

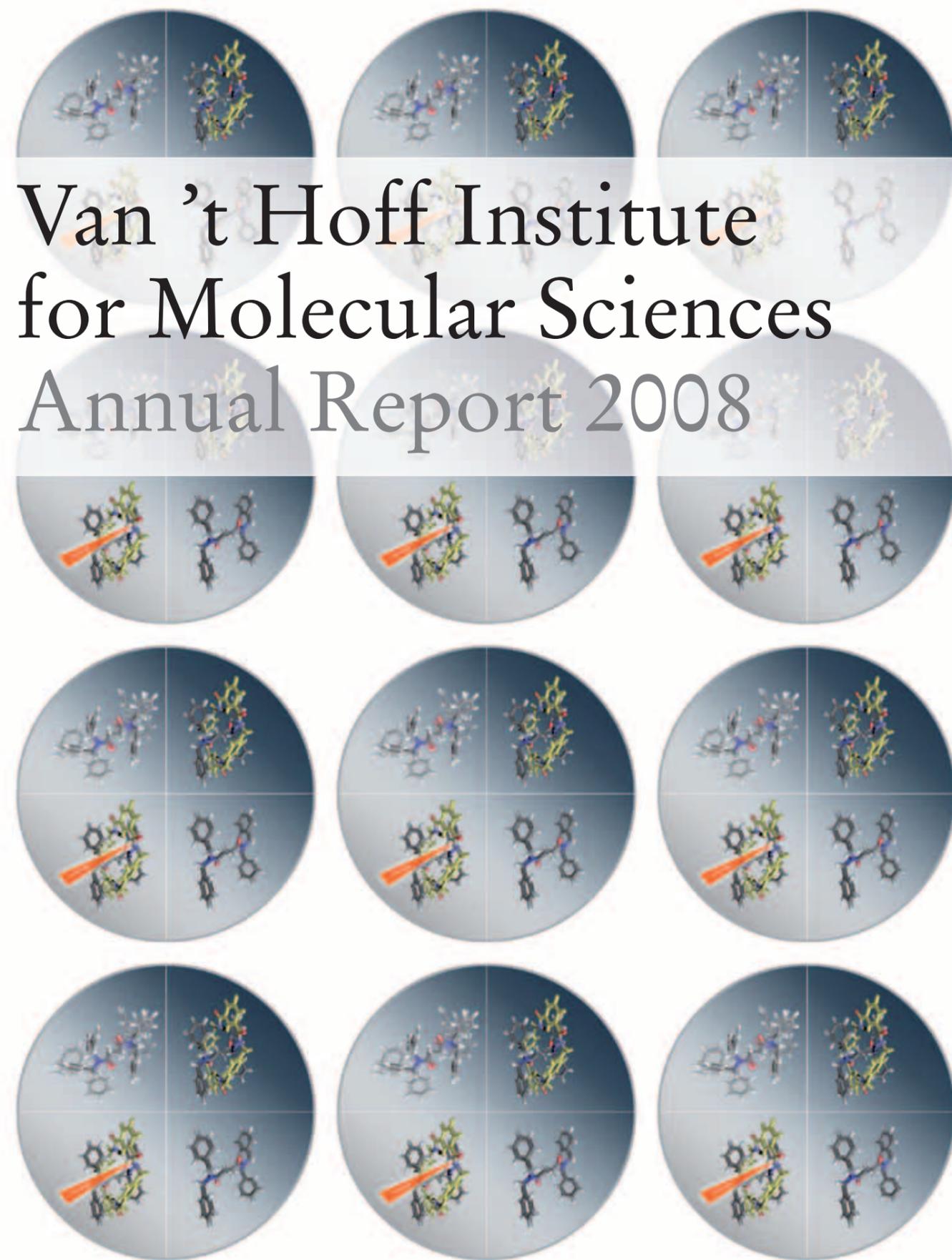


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University of Amsterdam

HIMS Annual Report 2008



Van 't Hoff Institute for Molecular Sciences Annual Report 2008

Colophon

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Structural characterization of large, floppy molecules is a difficult task. Due to their large conformational flexibility, these molecules can adopt many different structures which can not be resolved spectroscopically. The cover illustration shows a clever method, developed by Rijs & Buma of the Molecular Photonics group, to control, change, and decrease the conformational flexibility of a molecule by enclosing it with a macrocyclic mold as a [2]rotaxane. It behaves as an artificial molecular chaperone that forces the molecule into a specific shape. After rapid cooling the ring-shaped mold is removed with a laser pulse. The resulting frozen and molded molecule becomes a suitable candidate for structural characterization via high-resolution excitation spectroscopy.

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Van 't Hoff Institute for Molecular Sciences Annual Report 2008

Contents

8	Preface	
10	Summary	
17	1	Survey of the Institute
17	1.1	Introduction and perspective
17	1.2	Aim and mission
18	1.3	General overview and perspective of the research themes
18	1.3.1	Theme 1 'Macromolecular and Biosystems Analysis' (MBA)
18	1.3.2	Theme 2 'Bio-Molecular Synthesis' (BMS)
19	1.3.3	Theme 3 'Catalysis' (CAT)
20	1.3.4	Theme 4 'Computational Chemistry' (COMP)
21	1.3.5	Theme 5 'Molecular Photonics' (MOLP)
21	1.4	Dutch Research Schools and Technology Institutes & Networks
22	1.4.1	National Research School Combination-Catalysis (NRSC-C)
24	1.4.2	Holland Research School of Molecular Chemistry (HRSMC)
24	1.4.3	Nederlands Instituut voor Onderzoek in de Katalyse (NIOK)
25	1.4.4	Dutch Polymer Institute (DPI)
26	1.4.5	NanoImpuls and NanoNed
27	1.4.6	Amsterdam Center for Multiscale Modeling (ACMM)
27	1.4.7	Catalysis for Sustainable Chemicals from Biomass (CatchBio)
28	1.5	Recent and future developments
33	2	Fundamental and Applied Research
33	2.1	Introduction and research themes
35	2.2	Research quality assessments 2002 & 2008
36	2.3	Research output
36	2.3.1	Macromolecular and Biosystems Analysis
37	2.3.2	Bio-Molecular Synthesis
42	2.3.3	Catalysis
48	2.3.4	Computational Chemistry
51	2.3.5	Molecular Photonics
53	2.3.6.1	Polymer and Process Systems
54	2.3.6	Other activities
54	2.3.6.2	Röntgen Diffraction

55	3	Applied Research and Education
55	3.1	Social activities and education
55	3.1.1	Social activities
58	3.1.2	Education and promotion activities
60	3.1.3	New developments in education and related research activities
62	3.2	Results of large externally financed projects
64	4	Resources and management
64	4.1	Introduction
64	4.1.1	Management of the Institute
65	4.1.2	Management meetings
65	4.1.3	Decision making procedures and management style
66	4.1.4	Financial situation and personnel of HIMS (past and future)
67	4.2	Financial resources 2008
69	4.3	Human resources
71	4.4	Relations with external parties and innovations
73	5	Appendices
73	5.1	Research input, research output & external collaborations
73	5.1.1	Summary of external research budgets and personnel (from different sources of money) acquired in 2007, related projects started in 2008
74	5.1.2	External research funds acquired in 2007 and related projects started in 2008 (M€)
75	5.1.3	Summary of external research budgets and personnel (from different sources of money) acquired in 2008, related projects started in 2008
76	5.1.4	External research funds acquired in 2008 and related projects started in 2008
77	5.1.5	Summary of external research budgets and personnel (from different sources of money) acquired in 2008, related projects to be started in 2009
78	5.1.6	External research funds acquired in 2008, related projects to be started in 2009
79	5.1.7	Industrial collaborations per research theme
79	5.1.8	Research input and research output 2008
80	5.2	Internal and external collaborations
80	5.2.1	Collaborations of theme 1
80	5.2.2	Collaborations of theme 2
81	5.2.3	Collaborations of theme 3
84	5.2.4	Collaborations of theme 4
85	5.2.5	Collaborations of theme 5
87	5.2.6	Collaborations of other activities

88	5.3	Dissertations 2008
88	5.3.1	Dissertations of theme 1
88	5.3.2	Dissertations of theme 2
88	5.3.3	Dissertations of theme 3
88	5.3.4	Dissertations of theme 4
89	5.3.5	Dissertations of theme 5
89	5.3.6	Dissertations of other activities
89	5.4.	Science policy functions
89	5.4.1	Science policy functions of theme 1
90	5.4.2	Science policy functions of theme 2
90	5.4.3	Science policy functions of theme 3
91	5.4.4	Science policy functions of theme 4
92	5.4.5	Science policy functions of theme 5
93	5.4.6	Science policy functions of other activities
94	5.5	Financial report 2008
95	5.6	Personnel
95	5.6.1	Personnel of the research themes of HIMS (2008)
95	5.6.2	Personnel of the other research activities of HIMS (2008)
96	5.6.3	Management, supporting groups and other activities (2008)
97	5.6.4	HIMS personnel 2008 (Fte and persons)
97	5.6.5	HIMS PhD students and Postdocs 2008 (Fte)
98	5.6.6	HIMS personnel 2001 - 2008 (Fte)
98	5.6.7	HIMS personnel 2001 - 2009 (Persons; situation per January 1st)
99	5.6.8	The Scientific Advisory Committee (SAC, WAR)
100	6	Abbreviations

Preface

This Annual Report 2008 reflects the continuing efforts in the field of management, research and education and of the Van't Hoff Institute for Molecular Sciences (HIMS). The institute is a branch of the Faculty of Science (FNWI), where the Department of Chemistry unites the research institutes HIMS and SILS (biochemistry). HIMS has nine research groups, organized in five research themes. The research is involved in scientific problems of major importance for society and for the (fine-) chemical, pharmaceutical, agro, and electronic industry.

HIMS has been known for years as an institute where **MOLECULAR SCIENCES** take a predominant position. We additionally explore possibilities in application areas like Health, Durability (energy), as well as in Forensic- and Art (Restoration & Conservation) Sciences. The latter related with the new and unique educational programs recently started at the Universiteit van Amsterdam (UvA) in these fields.

The year 2008 was exceptionally successful for HIMS. The Molecular Photonics group of Prof. Wybren Jan Buma and Prof. Fred Brouwer received the very prestigious Descartes Prize, the most important Prize awarded by the European Union for Transnational Collaborative Research. Dr. G. Rothenberg could be appointed to professor in Heterogeneous Catalysis & Sustainable Chemistry. With this new chair UvA will be the only university in the Netherlands with internationally renowned active chairs in all areas of catalysis. Prof. Daan Frenkel, appointed in 2008 as Faculty of Science professor at the UvA, was elected Foreign Honorary Member of the American Academy of Arts & Sciences in Cambridge, Massachusetts. Last but not the least, Prof. Peter Bolhuis received a NWO-VICI grant. The master programme Chemistry was awarded the Euromaster label in 2008 by the European Chemistry Thematic Network (ECTN) organization. Also in external fund-raising 2008 again turned out to be very successful; a total of 7.22 M€ was externally acquired from important old and new subsidiaries such as NRSC-C, NWO (including various personnel grants), DPI, CatchBio, etc. Also the output of HIMS was on a high level in 2008. HIMS published 11 papers in absolute top journals (impact factor > 10). The number of HIMS publications (total 165) as well as the number of PhD dissertations (21) in 2008 was higher than in 2007, reflecting the increasing personnel input the last year.

The Scientific Advisory Committee (SAC) of HIMS performed a mid-term review of the research quality in 2008. On that occasion a bibliometric analysis was performed over the period 2001-2007. All five HIMS core research themes obtained individual scores well above the international standard for the CPP/FCSm value (an important indicator of a publication's impact compared to the international average). For HIMS as a whole the CPP/FCSm was 1.58.

For all these achievements HIMS was elected as **Institute of the year 2008** at the Dies of the Faculty, at which occasion Joost Reek and Peter Hauwert presented 'Het Chemisch Spektakel'.

Also the financial situation of HIMS has much improved as compared with the situation a few years ago. HIMS finished the year 2008 with a positive financial result of 0.9 M€. As a direct consequence, several important new scientific staff appointments could be realized in 2008, resulting, after years of decreasing numbers, in an increase in scientific staff members. We strongly hope to continue this positive trend for 2009.

New initiatives of HIMS to be mentioned are the ongoing explorations towards more intense forms of cooperation with other academic and non-academic partners, such as the Medical Faculty/Academisch Medisch Centrum (AMC) of the UvA, the Vrije Universiteit (in the framework of the Sectorplan Natuurwetenschappen), the FOM institutes AMOLF & Rijnhuizen, and important new country-wide initiatives such as CatchBio and TI-COAST.

I'm convinced that these promising and stimulating initiatives will lead to likely additional opportunities for funding on all levels and for collaborations, with both new and existing partners from universities, society and industries.



Rob Zsom,
director of HIMS

Summary

A short overview of the most interesting facts and highlights is given in this summary. The interested reader is referred to the chapters 1-4 and the appendices in chapter 5 for more detailed information.

Research output

HIMS produced 21 PhD dissertations in 2008 and the number of HIMS publications (165) in 2008 was some 6% higher than in 2007, reflecting the increasing personnel input the last year. HIMS published 11 papers in absolute top journals (impact factor > 10) and many more in high-impact journals (total 165 papers in 2008). The most striking publications were:

Bio-Molecular Synthesis

- A paper by Hiemstra c.s. in *Angew. Chem. Int. Ed.* (2008) on *Enantioselective copper-catalyzed propargylic amination*.
- A paper by Hiemstra c.s., together with colleagues from the VU (Lammertsma c.s), in *Organometallics* (2008) on Phosphascorpionate complexes by click chemistry using phenyl azide and ethynylphosphine oxides.
- A paper by Wever c.s. in *J. Appl. Microbiol.* (2008) on Bactericidal and virucidal activity of the alkalophilic P395D/L241V/T343A mutant of vanadium chloroperoxidase.

Catalysis

- A paper by Reek c.s. in *Chem. Soc. Rev.* (2008) on *Reactivity within a confined self-assembled nanospace*.
- A paper by Reek c.s. in *Angew. Chem. Int. Ed.* (2008) on *METAMORPhos: Adaptive supramolecular ligands and their mechanistic consequences for asymmetric hydrogenation*.
- A paper by Reek c.s. in *Adv. Synth. Catal.* (2008) on *Asymmetric synthesis of the Roche*

ester and its derivatives by Rhodium-INDOLPHOS-Catalyzed hydrogenation.

- A paper by de Bruin c.s. in *J. Am. Chem. Soc.* (2008) on *Exchange of organic radicals with organo-cobalt complexes formed in the living radical polymerization of vinyl acetate*.
- A paper by De Bruin c.s. in *J. Am. Chem. Soc.* (2008) on *Deprotonation induced ligand-to-metal electron transfer: Synthesis of a mixed-valence Rh(I,I) dinuclear compound and its reaction with dioxygen*.
- A paper by De Bruin c.s. in *J. Am. Chem. Soc.* (2008) on *Carbon-carbon bond activation of TEMPO by a RhII metallo-radical: a combined experimental and theoretical study*.
- A paper by Elsevier c.s. in *Angew. Chem. Int. Ed.* (2008) on *Transfer semihydrogenation of alkynes catalyzed by a zero-valent Palladium N-heterocyclic carbene complex*.
- A paper by Rothenberg c.s. in *Angew. Chem. Int. Ed.* (2008) on *Cat-in-a-cup: facile separation of large homogeneous catalysts*.
- A paper by Rothenberg c.s. in *J. Adv. Synth. Catal.* (2008) on *Selective Hydrogen oxidation catalysts via genetic algorithms*.

Macromolecular and Biosystems Analysis

- Two papers by Schoenmakers, Van der Wal, De Koster (SILS), c.s. in *J. Chromatography A* (2008) on *Low-molecular-weight model study of peroxide cross-linking of ethylene-propylene (-diene) rubber using gas chromatography and mass spectrometry - I. Combination reactions of alkanes*.
- A paper by Kok, Schoenmakers, c.s. in *J. Chromatography A* (2008) on *Topographic structures and chromatographic supports in microfluidic separate ion devices*.
- A paper by Janssen, c.s. in *H.J. Chromatography A* (2008) on *Extending the molecular application range of gas chromatography*.

Computational Sciences

- A paper by Smit c.s. in *Nature* (2008) on *Towards a molecular understanding of shape selectivity*
- A paper by Smit c.s. in *Chem. Rev.* (2008) on *Molecular simulations of zeolites: adsorption, diffusion, and shape selectivity*.
- A paper by Bolhuis c.s. in *Phys. Rev. Lett.* (2008) on *Phase transition to bundles of flexible supra-molecular polymers*.
- A paper by Vreede, Hellingwerf (SILS) and Bolhuis in *Proteins* (2008) on *Helix formation is a dynamical bottleneck in the recovery reaction of Photoactive Yellow Protein*.
- A paper by Krishna c.s. in *Chem. Eng. Sci.* on *Onsager coefficients for binary mixture diffusion in nanopores*.

Molecular Photonics

- Two papers by Buma c.s. in *Angew. Chem. Int. Ed.* (2008) on *Shaping of a conformationally flexible molecular structure for spectroscopy and Proton transfer with a twist? Femtosecond dynamics of 7-(2'-pyridyl)indole in condensed phase and in supersonic jets*.
- A paper by Brouwer c.s. in *J. Am. Chem. Soc.* (2008) on *A three state redox-active molecular shuttle that switches in solution and on a surface*.
- A paper by Woutersen and Bakker in *J. Chem. Phys.* on *Vibrational dynamics of ice in reverse micelles*.

Selected Research Highlights

Several remarkable research highlights of the year 2008, selected by the HIMS director are:

Macromolecular and Biosystems Analysis (MBA):

Industrial support for the MBA research group of Schoenmakers c.s. was again substantial in 2008, both through the DPI and directly from various companies. Two of these projects on the characterization of branched polymers and polymeric network structures were successfully completed. Together with the MKB company NLisis a research project was formulated on 'The next generation GC', and a PhD student will start January 2009. The Dutch NanoImpuls and NanoNed programs provided substantial support in terms of instrumentation and PhD positions. Mauro de Pra defended his PhD thesis on 'Pillar-structured micro-channels for liquid chromatography'. A number of new projects for the next nanotechnology program

NNI have been formulated together with other research groups from IBED and UTwente. An important factor for the future of the analytical chemistry groups at the UvA is the TI-COAST initiative: Top Institute for Comprehensive Analytical Science and Technology. Staff members Schoenmakers and Janssen of the Polymer-analysis group play an important role in this initiative. The UvA-VU combination is a candidate to play the role of lead-university.

Bio-Molecular Synthesis (BMS): Hiemstra c.s. completed the total synthesis of a natural pseudodipeptide (from *Philadelphus coronarius*, boerenjasmijn) in enantiomerically pure form by using nitrogen-stabilized carbocations (N-acyliminium ions) as reactive intermediates, and published the results in 2008. A vanadium chloroperoxidase was tested by Wever c.s. in collaboration with Crielaard (ACTA) for its effect on biofilms of *Streptococcus mutans*. The enzymatic products formed by vanadium chloroperoxidase significantly reduced the viability of biofilm cells. It is concluded that this enzyme and its reaction product form a potent antimicrobial system and that the enzyme could have potential as mouth rinse. Cross-links introduced between amino acid residues in close proximity can provide distant constraints to validate models of the 3D-structure of proteins. To facilitate mapping of cross-links in proteolytic digests, in close collaboration with the group De Koster/Back/De Jong (SILS, UvA), a new amine-type specific cross-linker, (bis)succinimidyl 3-azidomethyl glutarate (BAMG) has been developed by Van Maarseveen. Cross-linking of proteins by BAMG is followed by tryptic digestion. Treatment of the digest with the water soluble phosphine tris(carboxyethyl)phosphine leads to cleavage of the cross-linked and azide reduction without cleavage. Cross-linked peptides and peptides modified by BAMG without actual cross-linking yield distinct sets of TCEP-induced reaction products that can be isolated by reverse-phase diagonal chromatography and identified by mass spectrometry to reveal the identity of parent compounds.

Catalysis (CAT): The Heterogeneous Catalysis group was officially established as an independent research group with the appointment of Prof. Gadi Rothenberg as full professor and chair of Heterogeneous Catalysis and Sustainable Chemistry per

1 June 2008. With this appointment, the UvA became the only university in the Netherlands to have fulltime chairs in all catalysis subthemes. Reek c.s. further explored supramolecular approaches to arrive at novel transition metal catalysts. In previous years they have demonstrated that ligand libraries can be made by mixing functionalized ligand building blocks. In 2008 they have applied successfully the zinc-nitrogen interaction for the assembly of the building blocks and applied a part of the library in the rhodium-catalyzed hydrogenation of various substrates (collaboration with DSM). In this way they have extended the number of building blocks to 45 leading to about 450 chiral bidentate ligands. Elsevier c.s. studied ruthenium-based metallo-surfactants in collaboration with prof. De Cola (Universität Münster). Aggregates thereof combine unique spectroscopic and reactivity properties due to space confinement. The first inverted micelles with luminescent metallosurfactants have thus been obtained and were analyzed. The self-assembly of the metal complexes in solution was monitored by steady state and time-resolved absorption and emission spectroscopy. These compounds possess several long linear chains that favour the solubility of the highly water-soluble metal polar head in non-polar phases.

Computational Chemistry (COMP): Research in focused on computational studies of chemical, physical and biological systems. Our research on nanoporous materials has culminated in an accurate molecular understanding of adsorption behavior of zeolites as illustrated in the Nature publication of Smit & Maesen in 2008. In studies of a variety of (biological) macromolecules we revealed (i) the detailed mechanism and kinetics of Trp-cage protein folding, (ii) a novel insight into the formation of the signaling state and the recovery process of the photoactive yellow protein (PYP), and (iii) the hydrodynamic interactions between macromolecular filaments, explaining why spermatozoa swim in groups. In the field of nucleation and structure formation in liquids, we showed that formation of supramolecular fibers proceeds via a first-order phase transition, characterized by hysteresis and nucleation, and that diamond nucleation in liquid carbon requires pressures that are not reached in carbon-rich solar planets. Our ongoing effort to develop methods to study reactive events yielded a novel method to identify reaction pathways and an efficient method

to model activated processes that proceed via multiple intermediates.

Molecular Photonics (MOLP): Molecular Photonics has been one of the recipients of the Descartes Prize for Transnational Research. Research in the MOLP theme (Buma, Brouwer, Woutersen, Williams, Zhang) in the field of molecular nanotechnology has led to new rotaxanes that can be switched while being immobilized on a surface. The rotaxane architecture has also been employed to mold flexible molecules and make them accessible to high-resolution spectroscopy. Femtosecond laser spectroscopy has elucidated excited-state dynamics for fundamental and applied photoinduced processes. These include novel light harvesting materials developed for application in polymer solar cells. Examples are given by fullerene-perylenediimide dyads that show a quantitative photo-induced energy transfer from PDI to C_{60} . Very efficient light harvesting also occurs in arrays in which perylene bisimide chromophores are spatially arranged using calix[4]arene scaffolds. On a more fundamental chemical reaction level, it was shown that excited-state intramolecular proton transfer in 7-(2-pyridyl)indole is strongly coupled to the mutual twisting of the pyridine and indole moieties. Furthermore, it was found that the red upconversion luminescence of rare-earth nanocrystals designed for biomedical applications can be greatly enhanced by the use of citrate as a chelator. Water-dispersed semiconductor CdTe/CdS core/shell quantum dots were synthesized that showed an enhanced luminescence quantum yield from 8% of the bare core up to 40% after surface passivation by a CdS shell of optimal thickness.

Röntgen Diffraction (RD): In the Röntgen Diffraction group (Peschar) research was directed to structures and polymorphic phase behaviour of *cis*-mono-unsaturated structured lipids, a class of triacylglycerols (TAGs) designed for dietary purposes. A study of the structured lipid 1, 3-dilauroyl-2-oleoylglycerol (LaOLa) with time-resolved X-ray powder diffraction revealed crystal structures of two metastable polymorphs (β'_1 -2 and β^1 -3) and the stable β_2 -3 polymorph. LaOLa is now the first TAG for which both β' and β models are known. Both the β' polymorphs have an unexpected, novel type of packing in which the almost complete lauroyl chain at the glycerol *sn*-3 position is packed parallel to a part of the oleic chain. The packing of the β_2 -3 polymorph is quite different, with the two

lauroyl chains being packed parallel to each other, and this explains why the β_1 -2 β_2 -3 phase transition is slow and requires a liquid interface.

Social highlights

The work of the HIMS research groups has raised quite some national and international publicity, including publications in various newspapers and on various websites. Examples of HIMS' remarkable research highlights, awards and other measures of esteem with a high societal value that should be mentioned are:

In 2008 the Molecular Photonics group of Buma and Brouwer was recipient of the **Descartes Prize** for Transnational Collaborative Research as a member of the SynNanoMotor consortium for developing the first functional examples of synthetic motors on a molecular scale and many other useful and innovative nanomachines. The consortium in which - apart from the Molecular Photonics group - researchers from the University of Groningen and research institutes from the United Kingdom, France and Italy participated, received the prize for their trail-blazing work in the field of synthetic molecular motors and artificial nano-engines. Nano-engines and molecular motors, examples of molecular nanotechnology, form the basis of nearly every important biological process. Molecular nanotechnology offers unprecedented technological possibilities and can ultimately have an impact on economy and society that will transcend in scale and range those of the steam engine, electricity, and internet. The consortium was the first to build molecular engines that allow movements at the molecular level to be coupled to the macroscopic world, enabling them to be employed to various ends including storage of information in polymer films, or the transport of macroscopic objects, like drops of liquid over a surface. Another example concerns molecular systems that can be triggered to form spontaneously functional structures with a well-defined size and position on surfaces. These systems may be used for products in the fields of identification, security and health care.

The Molecular Photonics group will use their part of the Prize money to establish the *Molecular Photonics Descartes Fund*. The aim of this fund will be to promote undergraduate research in molecular

photonics by yearly awarding bursaries to excellent master students that perform their undergraduate research project in the field of molecular photochemistry and photophysics.

For the Computational Chemistry Group the most striking highlight of 2008 was the **VICI grant** awarded to Peter Bolhuis. It will allow him to carry out a state-of-the art research program addressing the influence of the environment on protein folding, binding and aggregation.

Some other highlights to be mentioned are:

- The **Amsterdam Center for Multiscale Modeling (ACMM)** was officially opened on June 26, 2008 during a special symposium at the KNAW Trippenhuis.
- Together with the Lorentz Center in Leiden the ACMM became a **node of CECAM**, the European center for computational science.
- The master program Chemistry was awarded the **Euromaster** label by the European Chemistry Thematic Network (ECTN) organization.
- In the Elsevier magazine annual academic survey students rated the UvA and UU **Chemistry bachelor programs** as being the best.
- **Prof. Daan Frenkel** was elected Foreign Honorary Member of the American Academy of Arts & Sciences in Cambridge, Massachusetts.
- **Dr. Jan van Maarseveen**, member of the Bio-Molecular-Synthesis theme, won the 2008 Onderwijsbokaal.
- **Dr. Gadi Rothenberg** was awarded the 2nd UvA ScienceParc innovation prize 2008 for his new concept for CO-resistant fuel cells: A practical solution to energy transfer problems.
- **Eveline Jansen** (NCCC conference) and **Linde Smeenk** (KNCV/PAC conference), both master students of HIMS, won 1st poster prizes in 2008.
- **Rob Edam**, PhD researcher of the group Schoenmakers, received poster prizes in 2008 at both the HTC-10 (Hyphenated Techniques in Chromatography) and the Dutch Polymer Days (KNCV, PTN and NWO).
- **Prof. Peter Schoenmakers** received the Eastern Analytical Symposium (EAS) award in recognition of his significant contributions to the field of Separation Science. The rewarding ceremony will take place in New Jersey, USA, in November 2009.



Prof. Wybren-Jan Buma



Prof. Fred Brouwer

External research funding

This year again turned out to be very successful in terms of external fund-raising; a total of 7.22 M€ was externally acquired from important old and new subsidiaries.

A number of external funding successes can be mentioned:

In 2008 The Dutch Polymer Institute (DPI) was positively evaluated again. HIMS participates in the DPI with the groups Schoenmakers, Reek, Brouwer and Iedema. They received together 1.4 M€ for projects from DPI in 2008.

The National Research School Combination-Catalysis (NRSC-C), was recently re-accredited for the period 2009-2013. In 2008 HIMS received a total of 2.7 M€ for new projects (groups Reek, Elsevier, Hiemstra, Rothenberg and Wever).

Catalysis for Sustainable Chemicals from Biomass (Catch-Bio) started in 2008 and aims to develop clean and efficient processes for the conversion of biomass into low-cost biofuels, chemicals and pharmaceuticals. In 2008 HIMS received a total of 0.7 M€ for projects (groups Reek, Elsevier and Rothenberg).

Prof. Peter Bolhuis of the Computational Chemistry group received a NWO-VICI grant of 1.25 M€.

After many years of decreasing numbers, the scientific staff numbers increased further with 4.7 Fte in 2008 (5.2 fte increase in 2007 compared to 2006). The numbers of externally funded PhD students and Postdocs in 2008 (102.5 Fte), by funding originating from the Research Schools NRSC-C, NWO-CW/STW/FOM, and EU, ERC, BSIK/NanoNed, CatchBio and Industry, was also higher than the year before (93.3 Fte in 2007). Since the number of vacancies at 01-01-2009 was exceptionally high (40), including vacancies for various staff positions, a further increase in external research funding (and scientific staff members) is expected in 2009.

Educational and promotional activities

The HIMS staff is largely responsible for teaching the courses in the bachelor Scheikunde and contributes to an important extent to the teaching in the bachelor Bio-exact and the b,g-bachelor study programme. The Master of Chemistry programme is divided in five tracks most of which are shared with other Master programmes of our university (UvA) or the Vrije Universiteit (VU) in

Amsterdam. Early 2008 it was decided that our master chemistry programme was accredited by the ECTN, so students who start(ed) their master in the period 2007 – 2012 will receive both the Euromaster certificate and a Master of Science diploma.

Dr. de Groot is the education director of the College of Science, encompassing all bachelor programmes of the Faculty of Science, while Dr. Ingemann Jørgensen (HIMS) is director of the bachelor programmes in scheikunde and bio-exact. Prof. Hiemstra (HIMS) is director of the master programmes of the Master School of Sciences.

He has been director of the master programme in Chemistry until August 31, 2008 after which date Prof. Elsevier (HIMS) took over this position.

In 2008, 5 students obtained their bachelor and 15 students their master degree in Chemistry. The number of 1st year chemistry students that started in 2008 amounted to 25. To reach a level of 50 1st year chemistry students, HIMS gives high priority to promotional activities and improvement of the bachelors programme.

The **Beta partner project** is based on collaboration of the FNWI (coordination Cor de Beurs/AMSTEL Institute) with 24 high-schools in the Amsterdam region that decided for a Beta-profile. Aim of this co-operation is raising young student's enthusiasm for science and technology and related professions. Science Lab is one of the initiatives of the Beta partner project, and in 2008 more than 500 students at the age of 15 years and higher attended one of HIMS science labs. The ITS Academy is another initiative that allows school teachers and university staff to develop new teaching subjects for upper level secondary school students. The purpose of the Betabrug project of the UvA-HvA is to teach science to upcoming students who intend to do a beta study, despite lacking qualifications; in 2008 some 20 participants attended this chemistry course. Traditionally, HIMS staff participates in the organization of masterclasses, educational information meetings and school visits for secondary school pupils to encourage and stimulate their interest in chemistry. In 2008 the institute organized the symposium **Viva Chemie** for the fourth time, the theme being 'From fascination to innovation'. Some hundred teachers attended the program, and were informed about recent developments.

The University of Amsterdam's Master program in **Forensic Science** is unique in the Netherlands and

has been developed with the Nederlands Forensisch Instituut (NFI). In the two-year master, the HIMS staff plays a significant part in educating forensic scientists with a chemistry profile. HIMS also participates in the only academic minor and master programs on **Conservation and Restoration Science** in the Netherlands, which is a joint effort of the UvA-faculties of Humanities and Science, the Instituut Collectie Nederland (ICN), and Stichting Restauratie Ateliers Limburg (SRAL). Since 2006 UvA/HIMS, the Ecole Normale Supérieure in Lyon, and La Sapienza University in Rome run a one-year MSc program on Atomic scale modeling of physical, chemical, and biomolecular systems coined **AtoSim**. It targets top students from all over the world, and is supported by the EU Erasmus Mundus program. **MolSim** is a 2 week international school on molecular simulation techniques for advanced MSc and starting PhD students that attracted 70 participants in 2008. The school was financially supported by CECAM and the ESF program SimBioMa, and organized with support from the HIMS secretariat.

Finances

Since 2006, the year of introduction of the new (integral costs) allocation model of the university board, the financial position of HIMS has much improved, reflecting the foreseen effect of the reorganization of the chemistry department that took place in the years 2002-2004. HIMS finished the year 2008 with a **financial result of +0.9 M€**, as it did in 2007 (+0.5 M€) and 2006 (+0.3 M€). As a direct consequence, several important new scientific staff appointments could be realized in 2008, resulting, after years of decreasing numbers, in an increase in scientific staff members. We strongly hope to continue this positive trend for 2009. However, notwithstanding the positive results of the years 2006-2008, the future financial prospects of HIMS (and the whole faculty) are uncertain, as a consequence of (to be expected) budget reductions both from the ministry and the university board in the years 2009-2012, as was announced late 2008 by the dean of the faculty.

Personnel

The following appointments of permanent personnel in the 1st money stream were effected in 2008:

- **Dr. G. Rothenberg** was appointed professor in Heterogeneous Catalysis and Sustainable Chemistry.
- **G. Zonneveld-de Boer** was appointed as institute manager.
- The appointment of **Dr. E. Eiser** at 01-02-2008 for 5 years (0.2 Fte) as UD (assistant professor) in the group Elsevier of the theme Catalysis.
- **Dr. B. de Bruin** was appointed as UHD in the group Reek of the theme Catalysis.
- **Dr. J. van der Vlugt** was appointed as UD in the group Reek of the theme Catalysis.
- **Dr. F. Hartl** was appointed for 5 years (0.0 Fte), as UD (assistant professor) in the group Reek of the theme Catalysis.
- **Prof. A. Fasolino** was appointed for 5 years (0.0 Fte) as professor in the group Bolhuis/Meijer of the theme Computational Chemistry.
- **Dr. S. Woutersen** was appointed as UD in the group Buma/Brouwer of theme Molecular Photonics.
- **Prof. C. Elsevier** was appointed as director of the master program chemistry of the Master School of Sciences.

Housing facilities

The Van 't Hoff Institute for Molecular Sciences is now housed in four different buildings located at the Roeterseiland complex. This situation is far from ideal and it is obvious, that HIMS is really looking forward to the realization of the newly planned buildings, which will unite HIMS with the complete Faculty of Science on one location, at the Science Park in the Watergraafsmeer. Three architects designed a 70.000 m² building that will be constructed in two phases. The construction of all the new buildings in this location has started in May 2007. After realizations of the first phase in February 2009, the constructors will start with the complete renovation of a number of existing buildings and with the second phase of the new complex. The laboratories for the research groups of Macromolecular and Biosystems Analysis, Computational Chemistry, Molecular Photonics, Biocatalysis (group Wever) and Röntgen Diffraction are planned in the second phase on two floors of the new

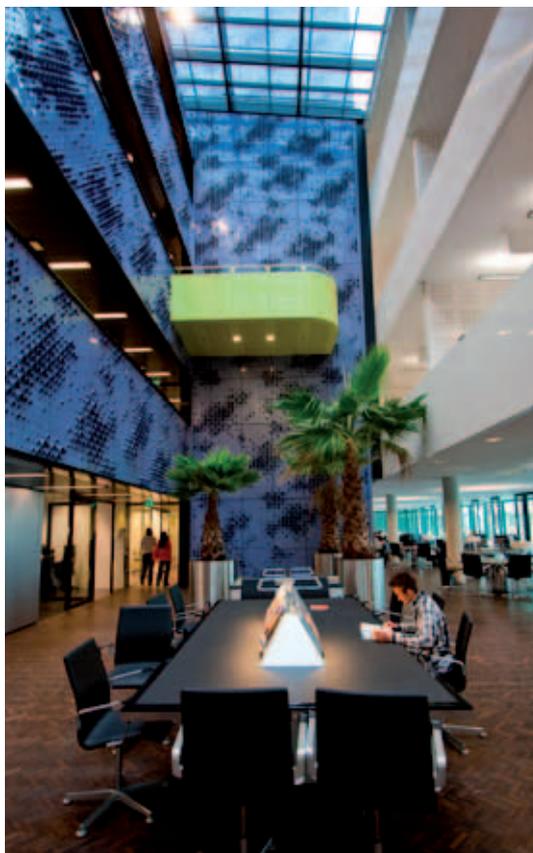


Prof. Gadi Rothenberg



Dr. Jarl van der Vlugt

Hall of the new faculty building (photo Hanne Nijhuis)



building D. For these groups 1566 m² lab space is available. Almost all offices and sitting rooms as well as the lecturing halls are located in the separate grey building in the middle, all on very short distance from the lab-space.

The research groups for Catalysis and Organic Synthesis (group Hiemstra), including the NMR-facilities, will be housed in the second phase in a separate building of in total three floors with 2052 m² area available for the laboratories only. This completely renovated building is attached on one side to the main building in which the other HIMS research groups will be located and on the other side to the bachelor student laboratories. In this way, the HIMS-space is more compact and all research groups will be in the near vicinity of each other. To avoid problems by changes in the research plans, housing of new groups and vanishing of others, all the labs in these new buildings are highly flexible and constructed in a uniform way. The completion of the total project is to be expected in September 2010. In this way the curriculum year 2010-2011 can start simultaneously on the same area for the complete Science Faculty. The main purpose of the movement and in-housing project is to guaranty the continuity of all the ongoing research in the institute.

Entrance of the new faculty building (photo Hanne Nijhuis)



1. Survey of the Institute

1.1 Introduction and perspective

The Van 't Hoff Institute for Molecular Sciences (HIMS) encompasses nine chairs (research groups), organized in the following five¹ research themes.

- Macromolecular and Biosystems Analysis (1 research group in HIMS; collaboration with 2 groups in SILS)
- Bio-Molecular Synthesis (2 research groups)
- Catalysis (3 research groups)
- Computational Chemistry (2 research groups)
- Molecular Photonics (1 research group)

The multidisciplinary themes of HIMS cover fields in chemical sciences where interesting new developments and important breakthroughs in our knowledge are anticipated in the next decade. The research program includes sophisticated design, synthesis, analysis and theoretical and fundamental understanding of (supra-) molecular systems with well-defined structural and physical properties and selective reactivity. Implementation of multidisciplinary themes within an institute with much internal and external co-operation is expected to initiate new developments at the frontier of chemical research. To cover a broad multidisciplinary research area, synergism will be established between the outstanding HIMS research programs in organic, inorganic, physical, biological, analytical and computational chemistry together with research programs in physics, biology and medicine (AMC). In Macromolecular and Biosystems Analysis, chemists from HIMS and SILS collaborate to develop integrated methodology, based on chromatographic separations, mass spectral analyses and statistical data analysis, to resolve basal problems related to the improvement of food and health. Supporting structural analysis is important for the existing research activities and is carried out in the

various research groups and in the NMR and Röntgen Diffraction departments of HIMS.

HIMS operates in interaction with FNWI institutes studying theoretical (SILS/Bio-Informatics, IHEF, ITFA) and experimental (WZI) physics and two institutes specializing in life sciences, at molecular (SILS) and at organism and ecosystem (IBED) level, respectively.

HIMS is involved in many scientific problems of major importance for society and for the (fine-) chemical-, pharmaceutical-, and electronic industry. Research in these directions is indispensable for deepening and broadening our knowledge of matter and of processes on a molecular level. The importance for society is found in research efforts of our themes in applications such as data transport, energy, health, storage in information technology, analytical techniques for medical and forensic purposes, sustainability (e.g. efficient transformations of fossil raw materials into useful compounds), design and synthesis of complex molecules for use as agro-chemicals and drugs and innovation. As a consequence, the major part of the HIMS research activities has a high societal character.

1.2 Aim and mission

Chemical research tries to resolve and rationalize the synthesis, structure, reactivity, specificity, kinetics, and thermodynamics of small and large molecular systems. Within this broad context, HIMS offers sufficient focus to perform high-level research, yet maintain sufficient diversity to support an outstanding education portfolio. The reactivity, (biological) activity and selectivity, and material properties of the systems studied at HIMS are ultimately determined by the (supra-) molecular structure; small electronic, steric and geometric changes on the molecular level, can have huge impact on meso- and macroscopic properties. Nowadays, and in future, the five themes of

¹ The Complex Fluids theme of HIMS was of subcritical size and discontinued on 01-02-2008. As such, HIMS follows the "Focus and Mass" policy of the Dutch universities; see also section 1.5.

research of HIMS will remain of great scientific, societal and industrial relevance.

In selecting research themes, HIMS will be driven by its proven strengths (technology drive), the relevance of molecules and molecular systems for science and society (application pull), and the possibilities to attract significant research funding (opportunity drive).

