

Annual Report 2010



Van 't Hoff Institute for Molecular Sciences



University of Amsterdam

Preface

2010 was a very eventful year for HIMS. After long preparations and discussions within the UvA for decades, finally HIMS did move mid 2010 as one of the last institutes to the Science Park in the Watergraafsmeer in the east of Amsterdam. Although the move was not entirely uneventful, it did go well thanks to the leadership of prof. Ad Oskam. The new labs look fantastic and will enable excellent molecular science in the coming decades.

The evaluation of the scientific program by a panel of international experts took place in September. Although the formal outcome was not communicated in 2010 it became clear that it was very good. The rejuvenation of HIMS in the last years certainly did not influence the performance of HIMS in any negative fashion. Also scientifically, HIMS is ready for the challenges of the coming decade.

After 12 years the directorship of HIMS changed. Dr. Rob Zsom stepped back to be replaced in October 2010 by prof. Aart Kleijn, surface scientist from the FOM Institute for Plasma Physics Rijnhuizen in Nieuwegein and also affiliated to Leiden University. Rob has led HIMS through turbulent times and left it in a splendid shape: with a young staff, a healthy budget, a new building and a strong scientific evaluation. HIMS expressed its gratitude in 2011 at a big farewell party. Rob remains active in HIMS.

Prof.dr. Aart W. Kleijn



Former and present director of HIMS: Dr. Rob L.J. Zsom and Prof.dr. Aart W. Kleijn

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1 General considerations

The year 2010 was a successful year for HIMS. A total of 5,01 M€ external funds (6,56 M€, including 2,70 M€ NRSC-C, in 2009) was acquired from subsidiaries such as NWO (1 Vidi, 1 TOP and 2 ECHO grants), EU, NanoNext (FES), Towards Biosolar (FES), NFI, etc. The output of HIMS was on a high level in 2010, comparable to 2009. HIMS published 7 papers (3 in 2009) in absolute top journals (impact factor > 15) and 11 papers (10 in 2009) in top journals (impact factor 10-15). The total number of refereed publications amounted to 178 (169 in 2009), including 3 patents (1 in 2009), reflecting the increased personnel input last year, while 14 PhD dissertations (16 in 2009) were produced.

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

- On the occasion of the 2010 assessment of research quality a bibliometric analysis was performed over the period 1999-2008. All five HIMS research themes obtained individual scores well above the international standard. For HIMS as a whole the **CPP/FCSm**¹ was **1.81**. The HIMS Scientific Advisory Committee concluded that the younger staff members are reaching the high quality level of their predecessors and re-established the international position of the individual research groups.
- The 'Nieuwe Ideeën Prijs 2010' for Dr. Raveendran Shiju & Prof. Gadi Rothenberg, received from the Science Park Amsterdam for their invention 'A new catalyst for making nylons'



Dr. Raveendran Shiju receives the 'Nieuwe Ideeën Prijs 2010'

- Dr. Sander Woutersen, Prof. Wybren Jan Buma and Prof. Fred Brouwer (Molecular Photonics) published in Science the article '*Operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy*'
- A Science publication by Prof Huib Bakker (Molecular Photonics and FOM/Amolf) on '*Cooperativity in ion hydration*'
- HIMS was assigned 4 new staff positions (0.58 mln €/year; total investment 2.9 mln €) from the Natuurkunde & Scheikunde (SNS; appointments can be realized as from 01-01-2011)
- Prof. Joost Reek (Catalysis) was highlighted in Angewandte Chemie because he published his 10th article since 2000 in this prestigious journal

Some other highlights to be mentioned are:

- The group Homogeneous and Supramolecular Catalysis (Reek/De Bruin/Van der Vlugt) was highlighted in Nature Chemistry for following publications in Angewandte Chemie and JACS in 2010
- Prof. Joost Reek (Catalysis) presented a NEMO lecture with the title '*Hoe wordt vuurwerk gemaakt?*' for an audience of young kids

¹ CPP/FCSm: impact of all articles, compared to the world citation average in the (sub) fields in which the institute is active



Prof. Joost Reek in NEMO

- The research of Dr. Jocelyne Vreede (Veni laureate of Computational Chemistry) was highlighted on the FNWI website
- Dr. Teunie van Herk (group Ron Wever/Bio-Molecular Synthesis) received the Martinus van Marum Prijs, from the Koninklijke Hollandsche Maatschappij der Wetenschappen, for her thesis on '*Bacterial class A acid phosphatases as versatile tools in organic synthesis*'
- Ira Saul Lurie (group Peter Schoenmakers/Macromolecular and Biosystems Analysis) received his doctoral degree for his thesis on '*Ultra High Performance Liquid Chromatography of Seized Drugs*', the first UvA thesis on a forensic subject
- Dr. Sander Woutersen (Molecular Photonics) explained in the broadcast program Noorderlicht of the VPRO the possible uses of molecular machines



Dr. Sander Woutersen

Since 2006, the year of introduction of the new integral costs allocation model of the university board, the financial position of HIMS has much improved. HIMS finished the year 2010 with a small negative financial result of -0.15 M€ (+0.05 M€ in 2009). This result is satisfactory, knowing that HIMS is confronted with a budget reduction of the structural university budgets (1^e geldstroom) of 10% (1 M€) for the years 2009-2012.

Although the financial prospects of HIMS and the faculty are negatively influenced by the budget reductions to be realized in the years 2009-2012 (and later?), increased revenues are expected from the realization of more PhD theses and the Sectorplan Natuurkunde & Scheikunde (SNS) in the coming years. Additional cost reductions will be realized in the years to come by early retirements and by discontinuation of the röntgen diffraction (RD) activities. Due to budgetary restrictions within the faculty, the RD activities were ended at 31-12-2010 as a part of the HIMS cost reduction plan *Chemie Financieel Duurzaam*.

As a direct consequence of the budgetary reductions no new scientific staff appointments in fixed positions through direct funding (1^e geldstroom) could be realized in 2010, with the exception of the appointment of the new HIMS director, Prof. A. (Aart) Kleyn at 15-10-2010. However, we expect several new (full-time) appointments in the course of 2011, e.g. a new professor in *Complex Molecular Simulations* and two new professors (*Supramolecular Analysis* and *Biocatalysis*) in the framework of the SNS.

The year 2010 again turned out to be very successful in terms of external fund raising; a total of 5,00 M€ was acquired from important old and new subsidiaries. A selection of projects acquired in 2010:

- Prof. Joost Reek (Catalysis) and Prof. Huib Bakker (Molecular Photonics/FOM-Amolf) both received a NWO-top GRANT of 0.78 mln €
- Dr. Bas de Bruin (Catalysis) and Prof.dr. Fred Brouwer (Molecular Photonics) both received a NWO-Echo grant of 0.26 mln €
- The Netherlands Forensic Institute (NFI) supplied Prof. Peter Schoenmakers (Macromolecular and Biomaterials Analysis) with a budget of 0.27 mln € for a research project on forensic explosives
- The groups of Prof. Joost Reek (catalysis) and Prof. Fred Brouwer (Molecular Photonics) received together a budget of 0.95 mln € from the related FES and FOM programmes *Towards Biosolar* for research on photocatalytic water splitting (hydrogen production)
- The groups of Prof. Peter Bolhuis (Computational Chemistry) and Profs Peter Schoenmakers and Hans Gerd Janssen (Macromolecular and Biomaterials Analysis) received together a budget of 0.89 mln € from the FES programme NanoNext for research in the fields of food and nutrition and micro/nano-fluidics.
- Dr. David Dubbeldam (Computational Chemistry) received a (0.8 M€) NWO-CW VIDI subsidy for the design of nanoporous materials with the computer



Dr. David Dubbeldam

- Dr. Hong Zhang (Molecular Photonics) received an IOP grant of almost 1.5 M€ for a collaborative project of HIMS with AMC and LUMC for research on cancer diagnosis and treatment

After many years of decreasing numbers, the scientific staff numbers in 2010 (170.8 fte) stabilized more or less on the level of 2009 (178.6 fte). Compared with the level 2007 (153.9 fte), and 2008 (158.6) an increase of ~20 fte. The number of externally funded PhD students and Postdocs in 2010 (112.4 fte), by funding originating from the Research Schools NRSC-C, NWO-CW/STW/FOM, and EU, ERC, BSIK/NanoNed, NFI, CatchBio and Industry, was a little bit lower than in 2009 (122.9 fte), but appreciably higher than in the forgoing years (102.6 fte in 2008, 93.3 fte in 2007). Since the number of 37 vacancies at 01-01-2011 was exceptionally high (including vacancies for various staff positions), a further increase in external research funding (and scientific staff members) is expected in 2011.

Mid 2010 the Van 't Hoff Institute for Molecular Sciences left the laboratories at the Roeterseiland.



Farewell from the Roeterseiland

Since mid 2010 the Van 't Hoff Institute for Molecular Sciences is located in the new buildings of the Faculty of Science at the Science Park in the Watergraafsmeer. The laboratories for the research groups of Macromolecular and Biosystems Analysis, Computational Chemistry, Molecular Photonics and Biocatalysis (group Wever) are placed in the new building D. For these groups 1566 m² lab space is available. Most offices and sitting rooms and the lecture halls are located in a separate building in the middle, all on a very short distance from the lab-space. The research groups for Catalysis and Organic Synthesis (group Hiemstra), including the NMR-facilities, are housed in a separate three floor building with 2052 m² available for the laboratories only. This renovated building is attached on one side to the main building in which the other HIMS research groups are located, and on the other side to the bachelor student laboratories.



