research output of the HIMS themes

Research output 2012 per type of publication

source: METIS

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint[1]	**Total**
Refereed articles	59	42	19	43	6	-4	**165**
Non-refereed articles	0	0	0	0	0		**0**
Books	0	0	0	0	0		**0**
Book chapters	3	0	0	0	0		**3**
PhD-theses	2	0	3	4	0		**9**
Conference papers	0	0	0	0	1		**1**
Patents	8	1	0	0	0		**9**
Professional publications	2	0	0	0	1		**3**
Publications general public	0	0	0	0	0		**0**
Other research output	0	0	0	1	0		**1**
Total	**74**	**43**	**22**	**48**	**8**	**-4**	**191**

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

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	PI	Joint[1]	**Total**
Refereed articles	8	6	29	1	11	4	18	4	20	19	32	11	6	-4	165
Non-ref. articles	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Books	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Book chapters	0	3	0	0	0	0	0	0	0	0	0	0	0		**3**
PhD-theses	0	0	2	0	0	0	0	0	0	3	4	0	0		**9**
Conference papers	0	0	0	0	0	0	0	0	0	0	0	0	1		**1**
Patents	1	0	1	0	6	0	0	0	1	0	0	0	0		**9**
Prof. publications	0	0	1	0	1	0	0	0	0	0	0	0	1		**3**
Publ. general public	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Other output	0	0	0	0	0	0	0	0	0	0	0	1	0		**1**
Total	**9**	**9**	**33**	**1**	**18**	**4**	**18**	**4**	**21**	**22**	**36**	**12**	**8**	**-4**	**191**

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

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

Number of refereed articles 2012, in ranges of different impact factor Source: METIS

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint[1]	**Total**
>15	3	2	0	0	0		**5**
10-15	1	2	0	5	0	-1	**7**
5-10	14	16	2	10	0	-1	**41**
<5	41	22	17	28	6	-2	**112**
Total	**59**	**42**	**19**	**43**	**6**	**-4**	**165**

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

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	Other	Joint[1]	**Total**
>15	0	2	1	0	0	0	0	0	2	0	0	0	0		**5**
10-15	0	0	1	0	0	0	1	0	1	0	5	0	0	-1	**7**
5-10	2	4	6	0	2	0	8	0	8	2	8	2	0	-1	**41**
<5	6	0	21	1	9	4	9	4	9	17	19	9	6	-2	**112**
Total	**8**	**6**	**29**	**1**	**11**	**4**	**18**	**4**	**20**	**19**	**32**	**11**	**6**	**-4**	**165**

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; Other: group Iedema

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

7.2.3 Efficiency of the doctoral research path

The following tables show the efficiency of the doctoral research path (period of appointment 2004-2008; planned PhD defense 2008-2012).

Employed PhD-candidates

Enrolment (-)				**Success rates of graduation**							
Starting Year	**Enrolment**		**Total (M+F)**	**< 4 years**	**4 - 5 years**	**5 - 6 years**	**6 -7 years**	**>7 years**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
	M	**F**									
2004	14	2	**16**	0	8	2	0	4	1	1	0
2005	7	3	**10**	1	3	1	1	0	0	1	3
2006	12	4	**16**	1	7	4	1	0	0	3	0
2007	2	6	**8**	0	2	1	0	0	0	5	0
2008	5	8	**13**	0	4	0	0	0	0	7	2
Total	**40**	**23**	**63**	**2**	**24**	**8**	**2**	**4**	**1**	**17**	**5**
Cumulative 2004-2008											
SC	21	7	**28**	2	14	4	1	1	0	3	3
COMP	5	5	**10**	0	4	1	0	0	0	5	0
ACF	3	7	**10**	0	0	1	1	2	0	4	2
MOLP	10	4	**14**	0	6	2	0	1	1	4	0
Other	1	0	**1**	0	0	0	0	0	0	1	0
Total	**40**	**23**	**63**	**2**	**24**	**8**	**2**	**4**	**1**	**17**	**5**
%	***63***	***37***	***100***	***3***	***38***	***13***	***3***	***6***	***2***	***27***	***8***

Non-employed PhD-candidates

Enrolment (-)				Success rates of graduation							
Starting Year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2004	0	1	**1**	0	1	0	0	0	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	1	0	0	0	1	2	0
2008	5	1	**6**	0	1	0	0	0	1	4	0
Total	**18**	**5**	**23**	**6**	**9**	**0**	**0**	**0**	**2**	**6**	**0**
Cumulative 2004-2008											
SC	1	0	**1**	0	0	0	0	0	0	1	0
COMP	1	2	**3**	0	3	0	0	0	0	0	0
ACF	7	2	**9**	4	2	0	0	0	0	3	0
MOLP	9	1	**10**	2	4	0	0	0	2	2	0
Other	0	0	**0**	0	0	0	0	0	0	0	0
Total	**18**	**5**	**23**	**6**	**9**	**0**	**0**	**0**	**2**	**6**	**0**
%	***78***	***22***	***100***	***26***	***39***	***0***	***0***	***0***	***9***	***26***	***0***

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

As can be seen from the tables, a number of PhD students have not received their doctor title within 6 years. Several delays are directly related to the reorganization of the chemistry department in 2002-2004 and the subsequent leave of PhD supervisors. Several PhD students completed their PhD for the same reason outside the UvA. 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