The proven strengths of HIMS are now focused in five research themes, as described above. In all five areas, we have demonstrated the potential to perform world-class research. Focus on relevance has a long tradition within Chemistry at the UvA. However, to rise to important challenges from society and, especially, to be a strong player in major research initiatives, researchers from the different themes within HIMS will combine forces. We can achieve great synergy if we can compute, understand, implement, demonstrate, and validate molecular solutions to important problems.

The mission of HIMS can be described as:

Addressing important issues in science and society through the design, synthesis, analysis, theoretical and fundamental understanding and application of novel functional (supra-) molecular systems with well-defined structural and physical properties and selective reactivity.

1.3 General overview and perspective of the research themes

1.3.1 Theme 1 'Macromolecular and Biosystems Analysis' (MBA)

The Macromolecular- and Biosystems Analysis research cluster is based on three areas of expertise, *viz.* analytical separations (group Schoenmakers, HIMS), mass spectrometry (group de Koster, SILS) and data analysis (group Smilde, SILS). In addition, there is a significant effort in environmental analysis within IBED (group de Voogt). Thus, only part of the effort in this area is made within HIMS. Originally, the main objective of the polymer-analysis group has been the characterization of complex samples of large molecules, with separations and mass spectrometry as the outstanding tools. The analytical knowledge and infrastructure are increasingly used in other application domains, such as forensic science.

Apart from the applications, strengthening the analytical discipline is an increasingly important area. A great deal of effort is devoted to the development of novel separation systems, including the application of nanotechnology to create superior separation channels (sponsored by NanoNed, see section 1.4.5), the preparation of tailor-made monolithic separation media, and studies into the principles of two- and three-dimensional chromatographic separations. This discipline-oriented part of the work may be boosted by the foundation of the TI-COAST (Comprehensive Analytical Science and Technology; see also section 1.5), which is a large-scale academic-industrial-government cooperation in this area.

The Dutch Polymer Institute (DPI, see section 1.4.4) continues to be one of the strongest sponsors for application-oriented research projects, including projects on the characterization of (long-chain) branched polymers, modified celluloses and polymer solubility. The first of these projects was completed in 2008, with very good results. A unique system for comprehensive two-dimensional liquid separations based on molecular-topology fractionation and size-exclusion chromatography (MTF×SEC) was developed and validated; see also section 2.3.1.

Great progress has been made on the application of gas-chromatographic techniques to non-volatile samples (Prof. Hans-Gerd Janssen). Pyrolysis and chemo-thermolysis (which is a combination of pyrolysis and chemical derivatization) have found many successful applications. Another area of greatly enhanced activity is the characterization of biomaterials (Prof. Sj. van der Wal).

The Polymer-Analysis Group is heavily involved in new education initiatives of the FNWI, notably on Forensic Sciences and Restoration Science (see chapter 3.1). In both areas analytical chemistry is a key discipline and the knowledge and infrastructure of the polymer-analysis group are eminently useful.

1.3.2 Theme 2 'Bio-Molecular Synthesis' (BMS)

Synthesis is an indispensable tool in molecular science to satisfy the continuing need for new molecules and novel synthetic methodologies. Further development of known reactions is necessary to arrive at milder and more sustainable

processes and at new reactions for the preparation of novel molecules and/or materials with desired properties. In the last decade synthetic methodologies are shifting towards the implementation of Bio-Molecular tools and to the target-oriented synthesis of molecules in order to interact with biological systems. Keywords related to the activities of the Bio-Molecular Synthesis theme are organic synthesis, homogeneous (organo) catalysis, chemical biology and biocatalysis.

Organic synthesis. The two key activities in organic synthesis are the development of new synthetic methodology and the target-oriented synthesis of bioactive natural products and related compounds. New synthetic methods should show maximal selectivity, efficiency and atom economy. Cationic intermediates play an important role in the methodological work, in particular N-acyliminium ions. Another key structure in the synthetic research is the allene moiety which is used in both metal-catalyzed processes and in photochemistry. Target molecules are alkaloids, medium-ring peptides and solanoclepin A, the hatching agent of potato cyst nematodes.

Homogeneous (organo)catalysis. New and more selective organocatalysts are developed based on privileged structures like the Cinchona alkaloids and binol species. Highly enantioselective variants were discovered for e.g. the Henry reaction and the Pictet-Spengler reaction. Moreover, the synthesis of novel chiral ligands for homogeneous enantioselective transition-metal catalysis is pursued by using our own synthetic methodology.

Chemical biology. In collaboration with the mass spectrometry group (SILS) non-natural amino acids containing biocompatible reactive groups are synthesized and incorporated into proteins *in vivo*. The resulting protein tagging can then be exploited to carry out time-resolved proteomics experiments.

Biocatalysis. There is a growing need for optically pure building blocks in the chemical industries. Enzymes play an important role in current industrial large-scale processes towards optically pure compounds. This theme's biocatalytic research focuses on vanadium haloperoxidases and the structurally related acid phosphatases, applying directed evolution techniques for the synthesis of versatile optically pure building blocks.

1.3.3 Theme 3 'Catalysis' (CAT)

The major aims of the catalysis groups are the design of new catalysts, the development of novel concepts in catalysis, catalyst immobilization on various supports to facilitate subsequent separations and the discovery and exploration of novel catalytic reactions. The challenge is to develop environmentally benign and atom-economic chemical conversions with high chemo-, regio-, and stereo-selectivities, which we approach in a multidisciplinary fashion based on transition metal coordination chemistry, homogeneous catalysis, heterogeneous catalysis, supramolecular chemistry and biocatalysis. Rational ligand design, the development of unusual, adaptive and non-innocent ligands, computational chemistry, *in situ* spectroscopy and combinatorial approaches are applied as very powerful tools to devise these new catalysts and to unravel their mechanistic basis. In addition, we have interest in the reactivity of metal complexes in unusual oxidation states, as they can display remarkable reactivity. An important goal is the development of new catalytic processes based on renewable resources, a research effort that is part of the national initiative CATCHBIO (see also section 1.5).

So far, most new reactions have been found by serendipity, and nowadays high-throughput catalyst screening plays an important role in this. Because combinatorial techniques are indispensable for this approach, new tools for combinatorial catalysis will be developed, which will include supramolecular ligand assembly, ligand synthesis on solid support, and catalyst formation using large libraries of biomolecules. Since these new approaches can lead to huge catalyst libraries, catalyst *selection* procedures are developed that will provide powerful tools for catalyst development. In addition, computational strategies combined with catalyst libraries also provide new ways to quickly find new catalysts.

Nature provides the ultimate example of complex and efficient catalytic performance, in which spatial organization leads to impressive selectivity and rate of conversion. This spatial organization is of utmost importance for living systems. For example, anabolic (i.e. biosynthetic) and catabolic processes occur simultaneously in the living cell. The conflicting demands of these two processes are managed by proper regulation of the respective metabolic

requirements and the physical separation of the competing pathways into different cellular compartments. To optimize catalytic efficiency in metabolic pathways these biocatalysts are often assembled in multi-enzyme complexes, also referred to as metabolons. This provides the great advantage that catalytic intermediates are not lost or diluted by diffusion.

To achieve a similar catalytic performance, with respect to selectivity and turnover rate, as the enzymes in a living cell, we will mimic some of the aspects of their spatial organization through supramolecular strategies. Unavoidably, the new catalytic systems will be conceptually different from those found in nature, for the simple reason that the current synthetic challenges are not similar to those of the living cell. A variety of strategies for this catalyst organization is explored. The use of catalysts located at different positions on various supports is also explored as a tool to improve one-pot cascade processes.

The important new strategies that are under investigation in the catalysis research program afford tools for the search of novel catalysts for known processes as well as 'unknown' conversions. Altogether, this program describes a unique combination of approaches that will provide the catalysts for the future.

1.3.4 Theme 4 'Computational Chemistry' (COMP)

Developments in computational chemistry focus on simulating more complex systems on increasingly longer time- and length scales. This trend is facilitated both by the continuous increase of computing power, and, more importantly, the application of new theoretical concepts and development of novel efficient computational methods. One of the important aspects is to use a hierarchical approach: link simulation techniques for different time and length scales. Suppose we want to model signal propagation in a photoactive protein. This involves various mutually coupled stages with a distinct spatial and temporal extent; (1) electronic excitation, (2) electron and chemical rearrangements, (3) local structural rearrangements, (4) protein structural transformation, (5) signal propagation to the environment. Modelling this process in full requires the use of a hybrid of quantum methods (1, 2), atomistic and molecular

dynamics (2, 3, and 4), and course grained modelling of the protein and its environment (4 and 5). The related scientific challenges are enormous since only in a few cases it is known how to link two different simulation techniques.

The Computational Chemistry group is one of the few molecular simulation groups that have expertise on all relevant length and time scales. At the quantum level we use DFT-approaches and ab-initio molecular dynamics to study reaction mechanisms and kinetics; at the molecular level we are involved in molecular dynamics and Monte Carlo simulations to compute thermodynamic and transport properties. At the mesoscopic level we focus on the link between the molecular scale and the mesoscopic or macroscopic scale. This includes course-grained description of colloidal systems and the application of computational fluid dynamics (CFD). Techniques that have been developed to extend the time- and length scale of conventional simulations include configurational-bias Monte Carlo and Transition Path and Interface Sampling. Crucial in the development of these techniques is a direct link with experiments.

In the near future this theme will continue its research along the lines indicated above, developing unifying, generic and novel concepts that will impact significantly on fundamental understanding but also (bio)technological applications. In the area of complex (bio)molecular systems we will focus on the role of macromolecules in the cell (e.g. photoactive protein complexes, protein aggregation and protein folding, cytoskeleton filaments) and catalysis in solution and semi-structured environments. In the field of materials and engineering we focus on carbonic materials and, on a larger scale, reactor intensification and -miniaturization.

The Amsterdam Center of Multiscale Modelling (ACMM) has strengthened our strategy; see also section 1.5. This centre combines the expertise of the group with that of the theoretical chemistry group of Baerends at the VU and the group of Frenkel at FOM-AMOLF. Together with the Lorentz Center the ACMM will become a CECAM node reflecting the recognition and internationally renowned computational expertise of all length and time scales relevant for chemistry and related fields in physics and biology.

1.3.5 Theme 5 'Molecular Photonics' (MOLP)

The interaction between light and matter is the leading research-theme of the Molecular Photonics group. The aim is to develop new molecular photonic materials through a profound understanding of the molecular factors that control phenomena such as photoinduced energy - and electron transfer within complex molecules. The systems studied range from rigidly bridged donor-acceptor systems to multi-chromophoric dye-arrays, polymers, and molecular aggregates, as well as chromophoric molecules at surfaces or in confined nano-spaces. By understanding the photoinduced processes we can gain control over the associated macroscopic properties of these materials. The Molecular Photonics theme is unique within the Netherlands because it combines the skills of internationally recognized experts in molecular synthesis, spectroscopy and theory. The knowledge generated is employed to design, synthesize, and characterize novel, intelligent materials with a priori determined photo-responsive properties, for application in e.g. photoconductive systems, optoelectronic devices, solar energy conversion materials, as molecular motors and molecular switches.

The Molecular Photonics group combines expertise in light-induced electron transfer in multifunctional organic molecules, electron and energy transfer in metal-organic systems, photochemistry and photophysics of metal-organic systems, spectro-electrochemistry, development of electroluminescent markers and probes, externally (light) controlled molecular machines, and industrial applications of photonic molecules. Over the years the group has acquired international recognition in the development and application of a wide variety of advanced spectroscopic methods in the frequency and time domain, investigating molecular systems in various environments and conditions, from gas phase to solid state, and from bulk measurements to the single molecule level.

Development of new spectroscopic techniques and molecular theory will extend the insight in light-driven processes, in the study of small molecules, but also in applications important to biology (such as luminescent probing of dynamic life processes and artificial photosynthesis). In parallel, new molecular photonic materials will be applied in data transport, data storage, luminescent materials, (electro-) luminescent devices, etc. With

the availability of rapidly scanning laser systems, it has become feasible to apply photochemical transformations to do chemistry on a spatially exactly defined scale, in e.g. the production of nanostructured objects and surfaces, or for labeling on a visually detectable scale. In these latter applications tuning of new materials to the wavelength of the writing laser beam and variation of the modulation of the resulting surface structure and -color are most challenging.

The multidisciplinary nature of the Molecular Photonics theme makes it an attractive partner for knowledge sharing and collaborations with other research groups within the Department. Within the context of the NRSC-C (see section 1.4.1), for example, the "Bio-Molecular Synthesis", "Catalysis", and "Molecular Photonics" research themes jointly aim at a strong synergy of their expertise in organic (ligand) synthesis, bio-catalysis, inorganic and transition metal chemistry, and molecular photonics to achieve major breakthroughs in the multidisciplinary area of catalysis. In this program, photonic techniques are increasingly employed as a catalyst activator, to monitor catalytic events, and to elucidate catalytic mechanisms. Similarly, there have been ample initiatives to establish research projects with the "Molecular Cell Biology" (SILS) and "Bio-Chemical Analysis" themes.

1.4 Dutch Research Schools and Technology Institutes & Networks

HIMS participates in various Dutch Research Schools and Technology Institutes & Networks. HIMS is the lead institution in one ECOS²-accredited National Research School (HRSMC, since 1994) and participates in two others (NIOK and Polymeren-PTN, since 1992). In 1997 the Dutch Minister of Economic Affairs established four new Leading Technology Institutes, as a public-private-partnership between industries in the Netherlands and knowledge institutes (universities and TNO). The Dutch Polymer Institute (DPI) is one of the four that were established. Moreover, the Dutch Government established in 1998 the National Research School Combination - Catalysis (NRSC-C), as a co-operation between three National Research Schools, NIOK, HRSMC, and Polymeren-PTN. NRSC-C is designed in such a way that it will favor added value to all these Graduate Research Schools,

² On request of the government, the Royal Netherlands Academy of Arts and Sciences (KNAW) is responsible for the accreditation of research schools. A Research School Accreditation Committee ECOS (Erkennings-commissie Onderzoekscholen) has been created for this purpose in 1992. Accreditation lapses after six years, when an application for follow-up accreditation may be submitted.

by which NRSC-C can really act as a combination of National Research Schools. In 2003 NanoImpuls was started as predecessor of NanoNed. NanoImpuls is a strategic initiative from the Ministry of Economic Affairs in the area of nanotechnology. NanoNed, the Nanotechnology network in the Netherlands, is an initiative of eight knowledge institutes and Philips and started in 2004. It clusters the nanotechnology and enabling technology strengths of the Dutch industrial and scientific nanotechnology knowledge infrastructure in a national network. The Amsterdam Center for Multiscale Modeling (ACMM) started in 2007 as a collaboration between the UvA/HIMS (Computational Chemistry), VU (Theoretical Chemistry) and the FOM/AMOLF (Theoretical Biophysics). ACMM is a new institute for theory and multiscale modeling in chemistry, physics and biology. In 2008 Catalysis for Sustainable Chemicals from Biomass (CatchBio) started with the aim to develop clean and efficient processes for biomass conversion into low-cost and sustainable biofuels, chemicals and pharmaceuticals. As from the early beginning the HIMS themes participated in various regionally and nationally organized Research Schools, viz. NRSC-C (Top Research School), DPI (Technology Institute), NanoImpuls/NanoNed, and CatchBio (and more are expected will follow; see section 1.5). Participation in (Top) Research Schools and Technology Institutes & Networks is considered of major importance for:

- Education of PhD students
- Research collaborations
- National - and International contacts
- External project funding

The HIMS participated in 2008 in the following (Top) Research Schools, and Technology Institutes & Networks, all active in the field of Chemical Sciences and Technology:

- National Research School Combination - Catalysis (NRSC-C)
- Holland Research School of Molecular Chemistry (HRSMC)
- Dutch Institute for Catalysis Research (NIOK)
- Dutch Polymer Institute (DPI)
- NanoImpuls/NanoNed
- Amsterdam Center for Multiscale Modeling (ACMM)
- Catalysis for Sustainable Chemicals from Biomass (CatchBio)

1.4.1 National Research School Combination-Catalysis (NRSC-C)

Top Research School

Accreditation in 1998, 2003 & 2008

The National Research School Combination Catalysis (NRSC-C), approved by the Minister in the course of 1998, is a co-operation between three National Research Schools, NIOK, HRSMC, and Polymeren-PTN, and is designed in such a way that it will favour added value to all these Graduate Research Schools, by which NRSC-Catalysis can really act as a combination of National Research Schools. The NRSC-C assembles research groups of eight Dutch Universities, the Technical University Eindhoven (legally representing the NRSC-C), the Universiteit van Amsterdam (HIMS), the Vrije Universiteit Amsterdam, the Universiteit Groningen, the Technische Universiteit Delft, the Universiteit Utrecht, the Universiteit Nijmegen and the Universiteit Leiden.

Experts in various key sub-disciplines from seven Dutch universities join forces in this new organization to execute a strong innovative research program of international standing in catalysis, to meet the challenge of a sustainable society in the next century. The mission of the NRSC-C is *to provide a strong innovative catalysis program to arrive at a full control of molecular recognition in complex chemical transformations*. This top research school is a meeting point of knowledge of catalysis in The Netherlands. Experts in various key sub-disciplines from eight Dutch universities join forces in this new organization to execute a strong innovative research program of international standing in catalysis, to meet the challenge of a sustainable society in the next century.

The NRSC-C is one of the six top research schools selected in 1998 by the Netherlands Organization for Scientific Research (NWO), and is supported financially by the Netherlands Ministry of Education, Culture and Sciences in the framework of their in-depth research strategy. This incentive furnishes a limited number of research schools with additional funding, to enable them to develop into research centers of international top quality. The research funding has a long-term character (for a period of 5 years, extended by another 5 years as of 2008). For the first periods 1999-2008 the NRSC-Catalysis budget amounted to 33.6 M€. The most characteristic aspect of the NRSC-C research

program is its fundamental and interdisciplinary approach. The ultimate aim involves an understanding of the dynamics of complex chemical transformations. Important examples include catalytic processes (homogeneous, heterogeneous and supramolecular), chemical transformations in confined space, controlled reactivity resulting from molecular pre-organization, and artificial self-instructed and self-replicating processes. The approaches will be both experimental and computational; much emphasis will be placed on the detailed understanding of the mechanism of the chemical transformations under study.

The interdisciplinary character of the NRSC-C is rooted in the three thrust areas of homogeneous catalysis, molecular heterogeneous catalysis and functional architectures, all governing integrated aspects, derived from the traditional disciplines organic, inorganic and physical chemistry. Each of these thrust areas with established expertise within the participating groups, providing the fundamental basis of this NRSC, will offer useful contributions to realize control of recognition in complex chemical transformations.

- Homogeneous catalysis: by combining organic and organometallic chemistry to achieve selectivity in chemical transformations and to prepare new catalytic species with specific functions towards controlled reactivity (thrust area leader: Prof. Dr. P.W.N.M. van Leeuwen/ Prof Dr. J.N.H. Reek (UvA).
- Molecular heterogeneous catalysis: by studying complex surfaces and the nanoscopic arrangements of active sites at these surfaces to promote both the induced assembly of reactants/molecules and their reactivity and functionality at these surfaces (thrust area leader: Prof. Dr. Ir. K.P.de Jong (UU).
- Functional architectures: by using all the new approaches that have become available to prepare, study and use (self-)assembled structures within the nanoscopic regime, thereby providing detailed insights into the role of co-operativity in the reactivity and structure of complex systems (thrust area leader: Prof. Dr. B.L. Feringa (RUG).

The long-term targets defined as Critical Research Issues of NRSC-Catalysis are:

- The determination and forecasting of the structural and electronic properties of the

catalytically active site (homo- as well as heterogeneous) during the recognition, binding and conversion of the substrate.

- The design and synthesis of molecular systems through self-instructed and self-reproducing chemical processes, involving templated-directed selectivity.
- The development of complex chemical transformations under environmentally friendly conditions, thus contributing the development of a society that uses its resources in a sustainable way.

Deriving from the critical research issues four sub-programs or research topics are defined:

- Catalyst design
- Closing the gap between homogeneous and heterogeneous catalysis
- Supramolecular catalysis
- Probing the event, theory and modeling

These sub-programs will bring man-made catalysis to a level of control that seems to be reserved for natural systems only. Although each of them has its focus in one or two of the three thrust areas, they obtain their surplus value due to the input of the other(s).

Control of reactivity, organization and regulation are collective objectives of the sub-programs that will benefit from the knowledge gathered in the three thrust areas. It is self-evident that the activities within NRSC-Catalysis will provide an excellent opportunity for the interdisciplinary training of young scientists developing skills in one of the most important aspects of modern chemistry with strong ties to physics and biology.

Approximately 60 researchers (PhD-students, post-docs, research fellows) are yearly working in the Top research School NRSC-C; besides NRSC-Catalysis invested in equipment to an amount of about 3,45 M€ (1999-2003).

In 2008 HIMS participated with four research groups (Reek, Elsevier, Hiemstra and Brouwer) in the NRSC-C. Reek is member of the management team since 2008. The total budget initially assigned to the UvA amounted to 4.2 (1999-2003, with internal competition) + 1.9 (2003-2008) = 6.1 M€ over the period 1999-2008. Funds from the NRSC-C are an important way of additional funding in the 1st money-stream, in addition to the gradually decreasing University budgets; see also section 1.5.

The NRSCC was recently re-accredited for the period 2009-2013. In 2008 HIMS received a total of 2.7 M€ in for new projects in the period 2009-2013 (groups Reek, Elsevier, Hiemstra, Rothenberg and Wever).

1.4.2 Holland Research School of Molecular Chemistry (HRSMC)

Accreditations in 1994, 1999 & 2006

The Holland Research School of Molecular Chemistry (HRSMC) was founded in 1994 and has been re-accredited in 2006 by the Royal Netherlands Academy of Arts and Sciences (KNAW) for the period 2006-2011 as a national Graduate School (Onderzoekschool). HRSMC comprises research groups of the Van 't Hoff Institute for Molecular Sciences (HIMS) at the Universiteit van Amsterdam, of the Leiden Institute of Chemistry (LIC) at the Universiteit Leiden, and of the Institute for Electrons and Molecular Structure (EMS) at the Vrije Universiteit Amsterdam. The research takes place in the heart of chemistry and focuses on the physical, chemical and biological properties of molecules in relation to their electronic and spatial structures. The main aims of HRSMC are:

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

The Universiteit van Amsterdam legally represents the HRSMC and currently prof. dr. W.J. Buma (HIMS) is the scientific director. Clearly, the HIMS beautifully fits in the heart of the HRSMC and its participation is a firm basis for extensive cooperation in research and in educational training of graduate students. The HIMS research groups Buma/Brouwer, Elsevier/Rothenberg, Hiemstra, Wever, Reek and Bolhuis/Meijer participated in the HRSMC in the year 2008. The HRSMC attracts special attention by the high quality of organic- and inorganic synthesis, catalysis, molecular spectroscopy, photochemistry, photonic materials and computational chemistry.

1.4.3 Nederlands Instituut voor Onderzoek in de Katalyse (NIOK)

Accreditations in 1992, 1997 & 2003

NIOK, which stands for 'Nederlands Instituut voor Onderzoek in de Katalyse' (Dutch Institute for Catalysis Research), is a virtual institute consisting of groups from eight Dutch Universities active in all areas of catalysis. As from 01-01-2001 the Universiteit Utrecht hosts the coordination of NIOK. Other participating Universities are the Technische Universiteit Eindhoven, the Universiteit van Amsterdam (HIMS), the Universiteit Groningen, the Technische Universiteit Delft, the Technische Universiteit Twente, the Universiteit Nijmegen and the Universiteit Leiden.

NIOK is a national Graduate School (Onderzoekschool), which acts as the platform and sparring partner for national and international contacts on catalysis with academia, industry and government. NIOK fosters the advancement of both higher education and research and stimulates collaboration between scientists of various disciplines and Universities. The major catalysis groups of seven Dutch Universities established NIOK in 1991. Later, NIOK was recognized by the Royal Netherlands Academy of Sciences (KNAW) and it is supported by an industrial advisory board VIRAN which consists of members from Dutch and multinational industries involved in many aspects of applied catalysis.

Graduate education is a prime activity of NIOK. An annual general catalysis course is given for all graduate students of NIOK groups. Guest speakers from academia and industry are no exception. In addition, each year a number of courses and workshops on special topics are organized, several examples are:

- Computational Catalysis
- Surface Characterization in Catalysis Research.
- Laser and Mass characterization techniques in catalysis and surface chemistry
- Catalytic Olefin Polymerization
- Catalysis, an integrated approach

The HIMS groups Reek, Elsevier/Rothenberg Hiemstra/van Maarseveen and Wever participate in NIOK. Elsevier is a Board Member of NIOK.

1.4.4 Dutch Polymer Institute (DPI)

Accreditations in 1997, 2002 & 2008

In the early nineties, the Dutch government launched the idea of so-called 'Leading Technological Institutes' (LTIs) in key areas of the Dutch industry. Reports, indicating that R&D activities in The Netherlands showed a relative decline compared to other countries, induced plans to establish LTIs as joint ventures between government, industry and the academia (public-private-partnership). The Dutch Polymer Institute (DPI) is one of the four LTIs that were established in 1997³. DPI is a foundation funded by industry, universities and government set up to perform exploratory research in the area of polymer materials. The entire Dutch polymer producing and converting industry is involved in DPI, including major producers such as DSM, Dow, Shell, Basell, Akzo Nobel and GE-Plastics, high-tech users of polymers such as Philips and Océ, and TNO. Now a total of 36 companies and 30 knowledge institutes (> 250 scientists) are executing challenging research programmes in the field of polymers. DPI operates at the interface of universities and industry, linking the scientific skills of university research groups to industrial need for innovation. DPI performs pre-competitive research projects to add value to the scientific community through scientific publications and to the industrial community through the creation of intellectual property. DPI provides a unique platform for new technology awareness in which participating industrial companies, commercial competitors in the market place, communicate on a pre-competitive basis to trigger innovation. DPI integrates the scientific disciplines and know-how of universities into the chain of knowledge to optimize the conditions for making breakthrough inventions and triggering industrial innovation. DPI aims to combine scientific excellence with a real innovative impact in industry, thereby creating a new mindset in both industrial and academic research. DPI aims to fill the innovation gap between industry and universities to resolve the Dutch paradox of scientific excellence and lack of innovation. DPI was initially established for a four-year period. The Dutch government (Ministry of Economic Affairs) supplied funds for a second period of six years (instead of the initially intended four years) up to 2008. The extra prolongation enabled DPI to expand in Europe, which was one of the original objectives. In 2008 DPI was positively

evaluated again and consequently the Polymer Innovation Programme (PIP) was started at September 11th, 2008 for a period of eight years (2008-2015). The PIP is one of the pillars of the chemistry key area of the Ministry of Economic Affairs and consists of two organizations, the Dutch Polymer Institute (DPI) and the DPI Value Centre. The PIP aims to keep the Netherlands at the front of industrial, scientific and social development. The programme has three tracks:

1. the accelerated creation of new business
2. carrying out pre-competitive research and joint development
3. securing a vital polymer community in the Netherlands as a driving force for future growth

The first and third track are being performed by the DPI Value Centre while the Dutch Polymer Institute is responsible for carrying out track 2. The Dutch government allocated a total of 49,6 M€ to execute the PIP in the next four years; 36 M€ is for research (DPI/track 2) and 13,55 M€ for new business and new companies, strengthening the valorisation from the research programme and community building (DPI Value Centre/tracks 1 and 3).

- In the new research programme (2008-2015), the focus lies on the following themes:
- Durable high-volume performance materials
- New polymers with properties that contribute to sustainability
- Coatings and membranes with high added value
- High-tech and biomaterials

These themes have been selected for their expected contribution to further improvement of the quality of life through the use of material technology, to develop more sustainable energy-efficient materials with a view to the rising scarcity of raw materials and energy and to open new economic opportunities through boosting competitiveness for the Dutch and European polymer industry. It is anticipated that the number of non-Dutch research groups involved in the DPI program will grow in the coming years and that DPI will evolve to a European Centre of Excellence.

HIMS started new initiatives and/or participates in 2008 with various research groups in the DPI: Schoenmakers/Kok, Reek/De Bruin, Brouwer and Iedema. The HIMS groups of Schoenmakers (theme Macromolecular and Biosystems Analysis), Reek/De Bruin (Catalysis), and Iedema received various DPI grants in 2008 (see chapter 3.2 and

³ In 2006 more LTIs were established: the Dutch Separation Technology Institute (DSTI), The Technology Institute Pharma (TI Pharma) and the centre of excellence for sustainable water technology (Wetsus). Next year the Comprehensive Analytical Science and Technology Institute (TI-COAST) will follow, with a strong HIMS participation and UvA/VU leadership (see section 1.5).

appendix 5.1). The HIMS director Zsom is a member of the DPI Advisory Board.

1.4.5 NanoImpuls and NanoNed

Started in 2003 (NanoImpuls) & 2004 (NanoNed)

NanoNed is a national nanotechnology R&D initiative that combines the Dutch strengths in nanoscience and technology in a national network with scientifically, economically and socially relevant research and infrastructure projects. The program began on January 1, 2004. The total budget for this NanoNed program amounts to 235 M€ and the program runs until 2009. NanoImpuls is a strategic initiative from the Dutch Ministry of Economic Affairs in the area of nanotechnology and the predecessor of NanoNed. This program started 2003 and ran until 2009; the investment comprised 18 M€. The objective of both NanoNed and NanoImpuls is to generate a strategic impulse for the Dutch scientific and industrial knowledge position in nanotechnology and will:

- Maintain and strengthen the strong nanotechnology position of the involved scientific/ industrial groups in the Netherlands
- Ensure the future availability of well trained workers for Dutch knowledge driven industry
- Strengthen the Dutch knowledge infrastructure through a comprehensive knowledge distribution/ transfer approach, leading to industrial nanotechnology applications

NanoNed is executed by a consortium of 9 partners, consisting of the main nanotechnology institutes of the Netherlands. The consortium and its representative consists of Mesa+ (UT), Kavli Institute of Nanoscience (TUD), BioMade (RUG), Fotonica Group Amsterdam (cooperation in the Amsterdam region between the FOM-Institute for Atomic and Molecular Physics/AMOLF and HIMS/UvA), IMM (RUN), TNO, Science & Industry (Delft), cNM (TUE), BioNT (WUR Research Center) and PREu (Philips Research Europe, Eindhoven).

The program is organized in 11 large interdependent programs called Flagships, based on national R&D strengths and industrial relevance. Each Flagship is a vehicle for national cooperation between different partners including industry, and is led by an independent scientific leader. The Flagships are:

- Advanced Nanoprobng

- Bottom-up Nano Electronics
- Chemistry and Physics of Individual Molecules
- BioNanoSystems
- NanoElectronic Materials
- NanoFabrication
- NanoFluidics
- NanoInstrumentation
- NanoPhotonics
- NanoSpintronics
- Quantum Computation

Generic, technology-oriented Flagships run together with more application-oriented programs, to create a cohesive nation-wide multidisciplinary program. The program covers about 200 research projects, which will represent more than 1200 man-years of research over a period of 5 years. As part of this initiative, NanoNed initiated NanoLab NL, a national nanotechnology facility that combines the existing facilities of Twente, Delft and Groningen. NanoLab NL coordinates the use of the facilities, tariffs, investments and the cooperation with industry, with a special emphasis on small and medium-sized high-tech enterprises. The NanoImpuls activities have been set up along the same lines as those within NanoNed and cover four of the Flagships (NanoFluidics, NanoSpintronics, NanoInstrumentation and NanoFabrication) and the infrastructure activity NanoLab. These were selected on the basis of their individual merits, the added value for the Dutch nanotechnology position, and on the fact that they could be easily incorporated into the NanoNed structure. The projects run parallel to and under the supervision of the NanoNed program. The NanoNed initiative should lead to new industrial nanotechnology applications (processes, products, services, general industrial activities). Extra attention will be paid to societal output and the innovation process. To this end, a Valorization Platform has been established that will play an important role in realizing the valorization targets by coaching and monitoring. Additionally, a Technology Assessment program is an integrated part of NanoNed. The assessment will result in a mapping of the societal impact of nanotechnology in close collaboration with the scientists involved. The NanoNed office at the Technology Foundation STW manages both the NanoNed and the NanoImpuls program. The NanoNed Board is also responsible for supervising the implementation of NanoImpuls.

HIMS participates in various Flagships with various research groups (Schoenmakers/Kok, Brouwer). The HIMS director Zsom is a member of the NanoNed Board.

1.4.6 Amsterdam Center for Multiscale Modeling (ACMM)

Started in 2007



The foundation of Amsterdam Center for Multiscale Modelling (ACMM) will be an important development that materializes the ambition of the computational group to create a computational centre with high visibility together with the theoretical chemistry group at the VU (Baerends, Visscher, Bickelhaupt) and the theoretical biology group at FOM-AMOLF (ten Wolde and Mulder). The three groups have achieved leading positions in complementary aspects of multiscale modelling. The Quantum Chemistry group at the Free University is an internationally recognized group that specializes in the development of novel quantum mechanical tools (in particular, density-functional theory) aimed at understanding and predicting properties and reactivity of small to medium-sized (bio) molecules. The group at the University of Amsterdam specializes in the development and application of Monte Carlo and Molecular Dynamics simulation techniques to study systems containing many thousands of particles, and on coarse-grained modelling of systems containing billions of particles. The group at AMOLF focuses on the development of novel computational tools to investigate ordering phenomena in colloidal systems and to model growth and regulation in living cells. In other words, internationally recognized expertise needed for multiscale modelling is available in Amsterdam. At present, no other region in the Netherlands has concentrated the same level of prominence in these three fields simultaneously.

At the national level the ACMM can act as the centre of reference for activities in the field of multiscale modelling and coordinate large-scale programs that involve simulation aspects. Recent

trends in funding of research increasingly tend towards large-scale projects. Often they focus on a specific topic (NWO programs, EU Thematic Priorities) or aim to support strong and viable research groups or consortia. The centre will be able to compete for the large scale projects as it houses high quality research, has a sufficiently broad size and focus, and has strong relations with industry. The ACMM has already been put forward in several national plans, showing that it is on track of being a serious competitor in large scale funding projects.

1.4.7 Catalysis for Sustainable Chemicals from Biomass (CatchBio)

Started in 2008

Accessible crude oil reserves are slowly but surely running out, and industrial processes capable of turning renewable biomass into a viable alternative for crude oil are urgently needed. With the appropriate catalytic conversions, biomass could replace crude oil as the primary source material for useful fuels and chemicals. CatchBio (Catalysis for Sustainable Chemicals from Biomass) aims to develop clean and efficient processes for biomass conversion into low-cost and sustainable biofuels, chemicals and pharmaceuticals.

Among the 22 partners of CatchBio are most of the Dutch universities (including UvA/HIMS), research institutes and industries, operating in the field of catalysis research. Industrial key players are involved but also more specialized SMEs take part in the consortium. CatchBio is part of a € 100 million investment program Smart Mix of the Dutch government aimed at boosting innovation in the Netherlands. Approximately half of the 29 M€ budget of CatchBio is financed through this investment program by the Dutch ministry of Economic Affairs and the ministry of Education, Culture and Science. The other half is financed by all the industrial and academic partners involved in CatchBio. CatchBio is an initiative of the Netherlands Institute for Catalysis Research (NIOK), legally represented by the commissioner Utrecht University. The program management is carried out by NWO-ACTS.

CatchBio initiates an ambitious research program of 8 years in the field of catalytic biomass conversion. It aims to process the various components present in biomass (cellulose, hemi-cellulose, lignin, proteins

and oils) in useful fuels, chemicals and pharmaceuticals. To tackle the different scientific and technological issues involved in biomass conversion, CatchBio is divided in five thematic clusters:

1. Energy
2. Bulk Chemicals
3. Fine Chemicals and Pharmaceuticals
4. Generic Research
5. Socio-economic and Ethical Research

The first three clusters are centered on the main production sectors. Research projects in these clusters will integrate fundamental, applied and industrial research to develop new homogeneous and heterogeneous catalysts, catalytic conversions, novel catalytic processes and their related reactor technologies. This research is carried out in close co-operation with industry. Since exploration of different catalytic options will have an important impact on future choices regarding energy conversion and chemicals production, research on the socio-economical and ethical aspects of the different technologies will also be undertaken. Prof. Elsevier is member of the program committee Fine Chemicals and Pharmaceuticals. In 2008 HIMS received a total funding of 0.7 M€ from CatchBio for projects in the groups Reek, Elsevier and Rothenberg.

1.5 Recent and future developments

Several (new) developments, related to the advice of the HIMS Scientific Advisory Committee (SAC), to new nation wide funding initiatives, to the priorities of NWO and the investments asked for in the Sectorplan Natuurwetenschappen, started in 2008, or are expected in the coming year(s). Important developments with a direct impact on HIMS are mentioned below:

A. Collaboration with the Vrije Universiteit Amsterdam (VU)

Formal research collaboration with VU is currently explored and has started already in part. In the framework of this strategic alliance it was decided to present joint chemistry programs in the Amsterdam area under four key research areas. These exhibit both excellence and critical mass in chemistry and provide the basis of future bachelor and master programmes at the Amsterdam universities and a joint investment plan to be offered in 2009 in the framework of the Sectorplan Chemistry (see also section B).

By investing in these areas of excellence the Amsterdam universities, HIMS and SILS being the major players from UvA, will be able to compete internationally and further boost their ambition with respect to valorisation.

The four selected key research areas are in line with the important research areas of NWO-CW, the advice of the SAC, the Sectorplan Chemistry, and recent discussions with the Regiegroep Chemie regarding TI-COAST (Analytical Chemistry & Spectroscopy; see also section E). The selected key research areas in chemistry are:

- Synthetic Chemistry & Catalysis (CAT & BMS with VU groups)
- Computational Chemistry (COMP with VU groups; ACMM, see section G)
- Analytical Chemistry & Spectroscopy (MBA & MOLP with VU groups, see section E)
- Chemistry of Life (SILS/Systems Biology with Molecular Pharmaceutical Sciences/VU groups)

In the area of computational chemistry the recently founded Amsterdam Center for Multiscale Modelling (ACMM, see section G) is the most illustrative and pronounced example of the collaborative initiatives of UvA (COMP), VU, and also FOM/AMOLF.

In analytical chemistry (MBA) and spectroscopy/ photonics (MOLP) a nationwide research initiative TI-COAST was initiated a few years ago by professors Schoenmakers and Janssen of HIMS, and Buydens from RU Nijmegen. This TI-COAST initiative is of great importance for the strong Amsterdam UvA/VU cluster (see also section E).

In synthetic chemistry (BMS) and catalysis (CAT) a strategic plan will be written in close collaboration with the colleagues of VU, which will lead to an Amsterdam Center of Sustainable Synthesis and Catalysis. In this framework, the present master track "Molecular Design, Synthesis and Catalysis" of the Amsterdam universities will be redirected towards "Sustainable Synthesis and Catalysis", to provide an optimum fit to the corresponding research theme. Regular research meetings of UvA/HIMS (Hiemstra) and VU (Orri) groups already are a first result of the new collaboration.

We expect to find financial support for this "Focus and Mass" initiative of the Amsterdam universities in the framework of the future investments of the Sectorplan Natuurwetenschappen (chemistry).

B. The Sectorplan Natuurwetenschappen

The Sectorplan Natuurwetenschappen (sciences sector plan) is drawn up by the Regiegroep Chemie (appointed by the Innovation Platform of the Dutch Government) together with the six general universities in the key area 'Chemistry' and was recently approved by the Dutch Minister of Education. Several specific areas in the field of chemistry are selected in this plan. Starting in 2011 at least 10 M€/year will be available on a basis of quality to achieve the necessary scale of university research, e.g. by investments in new chairs and equipment. The HIMS research activities in synthesis, catalysis, analysis, spectroscopy, photonics and multiscale modelling are all part of the joint investment plan of the Amsterdam universities UvA/VU (see section A).

C. Research quality assessment 2010

Seven Dutch universities, i.e. the 6 general universities plus Wageningen University and including UvA (HIMS) and the chemistry department of VU, will together organize the coming research quality assessment in 2010 for the period 2004-2009 through the Kamer Scheikunde of the VSNU.

Independently, the 3 technical universities will also organize their research quality assessment together. Part of the self-assessment to be made by HIMS is already available (years 2004-2006), and was discussed with the SAC in December 2008 during their visit to HIMS. The updated version (2004-2009) will be available early 2010.

D. Extension of existing research initiatives

In 2008 the funding periods of various existing national research initiatives (research schools, institutes and networks) were extended; see also section 1.4. A few important developments with HIMS participation to be mentioned are:

- In 2008 The **Dutch Polymer Institute (DPI)** was positively evaluated again and consequently the Polymer Innovation Programme (PIP) was started September 2008 for a period of eight years (2008-2015). The PIP is one of the pillars of the chemistry key area (Regiegroep Chemie) of the Ministry of Economic Affairs and consists of two organizations, viz. the DPI itself and the DPI Value Centre. The PIP aims to keep the Netherlands at the front of industrial, scientific and social development. HIMS participates in the DPI with the groups Schoenmakers, Reek,

Brouwer and Iedema; they received 1.4 M€ for projects from DPI.