2 Research themes

2.1 Bio-Molecular Synthesis

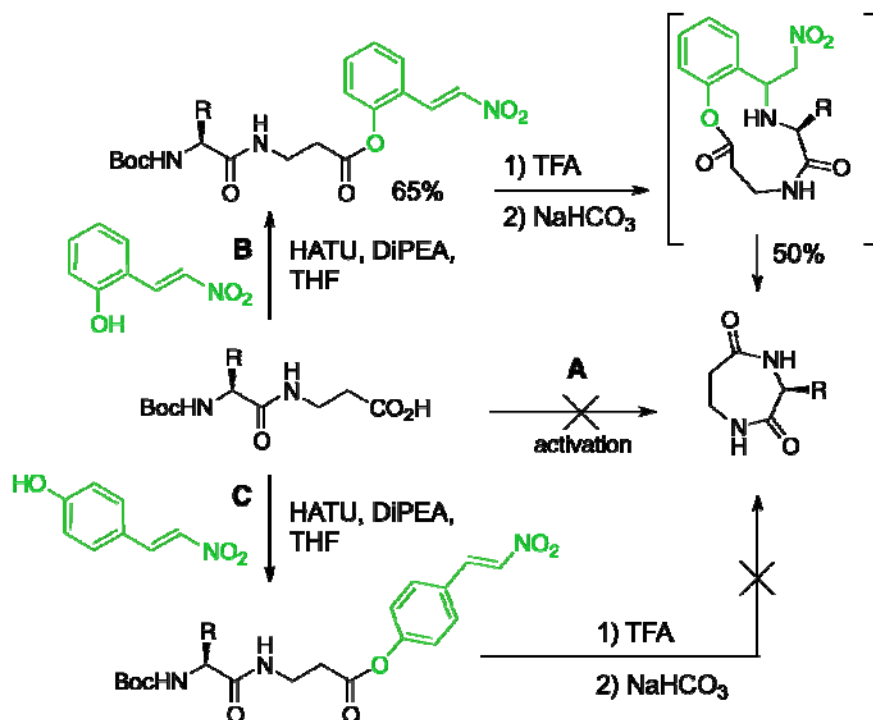
Two groups represent this research theme within HIMS, the Synthetic Organic Chemistry group (Hiemstra c.s) and the Biocatalysis group (Wever c.s). Their research is directed at the development of efficient and selective, diversity-oriented synthetic methodology, in particular organocatalytic and biocatalytic procedures, and the target-oriented preparation of molecules of relevance in chemistry, biology and medicine.

2.1.1 Synthetic Organic Chemistry

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

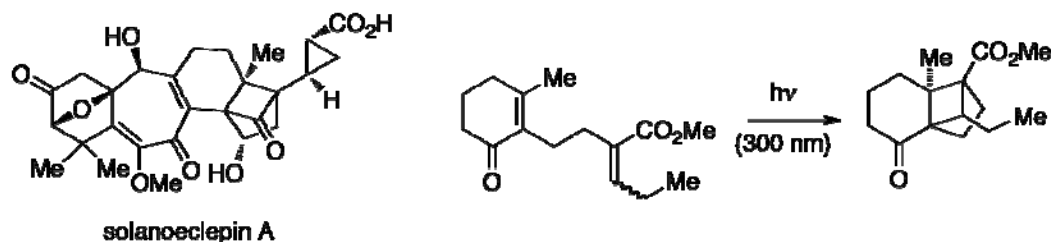
Summary of research activities

Synthetic methodology development: As is shown below, dipeptides containing one β -amino acid do not easily cyclize to 7-membered lactams (route A). Therefore, they are ideally suited for the development of methods to synthesize by ring-closure naturally occurring and biologically relevant strained lactams. It was found that esterification of N-terminal protected β -peptides with commercially available *o*-hydroxy- β -nitrostyrene, followed by liberation of the N-terminus is followed by facile 7-membered lactam formation (route B). Carrying out the same reaction sequence for *p*-hydroxy- β -nitrostyrene predominantly yields the unwanted cyclic dimer, as is found by lactamization attempts of the same β -peptides (route C). This result suggests in the case of *o*-hydroxy- β -nitrostyrene the intermediacy of an 11-membered macrocyclic intermediate, formed via an intramolecular aza-Michael reaction, which collapses to the 7-membered lactam via a ring-contractive O \rightarrow N acyl-transfer reaction, followed by a retro-aza-Michael reaction liberating the lactam. This method is now further developed for the ring-closure of naturally occurring small cyclic peptides that cannot be addressed using the current synthetic methodology.

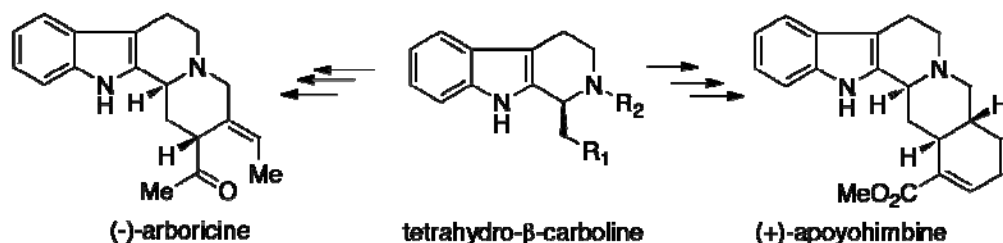


Target-oriented synthesis: Our research towards the total synthesis of the terpenoid hatching agent solanoelepin A should eventually lead to simple active analogues in order to combat potato cyst

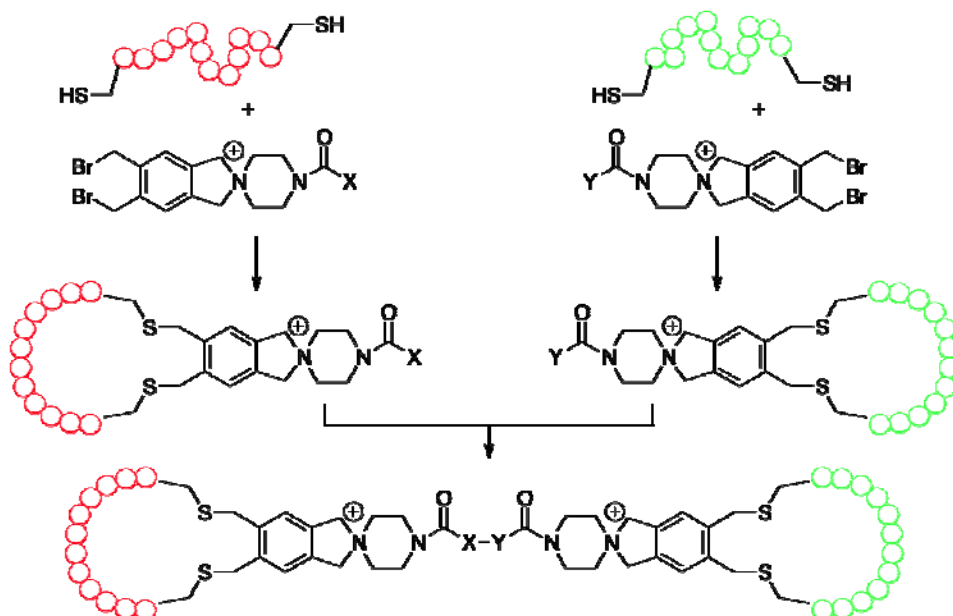
nematodes as parasites in potato production. In 2010 our insight into the [2+2]-photocycloaddition towards the tricyclic core of the natural product was considerably enhanced by the successful construction of the tricyclic ester from the cyclohexenone precursor in the correct regiochemical (crossed) sense.



Organocatalysis: Chiral biarylphosphoric acids were used to catalyse Pictet-Spengler reactions in order to prepare tetrahydro- β -carbolines in high ee's. These *N*-heterocycles are suitable substrates for the asymmetric synthesis of indole alkaloids through cyclization reactions between the C1 and N2 substituents, either via transition metal catalysis or Diels-Alder chemistry. In these ways the first total syntheses of (-)-arboricine and (+)-apoyohimbine were achieved.



Chemical biology: The CLIPS technology developed at Pepscan Therapeutics, Lelystad, by Timmerman and coworkers was further expanded by the introduction of additional reactive tags to the scaffolds to allow the covalent connection of different CLIPS-constrained peptides thus mimicking discontinuous protein epitopes. In addition, these tags were attached via an ammonium moiety to improve the water solubility. Covalent ligation of these highly functionalized *unprotected* CLIPS-peptides may be conducted by click-type transformations such as the CuAAC-reaction, oxime-formation or the thiol-ene reaction.



Key publications 2009-2010

1. Cinchona alkaloids in asymmetric organocatalysis, T. Marcelli, H. Hiemstra, *Synthesis* 1229-1279 (2010).
2. Selective enrichment of azide-containing peptides from complex mixtures,

- M.A. Nessen, G. Kramer, J.W. Back, J.M. Baskin, L.E.J. Smeenk, L.J. de Koning, J.H. van Maarseveen, L. de Jong, C.R. Bertozzi, H. Hiemstra, C.G. De Koster, *J. Proteome Res.* **8**, 3702-3711 (2009).
3. Expedient pyrrolizidine synthesis by propargylsilane addition to *N*-acyliminium ions followed by gold-catalyzed α -allenyl amides cyclization, A.C. Breman, J. Dijkink, J.H. van Maarseveen, S.S. Kinderman, H. Hiemstra, *J. Org. Chem.* **74**, 6327-6330 (2009).
 4. Binding of CDR-derived peptides is mechanistically different from that of high-affinity parental antibodies, P. Timmerman, S. Shochat, J. Desmet, R. Barderas, J.I. Casal, R.H. Meloen, D. Altschuh, *J. Mol. Recogn.* **23**, 559-568 (2010).

Highlights

H. Hiemstra

Distinction

- Novartis Lecturer Central Europe, autumn 2010.

Lectures on invitation

1. *Asymmetric catalysis by small organic Brønsted acids and bases*, Meeting of the KNCV “Organic Chemistry Division” and the three organic NWO-CW study groups, Wageningen, April 7th, 2010.
2. *Asymmetric Organocatalysis in the Henry Reaction and Pictet-Spengler Cyclization*, Invited Plenary Lecture at the 18th IUPAC Conference on Organic Synthesis, Bergen, Norway, August 6th, 2010.
3. *Asymmetric catalysis by small organic Brønsted acids and bases*, Adam Mickiewicz University of Poznan, Poland, October 18th, 2010. *Asymmetric catalysis by small organic Brønsted acids and bases*, Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland, October 20th, 2010.
4. *Asymmetric catalysis by small organic Brønsted acids and bases*, Jagiellonian University of Krakow, Poland, October 22nd, 2010.
5. *Asymmetric catalysis by small organic Brønsted acids and bases*, NOVARTIS lecture, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, November 1st, 2010.
6. *Synthetic studies toward solanoelepin A, a potato cyst nematode hatching agent*, NOVARTIS lecture, Institute of Biomolecular Chemistry, Hungarian Academy of Sciences, Budapest, November 3rd, 2010.
7. *Synthetic studies toward solanoelepin A, a potato cyst nematode hatching agent*, NOVARTIS lecture, Comenius University in Bratislava, Slovak Republic, November 4th, 2010.
8. *Chiral Brønsted acid base organocatalysis*, Plenary lecture at the annual HRSMC Symposium 2010, Leiden University, November 25th, 2010.