Sustainable Chemistry (SC)

Enrolment (-)				Success rates of graduation							
Starting year	Enrollment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2004	5	0	**5**	0	3	1	0	1	0	0	0
2005	7	1	**8**	1	3	1	1	0	0	1	1
2006	7	1	**8**	1	4	2	0	0	0	1	0
2007	0	1	**1**	0	0	0	0	0	0	1	0
2008	3	4	**7**	0	4	0	0	0	0	1	2
Total	**22**	**7**	**29**	**2**	**14**	**4**	**1**	**1**	**0**	**4**	**3**
%	***76***	***24***	***100***	***7***	***48***	***14***	***3***	***3***	***0***	***14***	***10***

Computational Chemistry (COMP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
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
2008	1	2	**3**	0	0	0	0	0	0	3	0
Total	**6**	**7**	**13**	**0**	**7**	**1**	**0**	**0**	**0**	**5**	**0**
%	***46***	***54***	***100***	***0***	***54***	***8***	***0***	***0***	***0***	***38***	***0***

Analytical Chemistry (including its application in Forensic Science) (ACF)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2004	2	0	**2**	0	0	0	0	2	0	0	0
2005	2	2	**4**	0	2	0	0	0	0	0	2
2006	2	1	**3**	2	0	0	1	0	0	0	0
2007	3	5	**8**	2	0	1	0	0	0	5	0
2008	1	1	**2**	0	0	0	0	0	0	2	0
Total	**10**	**9**	**19**	**4**	**2**	**1**	**1**	**2**	**0**	**7**	**2**
%	***53***	***47***	***100***	***21***	***11***	***5***	***5***	***11***	***0***	***37***	***11***

Molecular Photonics (MOLP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2004	5	1	**6**	0	2	1	0	1	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	2	0	0	0	1	0	0
2008	5	2	**7**	0	1	0	0	0	1	5	0
Total	**19**	**5**	**24**	**2**	**10**	**2**	**0**	**1**	**3**	**6**	**0**
%	***79***	***21***	***100***	***8***	***42***	***8***	***0***	***4***	***13***	***25***	***0***

Other (group Iedema)

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

Total HIMS

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2004	14	3	**17**	0	9	2	0	4	1	1	0
2005	11	4	**15**	1	8	1	1	0	0	1	3
2006	14	5	**19**	3	8	4	1	0	0	3	0
2007	9	7	**16**	4	3	1	0	0	1	7	0
2008	10	9	**19**	0	5	0	0	0	1	11	2
Total	**58**	**28**	**86**	**8**	**33**	**8**	**2**	**4**	**3**	**23**	**5**
%	14	3	**17**	0	9	2	0	4	1	1	0
Cumulative 2004-2008											
SC	22	7	**29**	2	14	4	1	1	0	4	3
COMP	6	7	**13**	0	7	1	0	0	0	5	0
ACF	10	9	**19**	4	2	1	1	2	0	7	2
MOLP	19	5	**24**	2	10	2	0	1	3	6	0
Other	1	0	**1**	0	0	0	0	0	0	1	0
Total	**58**	**28**	**86**	**8**	**33**	**8**	**2**	**4**	**3**	**23**	**5**
%	***67***	***33***	***100***	***9***	***38***	***9***	***2***	***5***	***3***	***27***	***6***

M = male; F = Female

7.3 Finance 2012

The table below shows the HIMS financial result 2012.

HIMS result 2012 (k€)

	1st (1 structural	1st (2 Other	1st total	2nd (3	3rd (4	Total
HIMS						
Budget (fixed)	4.090		4.090			**4.090**
Budget (variable[5])	4.397	814	5.211	2.392	2.577	**10.180**
Other income	528		528	16	30	**574**
Matching contract research	-4.139	271	-3.868	2.361	1.447	**-60**
Budget total	**4.876**	**1.085**	**5.961**	**4.769**	**4.054**	**14.784**
Percentage	***33***	***7***	***40***	***32***	***27***	***100***
Personal costs	-2.791	-440	-3.231	-1.567	-1.554	**-6.352**
Other costs (projects)	-923	-231	-1.154	-889	-737	**-2.780**
Overhead (central)	818		818	-460	-358	**0**
Overhead (faculty)	-740	-223	-936	-912	-710	**-2.585**
Overhead (institute)	1.499	191	1.690	-945	-745	**0**
Various costs	-2		-2			**-2**
Other (secundary) costs	-1.964		-1.964	-4	-26	**-1.994**
Costs total	**-4.103**	**-703**	**-4.806**	**-4.777**	**-4.130**	**-13.713**
Percentage	***30***	***5***	***35***	***35***	***30***	***100***
Result 2012	**773**	**382**	**1.155**	**-8**	**-76**	**1.071**
Reservation Sectorplan appointments		470	470			470
Result excluding reservation	**773**	**-88**	**685**	**-8**	**-76**	**601**

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

The HIMS result for 2012 amounts to + 1.071k€. This result includes a reservation of 470 k€ budget for appointments in the framework of the Sectorplan Natuurwetenschappen. It is a reservation for costs to be made in the coming years.