- The **National Research School Combination-Catalysis (NRSC-C)**, was recently re-accredited for the period 2009-2013. In 2008 HIMS received a total of 2.7 M€ for new projects (groups Reek, Elsevier, Hiemstra, Rothenberg and Wever).
- **Catalysis for Sustainable Chemicals from Biomass (Catch-Bio)** started in 2008 and aims to develop clean and efficient processes for the conversion of biomass into low-cost biofuels, chemicals and pharmaceuticals. Among the 22 partners are most Dutch universities, research institutes and industries operating in the field of catalysis research. Industrial key players are involved, but also more specialized SMEs take part in the consortium. In 2008 HIMS received a total of 0.7 M€ for projects (groups Reek, Elsevier and Rothenberg).

E. New national research initiatives

In 2008 several new research initiatives were started. A few important new nation wide developments in which HIMS participates are:

- **Comprehensive Analytical Science and Technology (TI-COAST)** is a new initiative to cluster existing and new techniques in the analytical and spectroscopy field with the main target to achieve breakthroughs using informatics and nanotechnology. Analytical chemistry is of tremendous importance to the other chemical sciences and society, and its impact is no less than that of ICT. The Regiegroep Chemie has proposed that an Analytical Chemistry Technology Roadmap will be drawn up to make an inventory of the strengths and to identify the challenges confronting the various stakeholders during the coming years, with an investment 11 M€ /year during 6 years. TI-COAST, a collaborative initiative of academia, industry and public institutes, will address the following critical factors:
 - Availability of well-trained/educated analytical scientists at bachelor, master and PhD level (quality & quantity)
 - Development of and access to new analytical & spectroscopic knowledge and know-how
 - Access to sophisticated and/or next generation analytical technologies (virtual lab)
 To achieve this TI-COAST will operate through Expertise Centers:

- Composition of complex mixtures
- Molecular structure assessment
- Solids characterization
- Data handling and chemometrics

The Amsterdam universities UvA/VU expressed they want to be the lead university of TI-COAST and will participate with 5-6 groups, including Schoenmakers and Buma/Brouwer of HIMS.

- The Netherlands **Nanotechnology Initiative-Strategic Research Agenda (NNI-SRA)** is an initiative of STW, FOM and NanoNed. Invited by the Dutch government in 2008, these organisations prepared a document based on the core of NanoNed (see section 1.4.5) that was much broader and more applied. It contains distinct recommendations for the development of nanotechnology for the coming 10 years. Many researchers from academia, technology institutes, government and industry contributed to this plan. The NNI-SRA selected the following themes of major importance for the Netherlands directed to new know-how (1-4), and important application areas (5-8):
 1. Beyond Moore's Law, chip technology beyond the possibilities of silicon
 2. Nanomaterials
 3. Bionanotechnology
 4. Nanofabrication, techniques to fabricate nanostructures and -materials
 5. Nanomedicine
 6. Food
 7. Energy
 8. Clean water

Within all themes various explicit research lines are chosen. The application areas are based on the selections of importance for the Netherlands as defined by the Dutch government in 2006 (Kabinetsvisie nanotechnologieën 'Van klein naar groots').

At the intersection of these themes 15% of the available budget is reserved for issues important for society such as ethical questions, impact and risk-assessment of nanomaterials.

The NNI-SRA was handed over to the Dutch ministry of Economic Affairs in September 2008. This led to nomination of NNI-SRA for the 2009 FES-investment round, and subsequently to a nation wide call for proposals in the 8 themes mentioned, and for societal issues (involving IVAM of the UvA Holding).

The HIMS groups of Bolhuis, Schoenmakers and Buma submitted projects that were selected for the final NNI-SRA plan. WZI, SILS and IBED are also involved. The next step will be the preparation of a business plan in 2009 in order to submit for the FES-round.

F. Extension of collaborations with the FOM institutes AMOLF and Rijnhuizen

The collaboration with FOM/AMOLF is illustrated by the extraordinary professorship of prof. Huib Bakker from FOM/AMOLF that was continued in 2008 for a second period of 5 years. Furthermore, Dr. Sander Woutersen (VIDI and ERC laureate), who came from FOM/AMOLF through the collaboration between Bakker, Woutersen and Buma, was recently appointed as UD/Assistant professor. Presently we are working on the appointment of an extraordinary professor from FOM/Rijnhuizen through the Stichting Fysica for 5 years.

G. Extension of Computational Science research (ACMM)

To strengthen the scientific environment of (molecular) computational science in Amsterdam the Amsterdam Center of Multiscale Modeling (ACMM) has been established in 2007. ACMM is well positioned to be a strong player in competition for research grants where focus and mass have become essential factors. Moreover, it will act as a seed for strengthening collaborative efforts in the field, both nationally and internationally. ACMM recently has been recognized as part of the spearhead e-Science of FNWI. It is also mentioned in various national research plans, e.g. the Sectorplan Natuurwetenschappen. Although the European research and training organization CECAM chose Lausanne as their new location, they decided last year Amsterdam will become a CECAM node.

H. Discontinuation of Complex Fluids

Since the Complex Fluids theme of HIMS is of sub critical size it was discontinued per 01-01-2008 as separate research theme, facilitated by the leave of the staff-members. Thereby, HIMS followed the 'Focus and Mass' policy of the Dutch universities and the advice of the SAC from 2006. Dr. E. Eiser was re-appointed 0.1 fte for 5 years and joined the group of Prof. Elsevier. The technician P. Verschuren was transferred to a vacancy in the group of Prof. Schoenmakers.

I. Extension of catalysis research via the new chair Heterogeneous Catalysis and Sustainable Chemistry

Based on the advice of the SAC and to extend the strategic Catalysis theme, Dr. G. Rothenberg was appointed full-time professor in Heterogeneous Catalysis and Sustainable Chemistry at 01-06-2008. Traditionally, catalysis is divided into heterogeneous, homogeneous, and bio-catalysis. With this new chair UvA will be the only university in the Netherlands with internationally renowned active chairs in all areas of catalysis and will become an important national focal point for catalysis. The new chair is financed from the funds that became available after the leave of the Complex Fluids staff-members, and illustrates the 'Focus and Mass' policy followed by HIMS. The new chair will focus on discovery, optimization, and application of new catalysts and processes for clean synthesis and green energy. Combining heterogeneous catalysis and bio-catalysis or heterogeneous and homogeneous catalysis in one process gives important advantages, including process intensification and more efficient overall processes. Our large research efforts in the broad spectrum of catalysis combined with valorization opportunities makes catalysis an attractive focused theme that aims to initiate a catalysis center of excellence.

J. Research in Forensic Sciences

The Faculty of Sciences started a new master course in Forensic Sciences in 2006, in an exclusive collaboration with the Netherlands Forensic Institute NFI. To create and sustain a master-level course, we believe it is essential to combine research with education. HIMS is in an excellent position to conduct research projects within forensic science and art science because of our knowledge on the analysis and characterization of highly complex samples, being the unique expertise of the group Schoenmakers. In forensic sciences we are aiming for intensive intrafaculty contacts, e.g. with IBED and IvI, as well as a close collaboration with NFI. The latter will be profitable for both parties and it will surely result in joint research projects. New appointments of an extraordinary professor, staff and technicians in the forensic field are expected within HIMS in the coming years, as well as part-time exchange of staff between HIMS and NFI. Prof. Schoenmakers will redirect the profile of his chair to encompass forensic sciences (50%).

K. Research in Art Conservation and Restoration Sciences,

The new teaching program is expected to give new impulses to related research in humanities and science, e.g. molecular chemistry. This research field is multidisciplinary and comprises art and cultural history, science and restoration-science and is being developed in collaboration between HIMS and the Faculty of Humanities. In recent years HIMS has already been involved in some research activities concerning Art Conservation and Restoration, including NWO-programs. In this respect the NWO-priority-project MolArt in 1996-2002 and its successor De Mayerne Project in 2002-2006 are significant. In these projects restorers, art historians and scientists collaborated to develop a molecular understanding of the changes of materials in works of art. This has proven to be of paramount importance for a rationalized restoration of art. The HIMS director Rob Zsom is member of the NWO-program committee De Mayerne. As a part of the Art-sciences initiative a Conservation Scientist will be appointed, partly within the Faculty of Humanities (0.6 fte) and partly in the Faculty of Sciences/HIMS (0.0 fte). Presently, Prof. Iedema is acting as coordinator for the educational program. In close collaboration with the group of Prof. Schoenmakers, new appointments of extraordinary professors and staff (including a future group leader) and technicians in Conservation and Restoration are expected within HIMS in the coming years. In addition, research collaborations of HIMS staff and researchers are foreseen with the Rijksmuseum and the Institute Collection Netherlands via co-worker exchange programs.

L. The Röntgen Diffraction department

After retirement of the chair holder Prof. Henk Schenk in 2004, the crystallography chair was discontinued. Since 2005 the HIMS Röntgen group is positioned in the WZI building in one facility with the Röntgen groups of WZI and IBED. Because we are of the opinion that the powder diffraction know-how and the equipment are unique in the Netherlands, we tried to position the group elsewhere in the Netherlands. In the framework of the Sectorplan Chemistry (see section B), we will continue these efforts. Another possibility is to find a place for the group in an existing or new chair at the UvA, e.g. within the new initiative of restoration

sciences. Although the faculty recently has endorsed this plan, implementation is only possible with financial support of NWO as a part of the plan for Conservation & Restoration Sciences described below.

Future plans regarding points K and L

HIMS considers the possibility to start a new research theme, comprising at least two chairs/groups:

- 1) The group Schoenmakers (Polymer Analysis and Forensic Sciences)
- 2) A new research group, combining the activities on Restoration Sciences and those of the Röntgen Diffraction department

Plans will be written in 2009, both for Forensic and Restoration sciences, in order to obtain external financial support from e.g. the Dutch Ministry of Justice, NWO, and the new matching fund of the faculty. The SAC of HIMS was asked to give advice on this plan in the course of 2008.

As mentioned later in this report (see chapter 4), the present and future financial prospects of HIMS are not certain. For this reason the institute is forced to be very selective with appointments in fixed positions. As a consequence, we follow a strategy of endowed chairs and make extensive research plans for people and equipment. With these plans we will apply for external funding, e.g. NWO for Conservation & Restoration Sciences, and NWO and the Ministry of Justice for Forensic Sciences. In case external finance cannot be found, HIMS very likely cannot execute these plans and will have to concentrate on its proven strength in the field of molecular chemistry.

Our policy on the longer term is that each chair should have enough financial possibilities for purposes such as matching, investment, maintenance of equipment and new activities. Regarding personnel, each HIMS chair will at least have the following composition:

- 1 professor
- 1-2 U(H)D's per chair
- 1 technician per 1-2 staff-members in experimental groups
- 1 PhD per chair (full time professor)

2. Fundamental and Applied Research

2.1 Introduction and research themes

In 2008 HIMS employed 14 professors, 5 extraordinary professors, 7 associate professors (UHD's, 1 of them is also part-time professor), 9 assistant professors (UD's), 94 PhD students (AIO/OIO's, including guest-aio's and outdoor-aio's), 47 postdocs (PD's), and 44 other personnel (OBP), all together a total of 220 persons (158.6 Fte).

Total personnel HIMS 2008

1 st (Fte)	NRSC-C (Fte) ¹⁾	2 nd (Fte)	3 rd (Fte)	External Fte	Total Fte	Total Persons
49.8	8.7	25.5	74.6	108.8	158.6	220
31.4%	5.5%	16.1%	47.0%	68.6%	100%	

¹⁾ 1st from NRSC-Catalysis (Top Research School)

Source of Funding

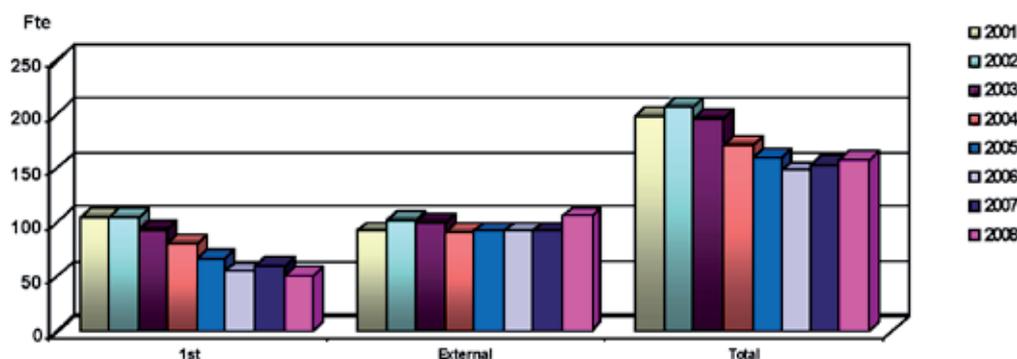
1st: University (direct) funding

1st: NRSC-Catalysis

2nd: NWO, FOM and STW

3rd: EU, BSIK and Industrial

External = NRSC-C + 2nd + 3rd



The five research themes of HIMS, cover a wide spread of activities, which all have in common the **(supra-) molecular** approach as is defined in the mission of HIMS. The rapid development of molecular sciences that has taken place in the recent years has also continued in the year 2008. Next to the research activities in the themes, HIMS also

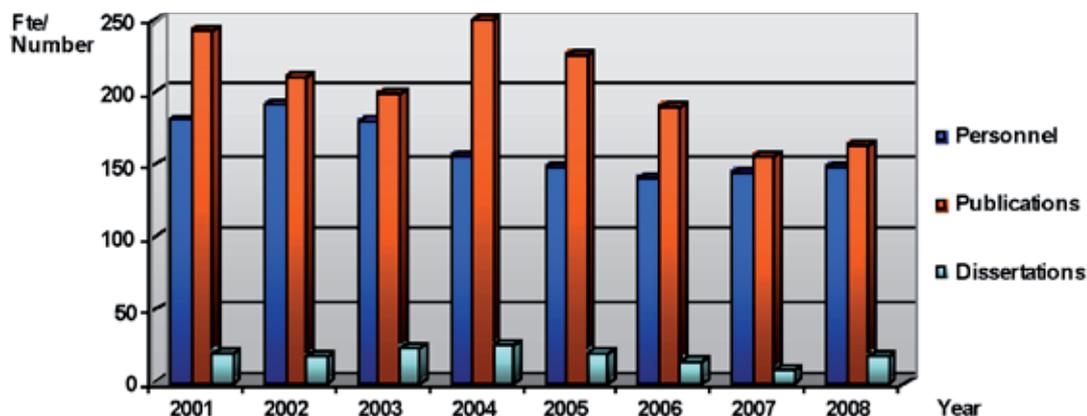
studies a number of activities on a more central level. A few to mention are: catalyst applications in (bio-) organic synthesis, nanotechnology, sustainability, energy, health, supra-molecular chemistry/catalysis, computational techniques, various (laser) spectroscopic techniques and use of biochemical approaches. In art sciences as well as in forensic

sciences, the new teaching program will give new impulses to related fundamental research within HIMS (e.g. molecular chemistry). HIMS is in an excellent position to conduct research projects in art sciences and forensic sciences, because of our unique knowledge on high-resolution and high-sensitivity (e.g. chromatographic/ spectroscopic) analysis of complex samples. Many of our research activities took place in close collaboration with other institutes of the FNWI. Those with groups from the Swammerdam Institute of Life Sciences (SILS) and the Van der Waals Zeeman Institute (WZI) are the most outstanding, as is described in more detail in the following sections with the research output of the themes. Collaborations are continuously growing with the Vrije Universiteit (VU), the Medical Faculty/Academisch Medisch Centrum (AMC) of the UvA, as well as with the NWO institutes FOM-AMOLF and FOM-Rijnhuizen (see chapter 1.5). This exchange of information and intensification of research collaborations over the borders of research groups, themes and institutes has been proven to be of increasing importance in exploring the field of **Molecular Sciences**, the core activity of HIMS. In addition, sharing of facilities for supporting structure determinations are also of great importance for our research groups. These facilities are embedded in the various research groups and in the two supporting departments of HIMS (NMR, IR, Raman and Röntgen Diffraction). Next to the activities as defined in the five research themes, other research activities were carried out in 2008 in the fields of 'Polymer and Process Systems' and

'Röntgen Diffraction'. The research output for these groups in 2008 will also be reflected in this annual report.

HIMS produced 21 PhD dissertations in 2008, an equal level as the numbers in 2005 (20) and 2006 (15), respectively. The low level of 2007 (9) was an incident, related with an (unwanted) peak in extension of the promotion period (longer 4 years) of several PhD students and with the reorganization of the chemistry department (2002-2004). Unfortunately, many PhD students defend their thesis not within the 4 years period, and as a consequence PhD-defences planned for 2007 were delayed to 2008 and some of them even later. In the period 2002-2004 the number of staff members decreased, and a stop in PhD appointments from direct funds (University budget) was introduced. As a consequence the average number of PhD students decreased from 20 (2001-2005) to 15 (2006-coming years). For the years to come the perspective is positive, however, due to an increase of PhD students to be expected in the coming years (22 PhD vacancies at 01-01-2009). Additionally, the decrease in PhD students in the last years was related with the matching demands by the Dutch- (e.g. BSIK/NanoNed, CatchBio, NNI, etc.) and EU subsidiaries. Fortunately, the matching demands have disappeared for the NWO-Vernieuwingsimpuls (VENI, VIDI and VICI) grants and the European Research Council (ERC) grants since 2008. Following the trend in dissertation output, the number of refereed papers in international journals

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



¹⁾ Professors, Associate Professors (UHD's), Assistant Professors (UD's), Postdocs, PhD students and Research Technicians; management and supporting staff not included

of the HIMS groups has increased again in 2008. In 2008 HIMS published 11 papers in absolute top journals (impact value > 10.0) such as Nature, Chemical Reviews, Chemical Society Reviews, Angewandte Chemie and Nature Physics, and 24 papers in top journals (impact value 5.0-10.0) such as Physics Review Letters, Advanced Synthesis & Catalysis, Advances in Catalysis, Coordination Chemistry Reviews, Chemical Communications, PLoS Computational Biology, Endocrine-Related Cancer, Chem.-A Eur. J., and J. Am. Chem. Soc. (total 165 papers in 2008). The output per theme is presented in more detail in the chapters 4 and 5. In the coming paragraphs of this chapter the research results of the HIMS groups will be given per theme and will be illustrated with highlights and key publications from 2008 for the specific projects.

2.2 Research quality assessments 2002 & 2008

The last VSNU research quality assessment in July 2002 showed that the ratings for quality, scientific productivity, scientific relevance and long-term viability data for the HIMS groups, are still at a good to excellent standard, indicating that the younger professors are reaching the high quality

level of their predecessors and re-established the international position of the individual research groups. This opinion is substantiated by the following conclusion taken from the 2002 VSNU report:

“... a number of changes of chair holders have taken place recently at the UvA, several of which offer good perspectives for the future”.

The Scientific Advisory Committee (SAC) of HIMS performed a mid-term review of the research quality in December 2008. On that occasion the Center for Science and Technology Studies (CWTS) conducted a bibliometric analysis over the period 2001-2007. In 2002 a comparable analysis was performed by the VSNU over the period 1991-2000. The ratio of the average number of citations per publication (corrected for self-citations) CCP and the mean field citation score FCSm is an important indicator of a publication's impact compared to the international average and allows rating of the international position of research groups.

For HIMS as a whole CPP/FCSm values were 1.51 and 1.58 over the periods 1991-2000 and 2001-2007, respectively, which is well above the international

Latest VSNU scores of the HIMS research themes and groups

Q = Quality, P = Productivity, R = Relevance, V = Viability

Research theme	Research group	Q	P	R	V	CPP/ FCSm ¹⁾ (1991-2000)	CPP/ FCSm (2001-2007)
Macromolecular and Biosystems Analysis	Schoenmakers	4	4	5	5	1.64	1.29
Bio-Molecular Synthesis	Hiemstra, Schoemaker, Rutjes	5	3	4	5	1.81	1.79
	Wever	4	3	4	3	1.19	1.39
Catalysis	Reek/Van Leeuwen	5	4	5	5	2.70	2.32
	Elsevier	4	4	4	4	2.08	1.37
Computational Chemistry	Krishna	5	5	5	5	3.00	1.31
	Smit	4	4	4	5	2.61	1.94
Molecular Photonics	Buma/Brouwer	4	4	4	5	0.96	1.17
Röntgen Diffraction	Peschar/Schenk					0.64	0.79
Polymer & Process Systems	Iedema					0.53	0.99
Total HIMS						1.58	1.51

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

Source: *Bibliometric analysis performed by the Center for Science and Technology Studies, 2008*

standard of 1.0. Furthermore, all five HIMS themes have individual scores well above 1.0 (see the table below).

At the moment this annual report of HIMS is written, the official midterm review report 2008 of the SAC was not yet available. However, the first verbal reaction of the SAC was very positive, substantiating their earlier conclusions from their 2006 report:

“All groups meet up with the quality demands needed to compete on the national level of fundamental chemistry research, and in most cases also on the international level. All groups have shown a considerable earning power by acquiring external research projects”.

2.3 Research output

2.3.1 Macromolecular and Biosystems Analysis

Staff: Prof. dr. ir. H.G. Janssen, dr. W. Th. Kok, Prof. dr. ir. P.J. Schoenmakers, Prof. dr. S. van der Wal

Research schools/Networks: DPI, NanoNed

Selected highlights of research activities 2008

The industrial support for the research group was again substantial in 2008. A number of PhD projects are sponsored by industrial partners through the DPI (e.g., DOW, Astra Zeneca, Waters) and there are also PhD projects financed directly by various companies (Unilever, DSM, Syngenta, ATAS GL, NLisis).

Rob Edam finished the experimental work on his DPI-project on the characterization of branched polymers, that was conducted in cooperation with DOW. He studied a completely new separation mechanism, molecular-topology fractionation (MTF), for separations of synthetic polymers according to branching parameters. He is expected to defend his thesis in 2009.

Ron Peters finished his external PhD project on the “Characterization of polymeric network structures”. He carried out the experimental work for his PhD thesis at DSM Research, while at the same time being busy with his ‘normal’ work there. His success in combining these tasks can be seen from the 14 papers already published of which he

was a (co)author. January 2009 Ron has obtained his doctorate from the University of Amsterdam, with Prof. van der Wal as promotor.

With the MKB company NLisis a research project has been formulated on “The next generation GC”. Smaller projects on gas chromatography carried out in 2008 and sponsored by a consortium of enterprises have paved the way for this project. Daniela Peroni will start as a PhD student in January 2009.

The Dutch nanotechnology programs (NanoImpuls and NanoNed) provided a large support for the research of the group, in terms of instrumentation and PhD positions. A number of papers from the PhD students involved (Mauro De Pra, Yuli Huo, Peter Pruijm) were published in 2008. Mauro De Pra defended his PhD thesis on “Pillar-structured microchannels for liquid chromatography” (promotor Prof. Schoenmakers). In his work he showed convincingly that microfabrication techniques can be applied to create separation devices that are really superior to conventional columns. Yuli Huo decided to leave the group; her research work on monolithic stationary phases will be continued by a newly appointed postdoc, Shane Seabrook. A number of projects have been formulated together with other research groups (from IBED and UTwente) for the new nanotechnology program NNI.

An important factor for the future of the analytical chemistry groups at the UvA is the TI-COAST initiative (Top Institute for Comprehensive Analytical Science and Technology). Staff members of the Polymer-analysis group (Schoenmakers, Janssen) play an important role in this initiative. After a number of years of conferring and promoting, COAST has now really taken off. Industry and universities started recognizing the importance of research and education in analytical chemistry. In 2008 steps were taken to start an organization. The UvA-VU combination is a candidate to play the role of “lead-university”.

Key publications

- Peters, R; Tonoli, D; van Duin, M; Mommers, J; Mengerink, Y; Wilbers, ATM; van Benthem, R; de Koster, C; Schoenmakers, PJ; van der Wal, S. 2008. Low-molecular-weight model study of peroxide cross-linking of ethylene-propylene (-diene) rubber using gas chromatography and

- mass spectrometry - I. Combination reactions of alkanes. *J. Chromatography A* 1201 (2): 141-150 (Part 1) and 151-160 (Part 2).
- Edam, R; Meunier, DM; Mes, EPC; Van Damme, FA; Schoenmakers, PJ. 2008. Branched-polymer separations using comprehensive two-dimensional molecular-topology fractionation x size-exclusion chromatography. *J. Chromatography A* 1201 (2): 208-214.
 - De Pra, M; Kok, WT; Schoenmakers, PJ. 2008. Topographic structures and chromatographic supports in microfluidic separation devices. *J. Chromatography A* 1184 (1-2): 560-572.
 - Kaal, E; Janssen, HG. 2008. Extending the molecular application range of gas chromatography. *J. Chromatography A* 1184 (1-2): 43-60.
 - Pruijm, P; Ohman, M; Huo, Y; Schoenmakers, PJ; Kok, WT. 2008. Methacrylate monolithic capillary columns for gradient peptide separations. *J. Chromatography A* 1208 (1-2): 109-115.
 - Huo, Y; Schoenmakers, PJ; Kok, WT. 2007. Efficiency of methacrylate monolithic columns in reversed-phase liquid chromatographic separations. *J. Chromatography A* 1175 (1): 81-88.

2.3.2 Bio-Molecular Synthesis

Staff: Prof. dr. H. Hiemstra, Prof. dr. H.E. Schoemaker/DSM, Prof. dr. R. Wever, Prof. dr. P. Timmerman/Pepsan, dr. J.H. van Maarseveen

Research schools: HRSMC, NIOK, NRSC-C

Selected highlights of research activities 2008

The Synthetic Organic group headed by Hiemstra carries out research in three main areas: Organic Synthesis, Homogeneous Catalysis and Chemical Biology.

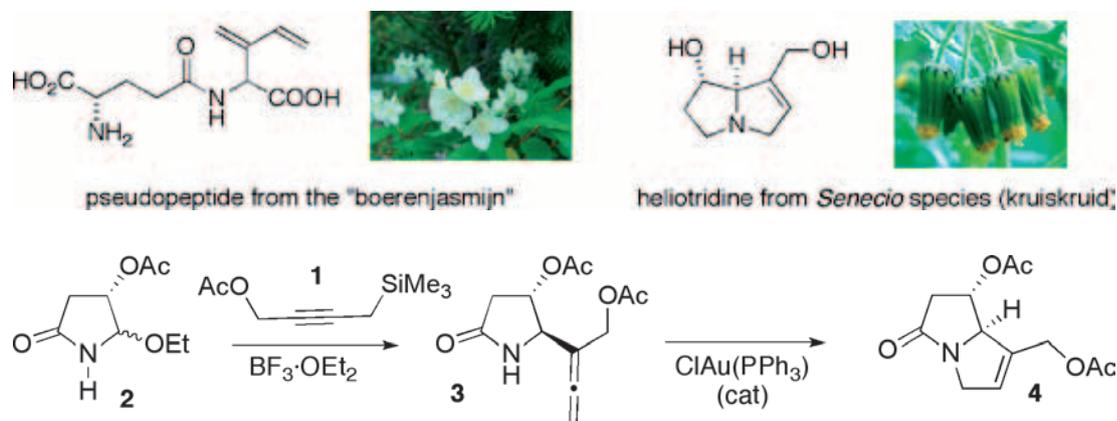
Organic synthesis: The group aims at (1) the development of new synthetic methodology and (2) the target-oriented synthesis of important natural and unnatural compounds, their relevance being associated with biological or catalytic activity. On several occasions these research areas overlap as we strive to apply our newly developed methodology for the synthesis of bioactive compounds. The use of nitrogen-stabilized carbocations (*N*-acyliminium ions) as reactive intermediates is

one of the historic subjects in our group to develop new synthetic pathways. The coupling of such species with allenylmethylsilanes provides novel dienic α -amino acid derivatives which are not readily accessible otherwise. In 2007, the total synthesis of a natural pseudodipeptide (from *Philadelphus coronarius*, boerenjasmijn) in enantiomerically pure form was completed using this methodology (Berkheij, CW/NWO-supported, PhD ceremony, April 10, 2008).

In related research the synthesis of allenes via *N*-acyliminium ions is combined with heterocyclization reactions catalyzed by gold complexes (Dijkink, Kinderman). This approach has led to an efficient total synthesis of the pyrrolizidine alkaloid (+)-heliotridine from (*S*)-malic acid. Thus, Lewis acid-mediated reaction of functionalized propargylsilane **1** with the *N*-acyliminium ion precursor **2** derived from (*S*)-malic acid provided allene **3** as a 4:1 diastereomeric mixture from which the trans isomer was easily purified. Cyclization of this compound with a gold(I) complex as catalyst provided bicyclic **4** in excellent yield. One more step gave the natural product. A similar process applied to cation precursor **5** led to 3,4-dehydroproline **6**.

A new project involves the Ferrier-type rearrangement of α -allenoxylactams of type **8** in the presence of trimethylsilyl triflate leading to the interesting lactam-substituted unsaturated aldehyde **9** (Kinderman, Dijkink). The starting allene is readily available by base-catalyzed isomerization of propargyloxylactam **7**. The scope and the stereoselectivity of this reaction which probably proceeds via a tight *N*-acyliminium ion is now under investigation.

Solanoeclepin A is a hatching agent of potato cyst nematodes which are a serious cause of losses in potato production. The natural product or simpler analogues thereof could serve as an environmentally benign nematocide which explains the great interest for a total synthesis of this complex terpene. Our synthetic approach toward solanoeclepin A includes an intramolecular photochemical [2+2] cycloaddition of an allene to access the most intricate cyclobutanone substructure (Lutteke). Novel synthetic pathways are developed to photochemical substrates in enantiopure state in order to access more suitable cyclobutanes. A key approach involves the tetracyclic cyclobutane **11**



which is obtained in good yield from irradiation of allenic butenolide **10**. Compound **10** arises in a few steps from alcohol **12** which is accessible in 93% ee by transfer hydrogenation of the corresponding ketone using Noyori's ruthenium catalyst. In a few steps including a Denmark cyclopropanation of an allylic alcohol cyclopropane **13** was obtained as the most advanced intermediate so far.

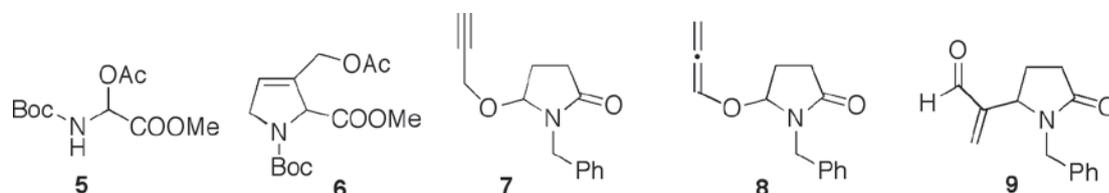
In a different approach to solanoeclepin A photochemical cycloadditions are studied of compounds of the type **14**, readily obtained from iodide **15**. [2+2]-Cycloaddition of **14** provides tricyclic **16** which is different from **13** in a sense that the lactone is replaced by the desired angular methyl group. The photocycloaddition of **14** appears to be extremely sensitive to the substitution pattern of the acyclic alkene.

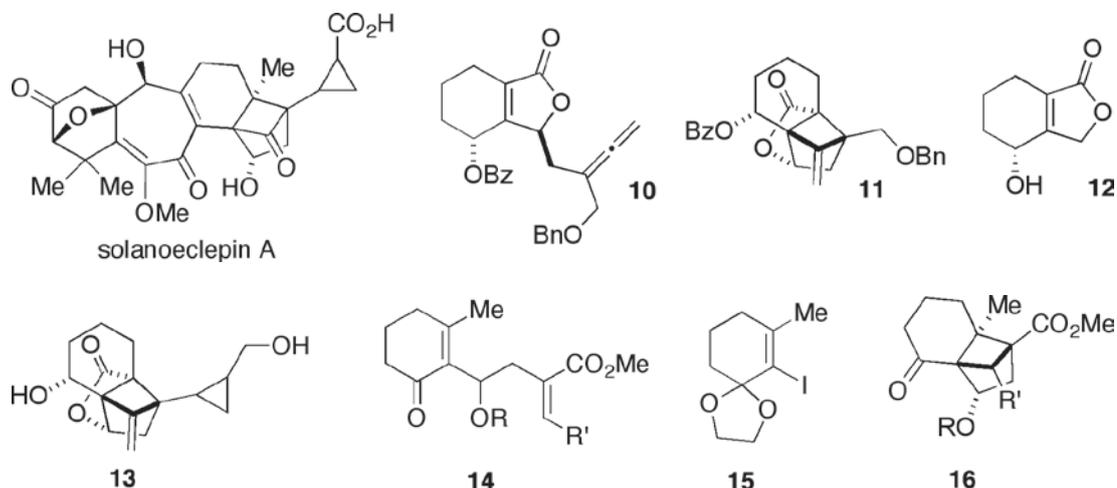
Another key research area of our group is the development of useful and robust methodology for preparing small cyclic peptides. Cyclic peptide-like molecules are highly desirable starting points for drug development.

The powerful copper(I)-catalyzed azide-alkyne "click" cycloaddition giving 1,4-connected-1,2,3-triazoles, acting as *trans*-amide bond surrogates, has been translated to the solid phase to enable cyclic

pseudo-peptide parallel synthesis (Springer, PhD ceremony November 6, 2008). As shown below, the key click cycloaddition could not be accomplished on the solid phase. Fortunately, detachment of the linear precursor gave a smooth intramolecular azide-alkyne cycloaddition furnishing the cyclic pseudo tetrapeptide.

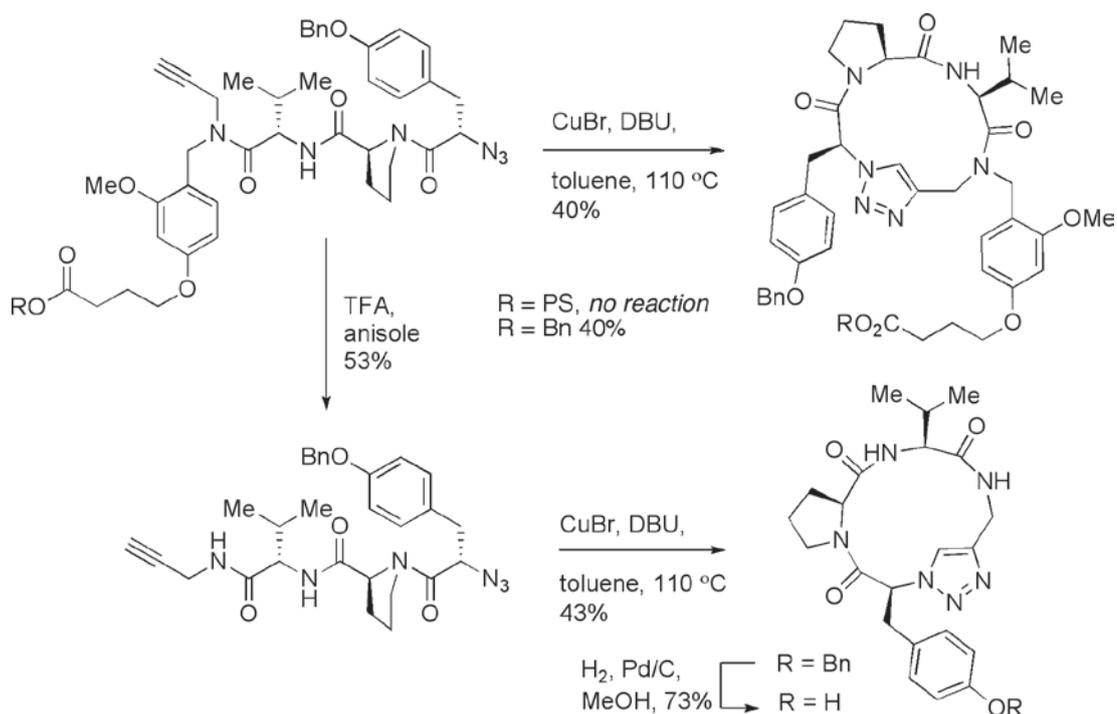
Homogeneous Catalysis: P,N-Ligands comprise a privileged class of compounds in the field of homogeneous catalysis. In this project a new class of P,N-ligands, named "ClickPhine", was disclosed in which the coordinating nitrogen atom is part of a 1,3-disubstituted 1,2,3-triazole, accessible via the powerful Cu(I)-catalyzed alkyne/azide "click" cycloaddition (Detz, NRSC-C-supported, PhD ceremony April 17, 2009). Complexes were made and characterized with metals such as Pd and Rh. In addition, the catalytic activity was shown in allylic alkylation reactions and hydrogenations. Preliminary results showing moderate enantioselectivities were obtained in Rh-catalyzed hydrogenations using chiral ClickPhine ligands. The chiral ClickPhine ligands were prepared from enantiopure α -substituted propargylic amines via the, for this purpose especially developed, Cu(I)-Pybox-catalyzed enantioselective propargylic amination reaction.

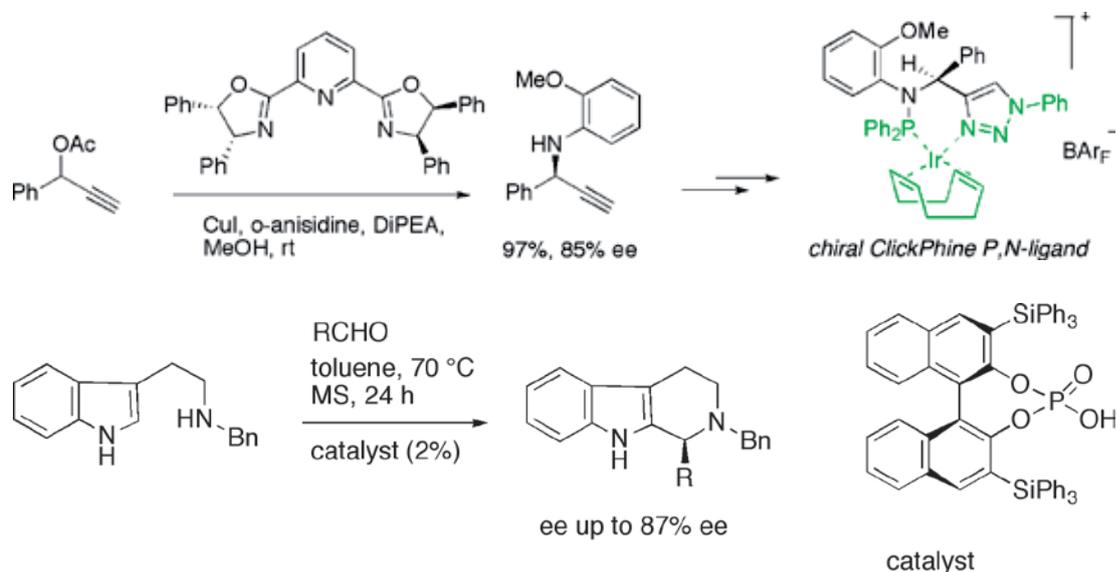




In our work in the area of organocatalysis (Wanner) enantiopure phosphoric acids are now generally used as Brønsted acid catalysts in enantioselective Pictet-Spengler cyclizations of a wide range of N-monosubstituted tryptamines. The key features of this reaction were carefully examined for N-benzyltryptamine. With p-bromobenzaldehyde as reaction partner and the bis-triphenylsilyl-substituted binolphosphoric acid (see structure) as catalyst the product β -carboline was obtained in 85% ee. This product was readily crystallized to enantiomerically pure crystals which

revealed the absolute configuration via X-ray crystallography (cooperation with De Gelder, RU Nijmegen). Another area of organocatalysis is the use of phosphines as catalysts. Kinderman (recipient of an NWO VENI grant) has continued his research with the study of the phosphine-catalyzed cycloaddition of allenic esters with activated imines leading to highly substituted piperidines. In future studies the influence of enantiopure phosphines on the stereochemical outcome of this process will be studied. Moreover, the product is a precursor for



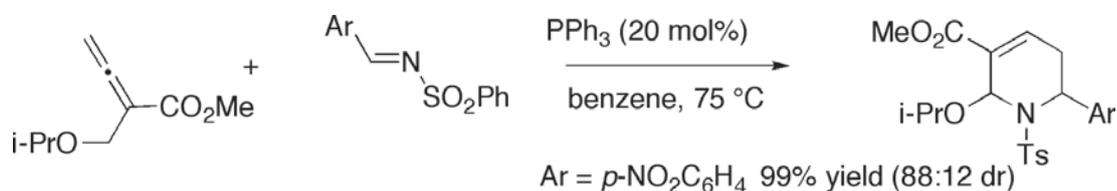


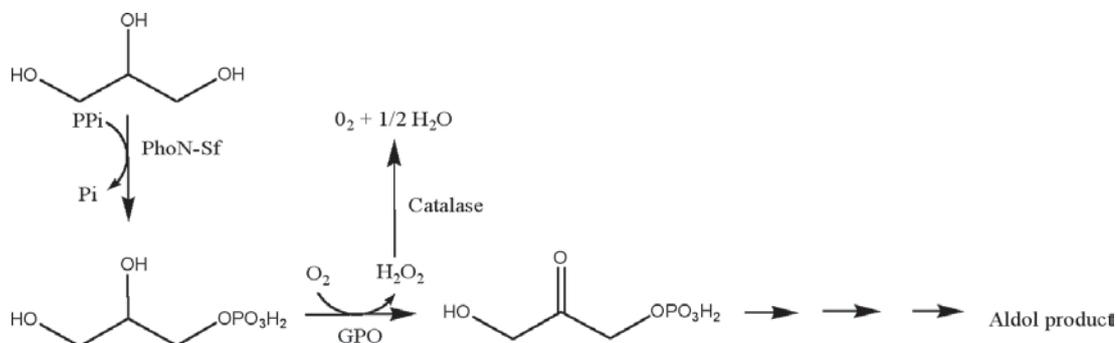
tosyliminium ion chemistry offering numerous opportunities for further functionalization.