J.H. van Maarseveen

Distinction

- Onderwijsbokaal, ACD (best chemistry teacher 2009-2010)

Lecture on invitation

1. *Catalytic asymmetric Pictet-Spengler condensations*, BIT’s 1st Annual World Congress of Catalytic Asymmetric Synthesis, Beijing, China, May 20th, 2010.

P. Timmerman

Lecture on invitation

1. *Reconstructing Protein Surfaces using Peptide Fixation Technologies*, Keynote lecture at the 1st International Conference on Molecular Recognition, Heraklion, Crete, Greece, June 6th-11th 2010.

Relevance

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

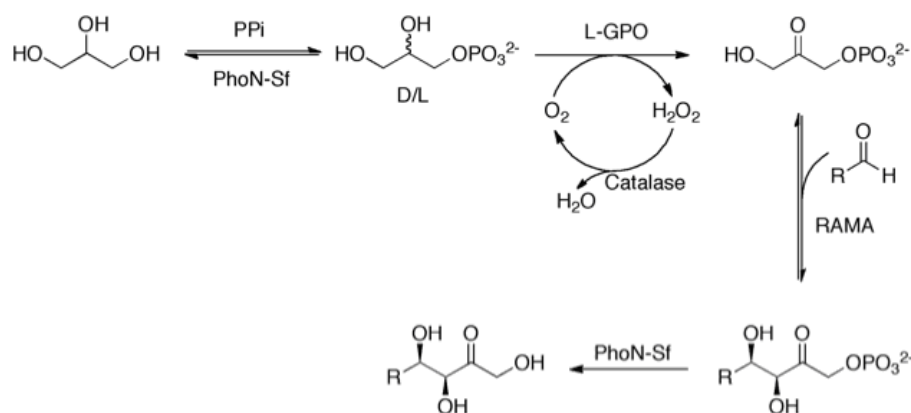
2.1.2 Biocatalysis

Prof.dr. R. Wever

Summary of research activities

A four enzyme one-pot cascade reaction was developed by which it was possible to synthesize a wide variety of non-natural carbohydrates starting from glycerol and a variety of aldehydes, using pyrophosphate as an energy rich phosphorylating agent to drive the reaction to completion. This was carried out in collaboration with the group of prof. Rutjes (RUN). Directed evolution was used to modify the enzymes (acid phosphatase, aldolases) involved. Immobilized enzymes in a flow reactor are now used to produce phosphorylated compounds and carbohydrates at a gram scale.

The antimicrobial and antiviral effect of the vanadium chloroperoxidase and a mutant obtained by directed evolution was also investigated. It is concluded that this enzyme and its reaction products form a potent antimicrobial system and that the enzyme could have potential as mouth rinse.



An enzyme-cascade reaction in which glycerol and an aldehyde are converted into non-natural carbohydrates by 4 enzymes

Publications 2010

1. R. Renirie, J.M. Charnock, C.D. Garner and R. Wever. Vanadium K-edge XAS studies on the native and peroxo-forms of vanadium chloroperoxidase from *Curvularia inaequalis*. *J. Inorg. Biochem.* 2010, 104, 657-664
2. R. Andre, F. Natalio, M. Humanes, J. Leppin, K. Heinze, R. Wever, H.-C. Schröder, W. E. G. Müller, and W. Tremel. V₂O₅ Nanowires with an intrinsic phosphatase-like activity. *Adv. Funct. Mater.* 2011, 21, 501-509

Key publications 2005- 2010

1. Van Herk T, Hartog AF, Schoemaker HE, Wever R. Simple enzymatic in situ generation of

dihydroxyacetone phosphate and its use in a cascade reaction for the production of carbohydrates: Increased efficiency by phosphate cycling. *J. Org. Chem.* : 2006, 71: 6244-6247; Times Cited: 7

2. Pooransingh-Margolis N, Renirie R, Hasan Z, Wever R, Vega AJ, Polenova T. V-51 solid-state magic angle spinning NMR spectroscopy of vanadium chloroperoxidase, *J. Am. Chem. Soc.* 2006 : 128 : 5190-5208; Times cited: 33

Highlights

1. Dr. T. van Herk received on May 28, 2010 the prestigious “Martinus van Marum prijs” for Biotechnology of the Koninklijke Hollandsche Maatschappij der Wetenschappen on biotechnology for her PhD thesis “Bacterial class A acid phosphatases as versatile tools in organic synthesis”.
2. R. Wever OHRI Seminar Series “Structural and functional properties of vanadium haloperoxidases, their physiological roles and possible applications”, April 12, 2010. Ottawa, Canada
3. R. Wever, Oral Session. “Structure and function of vanadium haloperoxidases”, 7th International symposium on the chemistry and biological chemistry of vanadium, October 6-9, 2010, Toyama, Japan

Relevance

A grant application has been submitted together with the University of Utrecht (Prof.dr. L. Jenneskens) and the SME van Loon Chemical innovations, Amsterdam to [www. Agentschap.nl](http://www.Agentschap.nl) (Ministry of Economic Affairs, Agriculture and Innovation). This application has been granted and this will allow further evaluation of the possibilities of enzyme-based antifouling coatings. The grant will also be used to find further support within EU programmes.

2.2 Catalysis

The catalysis theme consists of three research groups, *Organometallic chemistry and catalysis* (Prof. Elsevier), *Homogenous and supramolecular catalysis* (Prof. Reek), and *Heterogeneous catalysis and sustainable chemistry* (Prof. Rothenberg), while there are catalysis activities in the other themes as well.

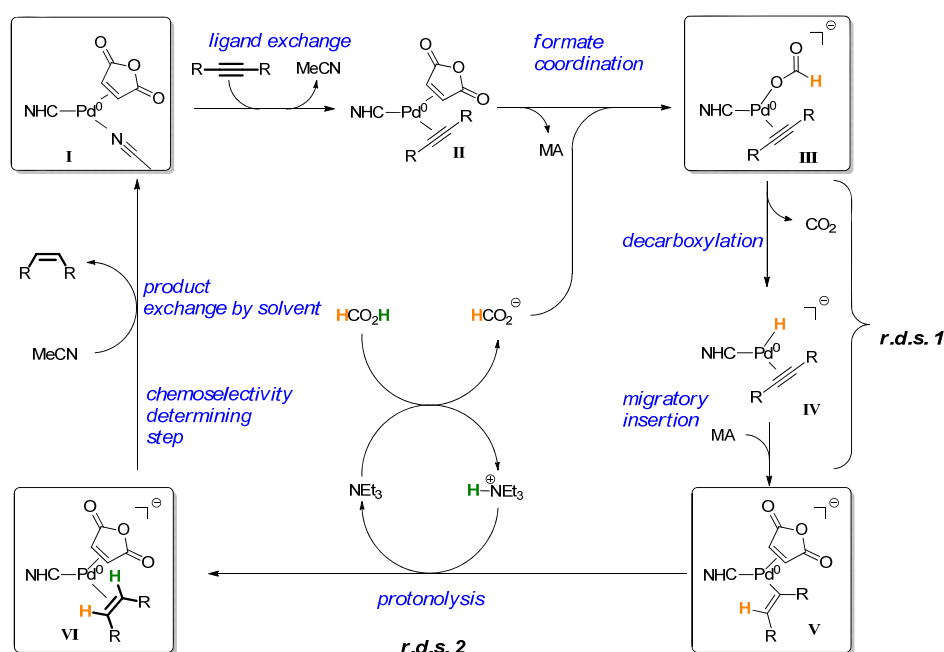
2.2.1 Organometallic Chemistry and Catalysis

Prof.dr. C. Elsevier

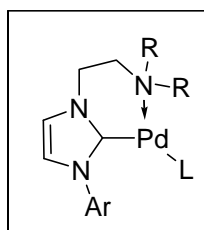
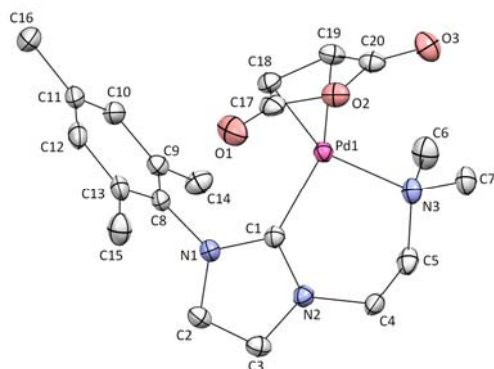
Summary of research activities

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

The design and implementation of N-heterocyclic carbene (NHC) ligands as well as rigid bidentate N-ligands in late transition metal compounds aimed at catalytic carbon-element bond forming reactions continues to be an important research topic in the group. This year, the studies concerning the mechanism of palladium(NHC)-catalyzed *transfer* hydrogenation of alkynes has been completed and published (*J. Am. Chem. Soc.* **2010**, *132*, 16900-16910). This methodology for the catalytic synthesis of Z-alkenes from alkynes *without* reduction to alkanes attracts a lot of interest. Our research provided insight in details of the mechanism due to careful kinetic measurements including deuterium isotope effects of all isotopomers of formic acid that is used as the hydrogen donor. In addition, *in situ* NMR measurements provided insight in the structure of accumulating intermediates. Altogether we were able to provide a convincing mechanism of this new reaction (Scheme below), proceeding by ligand exchange between **VI**, **I** and **II**, that critically depends on the coordinative properties of the solvent with respect to the substrate (stronger) and product (weaker). This feature ensures complete reduction of the alkynes to the alkenes, preventing further reduction from occurring.