Chemical Biology: Cross-links introduced between amino acid residues in close proximity can provide distant constraints to validate models of the 3D-structure of proteins. To facilitate mapping of cross-links in proteolytic digests, in close collaboration with the group De Koster/Back/De Jong (SILS, UvA), a new amine-type specific cross-linker, (bis) succinimidyl 3-azidomethyl glutarate (BAMG) has been developed. Cross-linking of proteins by BAMG is followed by tryptic digestion. Treatment of the digest with the water soluble phosphine tris(carboxyethyl)phosphine leads to cleavage of the cross-linked and azide reduction without cleavage. Cross-linked peptides and peptides modified by BAMG without actual cross-linking yield distinct sets of TCEP-induced reaction products that can be isolated by reverse-phase diagonal chromatography and identified by mass spectrometry to reveal the identity of parent compounds. Besides using the cleavage strategy,

currently also novel solid supports were developed incorporating highly strained cyclooctyne moieties that are able to sequester and characterize azide-containing peptides without the need for using Cu(I)-catalysis (Nessen, NWO-Echo grant).

Biocatalysis: This group (Wever, Schoemaker) focuses on the use and development of biocatalysts in synthetic organic chemistry as an alternative for existing chemical procedures. It uses directed evolution as a tool to create enzymes with novel or modified properties. To enhance the phosphorylating activity of the bacterial non-specific acid phosphatase from *Salmonella enterica* ser. *typhimurium* LT2 towards dihydroxyacetone (DHA), a mutant library was generated from the native enzyme (Van Herk). Three different variants were identified after one round of epPCR that showed enhanced activity. The single mutant V78L was the best and showed an increase in the maximal DHAP concentration that is 30% higher compared to the wild type enzyme at pH 5.0. This variant is 13 times more active at pH 7.0 compared to the WT acid phosphatase from *Shigella flexneri* that was





previously used by us in acid phosphatase – aldolase cascade reactions. Further we showed that this mutant is indeed far more effective in the cascade reaction in which DHAP is condensed to propionaldehyde is producing more of the desired aldol product in much less time. Further improvement in 3-carbon-unit primary alcohol phosphorylation by the acid phosphatase could be gained by saturation mutagenesis and more rounds of error prone PCR using this variant as parent strain. Hartog discovered that the new recombinant arylsulfotransferase is able to sulfate secondary alcohols enantioselective with a preference for hydrophobic compounds.

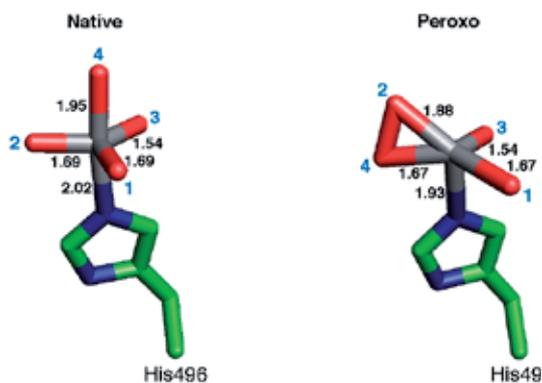
The cooperation with Rutjes (Radboud University, Nijmegen) and Franssen and Van der Oost (Wageningen University) within the framework of an IBOS-2/ACTS program has been very successful. A multi-enzyme cascade reaction has been developed in which we were able to convert glycerol and a number of aldehyde derivatives into chiral non-natural carbohydrates. Presently we are trying to upscale the cascade and to synthesize and characterize these compounds.

The vanadium chloroperoxidase was tested (Renirie) in collaboration with Crielaard (ACTA) for its effect on biofilms of *Streptococcus mutans*. The enzymatic products formed by vanadium chloroperoxidase significantly reduced the viability of biofilm cells. It is concluded that this enzyme and its reaction product form a potent antimicrobial system and that the enzyme could have potential as mouth rinse. In cooperation with Aubry and Renirie (University of Lille) it was shown that vanadium chloroperoxidase is active in chlorination and singlet oxygenation in non-ionic microemulsions. We propose that the chloroperoxidase can be used

as a green alternative for inorganic catalysts like molybdate and tungstate for which very high concentrations have to be used in oxygenation reactions.

In cooperation with Garner (University of Nottingham) Renirie has obtained vanadium *K*-edge X-ray absorption spectra of native, peroxy and reduced forms of the vanadium chloroperoxidase. The EXAFS regions provide a refinement of the crystallographic information previously reported for the native and peroxy-form of this enzyme: one short V=O bond (1.54 Å) is present in both forms. For the native enzyme, in addition to the oxo-group, the vanadium is coordinated to two other oxygen atoms at 1.69 Å, another oxygen atom at 1.95 Å and to the nitrogen of an imidazole group at 2.02 Å. The peroxide in the peroxyform of the enzyme is bound side-on.

Bio-organic Chemistry: The project leader Koomen has retired early 2006. The last PhD graduation (Koch) is expected in 2009. The thesis will deal with synthesis of nucleoside analogues and their activity on the different adenosine receptors.



Key publications

- Enantioselective BINOL-phosphoric acid catalyzed Pictet-Spengler reactions of N-benzyltryptamine, Sewgobind NV, Wanner MJ, Ingemann S, de Gelder R, van Maarseveen JH, Hiemstra H, *J. Org. Chem.* 2008, 73, 6405-6408.
- Phospha-scorpionate complexes by click chemistry using phenyl azide and ethynylphosphine oxides, van Assema SGA, Tazelaar CGJ, de Jong GB, van Maarseveen JH, Schakel M, Lutz M, Spek AL, Slootweg JC, Lammertsma K, *Organometallics* 2008, 27, 3210-3215.
- Bactericidal and virucidal activity of the alkalophilic P395D/L241V/T343A mutant of vanadium chloroperoxidase, Renirie R, Dewilde A, Pierlot C, Wever R, Hober D, Aubry JM, *J. Appl. Microbiol.* 2008, 105, 264-270.
- Backbone amide linker strategy for the synthesis of 1,4-triazole-containing cyclic tetra- and pentapeptides, Springer J, de Cuba KR, Calvet-Vitale S, Geenevasen JAJ, Hermkens PHH, Hiemstra H, van Maarseveen JH, *Eur. J. Org. Chem.* 2008, 2592-2600.
- Enantioselective copper-catalyzed propargylic amination, Detz RJ, Delville MME, Hiemstra H, van Maarseveen JH, *Angew. Chem. Int. Ed.* 2008, 47, 3777-3780.
- Probing FtsZ and tubulin with C8-substituted GTP analogs reveals differences in their nucleotide binding sites, Lappchen T, Pinas VA, Hartog AF, Koomen GJ, Schaffner-Barbero C, Andreu JM, Trambaiolo D, Lowe J, Juhem, Popov AV, den Blaauwen T, *Chem. & Biol.* 2008, 15, 189-199.
- Synthesis of a naturally occurring diene-containing amino acid and its glutamyl dipeptide via N-acyliminium ion chemistry, Berkheij M, Dijkink J, David ORP, Sonke T, IJzendoorn DR, Blaauw RH, van Maarseveen JH, Schoemaker HE, Hiemstra H, *Eur. J. Org. Chem.* 2008, 914-924.
- Formation of bicyclic pyrroles and furans through an enone allene photocycloaddition and fragmentation sequence, Lutteke G, AlHussainy R, Wrigstedt PJ, Hue BTB, de Gelder R, van Maarseveen JH, Hiemstra H, *Eur. J. Org. Chem.* 2008, 925-933.
- Crystal structure of a trapped phosphate intermediate in vanadium apochloroperoxidase catalyzing a dephosphorylation reaction, de Macedo-Ribeiro S, Renirie R, Wever R, Messerschmidt A, *Biochem.* 2008, 47, 929-934.

2.3.3 Catalysis

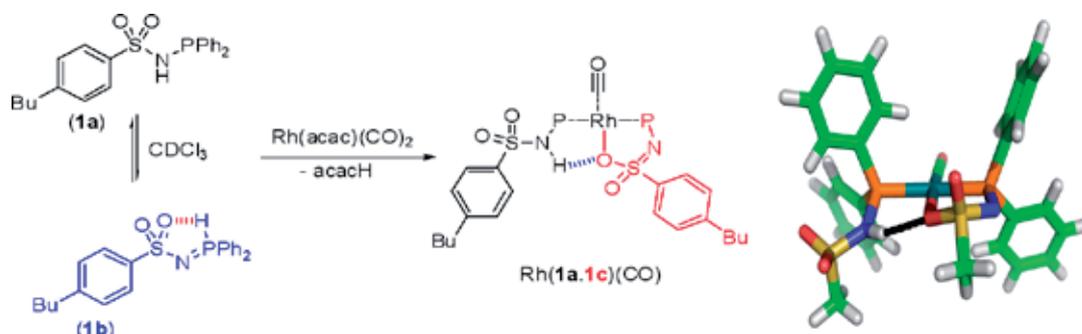
Staff: Dr. B. de Bruin, Prof.dr. C.J. Elsevier, Dr. F. Hartl, dr. J.C. v.d. Heuvel, Prof.dr. P.C.J. Kamer, Prof.dr. P.W.N.M. van Leeuwen, Prof.dr. J.N.H. Reek, Prof. dr. G. Rothenberg, dr. A.J. Sandee

Research schools: HRSMC, NRSC-C, NIOK

Selected highlights of research activities 2008

Development of supramolecular catalysts and their application in catalysis

We have further explored supramolecular approaches to arrive at novel transition metal catalysts. In previous years we have demonstrated that we can make ligand libraries by mixing functionalized ligand building blocks. We have applied successfully the zinc-nitrogen interaction for the assembly of the building blocks and applied a part of the library in the rhodium-catalyzed hydrogenation of various substrates (collaboration with DSM). We have extended the number of building blocks to 45 leading to about 450 chiral bidentate ligands. A part of the SUPRAphos ligand library was screened in a combinatorial fashion for the first time to search for novel catalysts for the symmetric hydroformylation of styrene. Some of the catalysts gave the product in high enantioselectivity, but at low conversion. Catalysts were found that give unusual high selectivity for the (non-chiral) linear aldehyde, which is unexpected as generally the branched aldehyde is formed with this substrate. We also have extended the approach to make supramolecular bidentate ligands to hydrogen bond based systems. As such we have introduced UREAphos, a new class of supramolecular bidentate phosphite ligands that was successfully applied in the rhodium-catalysed asymmetric hydrogenation of various substrates. The small series initially employed already provided hydrogenation catalysts that are highly selective. We have developed a fully automated preparation protocol for this new class of ligands, and over 100 ligands of this class have been prepared. In addition, we introduced METAMORPhos as a new class of supramolecular ligands that are adaptive through tautomerism. These properties give rise to new coordination



Tautomeric equilibrium of METAMORPhos ligand (1) and coordination behavior with Rh(acac)(CO)₂ (phenyl groups have been omitted in the complex for clarity) and the DFT calculated structure of Rh(1a.1c)(CO)

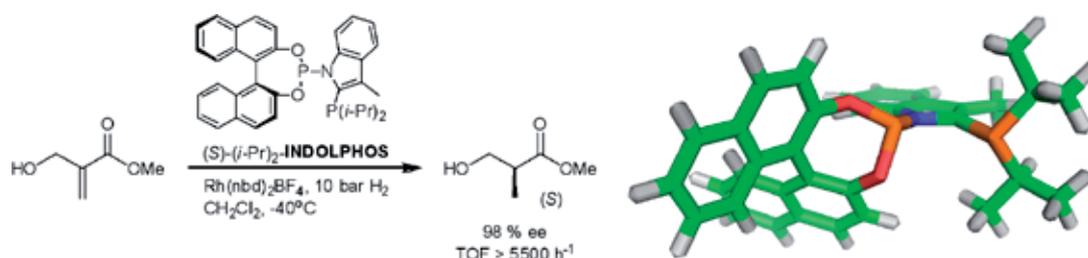
behavior, and the dual character also enables the selective formation of hydrogen bonded hetero-bis-ligated metal complexes. The adaptive behavior of the ligand when coordinated to the metal center, gives rise to rhodium complexes that show unique kinetics - zero order in H₂ and substrate - in the asymmetric rhodium-catalyzed hydrogenation of MAA. These kinetics let to the proposal of a new mechanism in the hydrogenation that is unique to this class of ligands and is attributed to the adaptive behaviour. Since the enantioselectivities obtained are high (above 90%) we are currently exploring if the strategy is suited to create large ligand libraries for fast catalyst discovery through combinatorial approaches (*Angew. Chem.* 2008).

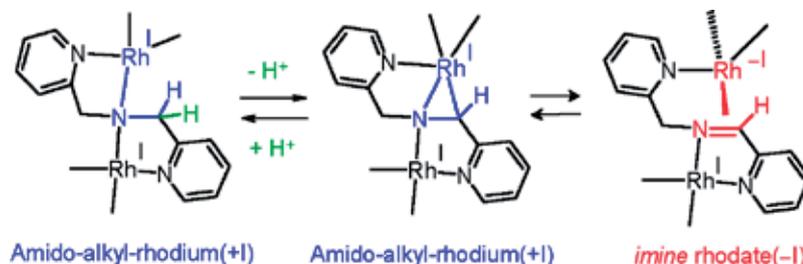
In the area of rational ligand design, we have developed a new class of hybrid bidentate phosphine-phosphoramidite ligands based on the indole backbone. The rigid backbone was chosen to enforce chiral environments around the metal complex. The coordination mode of the ligands to Rh is controlled by the steric properties of the ligand which has shown to play a major role in the asymmetric hydrogenation and hydroformylation. We have challenged the INDOLPhos library to the Roche ester precursor, and found that rhodium catalysts based on this ligand provides the product with the highest selectivity reported to date. Roche

ester 1a is successfully synthesized through asymmetric Rhodium catalyzed hydrogenation using INDOLPHOS in high yield and unprecedented enantioselectivity (up to 98% ee) on a preparative scale. The bidentate character of INDOLPHOS is of importance as all experiments with monodentate Monophos ligands resulted in poor ee of the product. A short study of the substrate scope revealed little sensitivity of the catalyst with regard to the ester group present in the substrate; both methyl as benzyl ester were converted in high selectivity. However, the primary alcohol function seems to have an important function as the acyl-protected substrate could not be hydrogenated in high selectivity (*Adv. Synt. Cat.* 2008).

Cooperative ligand concepts in catalysis

We recently reported that double deprotonation of cationic [(bpa)M'(diene)]⁺ complexes is unexpectedly easy and transforms the bpa ligand (bpa = bis-picolylamine) into a dianionic {bpa-2H}²⁻ ligand with unusual electronic properties. This led to a number of unexpected observations in which the N-ligands behave as 'non-innocent' and 'cooperative' ligands. The {bpa-2H}²⁻ ligand can be sequentially oxidized by up to two electrons, and thus serves as storage place for two reducing electrons. One electron oxidation of the ligand leads to ligand radical iridium complexes (*Chem. Eur. J.* 2008).





Analogous reactions of similar Rh species allowed us to prepare, for the first time ever reported, a mixed-valent Rh^{+1} , Rh^{-1} binuclear complex. This remarkable complex is formed via double electron transfer from the dianionic $\{\text{bpa-2H}\}^{2-}$ ligand to a Rh^{+1} center, thus producing a rare π -imine stabilized rhodium(-I) species (*JACS*, 2008).

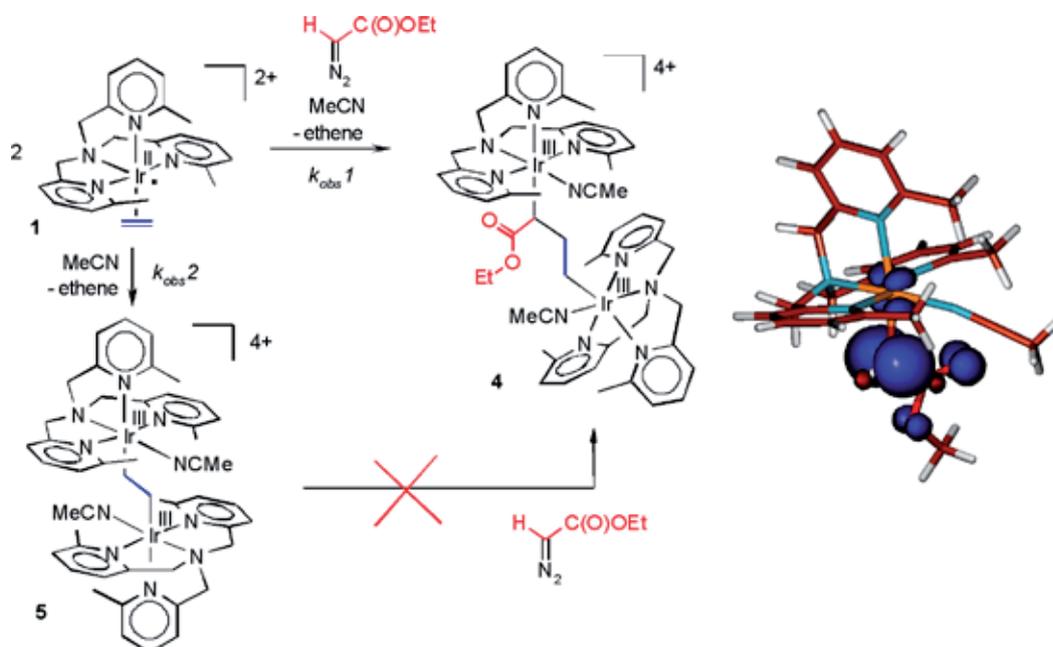
The ligand can thus be used to create metals with very unusual electronic properties. The impact of this concept on the catalytic properties of such species is currently not very clear, but the fact is that also these binuclear Rh complexes show activity in catalytic reactions, among which hydrogenation, polymerisation of acetylenes and polymerisation of carbenes from diazo-compounds.

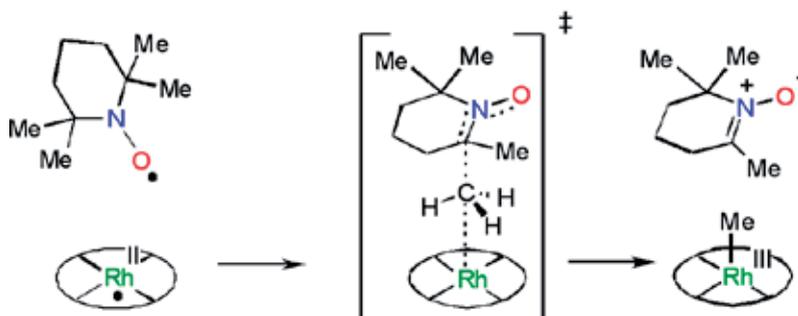
We demonstrated the cooperative action of the ligand and the rhodate(-I) metal ion in the

activation of molecular oxygen by these complexes. This reaction leads to the selective formation mononuclear carbonyl-amido $[(\text{bpam})\text{M}(\text{diene})]$ complexes (and $[\text{Rh}(\text{diene})\text{Cl}]_2$). This is a clear example of substrate activation by both the metal and the ligand.

Reactivity of metallo-radical complexes

Metallo-radical show special reactivity patterns expected to be useful in catalytic applications. We uncovered unusual C-C bond cleavage reactions as well as unusual C-C bond formation reactions using metallo-radical complexes. Although the PyMe groups shield the “vacant site” of $[\text{Ir}^{\text{II}}(\text{Me}_3\text{tpa})(\text{ethene})]^{2+}$ from attack by bulky reagents, acetonitrile is small enough to coordinate to iridium *trans* to the amine to form $[\text{Ir}^{\text{II}}(\text{Me}_3\text{tpa})(\text{NCMe})]^{2+}$. In the absence of other substrates, $[\text{Ir}^{\text{II}}(\text{Me}_3\text{tpa})(\text{NCMe})]^{2+}$ recombines with $[\text{Ir}^{\text{II}}(\text{Me}_3\text{tpa})(\text{CH}_2\text{CH}_2)]^{2+}$, or





perhaps more likely $[\text{Ir}^{\text{III}}(\text{CH}_2\text{CH}_2\bullet)(\text{Me}_3\text{tpa})(\text{MeCN})]^{2+}$ to form an ethylene bridged species.

Interestingly, and potentially relevant to carbene polymerisation reactions, entirely different selective reactions occur in the presence of diazo compounds. The reactivity towards ethyl diazoacetate (EDA) and trimethylsilyl-diazomethane (TMSDM) was investigated (*Chem. Eur. J.* 2008). The reaction with EDA gave rise to selective C-C bond formation, via radical coupling of the Ir-carbenoid radical species $[(\text{Me}_3\text{tpa})\text{Ir}^{\text{III}}(\text{CH}\bullet(\text{COOEt}))(\text{NCMe})]^{2+}$ and (the MeCN adduct of) $[\text{Ir}^{\text{II}}(\text{Me}_n\text{tpa})(\text{ethene})]^{2+}$ to give the tetra-cationic dinuclear complex $[(\text{Me}_3\text{tpa})(\text{NCMe})\text{Ir}^{\text{III}}\{\text{CH}(\text{COOEt})\text{CH}_2\text{CH}_2\}\text{Ir}^{\text{III}}(\text{Me}_3\text{tpa})(\text{NCMe})]^{2+}$.

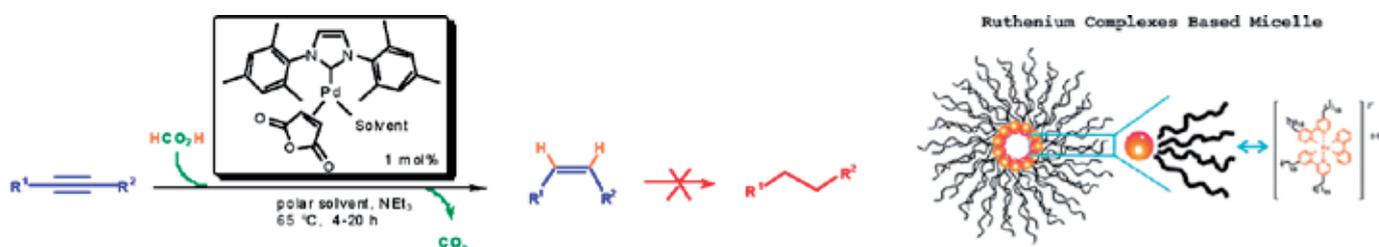
DFT calculations are in support of these pathways proceeding via the remarkably easily accessible Ir-carbenoid radicals. The electronic structure of the radical carbenoid species is best described as a carbon centered ligand radical obtained by one-electron reduction of a Fischer-type carbene. Spin density calculation reveal that these species are best described as carbon centred radicals.

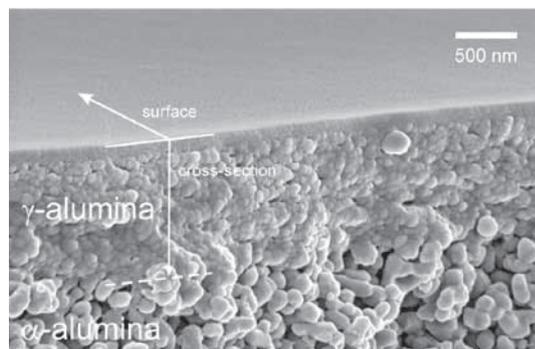
Reactivity of porphyrine stabilized metallo-radicals
Metallo-radicals can also be used to *break* C-C bonds. Porphyrine Rh^{II} species react with TEMPO, in which remarkably a methyl fragment of TEMPO is transferred to Rh through a C-C splitting reaction

producing (por)Rh^{III}-Me species. The mechanism of the TEMPO C-C bond activation was studied by means of kinetic investigations and DFT calculations. Both radical ($S_{\text{H}}2$) and ionic ($S_{\text{N}}2$) pathways are calculated to have barriers which are low enough to explain the experimental kinetic data (*JACS*, 2008). In another *JACS* paper we investigated the role of (por)Co radical systems in mediating radical polymerisation of methylacrylate and vinyl acetate (*JACS*, 2008). The cobalt radicals mediate polymerisation through a multitude of controlling reactions, which includes chain transfer catalysis, degenerative transfer polymerisation and some additional processes which are currently being further investigated.

Molecular inorganic chemistry and applications in catalysis

The design and implementation of N-heterocyclic carbene ligands as well as rigid bidentate N-ligands in late transition metal compounds aimed at catalytic carbon-element bond forming reactions continues to be an important research topic in the group. This year, the palladium-catalyzed hydrogenation of alkynes using Pd(0) complexes with an N-heterocyclic carbene ligand has been further studied. We found that we can go beyond Lindlar type catalysts by transfer hydrogenation of internal alkynes which gives excellent selectivity to Z-alkenes without reduction to alkanes. Ketones and other functional groups such as nitrile, nitro,





ester are not reduced. It is the first catalyst that shows excellent stereo- and chemoselectivity in semihydrogenation of alkynes without the need for hydrogen gas. Solvent effects were evaluated and isotope labeling studies were conducted to extend the scope, and a preliminary account was published (*Angew. Chem. Int. Ed.*, 2008, 47, 3223).

Based on our work coined metals@micelles we have studied ruthenium-based metallo-surfactants in collaboration with prof. De Cola (Universität Münster). Aggregates thereof combine unique spectroscopic and reactivity properties due to space confinement. The first inverted micelles with luminescent metallosurfactants have thus been obtained. These compounds possess several long linear chains that favour the solubility of the highly water-soluble metal polar head in non-polar phases. The size and shape of the aggregates was determined using dynamic light scattering. Atomic force microscopy allowed studying the dry structure of the aggregates on surfaces. Additionally, the self-assembly of the metal complexes in solution was monitored by steady state and time-resolved absorption and emission spectroscopy (*J. Mater. Chem.*, 2008, 18, 2762), an artist impression of the aggregates featured on the cover.

Furthermore, a paper has appeared on newly designed and synthesized amphiphilic iron and nickel compounds, which act as metallo-surfactants. These compounds contain modified diazoxa- and triaza-cyclononane ligands. In collaboration with dr. Eiser it was found that these molecules form inverse micelles as designed, and in some cases inverted vesicles, depending on the solvent. The size and structure of the aggregates was determined by dynamic light scattering and AFM (*Eur. J. Inorg. Chem.*). In a joint study with Prof. Keurentjes (TUE) we

have employed high-pressure NMR in our Amsterdam facilities for the study of interesting non-innocence of supercritical solvents during reactions. In this respect, we have studied the pressure and temperature dependence of equilibria involving carbon dioxide, and several amines with their respective carbamic acid (*J. Supercritical Fluids*). With Profs. Ragaini and Milani (Milano and Trieste, Italy) we have studied the synthesis of atactic polyketones catalyzed by Pd complexes with derivatives of our ubiquitous aryl-bian ligands; specifically meta-substituted analogues were used which exert a subtle balance of steric and electronic effects in the copolymerization reaction (*Organometallics*). Mechanistic organometallic chemistry of palladium compounds and kinetics were studied in collaboration with Profs. van Leeuwen and Kamer and with Prof. Canovese (Venezia, Italy), respectively.

Heterogeneous catalysis and sustainable chemistry
The Heterogeneous Catalysis group was officially established as an independent research group with the appointment of Prof. dr. Gadi Rothenberg as full professor and chair of Heterogeneous Catalysis and Sustainable Chemistry per 1 June 2008. With this appointment, the UvA became the only university in the Netherlands to have fulltime chairs in all of the catalysis subthemes. Collaborating with the materials science group at TU Twente, prof. Rothenberg and PhD student Anil Gaikwad designed and synthesised a dual-layer macroporous/nanoporous ceramic membrane cup. This is a simple and efficient device for separating large homogeneous catalysts in situ (*Angew. Chem. Int. Ed.*, 2008, 47, 5407). The figure below shows a scanning electron micrograph of a cross-section of the membrane.

Key publications

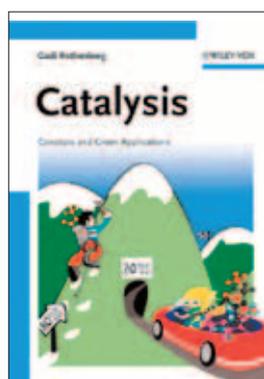
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- T.S. Koblenz, J. Wassenaar J. N. H. Reek, Reactivity within a confined self-assembled nanospace, *Chem. Soc. Rev.*, 2008, 37, 247 (inside cover)
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 - P. Hauwert, G. Maestri, J.W. Sprengers, M. Catellani, C.J. Elsevier. Transfer Semihydrogenation of Alkynes Catalyzed by a Zero-Valent Palladium N-Heterocyclic Carbene Complex. *Angew. Chem. Int. Ed.*, 2008, 47, 3223-3226.
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Snapshots showing location of isobutene in the zeolite MFI at loadings of (a) 2 and (b) 6 molecules per unit cell in MFI. The view is 2 unit cells deep. (Krishna et al., *Chem. Phys. Lett.* 459, 2008)

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- J. D. Holbrey, I. López-Martin, G. Rothenberg, K. R. Seddon, G. Silveroc and X. Zheng, Desulfurisation of oils using ionic liquids: Selection of cationic and anionic components to enhance extraction efficiency. *Green Chem.*, 2008, 10, 87-92.

Prof. Rothenberg published in 2008 an undergraduate/graduate textbook on catalysis (Catalysis: Concepts and green applications. G. Rothenberg, Wiley-VCH: Weinheim, ISBN 978-3-527-31824-7). This book combines for the first time all the aspects of catalysis (homogeneous, heterogeneous, biocatalysis and computer applications in catalysis research) in a single monograph.



2.3.4 Computational Chemistry

Staff: Prof. dr. B. Smit (until May 2008), Prof. dr. R. Krishna, Prof. dr. D. Frenkel (Amolf/Cambridge), Prof. Dr. P.G. Bolhuis, Prof. dr. A. Fasolino/RU, Dr. E.J. Meijer, dr. B. Ensing, dr. J. Vreede, dr. J. Ellenberger

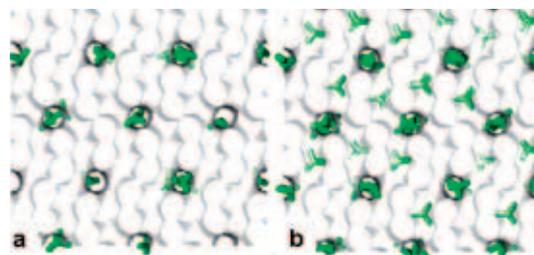
Research schools: HRSMC

Selected highlights of research activities 2008

Catalysis in nanoporous media and in homogeneous systems

Zeolites are aluminosilicates that are used in many applications involving catalysis, separation, and gas storage. Computer simulations are now at a stage where they can accurately provide a mechanistic explanation for the experimentally observed product distribution (Smit & Maesen, *Nature* 451, 2008).

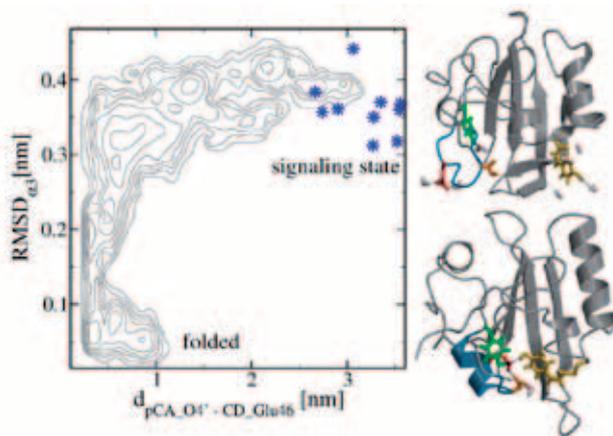
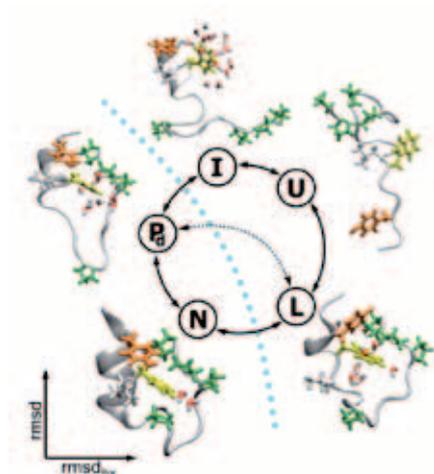
One recent focus has been on adsorption and diffusion in metal organic frame-works (MOFs). Molecular simulations have provided insights into a variety of phenomena, such as capillary condensation that occurs in such microporous structures. More interestingly, simulations have helped to interpret experimental data obtained at the University of Leipzig for intra-crystalline diffusion. (Krishna et al., *Phys. Rev. Lett.*, 102 2009).



Dynamics and structure of (biological) macromolecules

Fast folding proteins like the Trp-cage mini protein have contributed much to the understanding of generic folding mechanisms because they bridge the gap between experiments and computer simulation. Molecular dynamics simulations have investigated the stability of the protein, but folding pathways remained unknown because of the long timescales involved and solvent water has to be included explicitly. After we elucidated the mechanism of the folding of Trp-cage with an explicit solvent in an earlier study we determined the rate constant and analyzed the reaction mechanism in detail. (Jurazsek & Bolhuis *Biophys. J.*, 2008). The calculated folding rate agrees reasonably with experiment, while the unfolding rate is 10 times higher, a discrepancy we assign to the force field. We found that a combination of the root mean-square deviation of the helix and of the entire protein was, of the set of tried order parameters, the one that best describes the reaction coordination. The group of Sander Woutersen at HIMS using 2D-IR experiments is currently testing these prediction

The bacterial sensor Photoactive Yellow Protein (PYP) signals the presence of blue light by undergoing a series of conformational changes. Using parallel tempering simulations we have investigated the light-induced unfolding of PYP. We have shown that the formation of the signaling state is characterized by the solvent exposure of both the chromophore and Glu46 in agreement with NMR results. We also showed that the unfolding of helix alpha3 is part of the conformational change. As the NMR experiments were carried out on an N-terminally truncated mutant, we performed a simulation of this mutant to further substantiate our results. We compare simulations of the truncated PYP to the NMR structures, as well as to the wild type predictions. This comparison



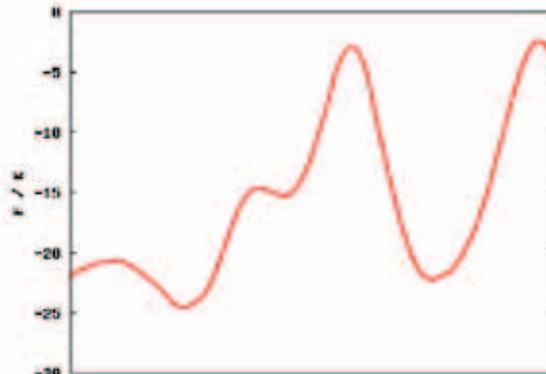
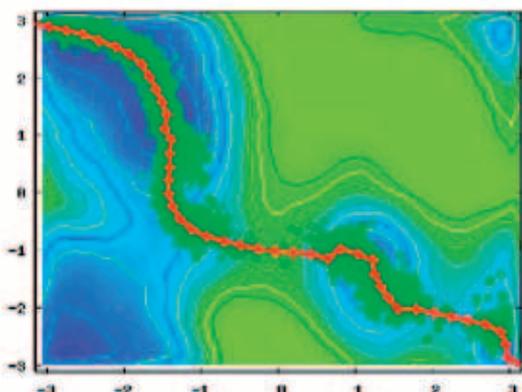
(Un)folding routes of Trp-cage protein. Two major routes between the native state N to the unfolded state U are possible: passing through state L or I. The rate-limiting barrier is represented by the light blue dotted line.

The free-energy profile of the transition from folded to signaling state for PYP, as sampled with parallel tempering.

also gives some insight into the role of the N-terminal domain of PYP, which restricts the movement of the chromophore binding pocket in the wild type. (Vreede et al., *Proteins* 72, 2008) Fixing the separation between the atoms of a molecule is a computationally efficient way of modelling chemical bonds. We developed a new algorithm (MILC SHAKE) that is orders of magnitude faster than existing methods such as SHAKE. This means that accurate molecular simulations of large linear molecules are now practical, where previously they were not. (Baily et al., *J. Comp. Phys.* 227, 2008) We further developed our model of flexible filaments moving in a viscous environment to study mechanisms for translational motion of pairs of these filaments. Importantly, the model takes into account the motion of the fluid caused by the filaments and how this in turn influences their motion. Our results show that then, if the waving motion of the

two filaments is synchronized in a particular way, they can move faster than if they were alone. That is, it can pay to swim with a friend. This offers one explanation as to why spermatozoa surprisingly behave co-operatively by usually swim in groups. (Lowe et al., *Comp. Phys. Comm.* 179, 2008)

Tracing complex reaction pathways
 Metadynamics is a molecular dynamics simulation technique aimed to enhance the sampling of activated processes, and is particularly useful for the calculation of the multidimensional free energy landscape of phenomena in terms of complex collective variables. The computational cost grows exponentially with the dimensionality. We have developed a combination of metadynamics with reaction path finding techniques that no longer depends on the number of collective variables. This is done by adding an extra variable, which is a function of all other collective variables. Initializing



Left: average reaction path (red line) computed in the free energy landscape of the alanine dipeptide.
 Right: free energy profile along the average reaction path.

this extra variable to represent a guess reaction pathway and steering the dynamics with the growing (one-dimensional) metadynamics bias potential along this variable, the extra variable efficiently evolves toward the locally most-likely reaction pathway, while simultaneously the biasing potential tends to an estimator of the free energy profile along the converged pathway. The algorithm is tested on the recovery of the reaction pathway and the free energy profile of a conformational transition in alanine dipeptide.

Transition Path Sampling (TPS) was developed for studying activated processes in complex systems with unknown reaction coordinate. Transition interface sampling (TIS) allows efficient evaluation of the rate constants. We developed extensions to these methods. The novel multiple state TPS approach allows for simultaneously sampling of pathways connecting a number of different stable states (Rogal & Bolhuis, *J. Chem. Phys.* 2008). The multiple state TPS approach is useful in complex systems exhibiting a number of intermediate stable states that are interconnected in phase space, such as proteins. Combining this approach with transition interface sampling we can also directly obtain an expression for the rate constants of all possible transitions within the system. However, when the transition can occur via more than one reaction channel separated by a high barrier, TPS and TIS are ineffective in sampling both channels. A second extension of path sampling allows for effective sampling of multiple reaction channels by combining the replica exchange method with TIS. (Bolhuis, *J. Chem. Phys.* 129 2008).

Structure, stability and nucleation of liquids

Fiber formation is an important process in material science as well as molecular biology. The phase behaviour of such supramolecular constructs is not well understood. We performed Monte Carlo simulations of the self-assembly of supramolecular polymers based on a model of patchy particles (Huisman et al., *Phys. Rev. Lett.* 100, 2008). We find a first-order phase transition, characterized by hysteresis and nucleation, toward a solid bundle of polymers, of length much greater than the average gas phase length. We argue that the bundling transition is the supramolecular equivalent of the sublimation transition, which results from a weak chain-chain interaction. We provide a qualitative equation of

state that gives physical insight beyond the specific values of the parameters used in our simulations.

Using a state-of-the-art model (LCBOP) we studied the phase diagram of carbon and diamond nucleation. Our results indicate that the ease of homogeneous crystal nucleation at constant super-saturation from one-and-the-same metastable liquid (liquid carbon) can be tuned by changing its pressure, and thereby its local structure. We used our results for the nucleation rate of liquid carbon to assess the existence of diamond inside carbon rich planets. We found that quite high carbon concentrations (over 15%) are needed to obtain homogeneous diamond nucleation. Such conditions do exist in white dwarfs, but certainly not in Uranus or Neptune.

Together with the group of M. Dijkstra (Utrecht) we studied the stability and interfacial properties of bulk and confined colloid-polymer mixtures incorporating polymer-polymer, colloid-polymer, and colloid-colloid interactions. (Fortini et al., *J. Chem. Phys.* 128, 2008) We compared our results with those of the Asakura-Oosawa-Vrij that treats the polymers as ideal particles. We find that the number of polymers needed to drive the demixing transition is larger for the interacting polymers, and that the gas-liquid interfacial tension is smaller. When the system is confined between two parallel hard plates, we find capillary condensation. Compared with the Asakura-Oosawa-Vrij model, we find that the excluded volume interactions between the polymers suppress the capillary condensation.

Key publications

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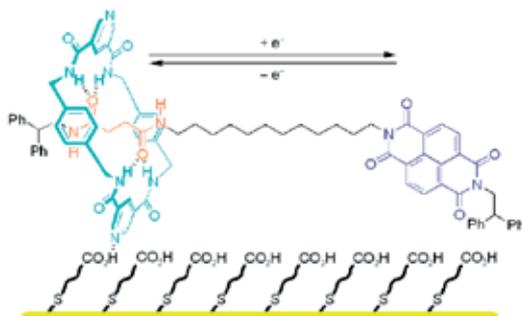
2.3.5 Molecular Photonics

Staff: Prof. dr. H.J. Bakker/FOM-Amolf, prof. dr. A.M. Brouwer, prof. dr. W.J. Buma, prof. dr. L. De Cola (guest), prof. dr. J.W. Hofstraat/Philips, dr. R.M. Williams, dr. S. Woutersen, dr. H. Zhang

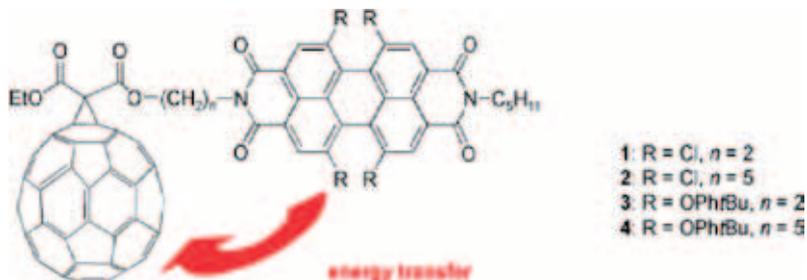
Research schools/Networks: HRSMC, NRSC-C, NanoNed/NanoImpuls

Selected highlights of research activities 2008

March 12, 2008 the Descartes Prize for Transnational Collaborative Research was awarded in Brussels to Molecular Photonics as member of the SynNanoMotor consortium for *developing the first functional examples of synthetic motors on a molecular scale and many other useful and innovative nanomachines.*



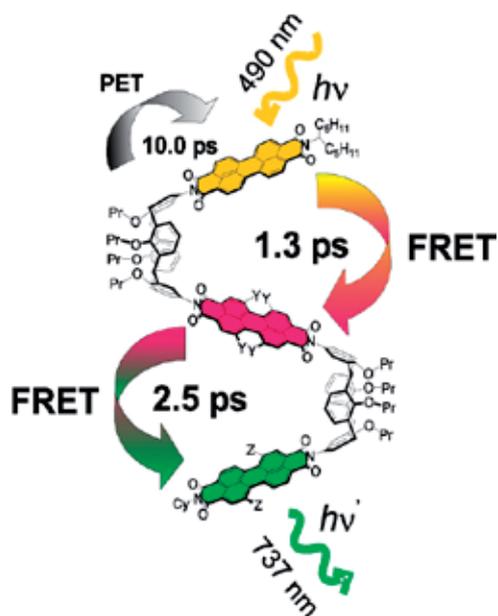
A rotaxane that shuttles on a surface. An important challenge in the field of molecular motors is immobilization on a surface without



compromising the molecular function. For the rotaxane shown, it could be demonstrated that the electrochemically induced structural switching occurs not only in the liquid phase but also when the molecule is hydrogen bonded to the surface (Fioravanti et al., *J. Am. Chem. Soc.* **130** 2008).

Light harvesting dyads. Two n-type molecular materials are covalently combined into a new photovoltaic component for polymer solar cells. Fullerene C_{60} - perylene-3,4:9,10-bis(dicarboximide) (C_{60} -PDI) dyads (1-4) show a quantitative photo-induced energy transfer from the PDI moiety acting as a light-harvesting antenna to the C_{60} -unit playing the role of energy acceptor. This results in very fast energy transfer to the C_{60} -unit, as shown with femtosecond transient absorption spectroscopy in toluene solution for 1. Two energy transfer rates are observed of $2.5 \times 10^{12} \text{ s}^{-1}$ (53 %) and $2 \times 10^{11} \text{ s}^{-1}$ (47 %), attributed to two conformations. The final excited state that is populated is a PDI based triplet state that is formed on the nanosecond timescale with a high quantum yield of 0.75-0.52 (Baffreau et al., *Chemistry - A Eur. J.* **14**(16) 2008).

FRET processes in Zigzag Arrays. Very efficient light harvesting also occurs in these calix[4]arene linked arrays composed of up to three different types of perylene bis(dicarboximide) chromophores (orange, red, and green PDI's; Y=phenoxy, Z=pyrrolidino). The specific optical properties of the individual chromophores facilitated the investigation of photoinduced processes by time-resolved emission and femtosecond transient absorption spectroscopy. These studies reveal very efficient energy transfer processes from the orange to the red PDI chromophoric unit ($k_{ET} = 6.4 \times 10^{11} \text{ s}^{-1}$ for array **or**), from the red to the green PDI ($k_{ET} = 4.0 \times 10^{11} \text{ s}^{-1}$ for array **rg**), and slightly less

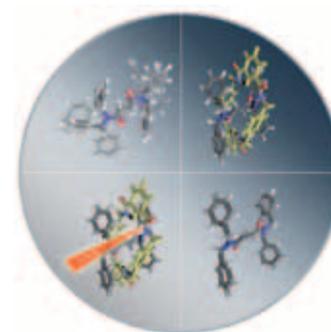


efficient from the orange to the green PDI ($k_{ET} = 1.5 \times 10^{11} \text{ s}^{-1}$ for array **og**) within these PDI-calix[4] arene arrays (Hippius, et al., *PCCP* 10(33) 2008).

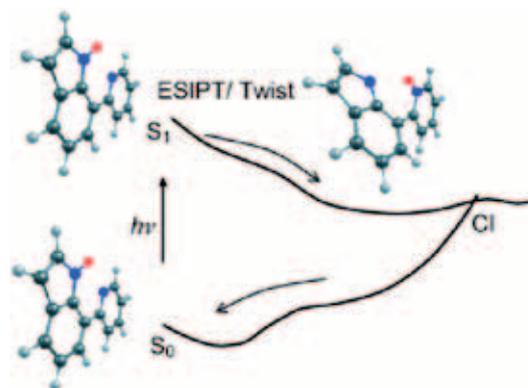
Enhancing red upconversion emission in rare-earth nanocrystals. Strong red upconversion luminescence of rare-earth ions doped in nanocrystals is desirable for the biological/biomedical applications. We have found that we can greatly enhance this emission associated with the $^4F_{9/2} \rightarrow ^4I_{15/2}$ transition of the Er^{3+} ion in $\text{NaYF}_4:\text{Yb}^{3+}, \text{Er}^{3+}$ nanocrystals at low doping level. This is ascribed to the effectiveness of multiphonon relaxation processes due to the existence of citrate as a chelator and cross relaxation between Er^{3+} ions (Zhao et al., 112 2008).

Ultrafast studies on the structural transition of CdTe/CdS core/shell nanosystems. Via the control of the shell thickness, 3-mercaptopropionic acid stabilized CdTe/CdS core/shell quantum dots (QDs) have been prepared that exhibit a spectacular increase of the photoluminescence quantum yield (up to 40% compared to 8% of the bare core). It has been shown that the CdTe/CdS QDs evolved from type I to type II core/shell structures with the increase of the shell thickness. Steady-state and time-resolved spectroscopy reveal that the evolution process is affected by the core size, shell thickness, and the surface quality of the core and shell (Zeng et al., *J. Phys. Chem. C* 112 2008).

Chaperones for wild molecules. We have shown how the conformational flexibility of floppy molecules can be significantly reduced by enclosing it with a macrocyclic mold as a [2]rotaxane that forces it into a specific shape. After rapid cooling, the mold is removed with a laser pulse. Through this process, the molded molecule becomes a suitable candidate for high-resolution electronic excitation spectroscopy. The article has been selected as one of the highlights of the issue of *Angewandte Chemie International Edition* in which it was published with the shown frontispiece (Rijs et al., *Angew. Chem. Int. Ed.* 47 2008).



Proton transfer with a twist. Excited-state intramolecular proton transfer (ESIPT) in 7-(2-pyridyl)indole has been studied with ultrafast spectroscopy which shows that it proceeds in a barrierless fashion and is coupled with mutual twisting of the pyridine and indole moieties. As a result, the reaction is slower in a condensed phase than in the supersonic jet-isolated molecule (1 ps vs. about 300 fs). Ultrafast radiationless deactivation of the phototautomer occurs via a conical intersection (CI). (Nosenko et al., *Angew. Chem. Int. Ed.* 47 2008).



Key publications

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- Hippus, C.; van Stokkum, I.H.M.; Gsaenger, M.; Groeneveld, M.M.; Williams, R.M.; Wuerthner, F., Sequential FRET processes in calix[4]arene-linked orange-red-green perylene bisimide dye zigzag arrays. *Journal of Physical Chemistry C* **2008**, *112*(7), 2476-2486.
- Benniston A.C., Harriman A., Verhoeven J.W., Comment: Electron-transfer reactions in the 9-mesityl-10-methylacridinium ion: impurities, triplet states and infinitely long-lived charge-shift states? *PCCP* **2008** *10*(33), 5156-5158.
- Zhao, J.; Sun, Y.; Kong, X.; Tian, L.; Wang Y.; Tu, L.; Zhang, H. Controlled synthesis, formation mechanism and great enhancement of red upconversion luminescence of NaYF₄:Yb³⁺, Er³⁺ nanocrystals/sub-microplates at low doping level, *J. Phys. Chem. B* **2008**, *112*, 15666-15672.
- Zeng, Q.; Kong, X.; Sun, Y.; Zhang, Y.; Tu, L.; Zhao J.; Zhang, H. Synthesis and optical properties of type-II CdTe/CdS core/shell quantum dots in aqueous solution via successive ion layer adsorption and reaction, *J. Phys. Chem. C* **2008**, *112*, 8587-8593.
- Rijs, A.M.; Crews, B.O.; de Vries, M.S.; Hannam, J.S.; Leigh, D.A.; Fanti, M.; Zerbetto, F.; Buma, W.J., Shaping of a conformationally flexible molecular structure for spectroscopy, *Angew. Chem. Int. Ed.* **2008**, *47*, 3174-3179.
- Nosenko, Y.; Wiosna-Sałyga, G.; Kunitski, M.; Petkova, I.; Singh, A.; Buma, W.J.; Thummel, R.P.; Brutschy, B.; Waluk, J., Proton transfer

with a twist? Femtosecond dynamics of 7-(2'-pyridyl)indole in condensed phase and in supersonic jets, *Angew. Chem. Int. Ed.* **2008**, *47*, 6037-6040.

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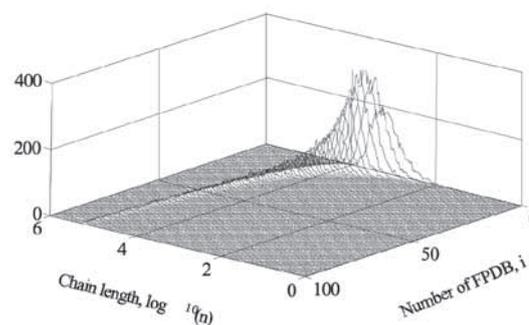
2.3.6.1 Polymer and Process Systems

Staff: Dr. A.C. Dimian, Prof. dr. P. Iedema

Research school: OSPT

Selected highlights of research activities 2008

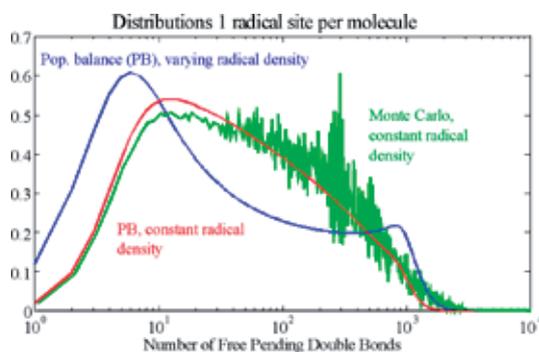
In the area of mathematical modeling of branched polymer architectures cross-linking radical polymerization as a new topic has been addressed. Di-vinyl monomer is incorporated in chains polymerized from mostly mono-vinyl monomer, leading to Free Pendant Double Bonds (FPDB) that are partially converted in backbone-to-backbone cross-links. A special variety of the 'pseudo-distribution' approach employing the FPDB as the distribution variable and the leading moments of the chain length has been developed to compute the two-dimensional degree of branching-chain length distribution.



2D distribution of chain length and free pending double bonds

The comparison to a Monte Carlo method turned out to yield good agreement for the case of negligible amounts of polymer molecules with more than one radical site. General simplifying assumptions made in previous work concerning the chain length independence of the FPDB and radical site density proved to be false, however.

Different distribution found for varying radical density



The contract research activities for industry continued in 2008 are:

- Sabic, Geleen: *Predicting molecular weight and branching distributions for controlled degradation of Ethylene-Propylene copolymers.* For this problem a new, powerful method of convoluting two distributions has been developed, drastically reducing computation time in a deterministic population balance model.
- BASF, Ludwigshafen (D) (Joint project with dr. Menno Dreischor, TIPb): *Predicting molecular weight, branching and sequence length distributions for mix-melting of linear and branched Polyamides.*

Key Publication

- Kim, D.M., Iedema, P.D. (2008). *Modeling of branching density and branching distribution in low-density polyethylene polymerization.* Chem. Eng. Sc., 63, 8, 2035-2046.

2.3.6 Other activities

2.3.6.2 Röntgen Diffraction

Staff Dr. R. Peschar
Research school HRSMC

Selected highlights of research activities 2008

Cis-mono-unsaturated structured lipids are attractive novel sources of calories and nutrients. Typically, these triacylglycerols have a small or medium-chain length fatty acid at the glycerol *sn*-1 and *sn*-3 positions (e.g. lauric acid, La, C12) and an unsaturated long-chain fatty acid (e.g. oleic acid, O) at the *sn*-2 position. Recently, the polymorphism of

1, 3-dilauroyl-2-oleoylglycerol (LaOLA) has been studied with temperature-dependent powder diffraction and crystal structures were solved of two metastable β' polymorphs (β'_1 -2 and β'_3) and the stable β_2 -3 polymorph from high-resolution powder diffraction data. This is the first type of triacylglycerol for which now both β' and β models have become available. Analysis of the crystal structures provided an explanation for the slow β'_1 -2 \rightarrow β_2 -3 phase transition. While the structure of β_2 -3 LaOLA is similar to that of related triple-chain monounsaturated triacylglycerols, in which the two saturated chains are packed parallel, both the β' structures turned out to have an unexpected, novel molecular conformation in which the almost complete saturated chain S3m (atoms C2c-C10c) at the *sn*-3 position is packed parallel to a part of the oleic chain. To achieve the β'_1 -2 \rightarrow β_2 -3 transition, and the change from a double chain to a triple chain length packing, the S3m chain has to rotate 180° around the glycerol chain (S2g, atoms C2c – C3). This major conformational change explains the slow transition and makes a solid-state conversion unlikely. This polymorph analysis and the structural models are expected to be useful in the future analysis and control of the $\beta' \rightarrow \beta_2$ phase transition of other *cis*-mono-unsaturated TAGs.

Key publications

- Van Mechelen, J.B., Peschar, R. and Schenk, H. Structures of mono-unsaturated triacylglycerols. IV. The highest melting β' -2 polymorphs of *trans*-monounsaturated triacylglycerols and related saturated TAGs and their polymorphic stability. *Acta Cryst.* **B64** (2008), 249-259.
- Van Mechelen, J.B., Goubitz, K., Pop, M., Peschar, R. and Schenk, H. Structures of mono-unsaturated triacylglycerols. V. The β'_1 -2, the β'_3 -3 and β_2 -3 polymorphs of 1, 3-dilauroyl-2-oleoylglycerol (LaOLA) from synchrotron and laboratory powder diffraction data. *Acta Cryst.* **B64** (2008), 771-779.
- Borodi, Gh., Bratu, I., Dragan, F., Peschar, R., Helmholtz, R.B. and Hernanz, A. Spectroscopic investigations and crystal structure from synchrotron powder data of the inclusion complex of β -cyclodextrin with atenolol. *Spectrochim. Acta* **A70** (2008), 1041-1048.

3. Applied Research and Education

3.1 Social activities and education

3.1.1 Social activities

Emphasis of the HIMS chemists in applied research is on many important scientific problems for the (fine-)chemical-, agro-, pharmaceutical- and electronic industry. The HIMS research program is directed to the synthesis and theoretical and spectroscopic investigation of new (supra) molecular systems in different themes. These themes are and will remain of great scientific, societal and industrial relevance. Research in these directions is indispensable for deepening and broadening our knowledge of matter and of processes on the molecular level. The importance for society is found in applications such as data transport, energy, health, storage in information technology, analytical techniques for medical, forensic - and restorative purposes, sustainability (e.g. efficient transformations of fossil raw materials into useful compounds), design and synthesis of complex molecules for use as agro-chemicals or drugs and innovation. The reactivity, biological activity and material properties of these systems are ultimately determined by the molecular structure; small electronic, steric and geometric changes on the molecular level can have huge impact on meso- and macroscopic properties. In addition to the present and new core activities of HIMS, all based on a molecular approach, HIMS is continuously active in fields of high societal importance. HIMS has been known for years as an institute where **MOLECULAR SCIENCES** take a predominant position. Nevertheless, we decided to explore the possibilities of new research profiles for HIMS, to combine forces in our relatively young institute. As a result of this internal discussion, **Health, Durability (energy) and Forensic & Art Sciences** were primarily selected as promising new profiles, to enhance our basis in molecular sciences.

We expect that these initiatives will lead to good additional opportunities for funding on all levels and for collaborations, with both new and existing partners from universities and industries. Although the discussion has not yet wended up completely, this new profiling will be continuously stimulated and monitored.

The work of some of our groups has raised quite some national and international publicity, including publications in various newspapers and on various websites. Examples of HIMS highlights with a high societal value that should be mentioned here are:

- **Prof. Wybren Jan Buma** and **Fred Brouwer** of the Molecular Photonics group and their partners in the SynNanoMotor Consortium received the EU Descartes Prize 2008.
- **Prof. Daan Frenkel** was elected Foreign Honorary Member of the American Academy of Arts & Sciences in Cambridge, Massachusetts (2008).
- **Prof. Daan Frenkel** was appointed as faculty professor in the faculty of Science of the UvA.
- **Prof. Peter Bolhuis** of the Computational Chemistry group received a NWO-VICI grant of 1.25 M€ that allows him to carry out a state-of-the art research program addressing the influence of the environment on protein folding, binding and aggregation.
- **Dr. Jocelyne Vreede** of the group Smit/Bolhuis in 2008 received a NWO-VENI grant of 0.21 M€ to study how proteins communicate.
- In 2008 HIMS received four NWO/CW-Echo grants (Timmerman/Van Maarseveen, Brouwer, Hartl and Reek⁴) and one NWO/FOM-Projectruimte grant (Zhang⁵), together having a value of more than 1.0 M€.



Dr. Jocelyne Vreede

⁴ With Bonn/FOM-AMOLF,

⁵ With Gregorkiewicz/WZI

EU Descartes Prize 2008

In 2008 the Molecular Photonics group was recipient of the Descartes Prize for Transnational Collaborative Research as a member of the SynNanoMotor consortium for developing the first functional examples of synthetic motors on a molecular scale and many other useful and innovative nanomachines. The announcement was made March 12, 2008 during the European Science Awards 2007 - ceremony in Brussels. The Descartes Prize is the most important Prize awarded by the European Union, and is given annually to transnational research teams from all fields of science that have achieved exceptional scientific or technological results through joint research. The selection committee judges all entries for the Prize for scientific excellence and quality. Additionally, they consider the quality of transnational cooperation, the synergy of expertise and available means, and the relevance of the research results for the policy and priorities of the European Union.

The consortium in which - apart from the Molecular Photonics group - researchers from the University of Groningen and research institutes from the United Kingdom, France and Italy participated, received the prize for their trail-blazing work in the field of synthetic molecular motors and artificial nano-engines. The collaboration was achieved through a series of European Union funded networks and other contracts of which two:

- Development of Rotaxane-based Unconventional Materials (DRUM)
- Hydrogen bond-gear Mechanically interlocked Molecular Motors (Hy3M) were coordinated by the University of Amsterdam.

Controlled movement of molecules or parts of molecules offers unprecedented technological possibilities. Nano-engines and molecular motors form the basis of nearly every important biological process. Scientists are therefore convinced that molecular nanotechnology can ultimately have an impact on economy and society that will transcend in scale and range those of the steam engine, electricity, and internet. Developing the full potential of molecular motors and nano-engines is still in its infancy, but the molecular systems developed by the SynNanoMotor Consortium have contributed significantly to the current state-of-the-art.

The researchers have introduced new approaches, including the incorporation of a ratchet mechanism, which has allowed the creation of molecular engines that transcend simple switches. The consortium was also the first to build molecular engines that allow movements at the molecular level to be coupled to the macroscopic world, enabling them to be employed to various ends including storage of information in polymer films, or the transport of macroscopic objects, like drops of liquid over a surface. Another example concerns molecular systems that can be triggered to form spontaneously functional structures with a well-defined size and position on surfaces. These systems may be used for products in the fields of identification, security and health care.

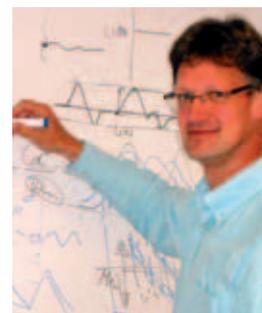
The Molecular Photonics group will use their part of the Prize money to establish the Molecular Photonics Descartes Fund. The aim of this fund will be to promote undergraduate research in molecular photonics by yearly awarding bursaries to excellent master students that perform their undergraduate research project in the field of molecular photochemistry and photophysics.

- The **Amsterdam Center for Multiscale Modeling** (ACMM) was officially opened on June 26, 2008 during a special symposium at the KNAW Trippenhuis.
- Together with the Lorentz Center in Leiden the ACMM became a **node of CECAM**, the European center for computational science.
- The master programme Chemistry was awarded the **Euromaster label** (2008) by the European Chemistry Thematic Network (ECTN) organization.
- In the Elsevier magazine annual academic survey students rated the UvA and UU Chemistry **bachelor programs** as being the best.
- **Dr. Jan van Maarseveen**, member of the Bio-Molecular-Synthesis theme, won the 2008 Onderwijsbokaal (best chemical teacher award). This prize is an initiative from the faculty chemistry students.
- **Dr. Gadi Rothenberg** was awarded the 2nd UvA ScienceParc innovation prize 2008 for his new concept for CO-resistant fuel cells: A practical solution to energy transfer problems.
- In recognition of his significant contributions to the field, the governing board of the Eastern Analytical Symposium (EAS) awarded **Prof. Peter Schoenmakers** for his achievements in Separation Science. The rewarding ceremony will take place in New Jersey, USA, in November 2009.
- October 2008 NWO published a popular book EXPERIMENT NL on the research of 100 Dutch top scientists, including the work of **Profs. Wybren Jan Buma and Fred Brouwer** on visualisation of rotaxane nanomachine movement.
- February 2008 **Prof. Daan Frenkel** presented a Sunday morning Wakker Worden Kinderlezing at NEMO on the 'secrets of gases, liquids and solids'. The audience were some 60 young children and their parents.
- A lecture and a spectacular laser light show for children (NEMO; 2008) was given by **Dr. Anouk Rijs**, entitled 'Is laser light always dangerous?'
- **Prof. Wybren Jan Buma** was guest in the 'Wetenschapscafé' broadcast of the 'Hoe? Zo!' radio and television program.
- HIMS was elected as **Institute of the year** at the Dies of the Faculty (2008), at which occasion Joost Reek and Peter Hauwert presented 'Het Chemisch Spektakel'.

- The work of **Sander Woutersen** on 'Protein Folding' was highlighted in the Annual Report 2007 (published July 2008) of the Universiteit van Amsterdam.
- **Eveline Jansen** (NCCC conference) and **Linde Smeenk** (KNCV/PAC conference), both master students of HIMS, won 1st poster prizes in 2008.
- **Rob Edam**, PhD researcher of the group Schoenmakers, received poster prizes in 2008 at both the HTC-10 (Hyphenated Techniques in Chromatography) and the Dutch Polymer Days (KNCV, PTN and NWO).

More highlights for HIMS were:

- The appointment of **Dr. G. Rothenberg** at 01-06-2008 to professor in Heterogeneous Catalysis and Sustainable Chemistry. With this new chair UvA will be the only university in the Netherlands with internationally renowned active chairs in all areas of catalysis. The new chair will focus on discovery, optimization, and application of new catalysts and processes for clean synthesis and green energy. Combining heterogeneous catalysis and bio-catalysis or heterogeneous and homogeneous catalysis in one process gives important advantages, including process intensification and more efficient overall processes. Our large research efforts in the broad spectrum of catalysis combined with valorization opportunities makes catalysis an attractive focused theme that aims to initiate a national catalysis center of excellence.
- The appointment of **G. Zonneveld-de Boer** as institute manager.
- The appointment of **Dr. E. Eiser** at 01-02-2008 for 5 years (0.2 Fte) as UD (assistant professor) in the group Elsevier of the theme Catalysis.
- The appointment of **Dr. B. de Bruin** at 01-10-2008 as UHD in the group Reek of the theme Catalysis.
- The appointment of **Dr. J. van der Vlugt** at 15-10-2008 as UD in the group Reek of the theme Catalysis.
- The appointment of **Dr. F. Hartl** at 01-09-2008 for 5 years (0.0 Fte), as UD (assistant professor) in the group Reek of the theme Catalysis.
- The appointment of **Prof. A. Fasolino** at 01-05-2008 for 5 years (0.0 Fte) as professor in the group Bolhuis/Meijer of the theme Computational Chemistry.



Prof. Peter Schoenmakers



- The appointment of **Dr. S. Woutersen** at 01-03-2008, as UD in the group Buma/Brouwer of theme Molecular Photonics.
- The appointment of **Prof. C. Elsevier** at 01-09-2008, as director of the master program chemistry of the Master School of Sciences.

3.1.2 Education and promotion activities

The HIMS staff is largely responsible for teaching the courses in the bachelor Scheikunde and contributes to an important extent to the teaching in the bachelor Bio-exact and the β, γ -bachelor study programme. Our PhD students supervise the laboratory courses and a number of tutorials. A detailed overview of the participation of HIMS co-workers in the regular chemistry and bio-exact study programmes is given in the bachelor study guide. Students who started or will start their bachelor Chemistry in the period 2006 - 2011 will receive the Eurobachelor certificate together with their Dutch diploma.

The present Master of Chemistry programme is divided in five tracks most of which are shared with other Master programmes of our university (UvA) or the Vrije Universiteit (VU) in Amsterdam:

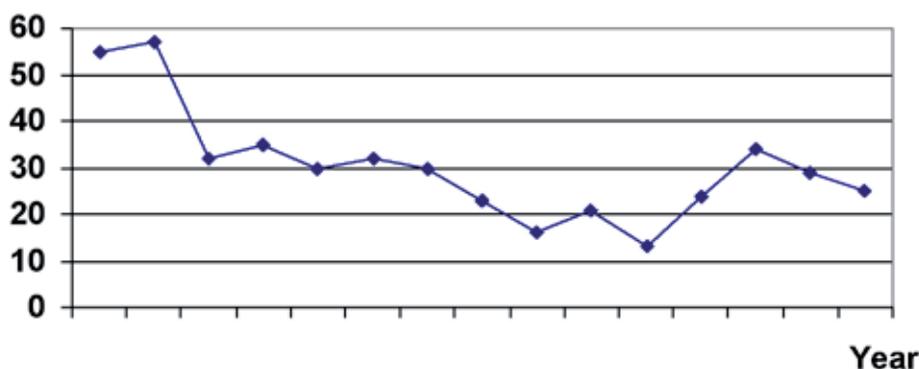
- Analytical Sciences (with VU)
- Molecular Design, Synthesis and Catalysis (with VU)
- Physical Sciences (with VU and Physics UvA)
- Environmental Sciences (with Earth Sciences UvA)
- Molecular Biosciences (with Biology UvA)

The HIMS staff is largely, or to a considerable extent, responsible for the first three tracks. IBED is the main organizer of the Environmental track while SILS is in charge of the Biomolecular track. Early 2008 it was decided that the master programme in Chemistry is also accredited by the ECTN, so students who started or will start their master in Chemistry in the period 2007 - 2012 will receive the Euromaster certificate together with their Master of Science diploma.

Dr. de Groot is the education director of the College of Science, encompassing all bachelor programmes of the Faculty of Science, while Dr. Ingemann Jørgensen (HIMS) is director of the bachelor programmes in scheikunde and bio-exact. Prof. Hiemstra (HIMS) is director of the master programmes of the Master School of Sciences. He has been director of the master programme in Chemistry until August 31, 2008 after which date Prof. Elsevier (HIMS) took over this position. In 2008, 5 chemistry students obtained their bachelor degree. Most (4) of these students performed their bachelor research project in one of the HIMS groups. Furthermore, 15 students gained their Master degree in Chemistry. Of these students, 10 acquired their degree after a research project in one of the HIMS groups. The students elected Dr. van Maarseveen as the best chemistry teacher of the year 2008.

The HIMS staff is regularly discussing and arranging educational matters, including coordination and control of the teaching tasks of the HIMS PhD students. HIMS has a Public Relations Committee with special promotional tasks, mainly to initiate and organize activities to increase the number of chemistry students. The number of 1st year chemistry students starting in 2008 amounted to 25, which seems to indicate a stabilization around 25-30.

Number

1st Year chemistry students of the UvA

Although our efforts to increase student numbers appear successful when compared to a couple of years ago, our ultimate goal to reach a level of 50 1st year chemistry students, can only be realized via combined promotional activities and improvement (increase of attractiveness) of the curriculum of the bachelors programme. Being strongly dependent on student numbers, now and in the future, it is obvious that both faculty and institutes must give high priority to these activities. For that reason student recruitment activities are now a regular part of the tasks of all FNWI staff members. It was decided in the FNWI management team that on the average all staff members should spend 40% of their time to teaching and promotion activities. For almost all HIMS staff-members this is already the case.

An overview of recent promotional activities with HIMS participation is given below:

The **Beta partner project** is a project based on collaboration of the FNWI (coordination Cor de Beurs/AMSTEL Institute) with 24 high-schools in the Amsterdam region that decided for a Beta-profile. Beta partner is a local network in the region of Amsterdam in which secondary schools co-operate with Universities, Technical Colleges, Industry and Science Centre NEMO. Aim of this co-operation is raising young student's enthusiasm for science and technology and related professions. This is done by improving school education and by offering challenging learning arrangements outside the schools. Lack of interest in science and technology can be ascribed partly to science teaching itself. Curricula deal with classical themes

and theories, and have difficulty in relating these to real life issues and active problem solving.

Furthermore, both students and their teachers have rather limited and biased ideas about what it means to be a scientist or an engineer in professional careers. In Beta partner we try to shift the focus of traditional science education from 'knowing the facts' to 'solving problems in real life and/or professional and authentic contexts' inside and outside school.

Science Lab is one of the initiatives of the Beta partner project. Within this framework HIMS offers practical courses on chemistry that exceed the possibilities of secondary schools in terms of equipment and time. Based on excellent evaluation results we have expanded our capacity, and in 2008 more than 500 students at the age of 15 years and higher attended one of science labs. HIMS technician Jan Fraanje is regularly involved in these activities. Based on the success of the Science Lab projects the municipal council of Amsterdam supported the UvA Science Lab initiative with an additional 0.5 M€ for the period 2008-2011.

The **ITS Academy** (Informatics, Technology and Science) is another initiative in the Beta partner project. In the ITS academy school teachers and university staff members work jointly on developing and teaching (new) subjects for upper level secondary school students. In 2008 almost 40 high schools participated in the ITS academy. The goal of this initiative is to stimulate the mobility of teachers from higher education to secondary education and reversed, to raise the quality of science and technology education and

above all to inspire students and teachers. HIMS Staff member Dr. Han van den Heuvel is regularly involved in this project.

The purpose of the **Betabrug** project of the UvA-HvA is to teach science to upcoming students who intend to do a beta study, despite lacking qualifications. In 2008 some 20 participants attended this chemistry course set up and taught by Dr. René Peschar (HIMS). Furthermore, this course is part of the minor Restoration and Conservation curriculum to supply these students (25 in 2008) with sufficient knowledge of chemistry

Traditionally, HIMS staff participated in the organization of masterclasses, educational information meetings and school visits for secondary school pupils to encourage and stimulate their interest in chemistry. In 2008 the institute organized - in cooperation with the Swammerdam Institute for Life Sciences (SILS) - the symposium *Viva Chemie* for the fourth time, this year's theme being 'From fascination to innovation'. Some hundred teachers attended the program, and were informed about the actual developments in chemical research by lectures, lab tours and demonstrations.

The composition of the Public Relations Committee HIMS in 2008 was:
Fred Brouwer (chairman, Molecular Photonics), Jan van Maarseveen (Bio-Molecular Synthesis), Gadi Rothenberg (Catalysis), Evert Jan Meijer (Computational Chemistry), Astrid Janmaat (FNWI) and Joost Teixeira de Mattos (Biochemistry/SILS).

3.1.3 New developments in education and related research activities

Within the faculty of science, broad education programs such as the beta-gamma bachelor play an important role. This program merges aspects of natural sciences, social science and philosophy and is highly popular among students. The HIMS institute and many of its staff members wholeheartedly participate in the development of new curricula, as we believe that **molecular chemistry** is an integral and vital part of modern interdisciplinary science.

Molecular chemistry is also embedded in several new teaching initiatives, i.e. a bachelor and master program on Art Restoration and Conservation Science and a master program on Forensic Sciences. Presently, discussions on a completely new master in Clinical Chemistry, together with SILS, AMC (medical faculty) and the VU counterparts are ongoing. The HIMS institute is enthusiastic about such developments, since they provide us with an opportunity to emphasize the central role of molecular chemistry in science and society.

Forensic sciences

The University of Amsterdam's Research Master's program in Forensic Science, offered by the Faculty of Science, is unique in The Netherlands. The program distinguishes itself from most international Master's programs in Forensic Science in that it builds on a range of general science backgrounds, not on a specific forensic science Bachelor's program. The goal of the program is to train good scientists, armed with forensic knowledge and skills. The study program has been developed together with the Nederlands Forensisch Instituut (NFI) (Netherlands Forensic Institute). Forensic research is technical, scientific research aimed at solving criminal offences. The research can consist of chemical analysis (bits of paint, fibres, tyre tracks), medical-biological analysis (hair, DNA, toxicology), analysis of handwriting, or the analysis of digital data (for example e-mail, photography and video). Forensic research is gaining in importance in the furnishing of proof of criminal trials, and the techniques applied are becoming more sophisticated. From this a need has arisen for scientists in chemistry, biology or computer science who can combine their knowledge with specific legal and criminological skills. The program in Forensic Science trains students to be innovative researchers with knowledge of forensic matters, which is made possible by a close cooperation with experts. In the two-year master, the HIMS staff plays a significant role in educating forensic scientists with a chemistry profile. Within the forensic program several (student) projects have been initiated in the HIMS laboratories, especially within the analytical chemistry group.

Restoration and conservation sciences

The Universiteit van Amsterdam (UvA) started a one-year Minor in Restoration and Conservation of objects of cultural heritage in September 2005, and a two-year Master in 2006. The Minor and the Master form the first three years in a full program for restorer-conservator of five years. The Minor/Master Programmes are followed by a two-year Post-Initial phase where students work and learn in accredited restoration-workshops. In the end the student will qualify according to international standards as an acknowledged professional restorer in one of the following fields: painting and painted surfaces, modern art, historical interior, metal, glass/ceramics, paper/book, wood/furniture and textiles. The program is a joint effort of the UvA-faculties of Humanities and Science, and of the Instituut Collectie Nederland (ICN) and Stichting Restauratie Ateliers Limburg (SRAL). It is the only academic program in conservation/restoration in the Netherlands. Courses taught by HIMS are partly existing ones: introductory chemistry for the RC Minor (Dr. Peschar) and Analytical chemistry (Prof. Schoenmakers) for the RC Master. New courses on Art Materials Science (Prof. Iedema) have been developed and during 2008 were taught to CR Minor and Master students.

AtoSim

Since 2006 the University of Amsterdam (via HIMS), the Ecole Normale Supérieure (Lyon), and La Sapienza University (Rome) together run a one-year MSc program 'Atomic scale modeling of physical, chemical, and biomolecular systems' (AtoSim) in the area of molecular simulation. AtoSim targets top students from all over the world, and provides an important source of well-trained PhD students. The EU Erasmus Mundus program supports AtoSim by providing 2 M€ for travel and accommodation of participating students and external scholars. The 2007/2008 AtoSim class consisted of 15 Erasmus Mundus students that were selected from 60 applications.

MolSim

The 2008 edition of MolSim took place in January and attracted about 70 participants from all over the world. MolSim is a 2 week international school

targeting advanced MSc and starting PhD students who want to learn molecular simulation techniques to study topics in physics, chemistry or biology. The course offers a recap of the statistical mechanics relevant for molecular simulation and covers basic and advanced simulation techniques including Monte Carlo, molecular dynamics, free energy calculations, rare events, and coarse graining. All techniques are illustrated by examples of present day research. The school consists of an integrated program of lectures and hands-on exercises. The book 'Understanding molecular simulation' by Frenkel and Smit provides the basis of the lectures, supplemented by handouts and copies of the lecture slides. The school was financially supported (45 k€) by CECAM and the ESF program SimBioMa, and organized with support from the HIMS secretariat.

New research activities in forensic and art sciences

To sustain a master-level course, we believe it is essential to combine research with education. HIMS is in an excellent position to conduct research projects in art sciences and forensic sciences, because of our unique knowledge on high-resolution and high-sensitivity analysis of complex samples. The data-analysis and chemometrics expertise of HIMS provide additional strength for both areas.

In forensic sciences we believe that a close collaboration with the Dutch Forensic Institute (NFI) will be profitable for both parties on the mid-longer term and no doubt it will lead to new research collaborations in both fundamental sciences (UvA/HIMS) and applied (NFI) sciences. New appointments of special chairs in the forensic field are expected in the coming years, as well as part-time activities of HIMS staff and researchers (PhD and PD's) at the NFI (exchange program of coworkers).

During 2008 the contours of a new partially NWO-funded research Programme 'Art and Science' became visible, as a follow-up of the successful Programmes MOLART and De Mayerne. HIMS has taken the initiative to participate in this future Programme in the area, among others, of chemical and physical reactivity and transport phenomena in oil paints. The new research activities will be embedded in Materials Science related research in the groups of Schoenmakers, Iedema and Peschar,

along with similar new activities in the area of Forensic Science. It is expected that the renewed appointment of Prof. Tennent in 2009 and the recruitment of Postdocs with experience from MOLART/De Mayerne will play a mayor role in the new Conservation and Restoration research at HIMS.

Continuation and revitalization of research programs is needed to give a firm backbone to the educational forensic and restoration programs. It is indispensable to support the academic claims of the profession of conservator/restorer or forensic scientist, which – internationally, and especially in

Europe – is emancipating from a vocational background to an academic future, including PhD training (which can either take place instead of or in addition to the post-initial phase in Art Sciences). The interest of students for the new educational programs is substantial and the importance of academic research and teaching in the field of conservation and restoration and forensic sciences is widely recognized. This provides a great new opportunity for research and teaching at the UvA. The new activities are expected to increase the number of bachelor chemistry students.

3.2 Results of large externally financed projects

External funds acquired 2007, related projects started 2008	Budget (M€)	
	Subsidy	Total ⁵⁾
1 st – NRSC-C ¹⁾	0.00	0.00
1 st – Others ²⁾	0.12	0.19
2 nd ³⁾	3.79	3.93
3 rd ⁴⁾	1.34	1.81
Total	5.25 ⁶⁾	5.93

External funds acquired 2008, related projects started 2008	Budget (M€)	
	Subsidy	Total ⁵⁾
1 st – NRSC-C ¹⁾	0.00	0.00
1 st – Others ²⁾	0.00	0.00
2 nd ³⁾	0.90	0.94
3 rd ⁴⁾	0.78	0.95
Total	1.68 ⁷⁾	1.89

External funds acquired 2008, related projects to be started 2009	Budget (M€)	
	HIMS	Total ⁵⁾
1 st – NRSC-C ¹⁾	2.70	2.70
1 st – Others ²⁾	0.00	0.00
2 nd ³⁾	1.76	1.86
3 rd ⁴⁾	1.08	1.27
Total	5.54 ⁸⁾	5.83

¹⁾ NRSC-C (TOP Research School Catalysis)

²⁾ COF, CvB (Funds from University Board), JvG (John van Geunsfonds)

³⁾ NWO-CW, FOM, STW, KNAW, DFG, ERC

⁴⁾ EU, DPI, Senter, NanoNed, Industry

⁵⁾ Including matching contributions UvA and own contributions HIMS (from reserves)

⁶⁾ Subsidy partners (total 0.00 M€) excluded

⁷⁾ Subsidy partners (total 0.53 M€) excluded

⁸⁾ Subsidy partners (total 0.00 M€) excluded

Vacancies per 01-01-2009: 22 PhD's, 14 Pd's, 3 Staff (1 Hgl, 2 UD), 1 Secretary.

Note: A complete overview of all in 2008 acquired externally funded projects, 2nd and 3rd is given in chapter 5.1.