Next, formate coordination (**III**) and CO₂ extrusion to give the active palladiumhydride **IV** occurs, which is followed by rate determining insertion of the alkyne in a palladium hydride to give Pd-alkenyl complex **V**. The second rate determining step concerns the protonolysis of the alkenyl intermediate providing the *cis*-alkene coordinated to palladium.



Currently, one of the focal points of our research concerns the design and application of late transition metal complexes with heterotopic carbene and N-ligands for coordination chemistry and applications in homogeneous catalysis. This year we have synthesized a number of heterobidentate NHC ligands containing a secondary nitrogen-donor. Combining a strong donor with a more weakly coordinating donor, we intend to gain access to a class of catalysts which benefits from the hemilabile behaviour of the weaker donor N-ligand. Additionally, the basicity of the secondary nitrogen-donor is easily varied to obtain the desired functionality. Various electron-rich palladium complexes bearing an NHC-ligand functionalized with N-donors such as a pyridyl, pyrimidyl, and pyrazolyl donors have been studied. Varying their basicity, hence coordinative properties, leads to specific behaviour in e.g. hydrogenation reactions. Several papers have appeared and will appear on this subject.

Part of this project has been carried out in collaboration with Taiwanese colleagues (in a project financed by NWO and NSC): this led to the synthesis of iridium-NHC complexes for catalytic indole synthesis and reductive amination (C-N bond formation), and palladium-NHC complexes for C-S bond formation. The palladium(NHC) systems with various tethers are unprecedented hydrogenation catalysts, since they catalyze *transfer* hydrogenation of alkynes to give *cis*-alkenes selectively. Usually transfer hydrogenation is restricted to ketones and imines. This collaboration has given rise to 13 papers, 6 of which appeared in 2010.

Furthermore, we have started a project on immobilization of NHC-transition metal complexes for catalysis, with the aim of recycling, on which we will report next year.

Key publications

1. S. Warsink, R.M. Drost, M. Lutz, A.L. Spek, C.J. Elsevier. Modular synthesis of bidentate triazolyl-functionalized *N*-heterocyclic carbenes and their Palladium complexes. *Organometallics*, **2010**, 29, 3109-3116. DOI: 10.1021/om100435x.
2. S. Warsink, P. Hauwert, I.-H. Chang, J.J. Weigand, J.-T. Chen, C.J. Elsevier. NHC-ligands with a secondary pyrimidyl donor for electron-rich palladium(0) complexes. *Organometallics*, **2010**, 29, 4555-4561. DOI: 10.1021/om100670u.
3. P. Hauwert, R. Boerleider, S. Warsink, J.J. Weigand, C.J. Elsevier. Mechanism of Pd(NHC)-catalyzed transfer hydrogenation of alkynes. *J. Am. Chem. Soc.*, **2010**, 132, 16900-16910. DOI: 10.1021/ja1062407.

Invited and keynote lectures 2010

1. C.J. Elsevier; July 22, 2010; Int. Conference on Organometallic Chemistry, Taipei, Taiwan, July 18-23, 2010. Invited keynote lecture. "Palladium-Carbene Species for Transfer Hydrogenation"
2. C.J. Elsevier; August 31, 2010, 3rd EUCHEMS Chemistry Congress, Neurenberg, Germany, Aug 29- Se 2, 2010. Invited lecture. "Catalytic Force of Late-Transition-Metal-NHC Complexes"

Highlights group

The group had a very fruitful year, especially regarding the ongoing NWO-NSC-project with the National Taiwan University at Taipei. Several joint papers came out and the whole group attended the international conference on Organometallic chemistry that was held in Taipei in summer. Kees Elsevier gave an invited lecture and all other group members presented well-received posters.

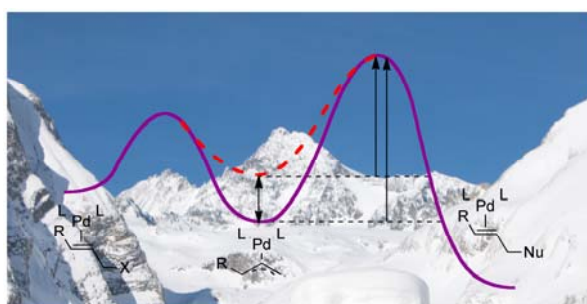
2.2.2 Homogenous and supramolecular catalysis

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

Summary of research activities

Charles Darwin proposed that evolution is based on "survival of the fittest." But in collaboration with Prof Bickelhaupt we just demonstrated that, when it comes to selecting the best catalysts, Darwin's dictum is misguided. We showed that one can select the best catalysts from combinatorial catalyst libraries by instead using the principle of "survival of the weakest"—the most unstable catalytic intermediates make for the best catalysts. The approach could make it possible to discover catalysts more quickly for syntheses of

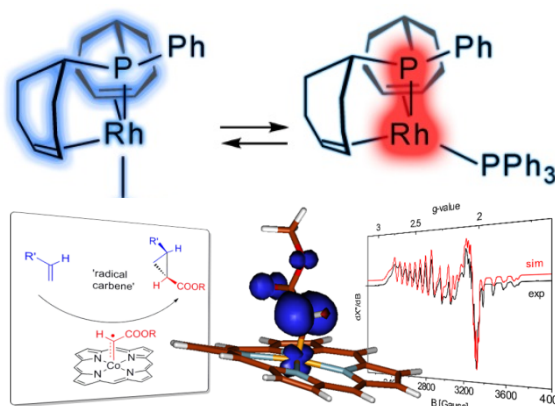
drugs and other products. Traditionally combinatorial libraries are screened to identify good catalysts, but this is a tedious process to separate the cream of the crop (the fastest catalysts) from the dross. In a *Nature Chemistry* contribution we report an innovative selection strategy for such experiments—"survival of the weakest". We have mixed limited amounts of a palladium complex that represents the resting state (lowest energy complex prior to the rate determining step) with an overabundance of phosphorus ligands. In the equilibrium mixture, different ligands bind this palladium complex, forming catalyst intermediates that differ in their ability to catalyze allylic alkylation of the starting material. The ligands that form the most stable Pd-ligand-substrate complexes become most abundant in solution, and those that form unstable complexes are scarce. Using electrospray mass spectrometry (ESI-MS) to determine the least abundant and therefore least stable complexes, the researchers were able to identify ligands that form the fastest catalysts. The study thus evaluates catalysts not in the conventional way—determining their ability to lower the reaction's activation barrier, the energy required to make it go—but instead by finding the least stable intermediates, which are by definition closer energetically to the top of the barrier and can therefore more easily traverse it. Hence "survival of the weakest."



In the area of catalyst recovery, we have reported new immobilization strategies using SBA 15 (*Chem. Commun*) and silica as support. In the latter case we studied the ligand immobilization process by employing the photophysical properties of the intrinsically fluorescent ligand nixantphos (*Angewandte Chemie*). The effect of the immobilization procedure on the catalyst distribution on the SiO₂ surface was investigated using the newly applied two-photon fluorescence microscopy (in collaboration with Prof Brouwer) at sub-micrometer level and correlated to the catalyst performance. To this end, an intrinsic fluorescence ligand was immobilized using different methods allowing identification of clustering of catalyst particles on a glass surface substrate. Independent techniques such as two-photon excitation fluorescence microscopy (solid support), GPC (solution) and intensity traces recorded of the reaction solution confirmed the growth of the ligand-aggregates/clusters *in solution* and subsequent deposition of the SiO₂-support. The industrially important rhodium-catalyzed hydroformylation reaction was taken as benchmark reaction. And it was found that the immobilization procedure could be rationally optimized such that the catalyst performance improved to a level that it becomes comparable to the homogeneous phase reaction.

In the field of metallo-radical reactivity, UvA researcher Bas de Bruin, in collaboration with Hansjörg Grützmacher at the ETH Zürich, investigated the reactivity of rare Rh⁰ complexes. This led to the discovery of a unique new type of isomerism (electro-isomerism) wherein two isomeric forms of the complex have a completely different electronic structure. One of them is best described as a ligand centered radical while the other is clearly a metal centered radical. These are in equilibrium with each other (*Angew. Chemie Int. Ed.*). The metal centered radical is furthermore capable of activating aromatic C-H bonds (*J. Am. Chem. Soc.*). This work was highlighted in *Nature Chemistry* (Bally, T.; *Nature Chemistry*, 2010, 2, 165-166), *C2W*, and *Chimia* (*CHIMIA*, 2010, 64(4), 266).

In collaboration with X. Peter Zhang of the USF in Florida, Bas de Bruin investigated in detail the



reaction mechanism of (por)Co catalyzed cyclopropanation of electron poor olefins (*J. Am. Chem. Soc.*). This reaction proceeds via a unique radical-type pathway in which ‘carbene radical ligands’ are formed from cobalt radicals. This plays a crucial role in the mechanism, and explains why: (1) electron deficient olefins can be cyclopropanated, (2) unwanted carbene dimerization is strongly suppressed, and (3) H-bonding accelerates the reaction. This work is currently attracting a lot of attention in the field of metallo-radical catalysis.

Key publications

- J. Wassenaar, E. Jansen, W.-J. van Zeist, F. M. Bickelhaupt,* M. A. Siegler, A. L. Spek, and J. N. H. Reek* Catalyst selection based on intermediate stability measured by mass spectrometry, *Nature Chemistry*, **2010**, 2,417, highlighted in C&E News en C2W.
- J. Meeuwissen and J.N.H Reek*, “Supramolecular catalysis beyond enzyme mimics,” *Nature Chemistry*, **2010**, 2, 615.
- W.I. Dzik, X. Xu, X.P. Zhang, J.N.H. Reek, B. de Bruin,* “Carbene radicals in Co-II(porphyrin)-catalyzed olefine cyclopropanation” *J. Am. Chem. Soc.* **2010**, 132, 10891-10902.

Grants

Dr. B. de Bruin

- **NWO-CW ECHO Grant** (1 PhD student, 4 yr, €260.000,-). Title: ‘Cooperative and redox non-innocent ligands in hydrogenation, dehydrogenation and dehydrogenative coupling reactions’.