The HIMS research themes were extremely successful in 2008 in the acquisition of externally financed projects. A total of 7.22 M€ was externally acquired, excluding 0.50 M€ matching and own contributions, as shown in the table. The amount of newly acquired external funds of which the related projects were started in 2008 (2nd 4.87 M€, 3rd 2.76 M€, total 7.63 M€) was twice as high as compared with the new projects started in 2006 (total 2nd and 3rd 3.22 M€) and 2007 (total 2nd and 3rd 3.12 M€). The total external funds acquired in 2008 for projects to be started in 2009 (5.54 M€) was higher compared to 2007 (5.25 M€), as partly reflected by the increased number of vacancies (40/ 01-01-2009; 30/01-01-2008).

Some selected examples of large externally funds for new projects acquired by the HIMS themes in 2008 to mention here are (without matching and own contributions; see also chapter 5 for a complete overview of all in 2008 acquired externally funded projects and chapter 2.2 for details on the research results obtained in 2008):

- NRSC-C projects for Reek/CAT (3 PhD's, 3 pd's), Hiemstra/Van Maarseveen/BMS (2 PhD's, 1 pd), Elsevier/CAT (2 PhD's, 2 pd's), Rothenberg/CAT (1 pd) and Wever/BMS (1 pd) for a total of 2.7 M€
- Application of droplet-based microfluidics for the screening of supramolecular catalysts (Reek/ CAT, EU grant, 0.16 M€)
- Hydrogenolysis of esters and amides (Elsevier/ CAT, CatchBio, 0.26 M€)
- Reactions to chiral amines from alcohols and ketones (Reek/CAT, CatchBio, 0.26 M€)
- How do proteins communicate? Predicting function, formation and interactions of coiled coil complexes at the molecular level (Vreede/ COMP, NWO-Veni grant, 0.21 M€).
- Hydrothermally stable organosilica-gased hybride membranes for molecular separations (Rothenberg/CAT, STW, 0.28 M€)
- Proteins out of isolation: simulating the influence of the environment on polypeptide self-assembly (Bolhuis/COMP, NWO-Vici grant, 1.25 M€)
- The next generation GC (Kok/MBA, NLSIS BV, 0.30 M€)
- 2nd Generation biofuel via heterogeneous catalysis (Rothenberg/CAT, Senter Novem, 0.29 M€)

- Rheology control by branching modeling (Iedema/Others, DPI, 0.36 M€)

Various projects, already acquired in 2007, were started in 2008. Other projects, mostly acquired in the last part of 2008, will be started in the beginning of 2009 (see chapter 5.1 for a complete overview of all in 2008 acquired externally funds and the funds acquired in 2007 and related projects started in 2008). At 01-01-2009 HIMS possessed vacancies for 22 PhD's, 14 PD's, 2 UD's and 1 secretary from various funds for projects acquired in 2008. Additionally, a vacancy exists for a chair 'Complex Molecular Simulations' related to the leave of the previous chair-holder. This vacancy will be fulfilled in 2009.

The number of direct industrially funded projects decreased appreciably in the last years. This is mainly related with the increased, highly interesting, possibilities for industrial parties in participating in new funding possibilities from the Dutch Ministry of Economic Affairs, such as the Technology Institutes (e.g. DPI, TI-Pharma and TI-COAST⁶), ACTS (e.g. IBOS) and the BSIK initiatives (e.g. NanoNed and NNI⁷). Industry prefers more and more an industrial matching contribution (mostly 25% financial participation) to direct (100%) funding. Nevertheless HIMS has several smaller and larger industrial collaborations. An overview of existing industrial collaborations of HIMS is given in chapter 5.1.7.

⁶ COAST (Comprehensive Analytical Science and Technology) is an initiative to cluster existing and new techniques in the analytical field (analytical chemistry and spectroscopy) with the main target to achieve breakthroughs using informatics and nano-technology (see also chapter 1.5).

⁷ NNI (the Dutch Strategic Research Agenda nano-technology) is the follow-up of NanoNed (the national nano-technology initiative; see chapter 1.4.5)

4. Resources and management

4.1 Introduction

At present Van 't Hoff Institute for Molecular Sciences (HIMS) is composed of nine chairs (research groups), organized in five research themes, each chair under the responsibility of a chair holder. In addition there is a NMR-facility situated in two different buildings, and as a consequence is part of two different research groups, and a Röntgen Diffraction (RD) facility, which is headed by an assistant professor. The organization scheme of HIMS is presented in chapters 1.1 and 5.6. A general overview and perspective of the research themes is described in chapter 1.3.

Each theme consists of one or more research groups, typically with a full professor and one or two tenured associate (UHD) or assistant (UD) professors (albeit with several exceptions), plus technicians, Post-docs and PhD students. In addition, there are several part-time chairs and extraordinary (endowed) chairs (bijzondere leerstoelen), usually scientists with an appointment elsewhere or paid by an external organization. Extraordinary (endowed) chair holders do not have a research group and tenured staff, but contribute to HIMS research by collaborating with other HIMS members and by supervising PhD students. They often participate in the teaching program of the University.

The five research themes function as clusters of expertise, with common interests in science, and shared facilities and approaches. The main goal of such a thematic organization is to create sufficient critical mass in different research areas and synergy by complementary expertise, to promote internal collaboration within HIMS and to have a structure in which opportunities for new research are identified and exploited and priorities can be set.

Within each theme the constituting research groups have their own research priorities and activities. In

fact, the actual management and allocation of resources is performed at the research group since research groups have a manageable size for personnel and financial management. Together, the five themes adequately cover the research mission of HIMS, with a firm basis for fundamental science, applied research projects, social activities, education and know-how validation activities (e.g. spin-offs; see section 4.4).

4.1.1 Management of the Institute

The HIMS director since 2004 is Dr R.L.J. (Rob) Zsom. The director is responsible for the scientific program and its quality, the contributions to the faculties educational program, for human and financial resource management, including investments in facilities and instrumentation. The actual financial and personnel management is delegated to the institute manager (bedrijfsvoerder Mrs. Gerda Zonneveld-de Boer, since May 2008). Together with the secretariat (2 persons) and the administration (2 persons) she forms the HIMS Office (Bedrijfsbureau). The institute manager is supported part-time by several laboratory technicians with special skills, e.g. an Arbo-veiligheid/Safety officer (Dr. Marjo Mittelmeijer), ICT officer (Paul Collignon), two facility officers (Mr. Joep Steeneken/REC and Mr. Jan Fraanje/New Buildings).

The Management of HIMS (dagelijks bestuur; DB) consists of the director, the business (institute) manager and the four special officers (ICT, Arbo and 2 for Facilities). The DB meets on a fortnight basis, and discusses finances, appointments, laboratory safety and security procedures, housing and facilities issues, and other matters related to the day-to-day management of the institute.

Two advisors for educational issues, Prof. dr. Henk Hiemstra (Master program), and Dr. Steen Ingemann

(Bachelor program) supported in 2008 the HIMS director in educational issues.

4.1.2 Management meetings

An internal Scientific Advisory Committee (Beleids Advies Raad/BAR), advises the HIMS director in matters concerning research priorities, education, investments, matching, PR and outreach, etc., and meets monthly. In the BAR the five HIMS research themes are represented by one of the staff-members (in principle one of the group leaders of the theme). The institute manager acts as secretary of the BAR in order to ensure efficient procedures. The director asks for the BAR's opinion, but the BAR can also take the initiative to advise the director. The BAR consisted in 2008 of Prof. Dr. Henk Hiemstra (BMS; also representing the educational institutes), Prof. Peter Schoenmakers (MBA), Prof. Joost Reek (CAT), Prof. Wybren Jan Buma (MOLP), Dr. Ever Jan Meijer (COMP), as well as the institute director Dr. Rob Zsom and the institute manager Mrs. Gerda Zonnevelde-de Boer.

A staff meeting (staff-lunch) takes place two-weekly. The aim of the meetings of the director with the staff is to inform the staff about developments, but also to obtain feedback. Most information disseminated in this way is subsequently communicated to the group members by the staff-members.

Several internal HIMS commissions meet on a regular basis. To be mentioned are the Public Relations commission (PR-commissie), the Safety and Health Commission (HIMS Arbo-veiligheids commissie; HAC) and the HIMS seminar commission (HIMS Seminar commissie). The PR-Commission consisted in 2008 of various staff members (also of SILS, representing biochemistry) representing the themes and an officer of the faculties PR-commission (Astrid Janmaat). On an ad-hoc basis the institute director is also attending the meetings. The present members are Prof. Fred Brouwer (MOLP, chairman), Dr. Jan van Maarseveen (BMS), Astrid Janmaat (FNWI; secretary), Prof. Joost Teixeira De Mattos, (SILS; biochemistry), Dr. Evert Jan Meijer (COMP), and Prof. Gadi Rothenberg. The HAC consist of the HIMS Arbo officer (Marjo Mittelmeijer; chairman) and various technicians representing the themes and labs. On an ad-hoc

basis the institute manager is also attending the meetings. The present members are Marjo Mittelmeijer (Chairman), Louis Hartog, Dorette Tromp, Jurg Ellenberger, Erik Bertelink, Peter Verschuren, Michiel Groeneveld, Jan Fraanje and Wim de Lange (FNWI).

The HIMS seminar committee organizes monthly a seminar. The purpose of the HIMS seminar is encouraging scientific discussion and enhancing collaboration in the institute, by bringing everyone together once a month for a stimulating lecture session followed by an informal 'borrel'. There are 10 seminars every year. The members of the seminar committee are Prof. Peter Bolhuis, Dr. Gadi Rothenberg, Dr. Sape Kinderman and Dr. Hong Zhang.

Finally, an international scientific advisory committee of HIMS (SAC) was installed in 2006 and visited the Institute for the first time in 2006. In 2008 the SAC meeting took place on December 12. The members are Prof.dr.ir. J.G.H. Joosten (DSM; chairman), Prof.dr.ir. D.N. Reinhoudt (UT), Prof. dr. R. Nolte (RUN), Prof.dr. M.L. Klein (LRSM - University of Pennsylvania, USA) and Dr. L.B.J. Vertegeal (NWO-CW/ACTS).

4.1.3 Decision making procedures and management style

The Van 't Hoff Institute for Molecular Sciences has two levels of leadership: that of the institute and that of the chairs (groups). At the institute level the director determines the scientific strategy and is responsible for the policy regarding finances, personnel, contracts and for the day-to-day management of the institute. The chairs (research groups) of the institute have a large degree of independence in arranging its affairs at the scientific and organizational level. The management style of HIMS is open there are many (formal and informal) possibilities for interaction between the director and the staff. This is important, because science can only thrive if scientists are given enough freedom to develop and pursue their ideas, given the boundaries set by the HIMS mission. HIMS scientists have great liberties in choosing their research topics. Their quantitative and qualitative research output (e.g. success in the acquisition of projects, and fit to the general HIMS mission), and educational performance are discussed in

formalized annual meetings between the director and the tenured full professors (jaargesprekken). The role of the institute's management (HIMS office) is to facilitate research.

In turn, professors have such meetings with the scientific staff members in their group. Thus, full professors have their own responsibility with respect to the quality of research within the scientific area of their respective chairs, and have their own budgets.

Collaboration at the theme level and also at the level of HIMS as a whole is greatly stimulated in a bottom-up approach, as it is more and more evident that complementary expertise is needed in modern research. More and more scientists with common interests and complementary expertise find each other in collaborative projects, of which there are many examples within HIMS and with other institutes (inside and outside the faculty and university). Shared, efficient facilities are another way to enhance collaboration, which is realized by the creation of general lab facilities (e.g. NMR facility) in which technicians and scientists interact closely. While academic freedom of individual researchers is highly valued, it is also clear that research priorities change, as well as budgets and funding opportunities. The style of management is to

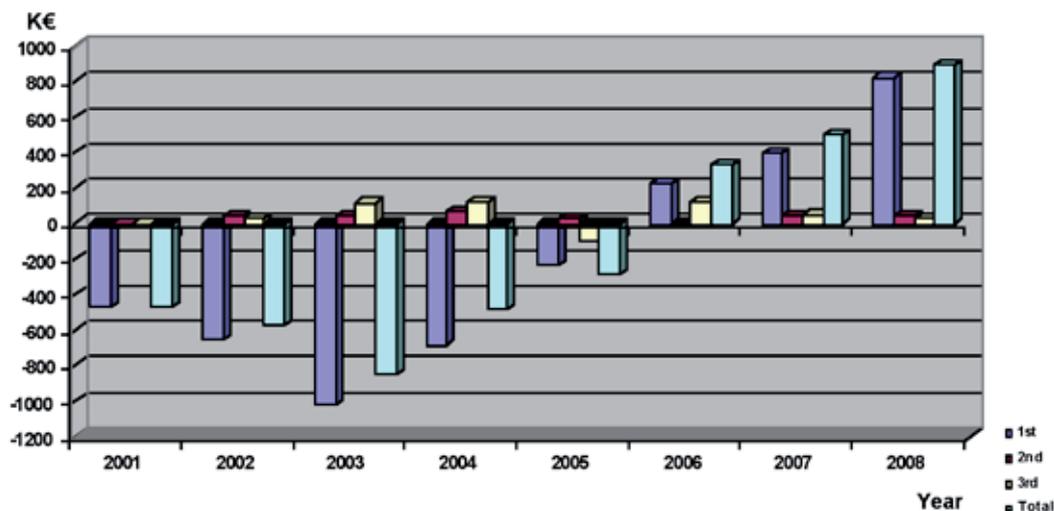
interact with the staff-members in the institute about such issues, and, if possible, seek consensus on and support for important developments affecting the future directions of the institute. This is realized by a number of formalized meetings as described before in section 4.1.2.

Apart from these formalized meetings, the director has ad-hoc contacts with individual professors and other staff members involved in important developments. The director has an active role in initiating and leading the discussion. He also discusses institute policies, both formally (in regular meetings) and informally with the faculty managers (the dean c.s. and chairperson of the department of chemistry), and is ultimately responsible for the decisions made.

4.1.4 Financial situation and personnel of HIMS (past and future)

Since 2006, the year of introduction of the new (integral costs) allocation model of the university board, the financial position of HIMS has much improved, reflecting the foreseen effect of the reorganization of the chemistry department that took place in the years 2002-2004, as is illustrated by the graph below.

HIMS Financial result 2001 - 2008 (all funding sources; k€)



Funding source

1st: University (direct) funding and NRSC-Catalysis

2nd: NWO, FOM and STW

3rd: EU, BSIK and Industrial

Notwithstanding the positive results of the years 2006-2008, the future financial prospects of HIMS (and the whole faculty) are uncertain. Furthermore, an adequate and balanced structural multi-year financial projection of institutes budgets and costs is still missing. The faculty is currently working on a new allocation model that will hopefully improve this situation.

In contrast with the expected result for the year 2008 (-233 k€), we succeeded to realize a positive result of 899 k€. Most likely the large difference between projection and realisation is related to financial uncertainties in the ~100 present and new external financed projects of HIMS in the new costs model. It seems that the expenses were correctly projected but the expected income seems to be projected too low, resulting in the negative result originally expected for 2008. This observation is still under study together with the financial department. In the course of the year 2008 quarterly financial reports were not made available, which hampered good financial and personnel management. Hopefully this will be improved in 2009.

In the past unexpected budget reductions and costs increases already forced the institute to take additional measures to lower the costs more than was planned, e.g. in the years directly after the reorganization of the chemistry department, which took place in the years 2002-2004. Late 2008 the dean announced that the future financial prospects of the faculty once again are uncertain, related to expected budget reductions from both the ministry and the university board in the years 2009-2012. Additionally an adequate and above all a structural

multi-year financial projection of institute budgets and costs is still missing. Based on these uncertainties, a further reduction in costs and external funds raising⁸, is needed for HIMS.

4.2 Financial resources 2008

During the years 2002-2004 the institute was confronted with substantial foreseen (e.g. as result of the reorganization of the chemistry department) financial measures and in the years 2003-2005 also with unforeseen lowering of university budgets and unforeseen increasing of costs (e.g. housing costs). These unexpected budget reductions and cost increases forced the institute to take additional measures to lower the costs even more than was planned in the reorganization of the chemistry department (2002-2004). As one of the direct consequences, even more reduction in personnel has taken place in the past years than was foreseen. Several vacancies could not be fulfilled and a temporarily stop in almost all appointments in the 1st money stream was still acting in 2008. Fortunately, an important extra cost increase (charged to the institute in the years 2003-2005), defined by the faculty as "housing costs", was not charged in the years 2006-2008 and as such contributed positively to the institutes results. Additionally, the institute remained very successful in external fund raising (especially in 2007 and 2008), which funds could partially be used to lower direct personnel costs as is shown in the table below.

⁸ Hopefully the HIMS spin-offs, under the umbrella of the UvA Holding (e.g. Cat-Fix and Cat-It/Reek or Yellow Diesel/Rothenberg; see also section 4.4), will also be profitable in the coming years. HIMS is presently working (together with the UvA Holding and the BKT/ Know-How Transfer Agency) to explore the possibilities of more spin-off and valorisation activities. HIMS has various patent positions (in different themes/ groups) that give us excellent possibilities.

Fte's of the HIMS staff in fixed positions^{a)} (2007, 2008) covered by external funds and other income

	2007 (Fte)	2008 (Fte)
Costs of the staff covered by projects ¹⁾	2.8	4.5
Costs of the staff covered by teaching tasks ²⁾	0.4	2.2
Costs of the staff covered by other sources ³⁾	2.4	2.0
Total	5.6	8.7

^{a)} Budgets for PhD students, postdocs and other temporary staff not included

¹⁾ Personnel grants of the staff from projects, e.g. FOM, NWO budgets, JvGeuns fund

²⁾ Personnel income of the staff from teaching tasks: bachelor and master schools, Amstel Institute/outreach and restoration programme)

³⁾ Personnel income of the staff from services for the faculty, research school, other institutes

A part of the extra income as shown in the table above was not projected and contributed considerably to the results of HIMS in 2007 and even more in 2008 (see the table below and chapter 5.6 for more details).

The table on the next page shows a survey of budgets versus expenditures 2008 for:

- The first money stream (1st; direct university funding).
- External funds 1st (NRSC-Catalysis, matching), 2nd (FOM, NWO-CW, STW) and 3rd (EU, BSIK and industrial funding).

In 2006 the university board introduces a new full costs (*integral costs*) allocation model used in the table.

The new integral costs model unfortunately shows various uncertainties and deficiencies:

- The costs for 1st and 1st-others funding category are calculated from the ratio taken from the budgets and are considered to have the same ratio.
Remark: This assumption is probably wrong, since incomes and spending (e.g. NRSC-C and matching contributions) usually do not follow the same pattern, or do not take place in the same year.

- Withdrawals from the reserves (bestemde, bekleemde reserves) were foreseen in the forecasts for 2008, but were not executed in the realization.
- The amount of overheads assigned by the faculty to the institute (both in budgets and costs) in the new model, which are related with the total number of Fte's in the reporting year, change from year to year.
- In the new model additional (overhead) budget is assigned in the 1st stream of money (University budget) as compensation budget for the integral costs charged to the institute by the UvA/FNWI for 2nd and 3rd stream projects.
- In the financial accounts 2008 (new allocation model), overhead assignments were not booked as additional budgets but as negative costs in the 2nd and 3rd stream of money reports.
- The costs assigned to HIMS contain in an unverifiable way costs for centralized services of the various supporting departments of the university (ICT, finances, personnel, etc.). These costs are appreciably higher than in the years before and increase from year to year without any control of the faculty and the institute.

HIMS financial account 2008 (*integral costs model*)

Benefits HIMS 2008 (k€)	1 st	1 st others	1 st total	2 nd	3 rd	Total
Budgets	10.431	887	11.318	1336	2151	14.804
Costs HIMS 2008 (k€)						
Personnel costs	4.396	321	4.717	1.212	1.159	7.088
Other costs	5.382	392	5.774	81	962	6.817
Total costs	9.778	713	10.491	1.293	2.121	13.905
Result HIMS 2008 (k€)						
Projected (1) ¹⁾	-822	450	-372	101	38	-233
Realized (2) ²⁾	653	173	827	43	30	899
Realized versus projection (2-1)	1.475	-276	1.199	-58	-8	1.132

Source of funding: 1st: University (direct) funding 1st-others ³⁾: (earmarked university budgets)
2nd: NWO, FOM and STW 3rd: EU, BSIK and Industrial

¹⁾ Projected result estimated including a contribution from the earmarked reserves (bestemde reserves) for NRSC-C and matching.

²⁾ Realized result estimated without a contribution from the earmarked reserves.

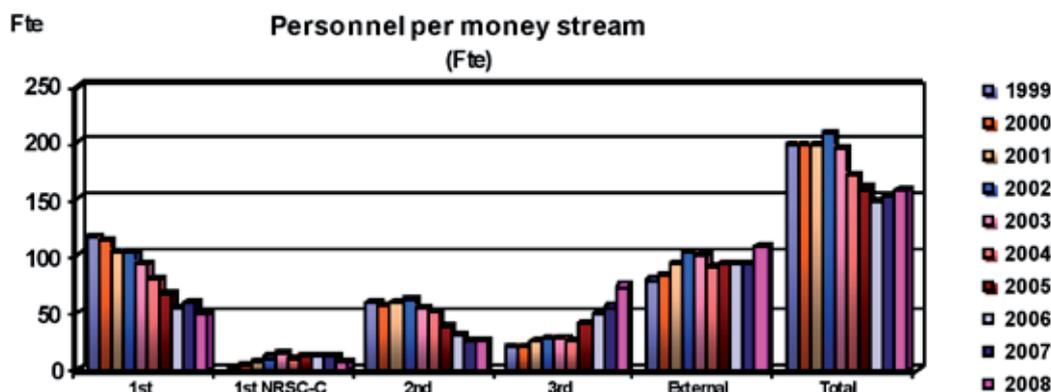
³⁾ Non-structural benefits and costs, which are earmarked contributions from external sources such as research schools (NRSC-C, HRSMC) and university board (matching for BSIK, equipment, vernieuwingsimpuls), etc.

The new integral costs model also shows some advantages in 2008. As is illustrated in the table above, HIMS obtained in 2008 (as well as in 2006 and 2007) a positive result, after years of negative results. Although the forecast for 2008, was negative (a result of -233 k€ was originally projected for 2008 by the faculty), a positive result was obtained in the new allocation model. Seemingly the new (integral costs) allocation model was beneficial for HIMS in the year 2008 (as it was in 2006 and 2007). Very probably the large difference between projection and realisation is related with errors in the projection (in the new integral costs model of the (~100) running and new externally financed projects of HIMS. It seems that the expenses were correctly projected but the expected income seems to be projected too low, resulting in the negative result originally expected for 2008. This observation is still under study together with the financial department.

HIMS has been very successful in 2008 in obtaining external funds especially in the last part of 2008, resulting in 40 vacancies on 01-01-2009. For 2008 the number of coworkers, both in numbers and in Fte's, increased as compared with the years 2006 and 2007 (see also chapter 2.1 and 4.3). A further increase in personnel numbers is expected for 2009. It is unknown for the coming years if the increase in costs in the new integral costs model (that certainly will be charged to HIMS) for the expected increase in personnel will be compensated by an increase in (overhead/compensation) budgets, to be assigned by the university board to the faculty and by the faculty to the institute.

Remark: In case the total number of personnel of the faculty increases problems can be expected. In

case the total number of personnel of the faculty remains constant, compensation budgets will be moved from institutes with decreasing personnel numbers to institutes with increasing numbers. End 2008 the dean of the faculty announced that, in addition to the uncertainties related with the introduction of the new (integral costs) allocation model, the faculty and concomitantly the institutes will be confronted again with serious budget reductions in the coming years (2009-2012), both from the ministry of education (e.g. budgets will be moved from direct funding of the universities towards indirect funding via NWO) and from the university board (e.g. budgets will move from our faculty to other faculties). Knowing all the uncertainties mentioned above, a further reduction in costs, most probably larger than in the last years, will be needed for HIMS in the coming years to be able to appoint young staff-members or technicians. The university budget (1st stream of money) is largely used for permanent positions. Only a few permanent positions were discontinued in 2008, most by the projected leave of the Complex Fluids staff. Several positions will be discontinued also in the coming years, e.g. by retirement or by other means. The HIMS policy will be to invest in its strengths, following the advice of the external Scientific Advisory Committee. Several coworkers were and will be transferred to other HIMS themes, e.g. in 2008 a technician from the discontinued theme Complex Fluids to the new research initiatives in forensic sciences (group Schoenmakers). The Röntgen Diffraction facility will be either transferred to the restoration sciences activities or to another university (when possible as a part of the 'sectorplan natuurwetenschappen', the national focus and mass activities).



Personnel 2008

	1 st (Fte)	NRSC-C ²⁾ (Fte)	2 nd (Fte)	3 rd (Fte)	Total Fte	Total Person ³
Management and support	7.5	0.0	0.0	1.8	9.3	12
Bio-Molecular Synthesis	7.4	1.7	3.4	5.0	17.5	26
Catalysis	11.9	5.4	9.4	22.6	49.4	67
Computational Chemistry	8.0	0.0	6.5	9.5	24.0	32
Molecular Photonics	6.1	1.6	5.9	13.9	27.5	42
Macrom. & Bios. Analysis	5.2	0.0	0.3	13.7	19.2	25
Complex Fluids	0.0	0.0	0.0	0.0	0.0	0
Others ¹⁾	2.1	0.0	0.0	2.3	4.4	7
Polymer Processing	1.5	0.0	0.0	5.8	7.2	9
Total	49.8	8.7	25.5	74.6	158.6	220
	31.4%	5.5%	16.1%	47.0%	100.0%	

¹⁾ Röntgen Diffraction department Source of Funding

²⁾ 1st from NRSC-Catalysis 1st: University (direct) funding 2nd: NWO, FOM and STW

³⁾ Number of co-workers in 2007 1st: NRSC-Catalysis 3rd: EU, BSIK and Industrial

4.3 Human resources

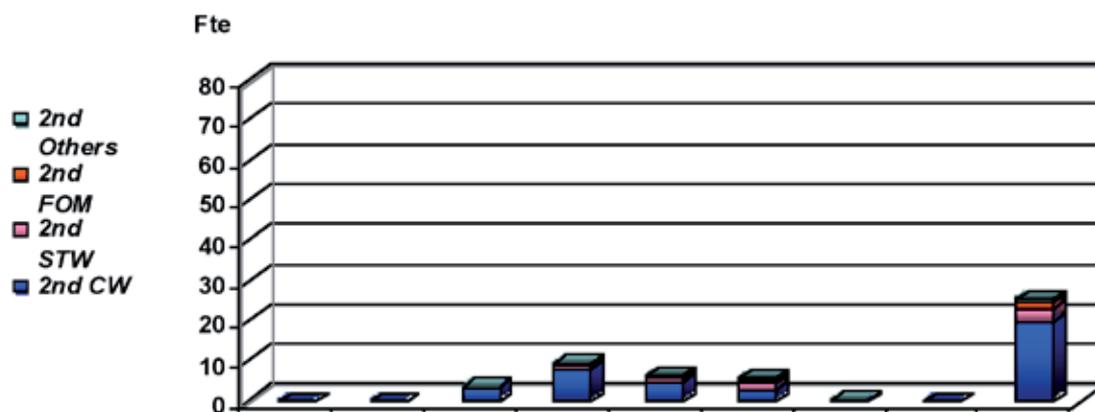
In 2008 HIMS employed 14 professors, 5 extraordinary professors, 7 associate professors (UHD's, 1 of them is also part-time professor), 9 assistant professors (UD's), 94 PhD students (AIO/OIO's, including guest-aio's and outdoor-aio's), 47 potdocs (PD's), and 44 other personnel (OBP), all together a total of 220 persons (158.6 Fte).

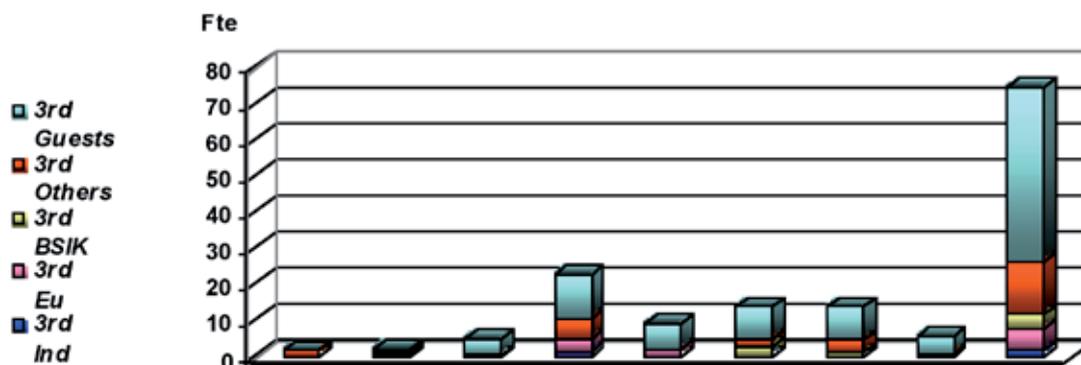
The externally financed projects count for more than 65% of our personnel in 2008 (in 2001 that was still much less, ~40%). HIMS personnel data for 2008 was 4.6 Fte higher than for 2007, mainly related with an increase in external funds obtained (see also chapter 5.6).

As can be seen from the figures below, where 2nd and 3rd money stream external funding of personnel is shown in more detail for 2008, NWO-CW is by large the most important funding agency in the 2nd money stream category, followed by STW. FOM is increasing in importance as funding agency.

In the 3rd money stream EU-funding is becoming more and more important, as is DPI (Others) and BSIK (NanoNed). The high number of guests includes PhD students employed elsewhere (buiten aio's), PhD students with finished contracts still awaiting their promotion, and guest researchers from different origins.

Personnel 2nd money stream HIMS 2008 (Fte)



Personnel 3rd money stream HIMS 2008 (Fte)

The figures also indicate that 3rd money stream funding is more important for the themes 'Catalysis' and 'Macromolecular and Biosystems Analysis'. For the other themes the difference is less outspoken. For more details on the data of 2008, see also the tables in chapter 5.6.

Although the present financial situation of HIMS is better than a few years ago, the present and future prospects, especially in HRM, are still uncertain. The institute was confronted in the last years with a stop in appointments of PhD students from direct university funds. Hopefully this will change in the years to come, depending on the financial situation.

4.4 Relations with external parties and innovations

Research innovations are increasingly important in creating benefits for society. The importance for society of the research efforts of the HIMS themes are found in applications such as, data transport, energy, health, storage in information technology, analytical techniques for medical, forensic- and restorative purposes, sustainability (e.g. efficient transformations of fossil raw materials into useful compounds), design and synthesis of complex molecules for use as catalysts, agro-chemicals or drugs and innovation. Research collaborations with external parties, especially with industrial parties, and since 2006 also spin-off activities, are important components of our strategy.

The importance of research collaborations with industry are clear from the many existing collaborations of the HIMS groups as well as from

the active participation of various part-time professors from industry in our research programs. HIMS follows an active policy to appoint part-time (endowed) professors, both internally and externally (from industry). Various new initiatives were started in 2008 and these efforts will hopefully result in new appointments in 2009.

In order to protect our intellectual properties, HIMS follows an active patenting policy, in most occasions directly with our industrial partners, but when possible also on our own. For the near future we are actively looking for new partnerships with industrial partners.

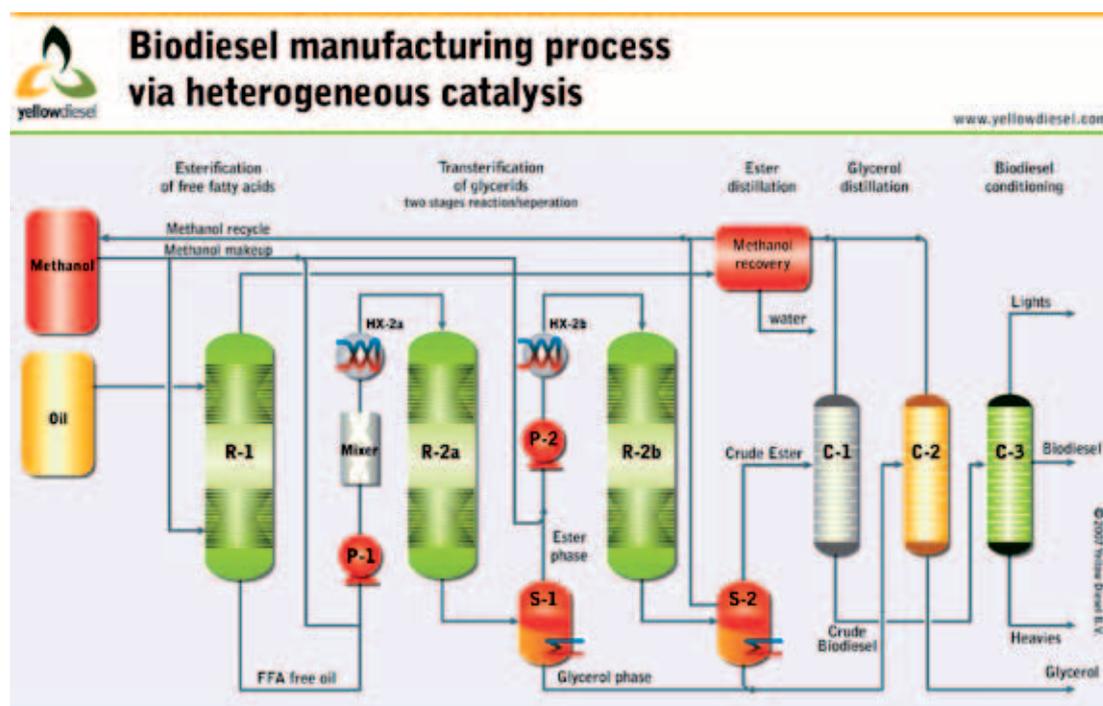
In 2006, HIMS started a spin-off activity in the area of Supramolecular Catalysis based on an own patent position generated via NRSC-C research (Reek et al., EP 03076827.9). The patent, now filed in many countries, claims the preparation, application and recycling of transition metal catalysts using self-assembly. With the help of a large subsidy of 2.7 M€ from Senter for the project 'Innovatiesubsidie Samenwerkingsprojecten Cat-It' and in collaboration with Engelhard (now BASF) it was demonstrated that with this new patented technology large libraries of chiral catalysts can be prepared partly by automated procedures. This research has resulted in the submission of another three patents to protect the developed technology. In 2009 the project is finished and this initiative should lead to commercial activities.

In addition, the patented technology also allows new concepts (Cat-fix) for the scavenging and recycling of homogeneous catalysts to be developed, both for bulk-chemistry and fine-

chemistry. The new catalyst scavenger-recycling concept can [1] clean industrial processes from polluting catalyst [2] recover the catalyst and [3] bring it back in the process. Cat-Fix combines these processes in one system, an 'ordinary' fixed-bed reactor with scavenger materials that recovers the active catalyst from the product flow and, when 'washed', can release the active catalyst for recycling. The core tangible Cat-Fix product will consist of scavenging/recycling particles. From the first phase project it was clear that several industries are interested in the Cat-Fix solutions and in 2007 the UvA Holding decided to further stimulate the activity in this area and the BV Cat-Fix was started as a part of the UvA Holding. In 2008 Cat-Fix has further developed the technology aiming at a stronger intellectual property position. Besides continuation along these lines, 2009 will be used to find customers for the Cat-Fix applications.

Another spin-off activity in the catalysis theme is the company Yellow Diesel BV, that was founded in July 2007 by Gadi Rothenberg and the UvA Holding BV. The core scientific idea behind the company is a new process for producing biodiesel, based on a combination of heterogeneous catalysts and advanced process technology. This process was

developed in Rothenberg's group together with Dr. Alexandre Dimian, an expert in process technology. In 2008, the Rothenberg group of HIMS and Yellow Diesel BV both strengthened their position in the area of biodiesel and biomass conversion research by forming a collaboration with the biodiesel manufacturing company Solarix BV. Together, the three parties succeeded in obtaining a 1 M€ EOS-subsidy as part of a 1.5 M€ project in total. In this innovative project, the two companies and HIMS will develop a new additive for diesel based on enhancing the value of biodiesel byproducts via heterogeneous catalysis. Further, Yellow Diesel has built up its IPR base by applying for two European Patents, one on the catalyst and one on the process.