Prof. J.N.H. Reek

- **NWO-CW TOP Grant** (3 PhD student, 4 yr, 1 PD, total €800.000,-). Title: ‘Enzyme inspired transition metal catalysis.

Prof. J.N.H. Reek/ Dr. J.I. van der Vlugt/Dr. D. Hetterscheit

- **TBSC Grant** (2 PhD students € 900.000,-). Title: ‘Solar-fuel: Supramolecular Catalysts for water oxidation and proton reduction’.
- **FOM TBSC Grant** (1 PDF student, 3 yr, €250.000,-). Title: ‘Photocatalytic Water Splitting in Microfluidic Devices’. Collaboration with group Brouwer (UvA; 1 PhD student) and prof. Gardeniers (U Twente; 1 PDF, 3 years)

Outreach

Prof. J.N.H. Reek

- NEMO zondagmorgen wakker worden lezing december 2010 “*Hoe werkt vuurwerk*“ (also published in NRC handelsblad)
- E-Dee lezing by ECN “*catalysis for green energy application*”

Dr. B. de Bruin

- NEMO Klokhuis vrijdagdag 14 November 2010 (including presentation “*Hoe werkt de motor van een auto?*“).

Invited Lectures

Prof. J.N.H. Reek

- Invited Lecture at the University of Köln January 2010: “New approaches to supramolecular transition metal catalysis”
- Invited lecture, Revolutionary catalysis conference 2010, Warsaw, Poland. “Supramolecular ligands in transition metal catalysis evolutionary ligand screening and a first approach to catalyst selection”
- Invited lecture Lorentz workshop Leiden, 2010. “Supramolecular catalysis for solar fuel devices”
- Invited lecture, ICIQ, September 2010 “Supramolecular approaches in transition metal catalysis”
- Invited lecture, University of Cambridge, October 2010 “New approaches to supramolecular transition metal catalysis”
- Invited lecture, supramolecular qua vadis?, conference 2010, Toarmina, Italy, “*Supramolecular control of selectivity in transition metal catalysis*”

- Invited lecture, Energy for the next generation, Beurs van Berlage, 2010, “Catalysis for green energy applications”

Dr. B. de Bruin

- International Symposium on Molecular Coordination Chemistry, Max Planck Institute for Bioinorganic Chemistry, Mülheim a/d Ruhr, Germany. November 7-9, 2010. Title: ‘Ligand Redox Non-innocence in Open-Shell Organometallic Chemistry’.
- International Conference on Porphyrins and Phthalocyanines (ICPP-6), New Mexico (USA), July 4-9, 2010. Title: ‘Radical Carbenes as Intermediates in C–C Bond Forming Reactions’
- Lorentz Workshop Multi-frequency EPR in the biosciences, University of Leiden, May 25-28, 2010, Title: ‘EPR spectroscopy and DFT computations: complementary tools to study paramagnetic organometallic compounds’
- GDCh lecture, Humboldt-Universität Berlin, May 31, 2010, Title: ‘Rhodium-mediated Stereoselective Carbene Polymerisation’

Dr. J.I. van der Vlugt

- Young Chemistry Lecturer Seminar Series, Ruhr-Universität Bochum, Germany (February 2010). Title: *Toward new avenues in bioinspired cooperative catalysis*

Patent Applications

Jellema, E. , Jongerius, A.L. Fransen, N.G.M. de Bruin, B. DPI-UvA patent application: DPI10005 EP-P0 FUNCTIONALIZED MATERIALS BY CATALYZED CARBENE COPOLYMERIZATION

Marras, F, Wang J., Coppens, M-O, Reek, JNH, EP14732, Mesoporous diphosphine-transition metal complexes for hydroformylation

N.b. DPI Invention Award 2010 awarded to de Bruin for patent 1

2.2.3 Heterogeneous catalysis and sustainable chemistry

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

Summary. of research activities

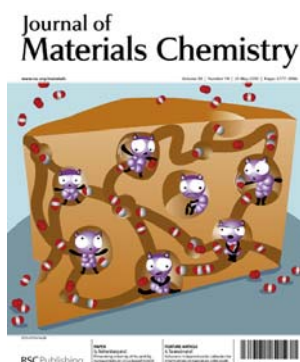
The year 2010 has been an excellent year for research in Heterogeneous catalysis and sustainable chemistry (HCSC). Thanks to the realisation of several large projects funded by CatchBio, Total G&P, NWO-Aspect and Avantium Technologies the group has recruited several excellent researchers and reached high-quality results. Moreover, the enthusiastic and motivated technicians, including the participation of Dr. J. Ellenberger for a period of 12 months (May 2010 – May 2011) has proved highly effective and helpful in the move to our new labs in Science Park Amsterdam.

Three representative research publications

- Finding furfural hydrogenation catalysts via predictive modeling. Z. Strassberger, M. Mooijman, E. Ruijter, A.H. Alberts, A.G. Maldonado, R.V.A. Orru and G. Rothenberg, *Adv. Synth. Catal.*, **2010**, 352, 2201-2210.
- Understanding catalytic biomass mining. E.J. Ras, G. Rothenberg and 53, 1202-1208.
- Interrelation of chemistry and process manufacturing by heterogeneous Srokol, M.C. Mittelmeijer-Hazeleger *Catal.*, **2010**, 53, 1197-1201.

conversion through data
B. McKay, *Top. Catal.*, **2010**,

design in biodiesel
catalysis. A.C. Dimian, Z.W.
and G. Rothenberg, *Top.*



Highlights

Trapping metal nanoparticles in “smart silica” cages

The collaboration between the research groups of Gadi Rothenberg (UvA) and Hubert Koller (Westfälische Wilhelms Universität Münster) has resulted in a new catalyst synthesis method. An article on this was published in 2010, and featured on the cover of Journal of Materials Chemistry (see image), as well as in a press release of the FNWI.

Many heterogeneous catalysts are made of metal nanoparticles on a porous support. In general, the smaller the particles, the better, because smaller particles mean higher surface area, and catalysis occurs on the particles' surface. Some chemical reactions work only on nano-sized particles. The latter have more unsaturated coordination sites, that exhibit much higher activity. This is the case for gold catalysis, where particles larger than five nanometer are generally inactive. These heterogeneous catalysts are often exposed to high temperatures and redox cycling. The metal nanoparticles often aggregate under such conditions, forming large metal chunks with a lower activity. This process is called 'sintering'.

Dr. Nina Wichner (Münster) has proposed an original solution for this problem during her PhD work, by trapping the metal nanoparticles in tailor-made cages of silica. The cages are just large enough for the particles to move and catalyse reactions, but they cannot grow further or aggregate. Wichner has made in Rothenberg's lab gold and silver nanoparticles coated with an amphiphilic "shell" covered in phenyl groups. She then synthesised porous silica via the sol-gel approach using a mixture of silica precursors that also contained phenyl groups. The phenyl-phenyl interactions resulted in a silica polymer with metal nanoparticles closely embedded in phenyl-phenyl shells. Calcining the materials at high temperature burned off the organic groups, leaving the metal nanoparticles trapped in the inorganic silica cages.

This synthesis method yielded a unique catalyst, with small metal nanoparticles that can catalyse reactions but cannot clump together and sinter. The application was demonstrated by Dr. Jurriaan Beckers (UvA), who showed that the 'trapped' gold and silver nanoparticles could catalyse CO oxidation under realistic process conditions without sintering.

The researchers of the two universities collaborated as part of the IRTG (International Research and Training Group) program, funded jointly by NWO and DFG. The program's objective is strengthening the collaboration between universities by exchanging lecturers and PhD students, and arranging special courses and 'summer schools'. Rothenberg and Koller received research funding from this program for designing and making robust solid catalysts. The IRTG is represented in the Netherlands by the Holland Research School for Molecular Chemistry (HRSMC).

Discovery of a new catalyst for making nylons, and Science Park Prize.

Dr. N.R. Shiju and Prof.dr. Gadi Rothenberg have won the UvA Science Park New Ideas Prize contest 2010 with their finding of 'A new catalyst for making nylons'. Their new catalyst and process gives a straightforward route to making nylons that reduces waste and demands less raw material. It is aimed at the caprolactam market for producing nylon 6 (the market for caprolactam is over \$3Bn per annum). The catalyst has also been patented by the University of Amsterdam. The researchers are now in dialogue with possible industrial partners in an effort to turn the discovery into a commercial process. The importance of the discovery is reflected by the seriousness by which it is treated by major industrial players. This is a true example of actual valorisation of basic research results.

Incidentally, this is the third time that researchers from the Heterogeneous Catalysis and Sustainable Chemistry group have won prizes in the New Ideas Contest (also in 2006 and 2008).

General data on publications and activities for 2010

We published in 2010 11 papers in peer-reviewed journals, and submitted three patent applications (one on ammoxidation, two others on biodiesel processing via our spin-off company Yellow Diesel BV).

Grant applications

Group members were highly active in applying for grants in 2010, but with disappointing results. Prof. Rothenberg applied for an NWO-vici grant, but although his proposal scored extremely high (A,A,A,A+), it was not granted. This proposal will be resubmitted in 2011. Similarly, applications by Dr. Shiju and Dr. Grecea for a NWO-vidi grant were rejected. We include these grant applications nevertheless in the scientific report because the time invested in writing the applications and preparing for the interviews is substantial, and so it reflects a major effort on the part of the group.

2.3 Computational Chemistry

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

Research topics

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

Summary. of research activities

The Computational Chemistry theme consists of three research groups, *Simulations of Bio-molecular Systems* (Prof. Bolhuis), *Chemische Reaktorkunde* (Prof. Krishna), and *Complex Molecular Simulations* (Vacancy, Dr. Meijer). The research in the Computational Physics and Chemistry groups of Krishna, Bolhuis and Meijer focuses on the study of materials, biological systems, and solution chemistry. Development and application of novel computational techniques are an essential part of the research. With many of the studied structures and processes intrinsically multiscale their computational approach focuses strongly on multiscale techniques. International collaboration with experimental and computational groups plays an important role.

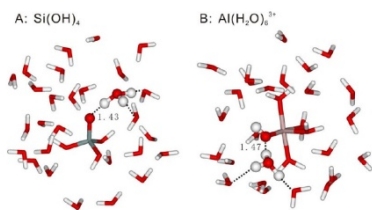
Highlights

The group has kept a strong record in modelling complex phenomena in chemical, physical, and biological systems.

Materials The design and development of novel nanoporous materials is of paramount importance in the areas as storage, separation, and catalysis. A targeted approach requires a proper quantitative description of the materials. We have focussed on zeolites, metal organic frameworks (MOFs) and carbon. In the area of zeolites we elucidated the how Al-substituted MFI zeolites containing nonframework cations can be used for enantioseparation. If one enantiomer is present in excess it will organize the nearby cations such that all adsorption sites become effectively chiral (van Erp, Caremans, Dubbeldam, Martin-Calvo, Calero, *Angew. Chem. Int. Ed.* **49**, 3010, 2010).

Carbon may adopt a large variety of structures. Using a state-of-the-art approach we have obtained an accurate picture of the thermal stability of carbon over a large range of pressures (Ghiringhelli and Meijer, *Springer Series on Carbon Materials*, **3**, 1, 2010).

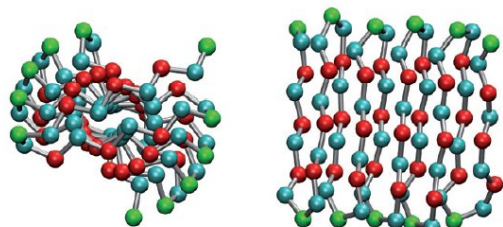
Chemical reactivity in complex environment Most (bio-)chemical processes occur in complex fluctuating environment, such as solvent, protein, or nanostructured cavities. We apply advanced *ab initio* molecular simulation techniques to address the role of the fluctuating environment. Silicic acid (Si(OH)_4) and the hexa-aqua of Al^{3+} are fundamental model aqueous species of chemical importance in nature. Combining *ab initio* molecular dynamics with rare events methods we determined the pKa of these components and elucidated their hydroxyl dissociation mechanism in aqueous solution. It provides an encouraging basis for applying the employed methodology to predict acidity constants. (Liu, Meijer, *et al.*, *Geochimica et Cosmochimica Acta* **74**, 510, 2010).



Cisplatin ($\text{cis-[Pt(NH}_3)_2\text{Cl}_2]$) is an important compound in cancer treatment. The mode of action of cisplatin starts inside the cell with the hydrolysis of Pt–Cl bonds to form a Pt–aqua complex. Our

metadynamics ab initio simulations show that hydrogen bonding between solvent water molecules and metal complexes in the hydrolyzed product systems is stronger than that in the reactant cisplatin system, and that the Second hydrolysis of cisplatin is thermodynamically more favorable than the first, which is in good agreement with experimental results. (Kai-Chi and Ensing, *PCCP* **12**, 10348, 2010)

Biomaterials (Bolhuis) Self-assembly of polypeptides into fibrils promises the development of new functional supra-molecular biomaterials. Here, prediction of structure and kinetics is crucial to control the design of such novel biomaterials. We studied the self-assembling fiber formation of a triblock copolymer



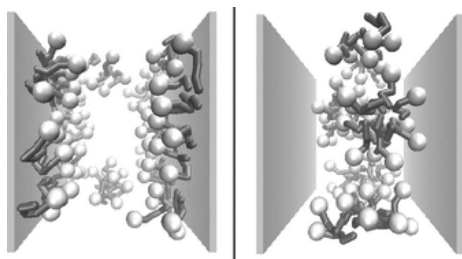
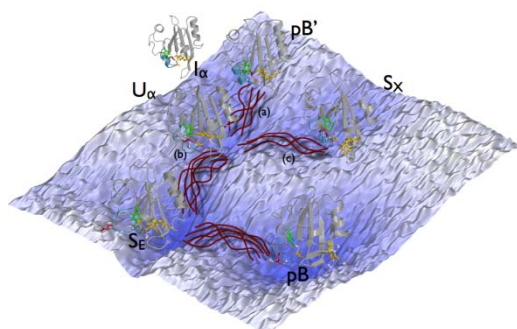
consisting of a middle silk-like block flanked by two hydrophilic end blocks. By extensive replica exchange molecular dynamics simulation we predicted the thermodynamically stable conformation of the middle block to be a β -roll. This all-atom approach was at the limit of what is feasible, and therefore we developed a coarse-grained force field to describe the assembled polypeptide including the hydrophilic flanks (Schor,

Ensing, Bolhuis, *Faraday Discuss.* **144**, 127, 201). Using this force field we predicted e.g. the fiber persistence length. These predictions are corroborated by experiments in Wageningen UR and facilitate the design of new self-assembling silk-like materials with novel functionality.

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

Protein conformational changes (Bolhuis, Vreede) Using a combination of four advanced rare event molecular simulation techniques we conducted a numerical study of the folding routes of the truncated FBP28 WW domain at ambient conditions (Juraszek, Bolhuis, *Biophysical Journal* **98**, 646, 2010) We explored the free energy landscape as well as the dynamical folding pathways with replica exchange molecular dynamics, bias-exchange metadynamics, transition path sampling and metadynamics. We find two major folding routes, differing in the formation order of the two main hairpins, and in hydrophobic side-chain interactions. The computed barriers are in agreement with experiments. Combining several powerful simulation techniques thus provides a more complete understanding of the kinetic mechanism of protein folding.

Understanding the dynamics of large-scale conformational changes in proteins still poses a challenge for molecular simulations. We employed transition path sampling of explicit solvent molecular dynamics trajectories to obtain atomistic insight in the reaction network of the millisecond timescale partial unfolding transition in the photo cycle of the bacterial sensor photoactive yellow protein. Likelihood maximization analysis predicts the best model for the reaction coordinates of each substep as well as tentative transition states, without further simulation. Our results open the way for studying millisecond conformational changes in other medium-sized (signaling) proteins (Vreede, Juraszek, Bolhuis, *Proc. Nat. Acad. Sci. USA* **107**, 2397, 2010)



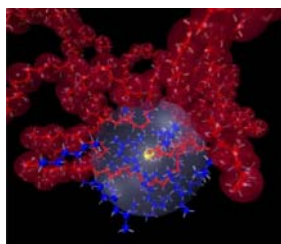
Soft matter systems (Bolhuis, Lowe) The stability of colloidal dispersions can be severely affected by the presence of surfactants. Because surfactants can adsorb at colloidal surfaces as well as form micelles, one can expect interplay between both phenomena. Using grand-canonical coarse-grained Monte Carlo simulations on surfactant solutions confined between two surfaces, we investigate how adsorption and micelle formation affects the effective

interaction between two colloidal particles, and hence, the stability of the colloidal dispersion. We find that the formation of micelles at concentrations above the CMC causes an additional depletion effect, resulting in an effective attraction, which in turn can destabilize a colloidal dispersion. (Pool, Bolhuis, PCCP **44**, 14789, 2010)

The stability of nanoparticle assemblies is strongly determined by the effective interactions between such particles. Together with the Kegel group in Utrecht we studied how hollow shells of nanoparticles can be stable through attractive and repulsive competing interactions (Mani, Sanz, Bolhuis, Kegel, J. Phys. Chem. C **114**, 7780 (2010)).

Methods for Simulating Complex Systems The multiple state transition path sampling aims to sample from an extended path ensemble including all possible trajectories between any pair of metastable states. We introduced a Wang–Landau based biasing approach to improve the sampling. We find that the biasing of the multiple state path ensemble does not influence the switching behavior, but does improve the sampling and thus the quality of the individual path ensembles (Rogal, Bolhuis, *J.Chem.Phys.* **133**, 034101, 2010). We also introduced a new reweighting scheme for the path ensembles in the transition interface sampling framework. The reweighting allows for the analysis of free energy landscapes and committor projections in any collective variable space (Rogal, Lechner, Juraszek, Ensing, Bolhuis, *J. Chem. Phys.* **133**, 2010). The reweighted path ensemble can be used to optimize possible nonlinear reaction coordinates based on a likelihood maximization approach in combination with a string projection method. While developed for use with path sampling, this analysis method can also be applied to regular molecular dynamics trajectories. (Lechner, Rogal, Juraszek, Ensing, B.; Bolhuis, P. G., *J.Chem.Phys.* **133**, **2010**, 133).

Finding the energy minima of systems with constraints is a challenging problem. We developed a minimization method based on the projection operator technique to enforce distance and angle constraints in minimization and reaction-path dynamics. Two case studies are presented: (1) A mode analysis of united-atom *n*-butane with various internal degrees of freedom kept frozen and (2) the minimization of chromene at a fixed approach toward the catalytic site of a (salen)Mn. The obtained information on energetics can be used to explain why specific enantioselectivity is observed. Previous minimization methods work for the free molecular case, but fail when molecules are tightly confined. (Dubbeldam, Oxford, Krishna, Broadbelt, and Snurr, *J.Chem.Phys.* **133**, 034114 (2010)).



Until now, adaptive atomistic–coarse-grain (A/CG) molecular dynamics simulations have had very limited applicability because the on-the-fly CG→A transformation is problematic for all but those molecules whose CG representation consists of a single particle. We have solve this problem by combining a transitional healing region with a rotational dynamics of rigid atomistic fragments in the CG region. The applicability of method is demonstrated with adaptive multiscale simulations of liquid hexane and of a dilute polymer solution (Nielsen, Moore, and Ensing, *Phys. Rev. Lett.* **105**,

237802, 2010).

Key publications 2010

- J. Vreede, J. Juraszek and P.G. Bolhuis, *Predicting the reaction coordinates of millisecond light-induced conformational changes in Photoactive Yellow Protein* Proc. Natl. Ac. Sci. USA **107**, 397, 2010. (Commentary by G. Hummer in the same issue and awarded the WiF best publication prize)
- S.O. Nielsen, P.B. Moore, and B. Ensing, *Adaptive multiscale molecular dynamics of macromolecular fluids*, *Phys. Rev. Lett.* **105** 237802 (2010).
- R. Krishna and J.M. van Baten, *In Silico Screening of Zeolite Membranes for CO₂ Capture*, *J. Membrane. Sci.* **360**, 323 (2010).
- D. Dubbeldam, G.A.E. Oxford, R. Krishna, L.J. Broadbelt, and R.Q. Snurr, *Distance and angular holonomic constraints in molecular simulations*, *J. Chem. Phys.* **133**, 034114 (2010).
- L. Ghiringhelli and E.J. Meijer, *Liquid carbon: Freezing line and structure near freezing*, *Springer Series on Carbon Materials*, **3**, 1, 2010.