5. Appendices

5.1 Research input, research output & external collaborations

5.1.1 Summary of external research budgets and personnel (from different sources of money) acquired in 2007, related projects started in 2008

	Budget (M€)			Personnel (Number)		Personnel (Fte)	
	Subsidy	Matching ⁵⁾	Total	PhD's [*]	Pd's ^{**}	Staff ⁶⁾	Techn ⁷⁾
1 st – NRSC-C ¹⁾	0.00	0.00	0.00	0	0	0.0	0.0
1 st – Others ²⁾	0.12	0.07	0.19	0	0	0.0	1.9
2 nd ³⁾	3.79	0.14	3.93	9	4	5.0	4.8
3 rd ⁴⁾	1.34	0.47	1.81	3	5	0.8	0.6
Total	5.25 ^{a)}	0.68	5.93	12	9	5.8	7.3

^{a)} Subsidy partners (total 0.00 M€) excluded

^{*} PhD's are appointed on a four years contract

^{**} Postdocs are mostly appointed on a two years contract

¹⁾ NRSC-C (TOP Research School Catalysis)

²⁾ COF, CvB (Funds from University Board), JvG (John van Geunsfonds)

³⁾ NWO-CW, FOM, STW, KNAW, DFG, ERC

⁴⁾ EU, DPI, Senter, NanoNed, Industry

⁵⁾ Matching contributions UvA/FNWI and own contributions HIMS (in kind and cash/from reserves)

⁶⁾ Tenured staff

⁷⁾ Lab technicians

5.1.2 External research funds acquired in 2007 and related projects started in 2008 (M€)

Project (nr)	PhD's (nr)	Pd's (nr)	Staff (fte)	Techn (fte)	Start date	End date	Source of funding	Theme	Project manager(s)	Subsidy (M€)	Matching (M€)	Total (M€)
1	0	0	0.00	1.94	02/01/2008	02/01/2011	JvG	MOLP	Brouwer & Buma	0.12	0.07	0.19
2	1	1	1.00	0.50	07/05/2007	01/01/2013	NWO	MOLP	Woutersen/Buma	0.40	0.11	0.51
3	0	0	0.00	0.00	07/05/2007	01/01/2013	JvG	MOLP	WoutersenBuma	0.08	0.00	0.08
4	1	0	0.00	2.00	10/01/2007	10/01/2007	NWO	BMS	Wever	0.35	0.00	0.35
5	5	2	0.00	0.00	07/01/2008	07/01/2013	ERC-grant	CAT	De Bruin	1.25	0.03	1.28
6	2	1	4.00	2.25	07/01/2008	07/01/2013	ERC-grant	MOLP	Woutersen	1.72	0.00	1.72
7	1	2	0.00	0.00	01/01/2008		DPI	CAT	Reek	0.53	0.20	0.74
8	0	0	0.00	0.00	01/01/2008		SenterN + Cat-Fix	CAT	Reek	0.02	0.00	0.02
9	1	0	0.00	0.00	01/01/2008	01/01/2012	DPI	CAT	De Bruin	0.28	0.11	0.39
10	0	2	0.00	0.00	01/01/2008		DPI	CAT	Reek	0.25	0.09	0.34
11	0	1	0.00	0.00	01/01/2008	01/01/2009	BASF	CAT	Reek	0.08	0.00	0.08
12	1	0	0.00	0.00	01/01/2008	01/01/2012	Avantium	CAT	Rothenberg	0.10	0.07	0.17
13	0	0	0.20	0.00	01/01/2008	02/29/2008	CECAM/ EU	COMP	Smit	0.03	0.00	0.03
14	0	0	0.00	0.02	01/01/2008		UvA Holding	CAT	Rothenberg	0.00	0.00	0.00
15	0	0	0.11	0.12	01/01/2008		SenterN + compagnies	MBA	Kok	0.05	0.00	0.05
Total	12	9	5.3	6.8						5.25^{a)}	0.68	5.93

^{a)} Subsidy partners (total 0.00 M€) excluded

- 1: External financing (dakpanfinanciering) of a technician
- 2: Vidi 'Molecular movies of protein folding'
- 3: Vidi 'Molecular movies of protein folding'
- 4: Industrially relevant heterocycles through biocatalytic cascades
- 5: Catalytic carbene insertion reactions; creating diversity in (material) synthesis
- 6: Vidi 'Molecular movies of protein folding'
- 7: New functionalized materials by Rh and Pd mediated carbene homo-polymerization and olefin/carbene co-polymerization
- 8: SenterNovem voucher Organo Cat. Recycling
- 9: Understanding structure/performance relationships for non-metallocene olefin polymerization catalyst
- 10: Green Rigid blocks for Engineering plastics with ENhanced pERformance
- 11: BASF Sandee
- 12: Descriptors for heterogeneous catalysis: rational design applied to the development of heterogeneous catalysts
- 13: CECAM director
- 14: Yellowdiesel (incidentele dienstverlening)
- 15: NLSis Voucher vervolg

5.1.3 Summary of external research budgets and personnel (from different sources of money) acquired in 2008, related projects started in 2008

	Budget (M€)			Personnel (Number)		Personnel (Fte)	
	Subsidy	Matching ⁵⁾	Total	PhD's [*]	Pd's ^{**}	Staff ⁶⁾	Techn ⁷⁾
1 st – NRSC-C ¹⁾	0.00	0.00	0.00	0	0	0.0	0.0
1 st – Others ²⁾	0.00	0.00	0.00	0	0	0.0	0.0
2 nd ³⁾	0.90	0.03	0.94	4	3	0.0	0.0
3 rd ⁴⁾	0.78	0.18	0.95	2	2	0.0	0.5
Total	1.68 ^{b)}	0.21	1.89	6	5	0.0	0.5

^{b)} Subsidy partners (total 0.53 M€) excluded

^{*} PhD's are appointed on a four years contract

^{**} Postdocs are mostly appointed on a two years contract

¹⁾ NRSC-C (TOP Research School Catalysis)

²⁾ COF, CvB (Funds from University Board), JvG (John van Geunsfonds)

³⁾ NWO-CW, FOM, STW, KNAW, DFG, ERC

⁴⁾ EU, DPI, Senter, NanoNed, Industry

⁵⁾ Matching contributions UvA/FNWI and own contributions HIMS (in kind and cash/from reserves)

⁶⁾ Tenured staff

⁷⁾ Lab technicians

5.1.4 External research funds acquired in 2008 and related projects started in 2008

Project (nr)	PhD's (nr)	Pd's (nr)	Staff (fte)	Techn (fte)	Start date	End date	Source of funding	Theme	Project manager(s)	Subsidy (M€)	Matching (M€)	Total (M€)
16	1	0	0.0	0.0	11/1/2008	10/31/2012	NWO	BMS	Timmerman	0.24	0.01	0.25
17	0	0	0.0	0.0			Pepscan	BMS	Timmerman	0.01	0.00	0.01
18	0	2	0.0	0.0	8/15/2008	11/10/2010	NWO	MOLP	Brouwer	0.24	0.00	0.24
19	1	0	0.0	0.0			NWO	CAT	Reek	0.01	0.00	0.01
20	1	0	0.0	0.0	9/1/2009	8/31/2012	NWO	CAT	Hartl, Reek	0.24	0.00	0.24
21	0	0	0.0	0.0			FOM	MOLP	Zhang	0.05	0.00	0.05
22	0	1	0.0	0.0	10/15/2008	4/15/2010	NWO	CAT	Vlugt	0.06	0.03	0.09
23	1	0	0.0	0.0	3/1/2009	2/28/2010	KNAW	MOLP	Zhang	0.05	0.00	0.05
24	0	0	0.0	0.0	7/13/2007	7/12/2009	NWO	BMS	Wever	0.01	0.00	0.01
25	0	0	0.00	0.00	10/1/2004	10/1/2008	DPI	MBA	Kok	0.02	0.01	0.03
26	0	1	0.00	0.00	7/1/2008	7/1/2010	EU	CAT	Reek	0.16	0.00	0.16
27	0	1	0.00	0.00	7/1/2008	9/30/2008	UCB Pharma	BMS	v. Maarseveen	0.02	0.00	0.02
28	1	0	0.00	0.00	4/1/2009	3/31/2013	CatchBio	CAT	Elsevier	0.26	0.09	0.35
29	1	0	0.00	0.00	?	?	CatchBio	CAT	Reek	0.26	0.09	0.35
30	0	0	0.00	0.51	1/1/2008	12/31/2008	Various	Others	Peschar	0.03	0.00	0.03
31	0	0	0.00	0.00	1/1/2008	2/19/2008	ECN	CAT	Mittelmeijer	0.02	0.00	0.02
32	0	0	0.00	0.00	1/1/2008	12/31/2008	NKI and NIOZ	BMS	Geenevasen	0.01	0.00	0.01
Total	6	5	0.0	0.5						1.68^{b)}	0.21	1.89

^{b)} Subsidy partners (total 0.53 M€) excluded

- 16: Functional mimicry of discontinuous protein binding sites using a combination of CLIPS-technology and CLICK-chemistry
 17: Functional mimicry of discontinuous protein binding sites using a combination of CLIPS-technology and CLICK-chemistry
 18: Translational motion in individual motor molecules
 19: Microreactor time-resolved operando spectroscopy for kinetic analysis of (ultra)fast reactions
 20: Light-driven dihydrogen production in [2Fe2S]-metalloporphyrin supramolecular assemblies
 21: Space-separated quantum cutting in Si nanocrystals
 22: Towards selective organometallic mediated amination of alkenes with ammonia
 23: Synthesis and spectroscopic studies of luminescence up-conversion nanoparticles doped with rare earth ions and their application in the diagnosis and therapy of cancer
 24: Enzymatic synthesis of enantio- and diastereomerically pure unsaturated B-hydroxy- α -amino acids and synthetic elaboration into biologically relevant derivatives
 25: Equipment
 26: Application of droplet-based microfluidics for the screening of supramolecular catalysts
 27: Peptidomimetic program 2008
 28: Hydrogenolysis of Esters and Amides
 29: New reactions to chiral amines from alcohols and ketones
 30: Various measurements
 31: High pressure absorption measurements
 32: NMR measurements

5.1.5 Summary of external research budgets and personnel (from different sources of money) acquired in 2008, related projects to be started in 2009

	Budget (M€)			Personnel (Number)		Personnel (Fte)	
	Subsidy	Matching ⁵⁾	Total	PhD's ⁶⁾	Pd's ^{**}	Staff ⁶⁾	Techn ⁷⁾
1st – NRSC-C ¹⁾	2.70	0.00	2.70	7	8	0.0	0.0
1st – Others ²⁾	0.00	0.00	0.00	0	0	0.0	0.0
2nd ³⁾	1.76	0.10	1.86	4	5	0.4	0.4
3rd ⁴⁾	1.08	0.19	1.27	3	0	0.2	0.3
Total	5.54 ^{c)}	0.29	5.83	14	13	0.6	0.7

^{c)} Subsidy partners (total 0.00 M€) excluded

^{*} PhD's are appointed on a four years contract

^{**} Postdocs are mostly appointed on a two years contract

¹⁾ NRSC-C (TOP Research School Catalysis)

²⁾ COF, CvB (Funds from University Board), JvG (John van Geunsfonds)

³⁾ NWO-CW, FOM, STW, KNAW, DFG, ERC

⁴⁾ EU, DPI, Senter, NanoNed, Industry

⁵⁾ Matching contributions UvA/FNWI and own contributions HIMS (in kind and cash/from reserves)

⁶⁾ Tenured staff

⁷⁾ Lab technicians

Vacancies per 01-01-2009: 22 PhD, 14 Pd, 3 Staff (1 Hgl, 2 UD), 1 Secretary

Vacancies per 01-01-2008 per theme:

Macromolecular & Biosystems Analysis: 1 UD, 1 PhD

Bio-Molecular Synthesis: 2 PhD, 2 Pd

Catalysis: 11 PhD, 8 Pd

Computational Chemistry: 1 Hgl, 4 PhD's, 4 Pd

Molecular Photonics: 3 PhD's, 1 Pd

Others: 1 PhD

General: 1 Secretary

5.1.6 External research funds acquired in 2008, related projects to be started in 2009

Project (nr)	PhD's (nr)	Pd's (nr)	Staff (fte)	Techn (fte)	Start date	End date	Source of funding	Theme	Project manager(s)	Subsidy (M€)	Matching (M€)	Total (M€)
33	3	3	0.00	0.00	2009	2012	NRSCC	CAT	Reek & d. Bruin & v.d. Vlugt	1.00	0.00	1.00
34	2	1	0.00	0.00	2009	2012	NRSCC	BMS	Hiemstra & Maarseveen	0.60	0.00	0.60
35	2	2	0.00	0.00	2009	2012	NRSCC	CAT	Elsevier	0.60	0.00	0.60
36	0	1	0.00	0.00	2009	2012	NRSCC	CAT	Rothenberg	0.25	0.00	0.25
37	0	1	0.00	0.00	2009	2012	NRSCC	CAT	Wever	0.25	0.00	0.25
38	0	1	0.00	0.00	2009	2012	NWO	COM	Vreede	0.21	0.00	0.21
39	0	1	0.00	0.00	2009	2013	STW	CAT	Rothenberg	0.28	0.01	0.29
40	0	0	0.00	0.00	2009	2012	ECN	CAT	Rothenberg	0.03	0.00	0.03
41	4	3	0.40	0.40	2009	2014	NWO	COM	Bolhuis	1.25	0.09	1.34
42	0	0	0.00	0.09	2009	2009	EU	MOLP	Buma	0.02	0.00	0.02
43	0	0	0.00	0.00	2009	2009	Various	MOLP	Buma	0.01	0.00	0.01
44	0	0	0.00	0.00	2009	2009	EU	COM	Meijer	0.03	0.00	0.03
45	0	0	0.00	0.00	2009	2009	CECAM	COM	Meijer	0.02	0.00	0.02
46	1	0	0.00	0.00	2009	2012	NLISIS BV	MBA	Kok	0.30	0.00	0.30
47	1	0	0.15	0.20	2009	2012	Senter Novem	CAT	Rothenberg	0.29	0.19	0.49
48	0	0	0	0	2009	2013	EU	MOLP	Buma	0.05	0.00	0.05
49	1	0	0.00	0.00	2009	2012	DPI	Others	Iedema	0.36	0.00	0.36
Total	14	13	0.6	0.7						5.54^{c)}	0.29	5.83

^{c)} Subsidy partners (total 0.00 M€) excluded

33: New catalytic processes

34: Organocatalysis

35: Multidentate carbene and aggregated transition metal catalysts

36: Developing descriptors for solids: heterogeneous catalysis by rational design

37: Integrated multi-step enzyme cascade reactions to form non-natural carbohydrates and N-heterocyclic compounds

38: How do proteins communicate? Predicting function, formation and interactions of coiled coil complexes at the molecular level.

39: Hydrothermally stable organosilica-gased hybride membranes for molecular separations

40: ECN contribution

41: Proteins out of isolation: simulating the influence of the environment on polypeptide self-assembly

42: Modern developments in spectroscopy

43: Modern developments in spectroscopy

44: Molecular simulations in biosystems and material science

45: Molecular simulations in biosystems and material science

46: The next generation GC

47: 2nd generation biofuel via heterogeneous catalysis

48: The realization of some of the world's first working synthetic molecular motors and mechanical nanomachines

49: Rheology control by branching modeling

Vacancies per 01-01-2009: 22 PhD, 14 Pd, 3 Staff (1 Hgl, 2 UD), 1 Secretary

5.2 Internal and external collaborations

5.2.1 Collaborations of theme 1

Macromolecular and Biosystems Analysis

HIMS

- (MALDI) Characterization of catalysts and polymers (Reek, Rothenberg, de Bruin/Catalysis).

FNWI/UvA

- Multivariate Calibration; Prof. dr. A. K. Smilde (SILS).
- Proteomics; Prof. dr. C. de Koster (SILS), shared PhD student (R Peters).
- Lipoprotein research, dr. J.A. Kuivenhoven, AMC, dept Vascular Medicine.

Dutch Research Schools and Technology Institutes

- DPI project: Combinatorial Screening of Polymer Solubility (COPS).
- DPI project: Comprehensive Characterization of Branched Polymers (CCBP).
- DPI project: Chemically Improved PolySaccharides (CHIMPS).
- DPI project: Ultra-Performance Polymer Separations (UPPS).

Dutch others

- NanoNed: 3 PhD projects (a) Nanostructures for separations on a chip (Mauro Depra) (b) Nanoliths (Yuli Huo), (c) 2D separations on a chip (Peter Pruijm).
- COAST Initiative (Comprehensive Analytical Science and Technology).
- NFI co-operation with forensic institute for education (Gerard van der Peijl, Huub Hardy, Henk Leijenhorst). Research is built around a number of MSc projects.

Industrial

- Intensive cooperation with Unilever (macromolecular food components, through Hans-Gerd Janssen) and DSM (biotericals, through Sjoerd van der Wal).
- Atas GL International 100% sponsoring of PhD student (Erwin Kaal).
- Gas Chromatography. NLis and Joint Analytical Systems, 100% sponsoring of a PhD student (Daniela Peroni).

- Characterization of cellulose derivatives. Dr. B. Wittgren, AstraZeneca (Möln Dahl, Sweden).
- Characterization of branched polymers. Dr. F. Van Damme en Dr. E.P.C. Mes, DOW Chemicals (Terneuzen).
- Ultra-performance polymer separations. Dr. J. Willis, Waters, (Milford, MA, USA).
- Syngenta (Guilford, UK), project "Characterization of lignosulfonate surfactants", 100% sponsoring of a PhD student (Stella Brudin).
- GL Sciences (Tokyo, Japan), "Extending the applicability of gas chromatography".
- Wyatt Technologies (Dernbach, D) project "Field-flow fractionation for the characterization of lipoproteins".

International

- Monolithic stationary phases for LC. Prof. Dr. F.Svec, University of Berkeley (CA, USA).
- Nanoscale Separations. Prof. Dr. G. Desmet, Dept. Chem. Eng., Vrije Universiteit Brussel (B).
- Chromatographic Data Analysis. Prof. Y. Van der Heyden, Dept. Pharmacy, Vrije Universiteit Brussel (B).
- Two-dimensional separations. Prof. Philip Marriott (RMIT, Melbourne, Australia).
- Performance limits of separations. Prof. P.W. Carr, University of Minnesota, Minneapolis, MN, USA.
- Chemometrics. Prof. R. Synovec, University of Washington, Seattle, WA, USA.

5.2.2 Collaborations of theme 2

Bio-Molecular Synthesis

HIMS

- Transition metal catalysis in a NRSC-C project. (Catalysis/Van Leeuwen, Reek).
- Cascade Chemo- and Biocatalytic Processes. (Catalysis/Reek).
- The possibility of coupling two separate reactions catalyzed by a phosphatase and a Pd catalyst in a one-pot synthesis. (Catalysis/Reek).
- Infrared spectroscopy of manganese acetyl and carbonyl complexes in the gas phase (Buma).

FNWI/UvA

- Development of Antibacterial Agents via Inhibition of FtsZ (de)polymerisation. Prof. N. Nanninga, Dr. T. den Blaauwen (CAIRE, Molecular Cell Biology/SILS).

- Development of small molecular organic tools for proteomics research. (Dr L. de Jong, Prof. C. de Koster, SILS).
- Combination of homogeneous and biocatalysis. (Prof. K. Hellingwerf, SILS).
- Development of novel cyclopeptide based tyrosinase inhibitors. (Dr. Speijer, Prof. Aerts, AMC).
- Structure of the insect repellent of tomato species (Prof. Haring, Dr Schuurink, SILS).
- Monitoring of reactions in microfluidic devices by CARS-spectroscopy (Prof. M. Bonn, Prof. M. Müller, SILS-Amolf).

Dutch Research Schools and Technology Institutes

- Synthetic bio-organic chemistry in general (joint group meetings with the group of prof. R.V.A. Orru, dr E. Ruijter, VU University, HRSMC).

Dutch others

- Synthesis and applications of enantiopure unusual amino acids. (Prof. F.P.J.T. Rutjes, RU Nijmegen).
- Industrially relevant heterocycles through biocatalytic cascades (Prof. F.P.J.T. Rutjes, RU Nijmegen, Prof. J van der Oost, University Wageningen, Dr. M.C. R. Franssen, University Nijmegen).

International

- Structure of vanadium haloperoxidase enzymes. Dr. A. Messerschmidt, Martinsried, Germany.
- Solid State NMR studies of vanadium sites in vanadium haloperoxidases. Dr T. Polenova, University of Delaware, Newark, USA.
- Application of vanadium haloperoxidases in organic synthesis. Prof. J.-M. Aubry, Laboratoire d' Oxydation et de Formulation, Lille, France.
- Cyclic peptides containing endocyclic triazoles. Prof. M. R. Ghadiri, The Scripps Research Institute (La Jolla, USA).
- Cu(I)-catalyzed azide/alkyne cycloaddition, combination with cationic chemistry. Prof. V. V. Fokin and Prof. K. B. Sharpless, The Scripps Research Institute (La Jolla, USA).
- Bioorthogonal synthesis. Prof. C. R. Bertozzi, University of California Berkeley (USA).
- Vanadium K-edge XAS studies on the vanadium chloroperoxidase. Prof. D. C. Garner, Nottingham University, UK.

- Hydrogen-bonding to alkyl radicals. Prof. S. Hammerum, University of Copenhagen, Denmark.

Industrial

- ACTS/IBOS project " Sulfatases: Use of sulfatases in the production of sulfated carbohydrates and steroids. Wever and Hiemstra in cooperation with Van Delft (Universiteit Nijmegen); 1 postdoc, 1 aio; Industrial partners Syncom, Organon, Diosynth.
- Industrially relevant heterocycles through biocatalytic cascades (Prof. F.P.J.T. Rutjes, RU Nijmegen, Prof. J van der Oost, University Wageningen, Dr. M.C. R. Franssen, University Nijmegen) Industrial partners Syncom, Organon and DSM, 3PhD students, 2 PD and 1 TA.
- ACTS/IBOS SME Project "Enzymatic synthesis of non-natural amino acids " together with F.P.J.T. Rutjes RU Nijmegen and Prof. Dr. J. van der Oost, Wageningen University. Industrial partner Chiralex. 1PD.
- Collaboration on several projects, Prof. Dr. C.G. Kruse, Dr. B. van Steen, Dr. L.A.J.M. Sliedregt, Mr. A. van den Hoogenband, Dep. of Chemical Design and Synthesis, Solvay Pharmaceuticals (Weesp).
- Combinatorial cyclopeptide synthesis. (Dr. P.H.H. Hermkens, Dept. of Medicinal Chemistry, Organon Int. N.V (Oss).
- Enzymatic resolution and application of unusual amino acids and analysis of enantiomeric purity. Dr. B. Kaptein, L. Duchateau, DSM Research (Geleen).
- Development of cyclopeptides as synthetic vaccines. Dr. P. Timmerman, Pepsan B.V. (Lelystad).

5.2.3 Collaborations of theme 3

Catalysis

HIMS

- Synthesis and catalysis with metal compounds in micelles and dendrimers (De Cola/Molecular Photonics till 2007, continued with Münster).
- Ligand design, dendrimers, click chemistry (Hiemstra and Van Maarseveen/Bio-Molecular Synthesis).
- Heteroannulation involving intramolecular C-N bond formation (Biomolecular Synthesis/Hiemstra).

- Identification of metal compounds in micelles by physical methods (Complex Fluids/Eiser).
- Sharing of equipment (electrochemistry, Raman, FT-IR, NMR) with Hiemstra/Bio-Molecular Synthesis and De Cola/Molecular Photonics.
- Photocatalysis (Dr. Brouwer Molecular Photonics).
- Cooperation with Berend Smit/Meijer Computational Chemistry.
- Cooperation with Dr. Alexandre Dimian and with Prof. R. Krishna.
- Cooperation with Prof. R. Wever: Bio-chemo cascade catalysis.
- Cooperation with Prof. Wybren Jan Buma: Laser spectroelectrochemistry.
- Cooperation with Prof. Peter Schoenmakers: Polymer analysis

FNWI/UvA

- Prof.dr. J. Boon (SILS/Amolf) and others involved in the NWO/De Mayerne program.
- Spectral tuning in Photoactive Yellow Protein (Hellingwerf/SILS).
- Cooperation with Johan Westerhuis/Age Smilde (SILS).

Dutch Research Schools and Technology Institutes

- NRSC-C: Hydroformylation, hydrocyanation, dendrimers, catalyst separation. Prof. dr. D. Vogt, Technische Universiteit Eindhoven.
- NRSC-C: Supramolecular chemistry and catalysis. Prof. dr. R. J. Nolte/Prof A.E. Rowan Radboud Universiteit Nijmegen and Prof. Dr. B. Feringa, Rijks Universiteit Groningen.
- NRSC-C: Dendrimers, supramolecular chemistry. Prof. dr. E. W. Meijer, Technische Universiteit Eindhoven.
- NRSC-C: Dendrimers. Prof. dr. G. van Koten, University of Utrecht.
- NRSC-C: Catalyst separation. Prof. dr. J. Moulijn, Technische Universiteit Delft.
- Dr. M. Bickelhaupt, VU, computational analysis of supramolecular transition metal catalysts.
- HRSMC: Prof.dr. K. Lammertsma; VU, applications of low-valent P-compounds.
- HRSMC: Transition metal NMR. Prof.dr. J. Reedijk (Leiden Institute of Chemistry, University of Leiden).
- HRSMC: Combinatorial catalysis, catalytic transformations of biomolecules. dr. G. van der

Marel, Leiden Institute of Chemistry, Rijksuniversiteit Leiden.

- HRSMC: Spectroelectrochemistry of biologically relevant radical species. Prof. Dr. J. Reedijk (Leiden Institute of Chemistry, University of Leiden).
- NIOK: Prof.dr. G. Van Koten, dr. B. Deelman, dr. B. Klein Gebbink; Transition Metal catalyzed carbonylations and development of biphasic catalysts.
- NIOK: Transition metal NMR. Prof.dr. J. Reedijk (Leiden Institute of Chemistry, University of Leiden).
- NIOK: Ligand design for polymerization catalysis. Prof. dr. B. Hessen, Rijks Universiteit Groningen.

Dutch others

- CW-NWO: New fluororous catalysts in supercritical media. Shared PhD position with Dr. B.J. Deelman/prof. G. van Koten (UU).
- Dr. R.P. Sijbesma, TUE (sonor catalysis/switchable catalysts).
- Prof A. de Haan TUE (CW scheiding).
- Dr. M. Bickelhaupt (Theoretical work in progress).
- Cooperation with Prof. Freek Kapteijn, TU Delft.
- Dr. van Eck, Institute for Molecules and Materials (IMM), Radboud University Nijmegen.
- Prof. Rutjes, IMM, Radboud University Nijmegen.
- Cooperation with Dr. Isabel Arends, TU Delft.
- Cooperation with Dr. André ten Elshof at TU Twente.

International

- NWO: Taiwan-Dutch international program; Study of basic insertion and addition reactions involving late transition metal compounds with heterotopic bidentate carbene ligands. Exchange of PhD's and staff.
- Optimisation of ionic liquid solvents for catalytic reactions; collaboration with Prof. Ken Seddon (Belfast) and Quest-ICI (project is fully funded by ICI).
- Pd-catalyzed hydrogenation of alkynes involving parahydrogen for elucidation of mechanism. Prof. J. Bargon, University of Bonn, Germany till 2004 and prof. K. Woelk, University of Lajolla/Missouri, USA. 3 joint papers.

- Computational approaches of transition metal NMR spectroscopy and C-element bond activation. Dr. M. Bühl, University of Zürich, Switzerland, MPI, Mülheim, Germany (1997-2007). 4 joint papers.
 - ⁹⁹Ru NMR of Ru-catalysts, various collaborations (prof. J. Vos, Dublin, 1 joint paper).
 - ¹⁵N NMR spectroscopy of copolymerization catalysts. Dr. B. Milani University of Trieste, Italy (1999-2007). 4 joint papers.
 - Theory and applications of palladacyclic compounds. Prof.dr. M. Pfeffer and prof.dr. A. Dedieu, Univ. Strasbourg, France (1996-2007) Since 2002 one joint PhD student (A. Holuigue), 4 joint papers.
 - Selective hydrogenation reactions of unsaturated compounds using Pd- and Ru catalysts with N-ligands. Dr. P. Pelagatti, prof. F. Pelizzi, Università di Parma, Italy (1998-2007) regular exchange of students for 3-6 months.
 - Prof Sanders, Cambridge (on porphyrin cages, and DCC).
 - Prof Berkessel, Universität zu Köln (On chiral porphyrins/salphens and organocatalysis, and separations, work in progress).
 - Prof Bolm, University of Aachen (On chiral sulfonamide based METAMorphos ligands).
 - Prof Le Floch, University of Paris (On INDOLphos based on phosphole components).
 - Prof Juge, University of Dijon, (On P-chiral ligands).
 - Prof F. Zerbetto University of Bologna (Theoretical studies on asymmetric catalysis).
 - Prof J. Kikuchi Nara Institute of science and technology Japan (Catalytically active Cerasomes, work in progress).
 - Prof R. Réau University of Rennes (Encapsulation of phosphazole ligands).
 - Hydroformylation. Collaboration with Claver, Tarragona, Spain, several joint papers.
 - Clusters in catalysis. Collaboration with Chaudret, Toulouse, France.
 - In-situ spectroscopic studies. Collaboration with Heaton, Liverpool, United Kingdom.
 - Hydroformylation in *sc* CO₂, catalyst separation. Collaboration with Poliakov, Nottingham, United Kingdom.
 - Combinatorial Chemistry. Collaboration with Prof. Claude Mirodatos, Lyon, France.
 - Combinatorial Catalysis. Collaboration with Prof. Selim Senkan, UCLA, Los Angeles.
 - Collaboration with Dr. Janet Scott, Green Chemistry Centre, Monash University, Melbourne, Australia.
 - Collaboration with Dr. Hubert de Jonge, Danish Institute for Agricultural Sciences, Viborg, Denmark.
 - Conjugated molecular bridges. Collaboration with Dr. Paul J. Low, University of Durham, UK.
 - Time-dependent DFT Calculations. Collaboration with Dr. Stanislav Zalis, J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic.
 - Ultrafast energy and electron transfer. Collaboration with Prof. Robin Perutz, University of York, UK.
 - Redox and photochemical activation of complexes with aromatic phosphorus ligands. Collaboration with Prof. Pascal Le Floch, Ecole Polytechnique, Palaiseau, France.
 - Reactivity of metallo-radicals. Collaboration with Prof. Hansjörg Grützmacher, ETH Zurich, Switzerland.
 - Controlled Radical Polymerisation. Collaboration with Prof. Bradford Wayland, Temple University, Philadelphia, USA.
 - Cooperative Ligands. Collaboration with Dr. Cristina Tejel and Prof. Miguel Ciriano, CSIC institute/University of Zaragoza, Spain.
 - Advanced Pulls Methods in EPR spectroscopy. Collaboration with Dr. Ed Reijerse (MPI für Bioorganische Chemie, Mülheim a/d Ruhr, Germany) and Dr. Jeffrey Harmer (University of Oxford, UK).
 - Cooperation with Prof. Herbert Plenio (TU Darmstadt, Germany).
- EU
- EU Palladium project (5th Framework) Palladium, the chameleon catalyst; with dr B. Milani, prof. P. Braunstein, prof. G. Consiglio, dr. C. Bianchini, prof. C. Claver.
 - Member of COST D29 working group with Dr. M. Haukka (Joensuu, Finland), Prof. A. Deronzier (Grenoble, France) and Prof. M. J. Calhorda (Lisbon, Portugal).
 - REVCAT research training network, started in 2007, coordinator Prof. Reek.
 - Artizymes: EU STREp project, coordinator Prof. Kamer, St. Andrews (participant group Reek).
 - ERC Starting Grant (7th framework Ideas Program) on Carbene Insertion Reactions (B. de Bruin).

- Member of COST Action CM0802 PhoSciNet (13 countries).

Industrial

- Ongoing interactions with prof.dr. J.G. de Vries (DSM) and Prof.dr. R. Hage (Unilever).
- Volatilization of metals by encapsulation with tentacle Cp ligands. URENCO.
- Project on new polymerization catalysts with Van Leeuwen, Hessen (RUG). De Bruin and DPI, consortium of industries.
- DSM (supports the CW-combinatorial chemistry project).
- Engelhard de Meern (Large joined IS project).
- Engelhard de Meern, Shell, DSM, Degussa and Sasol (support the CW-scheidingsstechnology project in collaboration with Prof de Haan TUE).
- Philips, TNO (support the STW-project on conjugated polymers).
- Catalytic aromatic amination. Collaboration with Shell.
- Copolymerization/carbonylation. Collaboration with Solvay.
- Synthron (supports IBOS project).
- Arkema; selective carbonylation of specified alkenes.

5.2.4 Collaborations of theme 4

Computational Chemistry

HIMS

- Transfer-hydrogenation, Reek.
- Structure and dynamics of polymeric systems, Jerome and Eiser.
- Protein folding mechanisms, S. Woutersen.

FNWI/UvA

- Light sensitive proteins: K. Hellingwerf, SILS.
- Complex fluids, Sprik and Wegdam, Van der Waals Zeeman Institute.

Dutch others

- P.-R. ten Wolde, FOM-AMOLF. Nucleation and rare event simulations in chemistry and biology.
- M. Dijkstra, Debye Institute, Utrecht University. Structure and phase transition in colloidal dispersions.
- T. Vlucht, Condensed Matter and Interfaces, Debye Institute, Utrecht University. Condensed matter and interfaces.

- A. Fasolino, Radboud University. Carbon materials, Fiber formation.
- B. Mulder, FOM-AMOLF and Wageningen University. Dynamics of cellular processes.
- A.M.C. Emmons, Wageningen University. Molecular motors and dynamics of cellular processes.
- S.W. de Leeuw, Delft University of Technology. Modeling biomolecular systems.
- H.L. Tepper, FOM-AMOLF. Membrane permeation.
- R.A. van Santen, TUE. Silica assembly.
- H. Bakker, FOM-AMOLF, Proton transport in confined systems.
- M. Cohen Stuart, Wageningen University, self-assembly of fiber of silk-like proteins.
- S. Tans, FOM-AMOLF, chaperonin effect on protein folding and association.
- Rosa Bulo and Luuk Visscher, Theoretical Chemistry, VU Amsterdam, Development of adaptive QM/MM multiscale molecular dynamics method.
- John Kennis, Biophysics group at the VU Amsterdam. Signal transduction in the BLUF photoreceptor protein.

International

- S. Calero, Universidad Pablo de Olavide, Seville, Spain.
- T.S. van Erp, Centre for Surface Chemistry and Catalysis, Univ. of Leuven, Belgium.
- F. Keil, Chemical Reaction Engineering, Hamburg University of Technology, Hamburg, Germany.
- P. Sautet, Ecole Normale Supérieure de Lyon (ENS), Lyon, France.
- K. Kremer, Max Planck Institute for Polymer Research, Mainz, Germany.
- J.P. Hansen, Centre for Computational Chemistry, Cambridge University, UK.
- G. Ciccotti, Dept. of Physics, University of Rome "La Sapienza", Italy.
- J.-L. Barrat, Univ. Claude Bernard Lyon 1, Lyon, France.
- S.I. Sandler, Dept. of Chemical Engineering, University of Delaware, USA.
- C. Dellago, Dept. of Experimental Physics, University of Vienna, Austria.
- A.A. Louis, Dept. of Physics, Oxford University, UK.
- M. Sprik, Centre for Computational Chemistry, Cambridge University, UK.

- D. Chandler, Dept. of Chemistry, Univ. of California Berkeley, USA.
- U. Roethlisberger, Institute of Chemical Sciences, EPF Lausanne, Switzerland.
- M.L. Klein, Faculty of Chemistry, Univ. of Pennsylvania, USA.
- R. Sear, Dept. of Physics, University of Surrey, UK.
- M.W. Deem, Rice University, USA.
- W.C. Poon, Univ. of Edinburgh, UK.
- G. Zerah, CEA, France.
- J. Anwar, University of Bradford, UK.
- I. Pagonabarraga, Dept. of Physics, Univ. of Barcelona, Spain.
- H. Loewen, Institute for Theoretical Physics, Univ. of Düsseldorf, Germany.
- A. Masters, Dept. of Chemistry, Manchester University, UK.
- C. Das, University of Leeds, UK.
- T. Schilling, University of Mainz, Germany.
- R. Blaak, Heinrich Heine University, Düsseldorf, Germany.
- F. Fraternali, Kings College – London, UK.
- D.A. Kofke, SUNY – Buffalo, USA.
- Juerg Hutter and Joos Vandevondele, University of Zurich, Silica assembly.
- A.P. Sutton, A. Bailey, Imperial College Department of Physics London SW7 2AZ, UK.
- M. Cosentino Lagomarsino, Dip. di Fisica, Universit di Milano, Via Celoria 16, 20133 Milano, Italy.
- J. Krager, Experimental Physics, University of Leipzig, Germany.
- M. Parrinello, ETH Zurich, Lugano, Switzerland.
- S. O. Nielsen, University of Texas, Dallas, USA.
- P. B. Moore, University of the Sciences, Philadelphia, USA.
- X. Liu, Nanjing University.

Industrial

- T. Maesen, Hydrocarbon, ChevronTexaco, Richmond, USA.
- V.B.F. Mathot, DSM, NL.
- M. Noro and P. Warren, Unilever, Port Sunlight, UK.
- K. Velikov, Unilever Research Vlaardingem.

5.2.5 Collaborations of theme 5

Molecular Photonics

HIMS

- Vibrational Circular Dichroism; (VCD); Ingemann/Bio-Molecular Synthesis and Reek/Catalysis.
- Fluorescent Organocatalysts: Hiemstra/Bio-Molecular Synthesis
- Sharing of infrastructure with Elsevier, Reek/Catalysis.
- Crystal structure determinations; Peschar/Röntgen Diffraction.
- Labeled peptide synthesis; van Maarseveen/Biomolecular synthesis.
- Ultrafast catalytic reaction dynamics; Reek/Catalysis.

FNWI/UvA

- T. Gregorkiewicz (WZI) on silicon nanocrystals.
- P. Schall and D. Bonn (WZI) on fluorescent probing of interparticle contacts.
- K. Hellingwerf (SILS) on photoactive proteins and protein folding.
- M. Aalders and T.G. van Leeuwen (AMC) on fluorescent up-conversion nanoparticles.

Dutch Research Schools and Technology Institutes

- NRSC-C: Reek (UvA) joint project on application of photophysical and spectroscopic techniques in homogeneous catalysis.
- HRSMC: Biannual HRSMC course on Photochemistry, Photophysics and Photobiology.
- HRSMC: Molecular Modeling. Series of joint HRSMC courses. K. Lammertsma, A. Ehlers, Vrije Universiteit Amsterdam.
- HRSMC: Bi(tri)annual Tulip Summer School on Modern Developments in Spectroscopy. W.J. Buma and M.H.M. Janssen (VU).
- HRSMC: Summer School on Photochemistry (every 5 years).
- HRSMC: Biennial HRSMC course on Physical Methods in Inorganic Chemistry (Reedijk, Glaser, Lammertsma, Williams, Haasnoot, Bouwman, Hartl, Kooijman, Ingemann).

Dutch others

- J. Broos (RUG) on decay excited states of tryptophan and related compounds.
- I.H.M. van Stokkum (VU) on global fitting dynamics of excited states.
- F. Ariese and C. Gooijer on pyridine N-oxides.
- E.J. Baerends on calculations of VCD spectra.
- FELIX facility (FOM-Rijnhuizen): use of FEL and construction of new facilities.
- A. Rijs (FOM-Rijnhuizen) on high-resolution spectroscopy on molecular machines.
- J. Oomens (FOM-Rijnhuizen) on energy and charge transport in isolated and aggregated triphenylenes and pyrenes.
- NanoNed Flagship Chemistry and Physics of Individual Molecules (with Feringa, Driessen, Dekker, Rowan).
- Rotational molecular motors. B.L. Feringa (RUG).
- Photophysics of silicon nanoparticles. H. Zuilhof (WUR).
- Photoinduced processes in non-covalently linked multicomponent systems. R. Nolte, M. C. Feiters, University of Nijmegen.
- Collaboration with M. Bonn, Amolf, Amsterdam on photoelectric dynamics in nanocrystals and solar cell materials (ZnO).
- Collaboration with R.A.J. Janssen en A.P.H.J. Schenning (TU/e) on energy and electron transfer in organized dye systems.
- Collaboration with R.J.M. Nolte and A.E. Rowan on α -sheet helices.
- Collaboration with H.J. Bakker and M. Bonn on proton transport.

International

- M. Blanchard-Desce (Rennes) on excited state properties of systems with large cross-sections for two-photon excited fluorescence.
- B. Mennucci (Pisa) on calculations of solvatochromic dyes.
- J. Hofkens (Leuven) on single molecule spectroscopy.
- Photoinduced matter migration, photochemical and photophysical aspects. E. Ishow, ENS Cachan.
- Electrochemistry of rotaxanes. F. Paolucci, Bologna.
- Tetraxanes. P. Audebert (ENS Cachan).
- Flavin rotaxanes. G. Cooke (Glasgow).
- Excited state dynamics of rotaxanes. F. Zerbetto and M. Garavelli (Università di Bologna).

- Quantum chemical calculations on excited states of chromophores of PYP. H. Köppel (University of Heidelberg).
- Vibronic coupling in excited states of acetylene. R.W. Field (MIT).
- Spectroscopy and dynamics of excited states of chromophores of PYP and GFP. Prof. D. Pratt (University of Pittsburgh).
- Development of new laser desorption techniques. M.S. de Vries (UCSB).
- Excited-state intramolecular proton transfer reactions. J. Waluk (Polish Academy of Sciences) and I. Petkova (Bulgarian Academy of Sciences).
- Excited-state dynamics of pyridine N-oxides. A. Szemik-Hojniak (University of Wrocław).
- Vibrational circular dichroism. L. Nafie (Syracuse University).
- Molecular imprinting of polymers. B. Wandelt (University of Lodz).
- Modeling of Cu/ZnO/SiO₂ Catalysts. Catlow (The Royal Institution of Great Britain) and Frost (Johnson Matthey; Fuel Cells).
- Collaboration with X.G. Kong, CIOMP, Changchun, China on bioactive luminescence up-conversion nanocrystals.
- Collaboration with M. Casalboni, P. Proposito (University of Rome 'Tor Vergata', Rome, Italy) on ultrafast dynamics in sol-gel materials.
- Collaboration with M. Kubinyi (Budapest University of technology and Economics, Budapest, Hungary) on intramolecular proton transfer dynamics.
- Collaboration with F.k Würthner (Würzburg) on photophysical properties of perylene imides and related dyes in supramolecular complexes.
- Collaboration with P. Hudhomme (Angers) on perylenebisimide-fullerene dyads.
- Photoactive multimetallic assemblies. Royal Chemical Society grant with Pikramenou, University of Edinburgh., UK.
- Photophysical properties of novel tripod systems. P. Belser, University of Fribourg, Switzerland.
- Development of new 2D-IR techniques. P. Hamm, University of Zürich, Switzerland.

EU

- STREP Network Hydrogen-bond assembled mechanically interlocked molecular motors: University of Amsterdam (coordinator), University of Edinburgh (Prof. David Leigh),

Commissariat à l'Énergie Atomique (Prof. Francois Kajzar), University of Bologna (Prof. Francesco Zerbetto), University of Groningen (Prof. Petra Rudolf), Consiglio Nazionale delle Ricerche, Bologna (Dr. Fabio Biscarini), Intertek ASG (Dr. Philip Nash)(2005-2008).

- STREP Network Switch-able materials and their fabrication technology for Multifunctional TAG: Consorzio INSTM, Florence (coordinator), Universiteit van Amsterdam, University of Edinburgh (Prof. David Leigh), Université Libre de Bruxelles (Prof. Yves Geerts), BASELL Poliolefine Italia Srl, SCRIBA Nanotecnologie Srl (2007-2009).
- RTN Network UNIdirectional NANOscale molecular wires assembled with cyclodextrin CUPS (UNI-NANOCUPS): Birmingham: Dr. Zoe Pikramenou (project leader), Warwick: Prof. Pat Unwin, Dr. Mike Hannon, Dr. Julie Macpherson Nijmegen: Dr. Martin C. Feiters. Dublin: Prof. Robert J. Forster Kassel: Dr. Frank Hubenthal, Prof Frank Träger Demokritos: Dr. Irene M. Mavridis, Dr. Konstantina, Dr. Nikos Glezos.
- ERA Nanosciences project Molecules and Light in Individual Metallic Nanostructures (MOLIMEN): Dr. A. Débarre (Orsay), Prof. B. Mennucci (Pisa) and Dr. M.H.V. Werts (Rennes).

Industrial

- Laser decoration of polymer surfaces and on the development of rotaxane based unconventional materials; T. Loontjens, DSM, Geleen.
- Vibrational Circular Dichroism (VCD) and photophysics and photochemistry of steroids; R. Bursi, M. Honing and E. Kellenbach (Schering Plough).
- Dynamics of film formation of coatings; T. Nabuurs, DSM Neoresins, Waalwijk. Project supported by Dutch Polymer Institute.

5.2.6 Collaborations of other activities

5.2.6.1 Collaborations of Polymer and Process Systems

HIMS

- Schoenmakers/Macromolecular and Biosystems Analysis.

Dutch Research Schools and Technology Institutes

- Collaboration with Dutch Research School Process Technology (OSPT), member of management-team.

Dutch others

- Partnership in TIPb (Toegepaste Industriële Procesbeheersing, Amsterdam).
- Collaboration with DSM/Sabic.
- Collaboration with Dow Chemicals, Terneuzen.
- Collaboration with Dutch Polymer Institute (DPI).
- Cooperation with Polymer groups TUE.

International

- Collaboration with BASF, Ludwigshafen.
- Collaboration with Dr. Wulkow, CIT GmbH, Rastede, D.
- Collaboration with Programa de Engenharia Química/COPPE, Universidade Federal do Rio de Janeiro (visiting researcher: Dr. Priamo Melo).
- Collaboration with European Federation of Chemical Engineering, Working Party Polymer Reaction Engineering.
- Collaboration with the European Graduate School on Control of Microstructural Properties in Radical Polymerization (with TUE, Univ. Goettingen, Univ. Clausthal).