Highlights

Grants and Prizes

- VIDI grant; D. Dubbeldam
- FOM Free Research Program; Bolhuis
- FOM Free Research Program; Meijer, Ensing
- DEISA Extreme Computing Initiative Grant; Bolhuis, Vreede
- HPC Travel Grant; Ensing
- ESF Scientific Meeting; Meijer, Ensing
- WiF Best Publication Prize 2010; Vreede
- Glasser Visiting Professor 2010, Philadelphia; Ensing

Collaborations

- Krishna – Karger (Leipzig), Smit (Berkeley)
- Bolhuis – Kegel (Utrecht), Dellago (Vienna), Cohen Stuart (Wageningen)
- Meijer – van Santen (Eindhoven), Sprik (Cambridge), van Erp (Leuven), Bakker (AMOLF), Sautet (Lyon), Liu (Nanjing)
- Lowe – Pagonabarraga (Barcelona)
- Ensing- Nielsen (U Texas), Moore (Philadelphia), Visscher (VU-Amsterdam)
- Dubbeldam – Snurr (Northwestern), T. van Erp (Leuven)
- Vreede – Dame (Leiden), Groenhof (Göttingen), Groot (VU-Amsterdam), Lupas (Max Planck Institute Tübingen)

Invited plenary lectures

- Bolhuis – Conference on Multiscale Molecular Modeling, Edinburgh, 30 June -3 July 2010
- Vreede – Gordon Research Conference on Photosensory Receptors and Signal Transduction, April 2010, Lucca, Italy.

Organized conferences/schools

- Ensing – Winterschool Theoretical Chemistry and Spectroscopy (Han-sur-Lesse)
- Meijer, Ensing, Dubbeldam – Winterschool MolSim 2010 (Amsterdam)
- Bolhuis – ACMM Spring and Fall symposia (Amsterdam)
- Bolhuis – FOM Biophysics meeting 4-5 October 2010 (Veldhoven)
- Ensing, Vreede – Amsterdam Photoreceptor Meeting (Amsterdam)

Membership committees

R. Krishna

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

P.G. Bolhuis

- Member NWO TOP/Echo committee 2010
- Member FOM BRM program committee
- FOM-workgroup leader (A-23)
- Member of FOM network “Statistische Fysica”.

E.J. Meijer

- UvA representative Scientific Council CECAM.
- Member Selection Committee CECAM Berni Alder Prize.
- Coordinator Erasmus Mundus program ATOSIM (2006-2011).
- Member of FOM network “Statistische Fysica”.
- Member NWO/CW Study group "Spectroscopy and Theoretical Chemistry".

C.P. Lowe

- Co-organizer "write it right". International workshops 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)

Outreach activities

- Vreede, Ensing – Open day UvA.

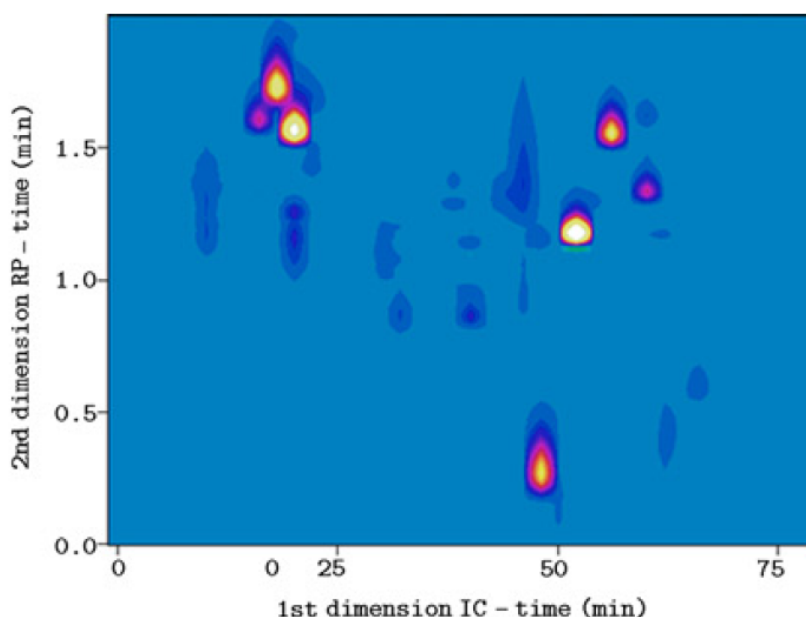
2.4 Macromolecular and Biosystems Analysis

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

Summary of research activities

In 2010, Erwin Kaal defended his PhD thesis on "Extending the applicability of GC" (promotor Prof.dr. Hans-Gerd Janssen). His research project, directly sponsored by industry, resulted in 9 publications in scientific journals.

Stella S. Brudin defended her PhD thesis on "One- and two-dimensional analysis of complex anionic mixtures". Her project had been sponsored directly by industry. Part of her work had been carried out at the University of Tasmania, Australia, in the group of her co-promotor Prof.dr. Paul Haddad.



Two-dimensional separation of the organic acids in a yoghurt sample. From the thesis of Stella Brudin.

In the field of Forensic Science, Ira.S. Lurie defended his PhD thesis on "UHPLC of Seized Drugs" (promotor Prof.dr. Peter Schoenmakers). A start was made with experimental research on forensic analysis, in a project conducted in cooperation with NFI and TNO (Analysis of Explosives, H. Brust).

The project on "Two- and three-dimensional spatial liquid chromatography for biomarker discovery" (DiscoverIE), in which the UvA analytical-chemistry group collaborates with the Free University of Brussels (Profs. Gert Desmet and Sebastiaan Eeltink) and the University of Ghent (Prof. Bart Devreeze) in a consortium led by ThermoFisher Scientific / Dionex was awarded a subsidy of 965 k€.

Our research on the development of rapid, reliable and simple methods for the diagnosis of Tuberculosis and other pulmonary diseases could be further strengthened by a research grant in the Nanonext program

‘Integrated Microsystems for Biosensing’. The research work will focus on pathogens present in sputum, breath, serum and urine from patients with pulmonary diseases. With the devices under study patients can be screened for pathogens in a direct way, providing results within an hour, while this currently takes up to many days. Partners in the project are ATAS - GL International, C2V and Our group (Arend Kolk and Hans-Gerd Janssen).

In the same program a proposal on “Nanofluidic devices for the separation of biomacromolecules” was granted (Dr. Wim Th. Kok together with Twente University). This project builds on previous NanoNed projects conducted in the Analytical Chemistry group.

A proposal for the STW program SmartSep was also granted (Dr. Wim Th. Kok). This project is directed on the development of methods and devices for the industrial-scale purification of biopharmaceuticals such as recombinant proteins and antibodies.

Key publications 2010

- S. Peters, H.-G. Janssen, G. Vivó-Truyols, “Trend analysis of time-series data: a novel method for untargeted metabolite discovery”, *Anal. Chim. Acta* 633 (2010) 98-104.
- W.Th. Kok, A.G. Shepherd, A.J. Tüdös, M. Grutters, "Characterization of asphaltenes by non-aqueous capillary electrophoresis", *Energy&Fuels*, 25 (2011) 208-214.
- G. Vivó-Truyols, S. van der Wal, P.J. Schoenmakers, “Comprehensive study on the optimization of online two-dimensional liquid chromatographic systems considering losses in theoretical peak capacity in first- and second-dimensions: A pareto-optimality approach”, *Analytical Chemistry*, 82 (2010) 8525-8536.

Highlights

COAST (Comprehensive Analytical Science and Technology) was officially launched on November 1st, 2010. This national initiative on strengthening the foundations of analytical science took many years of preparation by a number of people, including Peter Schoenmakers and Hans-Gerd Janssen. COAST has elected Science Park Amsterdam as its headquarters and Peter Schoenmakers is its Education Director. The HTC-11 (Hyphenated Techniques in Chromatography) and (HTSP) Hyphenated Techniques for Sample Preparation took place in early 2010, with Peter Schoenmakers (Chairman) and Petra Aarnoutse carrying most of the organization. The two conferences drew more than 500 people to Bruges (Belgium). Peter Schoenmakers presented plenary lectures at HTC-11 (Bruges, Belgium) and Simcro 2010 (Campos do Jordão, Brazil), keynote lectures at HPLC2010 (Boston, MA, USA) and PittCon (Orlando, FL, USA) and an honorary lecture for the MassSep society in Boston. Hans-Gerd Janssen presented a state-of-the-art overview lecture at HTC 11 and a plenary lecture at the GCxGC conference in Riva del Garda.

Patents

Together with Sebastiaan Eeltink (Dionex) Peter Schoenmakers filed several patents on Spatial Chromatography.

2.5 Molecular Photonics

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

Summary of research activities

Light-induced chemical conversions play a key role in many technological and biological processes, the most important of all being photosynthesis. Understanding the interaction of light and molecular matter is therefore highly significant. *Molecular Photonics* aims to advance the fundamental knowledge of the dynamics of excited states in molecules and nano-sized objects, and to contribute with its expertise to applications of the photosciences. The *Molecular Photonics* group is unique within the Netherlands because it combines the skills of internationally recognized experts in molecular synthesis, spectroscopy and theory. Fields of research are energy and electron transfer, catalytic reactions, and conformational dynamics. This leads to investigations of molecular switches and motors, nanoparticles and photochemical

reactions. Topical application areas are found in photochemical energy conversion, polymer science, mechanisms of catalysis, biomedical imaging, and phototherapies. The *Molecular Photonics* group is a full partner in *LaserLab Amsterdam*, a European facility (Laser Lab Europe) and participates in the *Holland Research School of Molecular Chemistry*. In 2010 the group has been active in the following research areas.