5.2.6.2 Collaborations of Röntgen Diffraction

Dutch others

- Phase behaviour of fats in dynamic systems, in relation to the atomic structure of triacylglycerols. ADM Cocoa (Koog aan de Zaan), Gerken's Cacao (Wormer), Koninklijke De Ruyter (Baarn), Nestlé Nederland (Nunspeet).
- Effect of additives on the phase behaviour of lipids. Dr. I. 't Zandt (Loders Croklaan, Wormerveer).
- Development of environmental-friendly flame retardants based on melamine and its derivatives. Prof. A. Kentgens, Dr. E. van Eck, Dr. A. Brinkmann (all Solid-State NMR group, KUN).
- Examination of painting pigments. Dr. J. Dik (TU Delft).

International

- Structure determination of cyclodextrin inclusion compounds, Dr. Gh. Borodi

(National Institute for R&D of Isotopic and Molecular Technologies (Cluj-Napoca, Romania).

- Dipertenes. Prof. L. Pieters (University of Antwerp, Belgium).
- Organic compounds. Prof. B. Maes, Dr. S. Hostyn (University of Antwerp, Belgium).

Industrial

- PANalytical (Almelo), research in the field of powder diffraction.
- Crystallization of cream and milkproducts. Campina. (Oud Gastel).
- Cocoa butter replacing materials. Cargill (Vilvoorde, Belgium).
- Chocolate analysis. Kraft Foods R&D Inc. (Muenchen, Germany).
- Analysis of palmoilfractions. CSM Unipro (Merksem, Belgium).
- Aluminum hydroxides. Hal Allergy (Haarlem).

5.3 Dissertations 2008

5.3.1 Dissertations of theme 1

Macromolecular and Biosystems Analysis

- Pra, M. de (2008, October 24). Pillar-structured microchannels for liquid chromatography.
- Prom./coprom.: Prof. dr. ir. P.J. Schoenmakers & dr. W.Th. Kok.
- Stanimirovic, O. (2008, December 4). Optimal sensor placement and timing. Where and when to measure?
Prom./coprom.: Prof. dr. A.K. Smilde

5.3.2 Dissertations of theme 2

Bio-Molecular Synthesis

- Berkheij, M. (2008, April 10). Synthesis of 1,3-diene-containing alpha-amino acids and peptides via N-acyliminium ions.
Prom./coprom.: Prof. dr. H. Hiemstra, Prof. dr. H.E. Schoemaker & dr. J.H. van Maarseveen.
- Herk, T. van (2008, March 6). Bacterial class A acid phosphatases as versatile tools in organic synthesis.
Prom./coprom.: Prof. dr. R. Wever.
- Sonke, T. (2008, March 13). Novel developments in the chemo-enzymatic synthesis of enantiopure alpha-hydrogen-and alph,

alpha-disubstituted alpha-amino acids and derivatives.

Prom./coprom.: Prof. dr. H.E. Schoemaker & Prof. dr. R. Wever.

- Springer, J. (2008, November 6). A combinatorial approach towards pharmaceutically relevant cyclic peptides.
Prom./coprom.: Prof. dr. H. Hiemstra & dr. J.H. van Maarseveen.

5.3.3 Dissertations of theme 3

Catalysis

- Duran Pachon, L. (2008, April 10). Synthesis and application of nano-structured metal catalysts.
Prom./coprom.: Prof. dr. C.J. Elsevier & Prof. dr. G. Rothenberg.
- Holuigue, A.F. (2008, February 29). Palladacycles: Synthesis and Catalysis.
Prom./coprom.: Prof. dr. C.J. Elsevier & M. Pfeffer.

5.3.4 Dissertations of theme 4

Computational Chemistry

- Argentini, R. (2008, June 19). Flow and flexibility: applications in biophysics.
Prom./coprom.: Prof. dr. D. Frenkel & dr. C.P. Lowe.
- Berkenbos, A. (2008, September 9). The dynamics of polymers by novel mesoscopic methods.
Prom./coprom.: Prof. dr. D. Frenkel & dr. C.P. Lowe.
- Bozorgui, B. (2008, December 9). Computational methods to study strongly-binding polymer-colloid systems.
Prom./coprom.: Prof. dr. D. Frenkel.
- Huisman, B.A.H. (2008, September 30). Dynamical and structural self-organization.
Prom./coprom.: Prof. dr. A. Fasolino.
- Leenders, E.J.M. (2008, September 12). Proton transfer in the photocycle of the photoactive yellow protein.
Prom./coprom.: Prof. dr. P.G. Bolhuis & dr. E.J. Mayjer.
- Liu, B. (2008, November 4). Molecular simulation studies of adsorption and diffusion phenomena of gases in porous materials.
Prom./coprom.: Prof. dr. ir. B. Smit.

- Poelwijk, F.J. (2008, May 29). Fitness landscapes of gene regulation in variable environments. Prom./coprom.: Prof. dr. D. Frenkel & dr. ir. S.J. Tans.
- Juraszek, J. (2008, May 29). Proteins in action. Prom./coprom.: Prof. dr. P.G. Bolhuis.

5.3.5 Dissertations of theme 5

Molecular Photonics

- Balkowski, G.M. (2008, October 16). Ultrafast excited state dynamics of the proton sponge, oligodiacetylenes and supramolecular assemblies. Prom./coprom.: Prof. dr. W.J. Buma & dr. H. Zhang.
- Dokter, A.M. (2008, March 19). Water in confinement (ultrafast dynamics of water in reverse micelles). Prom./coprom.: Prof. dr. H.J. Bakker & dr. S. Woutersen.
- Jukes, R.T.F. (2008, April 15). Photochromic systems for energy transfer switching. Prom./coprom.: Prof. dr. L. De Cola.
- Rezus, Y.L.A. (2008, januari 10). Snapshots of water. Prom./coprom.: Prof. dr. H.J. Bakker.
- Vasic, M. (2008, December 1). Synthesis and photophysics of functionalized silicon nanoparticles. Prom./coprom.: Prof. dr. L. De Cola & Prof. H. Zuilhof (Universiteit Wageningen).

5.3.6 Dissertations of other activities

- Van Mechelen, J.B. (2008, September 9). Triacylglycerol structures and the chocolate fat bloom mechanism. Prom./coprom.: Prof. dr. H. Schenk & dr. R. Peschar.

5.4 Science policy functions

5.4.1 Science policy functions of theme 1

Macromolecular and Biosystems Analysis

P.J. Schoenmakers

- Instigator and coordinator of national initiative on Comprehensive Analytical Science and Technology (COAST).

- Member of European Graduate School on Free-Radical Polymerization.
- DPI coordinator Polymer Analysis and Characterization.
- Consultant to Dow Chemical.
- Consultant to AstraZeneca (Sweden).
- Consultant to Institute for Food Science University of Messina, Italy.
- Consultant to Australian Centre of Excellence in Research on Separation Science (ACROSS).
- Consultant to Teijin Twaron (Arnhem).
- Member BAR HIMS.
- Chairman Onderwijs Commissie Scheikunde (OCS).
- Member of the Permanent Scientific Committee of the International Symposium on Liquid-Phase Separations.
- Initiator and chairman of the “International Symposium on the Separation and Characterization of Natural and Synthetic Macromolecules”, a biennial series of meetings held in Amsterdam (2003, 2006, 2007, 2009).
- Member of the organization committee and scientific committees of the HTC symposium series.
- Member of scientific committee and advisor of several other conferences, including the Balaton Symposium on High-Performance separation methods, and the International Symposium on Separation Sciences.
- Ed. Board (from ca. 1992) and editor (from 2003) of the Journal of Chromatography (ranked 2nd).
- Ed. Board of Separation Science.
- Ed. Board of Chromatographia.
- Ed. Board of LC-GC.
- Ed. Board Encyclopedia of Separation Science.
- Consultant and Ed.-Board member of Chromedia.

W. Th. Kok

- Coordinator of the UvA-VU MSc program Analytical Sciences.
- Treasurer MacroMol International Symposium Series on the Separation and Characterization of Macromolecules.
- Treasurer of HPLC 2013, the International Symposium on Liquid Phase Separations, Amsterdam, June 2013.
- Member Editorial Board Chromatographia.
- Member of the Advisory Board of the Hogeschool Utrecht, Inst. Life Sci. & Chemistry.

5.4.2 Science policy functions of theme 2

Bio-Molecular Synthesis

H. Hiemstra

- Member of the International Society of Heterocyclic Chemistry (ISHC).
- Member of the American Chemical Society.
- Member of the Scientific Committee National Research School Combination Catalysis (NRSC-C).
- Member research committee HRSMC.
- Member Genootschap ter bevordering van Natuur-, Genees- en Heelkunde.
- Member Nederlands Instituut voor Onderzoek in de Katalyse (NIOK).
- Member of the KNCV, section Organic Chemistry.
- Member of the Kamer Scheikunde, VSNU.
- Member directorium HIMS.
- Member of the International Scientific Committee, European Symposia on Organic Chemistry (ESOC).
- Member of the Editorial Board European Journal of Organic Chemistry (since 2006).
- Guest Editor of Volume 48 of Science of Synthesis, Houben-Weyl Methods of Molecular Transformations.
- Educational director Master School of Sciences, Faculty of Sciences, UvA.
- Program director Master Chemistry, Faculty of Sciences, UvA.

H. E. Schoemaker

- Member of the industrial advisory board of Advanced Synthesis and Catalysis.

R. Wever

- Chairman Examencommissie Scheikunde en Bio-exact.
- Chairman Opleidingscommissie beta-gamma bachelor.
- Co-organizer 4th Japanese-Netherlands Joint Seminar, September 2008, Japan.
- Member of the Board Genootschap ter bevordering van Natuur-, Genees- en Heelkunde.
- Member Board of the Netherlands Society for Biochemistry and Molecular Biology (NVBMB).

J.H. van Maarseveen

- Treasurer KNCV, Section Organic Chemistry.
- Member Genootschap ter bevordering van Natuur-, Genees- en Heelkunde.

- Member of the KNCV, section Organic Chemistry.

S. Ingemann

- Member of the KNCV.
- Member Genootschap ter bevordering van Natuur-, Genees- en Heelkunde.
- Member of the Dutch Society for Mass Spectrometry.
- Program director for the Bachelor Chemistry and the Bachelor Life-sciences (Bio-exact), Faculty of Sciences, UvA.

5.4.3 Science policy functions of theme 3

Catalysis

P.W.N.M. van Leeuwen

- Member of the editorial board of Dalton Transactions.
- Member International Advisory Board Advanced Synthesis and Catalysis.
- Series editor Catalysis by Metal Complexes, Springer.
- Consultant to Cataluña Network on Homogeneous Catalysis.
- Member of the Advisory board International Symposium on Relations between Heterogeneous and Homogeneous Catalysis.
- Member 'Academie-Commissie Chemie', KNAW
- Member Advisory Board Netherlands Congress for Chemistry and Catalysis.
- Chairman advisory board Faculty of Chemistry Tarragona (URV).
- Consultant to Sasol S.A.

C.J. Elsevier

- Scientific Director of the Holland Research School of Molecular Chemistry (HRSMC), since 01-10-2001.
- Member of the Board of NIOK.
- Member of the management committee and project group EU COST D30.
- Member education committee NIOK
- Initiator and Coordinator Master "Molecular Design, Synthesis & Catalysis" (together with VU).
- HRSMC Autumn School (organization and development curriculum courses 2007-6).
- Consultant to Sasol South-Africa (high pressure NMR).

- Consultant to ICI (Benelux) NMR advice.
- Consultant to Unilever (ad hoc).
- NWO (various NWO-panels; chair NWO-groot, middelgroot (2007-7).
- Member of the Board of EUCHEMS conferences Organometallic Chemistry.
- Vice-chair NCCC conferences.
- Member of the editorial board of Magnetic Resonance in Chemistry (2003-).
- Member of the editorial board of European Journal of Inorganic Chemistry. (1997-).
- Member of the editorial board Collection Czechoslovak Chemical Communications/ Czechoslovakian Academy of Sciences. (1998-).

G. Rothenberg

- Member of the NRSC-C workgroup 'bridging the gap' (between homogeneous and heterogeneous catalysis).
- Member of the NWO-CW VENI committee.
- Scientific director and co-founder of the spin-off company Yellow Diesel BV.
- Secretary of the Exams committee chemistry and bio-exact.

J. Reek

- Invited visiting professor University of Rennes
- Elected member of the young Royal Dutch Academy of Sciences (KNAW).
- Member of VIDI committee 2006.
- Member of various NWO-committees.
- Member of Royal Dutch Chemical Society (various sections).
- Member of the NIOK-research committee.
- Member Scientific Council NRSC-C. Top Research School Combination Catalysis.
- Member of the management committee of the NRSC-C since 2007.
- Member of the editorial board of European Journal of Inorganic Chemistry.
- Consultant to Shell.
- Scientific director and founder of spin-off company Cat-fix.
- Member of the committee of various academic functions.
- Member of the KNAW recognition committee for research schools.

B. de Bruin

- Member of the Board of NIOK (on behalf of the University of Nijmegen).

- Member of the Board of the KNCV-NWO/CW section 'Coordination chemistry and homogeneous catalysis'.

F. Hartl

- Invited visiting professor, Chuo University, Tokyo, Japan.
- Invited visiting professor, Joseph Fourier University, Grenoble, France.
- Member of the Royal Society of Chemistry, UK.
- Member of the European Photochemistry Association.
- Consultant to Bruker Optics Ltd.
- Associate editor and member of the editorial board of the Collection of Czechoslovak Chemical Communications (since 1998).

J.I. van der Vlugt

- Member of Royal Dutch Chemical Society.
- Member of the Board of the KNCV-NWO/CW section 'Coordination chemistry and homogeneous catalysis'.

5.4.4 Science policy functions of theme 4

Computational Chemistry

B. Smit

- Elected director of CECAM, Lyon (2006-2008).
- FOM- vice chairman FOM/v program Women in Physics.
- Editor of Computational Science Series.
- Member of DFG/NWO sponsored Graduate School on Diffusion in Zeolites, linking University of Leipzig with research groups in Amsterdam, Delft and Eindhoven.
- Advisory Board, Physical Chemistry Chemical Physics (PCCP).
- Vice chair ESF-COST program MolSimu.
- Coordinator Marie Curie program series of events MolSimu 2004-2008.
- Coordinator Marie Curie program series of events Psi-k Training 2006-2009.
- Coordinator Marie Curie early stage training program EuroSim 2006-2010.
- Team leader Marie Curie excellence grant BiMaMoSi 2006-2008.
- Member of the international steering committee of the Thomas Young Centre, London.

A. Fasolino

- Board Member Semiconductor and Insulators Section of the Condensed Matter Division of European Physical Society.
- Member of several evaluation panels of the Swedish Research Council, Istituto Nazionale della Materia (Italy), Italian Ministry of University and Scientific Research.
- Coorganizer (with H. van Beijeren) of the yearly course of the landelijke onderzoeksschool Theoretische Fysica, Jonkerbosch.

R. Krishna

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

D. Frenkel

- Dutch representative Scientific Council Centre Européen de Calcul Atomique et Moleculaire.
- Member of the EPS Liquids Board.
- Voorzitter KNAW Commissie voor Biochemie en Biofysica.
- Member external Advisory Board INFM Research and Development Center SMC at La Sapienza University, Rome.
- Member advisory board John van Neumann Center (Germany).
- Partner EU network NUCLEUS.
- Member editorial board Molecular Physics.
- Member editorial board Soft Matter.
- Coordinator of the FOM program on Structure and function of soft materials, Physical Biology I and II, FOM-Shell IPP Innovative Physics for Oil and Gas.
- Honorary Professor, Beijing University of Chemical Technology.
- Member of the Royal Society in London.
- Honorary Doctorate, University of Edinburgh.
- Professor of Chemistry, University of Cambridge.

E.J. Meijer

- Member NWO/CW Study group Spectroscopy and Theoretical Chemistry.
- Member of FOM network Statistische Fysica.
- Workgroup chair ESF-COST program MolSimu.
- Coordinator Erasmus Mundus program AtoSim (2006-2011).
- Member ESF-COST AIDM4GRID.

- UvA representative Scientific Council CECAM (Centre Européen de Calcul Atomique et Moleculaire).

P.G. Bolhuis

- Co-organizer CECAM workshop Conformational dynamics in complex systems.
- Co-organizer 3-months programme Metastability and Rare Events in Complex Systems, held at the Erwin Schrödinger Institut in Vienna, Feb-April 2008.
- FOM-coordinator group A-23.
- Member of FOM network Statistische Fysica.

C.P. Lowe

- Co-organizer Write it right, international workshop on writing scientific papers (with Gadi Rothemberg).

B. Ensing

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

5.4.5 Science policy functions of theme 5**Molecular Photonics**

W.J. Buma

- Initiator and co-ordinator EC-funded STREP Hy3M (2005-2008).
- Co-initiator EC-funded STREP STAG (2006-2009).
- Member transnational Micro- en Nanotechnology network organized from Università degli Studi di Bologna, Italy, for co-tutoring PhD students.
- Scientific Director HRSMC.
- Chairman NWO-CW Study group Spectroscopy and Theory.
- Member Beleidsadviesraad HIMS.
- Senate member University of Amsterdam.
- Co-coordinator Amsterdam Master in Physical Sciences.
- HRSMC Biannual HRSMC course on Photochemistry, Photophysics and Photobiology.
- Co-chairman of the HRSMC and ESF Dyna Program Graduate School on Modern Developments in Spectroscopy, Noordwijk, The Netherlands, April 15-18, 2009.

- Associate editor Research Letters in Physical Chemistry.
- Member International Advisory Committee ERPOS-11, July 13-17 (2008), Piechowice, Poland.

A.M. Brouwer

- Bijzonder Hoogleraar Molecuulspectroscopie via het John van Geunsfonds (2006-2011).
- Member of Intersociety Committee on Photochemistry.
- Co-chairman of the IUPAC project Reference methods, standards and applications of photoluminescence (2002-2008).
- Member PR en Studentenweringscommissie Scheikunde.
- Chairman Opleidingscommissie Scheikunde
- Member universitaire bibliotheekcommissie (2006-).
- HRSMC Molecular Modeling. Series of joint HRSMC courses with Dr. A. Ehlers and Prof. dr. K. Lammertsma, Vrije Universiteit Amsterdam.
- Member of the international organizing committee of the IUPAC Symposium on Photochemistry, Gothenburg, 2008.
- Member of the organizing committee of HRSMC/EPA Summer School on Photochemistry (2008).
- Project leader of ERA Nanoscience network MOLIMEN (2006-2011).
- Member of editorial board of International Journal of Spectroscopy.
- Invited professor at Ecole Normale Supérieure de Cachan, France (2008-2009).

R.M. Williams

- Member of the Editorial Advisory Board of The Open Inorganic Chemistry Journal.
- Local Treasurer of the European Photochemistry Association.
- Auditor to the International Treasurer of the European Photochemistry Association.
- Member of the International Scientific Organizing committee of EURESCO conference Supramolecular Chemistry, EuroConference on Molecular Rods, Wires and Switches, 14-19 September 2002, San Felui, Spain.
- Member of the International Scientific Organizing committee of IUPAC Photochemistry, 2004, Granada, Spain.
- Member of the International Scientific Organizing committee of IUPAC Photochemistry, 2-7 April 2006, Kyoto, Japan.

- Co-initiator of EC-funded Research and Training Network UNI-NANOCUPS (2004-2008).
- Member of the Habilitation à Diriger des Recherches committee of Martijn H.V. Werts in Rennes, 23 May 2008.
- Member of the American Chemical Society.
- Member of the European Photochemistry Association.
- Member of the FNWI library committee.

H. Zhang

- Member of the organizing committee of the International conference on luminescent properties of doped nanomaterials, 11-16 November 2008, Zhuhai, China.
- Professor at Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences.
- Guest professor at Suzhou Institute of Nanotech and Nanobionics, Chinese Academy of Sciences and Northeast Normal University, China.
- Coordinator of KNAW (the Netherlands) – CAS (China) exchange programme on cancer cell detection and therapy via upconversion nanocrystals.
- Member of HIMS seminar committee.

S. Woutersen

- Member VENI jury 2008.
- Coach for NWO for new VENI applicants.

5.4.6 Science policy functions of other activities

R. Peschar

- Co-editor of Zeitschrift für Kristallografie.
- Member of the NWO study group Chemie van de vaste stof en materiaalkunde.
- Secretary of the NWO study group Kristal- en Structuuronderzoek.
- Secretary of the National Committee for Crystallography in the Netherlands.
- Executive Director of the NWO/CW AIO School Kristal en Structuuronderzoek.

P. Iedema

- Member scientific committees on WP-CAPE events ESCAPE.
- Member Management team Dutch Research School Process Technology (OSPT).

5.5 Financial report 2008

This chapter shows a survey of benefits versus expenditures for The first stream of money (1st; direct university funding)

External funds 1st (NRSC-Catalysis, HRSMC), 2nd (FOM, NWO-CW, STW) and 3rd (EU, BSIK, industrial funding)

HIMS 2007 – 1 st , 2 nd and 3 rd	Budget (k€)	Costs (k€)					(k€)
Source of funding	Total	Personnel	Equipment/ Consumables	Compensation Costs 5)	Housing, IC, etc	Total	Result
Direct/UvA, 1 st	10431	4396	723	2092	2566	9778	653
External funding, 1 st 1)	126				187	187	-61
HRSMC 2), 1 st	50	50				50	0
NRSC-C 3), 1 st	380	271	53			324	56
Matching running projects 4), 1 st	331			153		153	178
Total UvA funding, 1 st	11318	4717	776	2245	2753	10491	827
External funding, 2 nd	1336	1212	241	-1296	1136	1293	43
External funding, 3 rd	2151	1159	733	-949	1178	2121	30
Total	14804	7088	1750	0	5067	13905	899

1) Additional 1st money stream income (teaching income, interest, etc.)

2) HRSMC = Holland Research School of Molecular Chemistry

3) NRSC-C = Top Research School NRSC-Catalysis

4) Matching for Veni, Vidi, Vici projects, NanoNed and NanoImpuls projects, etc.

5) Compensation costs (needed to compensate the overhead costs of external, e.g. 2nd and 3rd stream of money, projects)

Concluding remark

Several positions of staff members with permanent positions are temporarily financed with external funds (8.7 Fte; > 500 k€ in 2008).

5.6 Personnel

5.6.1 Personnel of the research themes of HIMS (2008)

Internally/UvA funded personnel and externally funded professors

Macromolecular and Biosystems Analysis: 1 chair, collaboration with SILS ¹⁾

Staff: Prof. dr. P.J. Schoenmakers (chair holder 'Polymeeranalyse' ²⁾), Prof. dr. H.G. Janssen/Unilever (0.2 Fte; 'Analytische Scheidingen van Biomacromoleculen'), Prof. Dr. S. van der Wal/DSM (0.2 Fte; 'Bioterials Analysis', Dr. W.Th.Kok (UHD), vacancy (UD).

Supporting staff: P.J. Aarnoutse, T. Aalbers, P. Verschuren.

¹⁾ Collaborations with De Koster/SILS & Smilde/SILS)

²⁾ Teaching and research activities also partly in the field of forensic sciences

Bio-Molecular Synthesis: 2 chairs

Staff: Prof. dr. H. Hiemstra (chair holder 'Synthetische Organische Chemie'), Prof. dr. R. Wever (chair holder 'Biokatalysatoren en Bio-Anorganische Chemie'), Prof. dr. H.E. Schoemaker/DSM (0.2 Fte; 'Industriële Fijnchemie'), Prof. dr. P. Timmerman/Pepsan (0.2 Fte; 'Protein-mimetic Chemistry'), Dr. J.H. van Maarseveen (UHD), Dr. S. Ingemann Jørgensen (UD), Dr. S.S. Kinderman (Veni Laureate).

Supporting staff: M.J. Wanner, H. Bieraugel, J. Dijkink, A.F. Hartog.
Added to the theme BMS with tasks for HIMS as a whole: J.A.J. Geenevasen (NMR department), J.C.M. Steeneken (Electronics and NMR equipment).

Catalysis: 3 chairs

Staff: Prof. dr. J.N.H. Reek (chair holder 'Supramoleculaire Chemie'; Vici Laureate), Prof. dr. C.J. Elsevier (chair holder 'Coördinatie- en Organometaalchemie'), Prof. dr. P.C.J. Kamer (0,1 fte; Homogene Katalyse), Prof. dr. G. Rothenberg (chair holder 'Heterogen katlyse en Duurzame Chemie'; Vidi Laureate). Dr. B. de Bruin (UHD; Vidi and ERC Laureate:), Dr. J. Van der Vlugt (UD;

Veni Laureate), Dr. E. Eiser (UD; 0.1 Fte), vacancy (UD).

Supporting staff: F. ait el Maate, E. Bertelink, M. Mittelmeijer, D. Tromp, C. Mahabiersing, A.M. van der Burg.

Added to the theme with tasks for HIMS as a whole: J.M. Ernsting (NMR department), P.F. Collignon (Electronics and process automation).

Molecular Photonics: 1 chair

Staff: Prof. dr. W.J. Buma (chair holder; 'Molecuulspectroscopie'), Prof. dr. H.J. Bakker/FOM-Amolf (0.2 Fte; 'Ultrasnelle Spectroscopie van Moleculen in de Gecondenseerde Fase'), Prof. dr. A.M. Brouwer (0.2 Fte; Molecuulspectroscopie), Dr. H. Zhang (UD), Dr. R.M. Williams (UD), Dr. S. Woutersen (UD; Vidi and ERC Laureate).

Supporting staff: M.M. Groeneveld, Drs. M. Hilbers, S. Kettelarij, P. Reinders.

Computational Sciences: 2 chairs

Staff: Vacancy (chair holder; 'Complex Molecular Simulations'), Prof. dr. R. Krishna (chair holder; 'Chemische Reaktorkunde'), Prof. dr. D. Frenkel/FOM-Amolf (0.2 Fte; 'Macromoleculaire Simulaties'; Spinoza Laureate), Prof. dr. A. Fasolino/KUN (0.0 Fte; Computationale Fysica van de Gecondenseerde Materie'), Prof. dr. P.G. Bolhuis (0.2 Fte; 'Simulations of Bio-molecular Systems'; Vidi, Vici and FOM Springplank Laureate); Dr. E.J. Meijer (UHD), Dr. C.P. Lowe (UHD), vacancy (UD), dr. B. Ensing (Vidi Laureate).

Supporting staff: Dr. J. Ellenberger.

5.6.2 Personnel of the other research activities of HIMS (2008)

Internally/UvA funded personnel and externally funded professors

Polymer and Process Systems: 1 chair ³⁾

Prof. Dr. P. Iedema (Fysische Technologie, associated with group Schoenmakers).

³⁾ As a consequence of the reorganization of the chemistry department the chair was discontinued in December 2002. Research and teaching activities were continued in 2008 on a personnel basis, mainly in the field of restoration sciences.

Scanning Tunneling Microscopy

Dr. J.C. v.d. Heuvel (UHD, associated with the group Reek).

Research and teaching activities were continued in 2008 on a personnel basis, including outreach activities in collaboration with the Amstel Institute.

Röntgen Diffraction department ⁴⁾,
collaborations with WZI and IBED

Staff: Dr. R. Peschar (UD).

Supporting staff: Drs. K. Goubitz, E.J. Sonneveld, and Drs. J. Fraanje.

⁴⁾ Former research group Crystallography, the chair holder Prof. Dr. H. Schenk retired at 01-01-2006.

5.6.3 Management, supporting groups and other activities (2008)

Internally/UvA funded personnel

Management of HIM5

Scientific Director: Dr. R.L.J. Zsom.

Management team (bedrijfsvoering):

G.J.J. Zonneveld - De Boer, Mrs. Drs. H.E. Zwaan
- Van der Plas (HRSMC).

Supporting team: Mrs. P.J.E. Hagen, Mrs. S. Weijer (0.4 Fte HRSMC), Mrs. R.B. Hippert, Mrs. M.P.C. Sabandar-Mumu, Mrs. J.L. Pentinga, M.J. Moolenaar.

Special tasks: M. Mittelmeijer (Safety and Health), P.F. Collignon (ICT), J.C.M. Steeneken (Buildings and Housing), J. Fraanje (New buildings), P. Verschuren (Website).

5.6.4 HIMS personnel 2008 (Fte and persons)

<i>HIMS Total</i> Money category	1 st	1 st	1 st	2 nd	3 rd	Total Fte	Total persons									
		NRSC-C	Total	CW	STW	FOM	Others	Total	Ind	Eu	BSIK	Others	Guests	Total		
Chairs/profs	8.6	0.0	8.6	0.0	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.7	0.0	0.7	9.4	14
Spec. Profs	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	5
UHD	6.9	0.0	6.9	0.0	0.0	0.2	0.0	0.2	0.2	0.0	0.0	0.0	0.0	0.2	7.3	7
UD	5.2	0.0	5.2	0.4	0.0	0.0	0.6	1.0	0.0	0.0	0.0	0.4	0.0	0.4	6.6	9
Postdoc	1.8	0.5	2.3	6.0	0.0	0.5	0.2	6.7	1.0	1.9	0.1	2.3	16.6	21.9	30.9	47
AIO/OIO	2.7	8.2	10.9	12.9	2.3	0.8	0.0	16.0	0.0	4.2	3.8	6.7	30.0	44.8	71.6	94
OBP	24.5	0.0	24.5	0.5	1.0	0.0	0.0	1.5	0.7	0.0	0.0	4.4	0.6	5.7	31.7	44
Total	49.8	8.7	58.5	19.8	3.3	1.5	0.8	25.5	1.8	6.1	3.9	14.5	48.2	74.6	158.6	220

<i>HIMS Total</i> Money category	1 st	1 st	1 st	2 nd	3 rd	Total Fte	Total persons									
		NRSC-C	Total	CW	STW	FOM	Others	Total	Ind	Eu	BSIK	Others	Guests	Total		
Management	7.5	0.0	7.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	0.0	1.8	9.3	12
Röntgen Diffraction	2.1	0.0	2.1	0.0	0.0	0.0	0.0	0.0	0.5	0.0	0.0	0.5	1.3	2.3	4.4	7
Bio-Molecular Synthesis	7.4	1.7	9.1	3.4	0.0	0.0	0.0	3.4	0.0	0.0	0.0	0.5	4.5	5.0	17.5	26
Catalysis	11.9	5.4	17.3	8.3	1.0	0.0	0.2	9.4	1.3	3.8	0.0	5.5	12.1	22.6	49.4	67
Computational Science	8.0	0.0	8.0	5.1	0.7	0.8	0.0	6.5	0.0	2.2	0.0	0.0	7.3	9.5	24.0	32
Molecular Photonics	6.1	1.6	7.7	2.9	1.7	0.8	0.6	5.9	0.0	0.2	2.8	2.0	8.9	13.9	27.5	42
Bio-Analytical Chemistry	5.2	0.0	5.2	0.3	0.0	0.0	0.0	0.3	0.0	0.0	1.1	3.7	9.0	13.7	19.2	25
Polymer Processing	1.5	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.6	5.2	5.8	7.2	9
Total	49.8	8.7	58.5	19.8	3.3	1.5	0.8	25.5	1.8	6.1	3.9	14.5	48.2	74.6	158.6	220

5.6.5 HIMS PhD students and Postdocs 2008 (Fte)

PhD students 2008 (Fte)	1 st	1 st	2 nd	3 rd	Total	Postdocs 2008 (Fte)	1 st	1 st	2 nd	3 rd	Total
Money category		NRSC-C				Money category		NRSC-C			
Bio-Molecular Synthesis	0.0	1.7	2.1	2.4	6.1	Bio-Molecular Synthesis	0.0	0.0	0.8	1.8	2.6
Catalysis	0.3	5.0	8.5	7.8	21.5	Catalysis	0.0	0.4	0.9	13.1	14.4
Computational Chemistry	1.0	0.0	2.5	8.5	12.0	Computational Chemistry	1.8	0.0	3.7	1.0	6.5
Molecular Photonics	0.5	1.5	2.6	11.4	16.0	Molecular Photonics	0.0	0.1	1.3	1.3	2.6
Macromolecular & Biosystems Analysis	1.0	0.0	0.3	11.1	12.4	Macromolecular & Biosystems Analysis	0.0	0.0	0.0	2.2	2.2
Complex Fluids	0.0	0.0	0.0	0.0	0.0	Complex Fluids	0.0	0.0	0.0	0.0	0.0
Röntgen Diffraction	0.0	0.0	0.0	1.1	1.1	Röntgen Diffraction	0.0	0.0	0.0	0.0	0.0
Core activities	2.7	8.2	16.0	42.2	69.0	Core activities	1.8	0.5	6.7	19.3	28.3
Polymer Processing	0.0	0.0	0.0	2.6	2.6	Polymer processing	0.0	0.0	0.0	2.6	2.6
Other activities	0.0	0.0	0.0	2.6	2.6	Other activities	0.0	0.0	0.0	2.6	2.6
Total HIMS	2.7	8.2	16.0	44.8	71.6	Total HIMS	1.8	0.5	6.7	21.9	30.9

5.6.6 HIMS personnel 2001 - 2008 (Fte)

	1 st	1 st NRSC-C	2 nd	3 rd	Ext. ¹⁾ (Fte)	Total (Fte)	1 st (%)	Ext. ¹⁾ (%)
2001	105.4	8.1	59.4	25.5	93.0	198.4	53.1	46.9
2002	104.7	11.6	63.5	28.7	103.8	208.4	50.2	49.8
2003	94.8	16.0	55.6	29.8	101.5	196.2	48.3	51.7
2004	81.1	11.5	52.7	27.2	91.4	172.5	47.0	53.0
2005	67.8	12.0	40.2	41.0	93.2	161.1	42.1	57.9
2006	55.5	13.1	31.2	49.0	93.3	148.8	37.3	62.7
2007	60.6	12.2	25.0	56.2	93.3	153.9	39.4	60.6
2008	49.8	8.7	25.5	74.6	108.8	158.6	31.4	68.6

¹⁾ External = 1st + 1st NRSC-C + 2nd + 3rd

5.6.7 HIMS personnel 2001 - 2009 (Persons; situation per January 1st)

Category	2001	2002	2003	2004	2005	2006	2007	2008	2009 ¹⁾
Chairs/profs	17	17	17	13	12	10	12	12	11
Spec. Profs	3	5	6	7	7	7	4	5	5
U(H)D	11	10	10	11	10	7	10	9	6
UD	10	10	12	9	9	10	9	7	8
Postdoc	29	27	29	38	43	22	23	27	42
AIO/OIO	94	102	94	85	74	73	70	72	81
OBP	57	54	47	50	39	38	39	34	41
Total	221	225	215	213	194	167	167	166	194

Theme	2001	2002	2003	2004	2005	2006	2007	2008	2009 ¹⁾
Management	19	18	15	18	14	14	10	9	12
Support	13	12	13	19	15	8	4	7	6
Bio-Molecular Synthesis	33	34	31	29	25	20	21	22	21
Catalysis	46	48	48	43	49	48	47	44	62
Computational Chemistry	27	30	27	27	22	22	24	25	21
Molecular Photonics	29	32	31	33	37	29	30	26	38
Macromolecular & Biosystems Anal.	25	22	21	21	16	15	21	24	28
Complex Fluids	10	12	15	13	10	6	6	4	0
Others	19	17	14	11	6	5	4	5	6
Total	221	225	215	213	194	167	167	166	194

¹⁾ 40 Vacancies at 01-01-2009 (22 PhD's, 14 Pd's, 1 Hgl, 2 UD's, 1 Secretary) are not included

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6. Abbreviations

ACTS	Advanced Catalytic Technologies for Sustainability (NWO program)
AIMS	Amsterdams Instituut voor Moleculaire Scheikunde
AIO	PhD student (Assistant in opleiding)
AMC	Academisch Medisch Centrum
Amolf	Instituut voor Atoom & Molecuul Fysica (FOM)
ASPECT	Advanced Sustainable Processes by Engaging Catalytic Technologies (program of ACTS)
AvL	Antoni van Leeuwenhoek Ziekenhuis
BAR	Science Advisory Board (Beleids Advies Raad) of HIMS
BMS	Bio-Molecular Synthesis (HIMS research theme)
CAIRE	Center for Anti-infectives, Research and Education.
CAT	Catalysis (HIMS research theme)
CERC3	Chairmen of the European Research Councils' Chemistry Committees.
CF	Complex Fluids (HIMS research theme)
CoF	Centraal Onderzoeksfonds (Research fund of the University Board)
COMP	Computational Chemistry (HIMS research theme)
COST	European program
CPP	The average number of citations per publication corrected for self-citations (VSNU bibliometric analysis)
CvB	University Board (College van Bestuur)
CW/NWO	Chemische Wetenschappen/Nederlandse Stichting voor Wetenschappelijk Onderzoek (National Research Foundation)
DFG	Deutsche Forschungs Gemeinschaft
DPI	Dutch Polymer Institute
DSM	Dutch State Mines
EE	Enantiomeric excess
ECN	Energie Centrum Nederland
ECOS	Erkenningcommissie Onderzoekscholen (Accreditation Committee for Research Schools)
EC-TMR	European network program
EMMMA	Exploiting Mechanical Motion of Molecular Architectures
EMS	Institute for Electrons and Molecular Structure (VU).
EU	European Union
FCS _m	The mean Field Citation Score (VSNU bibliometric analysis)
FOM	Stichting voor Fundamenteel Onderzoek der Materie
FNWI	Faculty of Science (Faculteit der Natuurwetenschappen, Wiskunde en Informatica)
HBO	Hoger Beroeps Onderwijs
HIMS	Van 't Hoff Institute for Molecular Sciences
HRI	Van 't Hoff Research Instituut
HRM	Human Resources Management
HRSMC	Holland Research School of Molecular Chemistry (National Research School), part of NRSC-C
IBED	Instituut for Biodiversity and Eco-Dynamics

IBOS	Integration of Biocatalysis and Organic Synthesis (program of ACTS)
ICN	Instituut Collectie Nederland
IMC	Institute for Molecular Chemistry
ITS	Instituut voor Technische Scheikunde
KNAW	Royal Netherlands Academy of Arts and Sciences (Koninklijke Nederlandse Academie van Wetenschappen)
LACDR	Leiden Amsterdam Centre for Drug Research
LIC	Leiden Institute of Chemistry
MBA	Macromolecular and Biosystems Analysis (HIMS research theme)
MechMol	MechMol (MECHAnized MOLEcules), the EU 5th Framework Program project started in July 2002.
Mesa+	Top research Institute University of Twente
MOLP	Molecular Photonics (HIMS research theme)
NanoNed	Dutch nanotechnology initiative (HIMS is partner of NanoNed)
NFI	Nederlands Forensisch Instituut
NIOK	Dutch Institute for Catalysis Research; Nederlands Instituut voor Onderzoek in de Katalyse, (National Research School), part of NRSC-C
NKI	Nederlands Kanker Instituut
NMR	Nuclear Magnetic Resonance
NRSC-C	National Research School Combination - Catalysis
NWO-CW	National Research Foundation (Nederlandse Stichting voor Wetenschappelijk Onderzoek - Chemische Wetenschappen)
OBP	Technical assistant
OC&W	Ministerie van Onderwijs, Cultuur & Wetenschappen (Ministry of Culture and Education)
OIO	PhD student (Onderzoeker in opleiding) of NWO
OL	Other costs (Operational costs, overige lasten)
OSPT	OnderzoekSchool ProcesTechnologie
OWC	HIMS Education Committee (OWC; Onderwijscommissie)
OWP	Other Scientific Personnel (Overig wetenschappelijk personeel)
OZC	HIMS Research Committee 'Molecules in Action' (OZC; Onderzoekscommissie)
OZIS	Concern information system (performance indicators; kengetallenrapportage)
P	Professor
Pd	Postdoc
PhD	PhD student (AIO, OIO)
PL	Personnel costs (Personele lasten)
PNAS	Proceedings of the National Academy of Sciences
PTN	Polymeer Technologie Nederland (National Research School), part of NRSC-C
RCM	Ring Closure Methathesis
RUN	Radboud Universiteit Nijmegen
RUG	Rijks Universiteit Groningen
SAP	Financial administration system of the UvA

SILS	Swammerdam Institute for Life Sciences
STW	Stichting Technische Wetenschappen (part of NWO)
TNO	Dutch Institute for Applied Research (Nederland Instituut voor Toegepast Onderzoek)
TUe	Technische Universiteit Eindhoven
UD	Assistent Professor (Universitair docent)
UFO	VSNU function classification system (Universitair Functie Ordenen)
UHD	Associate Professor (Universitair hoofddocent)
UL	Universiteit Leiden
UOC	Research Committee of the UvA (Universitaire Onderzoekscommissie)
UOF	University Research Fund of the UvA (Universitair Onderzoeks Fonds)
UU	Universiteit Utrecht
UvA	Universiteit van Amsterdam
VIRAN	Industrial advisory board for Catalysis
VSNU	Association of Universities in The Netherlands (Vereniging van Samenwerkende Nederlandse Universiteiten)
VWO	Voorbereidend Wetenschappelijk Onderwijs
VU	Vrije Universiteit (Amsterdam)
WU	Wageningen University
WTCW	Wetenschap en Technologie Centrum Watergraafsmeer
WZI	Van der Waals Zeeman Institute
XRD	X-Ray Diffraction