Molecular nanotechnology. We have shown how in the gas phase binding interactions between the thread and the macrocycle of a [2]rotaxane can be tuned in a quasi-continuous manner by adding hydrogen-bond-forming solvent molecules one at a time to an isolated [2]rotaxane molecule. In this way conformational changes have been induced that detach controllably the thread from the macrocycle (*Angew. Chem. Int. Ed.* **2010**, *49*, 3896-3900).

Molecular machines in motion. Using time-resolved vibrational spectroscopy, we have investigated the operation mechanism of a rotaxane-based molecular shuttle. The shuttling involves two steps: thermally driven escape from the initial station, followed by fast motion along the track ending either at the initial or final station. The fast motion approximates a biased random walk. Surprisingly, the direction of the overall motion is opposite that of the bias (*Science* **2010**, *328*, 1255-1258). A modification of the molecular design led to a bistable molecular shuttle. The thermodynamics of this system could be studied with high precision, which revealed the importance of entropy and heat capacity differences between the two co-conformational states (*Chem. Commun.* **2010**, *46*, 2061-2063).

Tunneling electrons through bends and around corners. A simple theoretical model has been developed that describes orientation effects in electron transfer. In this model the twist and dihedral angles between electron donor (D) and acceptor (A) play a role in the distance dependence of charge transfer (CT), next to the conventional distance dependence of electron transfer that is not influenced by the angles between D and A. This can be applied to, for example, helical bridges, when twist and dihedral angles can modulate the rate. The new equation is dubbed: Karplus Relation for Charge Transfer Interaction. It can be used to describe orientation effects and non-linear plots of $\ln(k_{\text{CT}})$ vs. distance (*Photochem. Photobiol. Sci.* **2010**, *9*, 1018-1026). Furthermore, charge separation processes in two low-band gap oligomer/fullerene C₆₀ triads that are models for new organic solar cell materials were studied in collaboration with TU-Eindhoven (*Photochem. Photobiol. Sci.* **2010**, *9*, 1055-1065; *J. Phys. Chem. B* **2010**, *114*, 14149-14156).

Photoactive proteins. A series of high-resolution laser spectroscopic studies have been performed on *para*-coumaric acid and derivatives, chromophores of the Photoactive Yellow Protein. These have led to the first characterization of their electronically excited-state manifold under isolated-molecule conditions (*J. Am. Chem. Soc.* **2010**, *132*, 6315-6317).

Ion spectroscopy. A new method has been developed that allows for the observation of IR and UV/Vis spectra of cold and isolated molecular ions with unprecedented sensitivity. To this purpose ions are captured in nanodroplets of superfluid helium. The study opens up exciting new opportunities for the investigation of ionic that may range from biomolecular ions such as polypeptides and proteins to ionic clusters (*J. Am. Chem. Soc.* **2010**, *132*, 14086-14091).

Silicon nanocrystals. In collaboration with the group of T. Gregorkiewicz (Van der Waals – Zeeman Institute, UvA), no-phonon optical transitions that are tunable into the visible range have been identified in silicon nanocrystals. The enhanced quantum efficiency of this emission compared to bulk silicon (three orders of magnitude for 2.5-nm-diameter nanocrystals) creates new opportunities in photonic, photovoltaic and optoelectronic applications of silicon nanocrystals (*Nature Nanotech.* **2010**, *5*, 878-884).

Designing nanoplatfroms for homogeneous assay and cancer detection and therapy. Various nanostructures/complexes have been tailor-designed for the biological application. Au/SiO₂ core/shell nanoparticles have been designed to enhance significantly sensitivity of the homogeneous assay based on FRET from QDs to organic fluorophores in solution (*Chem. Comm.* **2010**, *46*, 6479-6481). Multi-targeting single fiber-optic biosensor based on evanescent wave and quantum dots was realized for the first time (*Biosensors and Bioelectronics* **2010**, *26*, 149-154).

Single molecular spies. A new mechanism for single molecule fluorescence switching based on photoinduced electron transfer was exploited to detect spatial and temporal heterogeneities in thin polymer films. The electron transfer process requires a sufficiently large free volume to occur. As a result, fluorescence is switched off when heating the material from temperatures below the glass transition to a few degrees above it (*J. Am. Chem. Soc.* **2010**, 132, 1240-1242).

Fluorescence microscopy assists catalyst development. In a collaboration with the HIMS homogeneous catalysis group, two-photon fluorescence imaging pointed the way to a large improvement in the preparation of immobilized catalysts. A simple change in the experimental procedure avoided the formation of clusters of ligands in solution, prior to condensation on the substrate. The catalyst thus produced was very active and could be recycled effectively (*Angew. Chem. Int. Ed.* **2010**, 49, 5480–5484).

Key publications 2010

1. M.R. Panman, P. Bodis, D.J. Shaw, B.H. Bakker, A.C. Newton, E.R. Kay, A.M. Brouwer, W.J. Buma, D.A. Leigh, S. Woutersen; Operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy. *Science* **328** (2010), 1255-1258.

2. W.D.A.M. de Boer, D. Timmerman, K. Dohnalova, I.N. Yassievich, H. Zhang, W.J. Buma, T. Gregorkiewicz; Red spectral shift and enhanced quantum efficiency in phonon-free photoluminescence from silicon nanocrystals. *Nature Nanotech.* **5** (2010), 878-884.

3. F. Marras, A.M. Kluwer, J.R. Siekierzycka, A. Vozza, A.M. Brouwer, J.N.H. Reek; Phosphorus ligand imaging with two-photon fluorescence spectroscopy: towards rational catalyst immobilization. *Angew. Chem. Int. Ed.* **49** (2010), 5480–5484.

Highlights

In 2010 Brouwer obtained an ECHO grant on “Fluorescence monitoring of organocatalytic events”. Oomens and Buma are part of the NWO Astrochemistry Programme approved in 2010. A large part of the key publications has attracted the attention of the popular press, leading to articles and commentaries in popular journals and on the web. Promotional activities included radio interviews with Sander Woutersen (Noorderlicht, April 12 and June 17, 2010), contributions to popular scientific journals (*e.g.* *Nederlands Tijdschrift voor Natuurkunde* **2010**, 76, 350-355), and popular lectures (PAC Symposium *Chemistry makes Sense*).

2.6 Other activities (Polymer Systems)

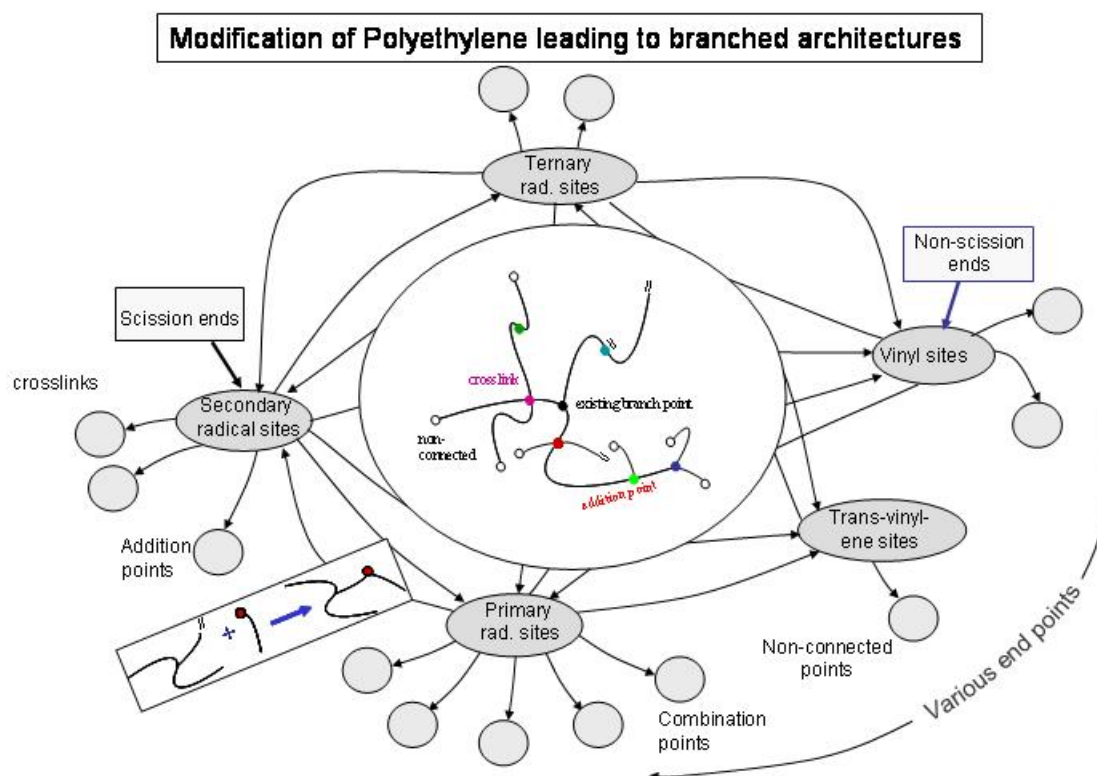
Prof.dr. P. Iedema

Summary of research activities

Research activities have continued in the area of modeling branched polymer architectures. A research contract project in cooperation with TIPb (Toegepaste Industriële Procesbeheersing) has been finalized with an end report (confidential). This project was concerned with the reactive modification of Polyethylene and Polypropylene homo-and copolymers (see highlight below). A start has been made with two new projects being co-financed by a Marie Curie ITN Programme “NANOPOLY” and a Dutch Polymer Institute, Polyolefins Project #674, “RheoConBran”. The latter is part of a larger project in cooperation with Prof.dr. H. Slot, TU Eindhoven. The Polymer Systems group provides information concerning the branching architectures and TUE employs this information to predict the melt rheology. In May and September two new PhD students have been appointed on the NANOPOLY/DPI-project: Nazila Yaghini and Ivan Kryven, respectively working on “Prediction of Branched Polymer Structures by conditional Monte Carlo simulation”, and “Hybrid Deterministic/MC approach of Polymer Modification with Scission and Branching”.

A new research activity is in preparation in the area of Conservation and Restoration of Art objects. During the 90's of the last century the NWO-funded Programmes MOLART and De Mayerne have been carried out, revealing the important role of certain mobile components the metal-coordinated network of 17th century oil paintings. End 2010 NWO has announced a new Programme, Science4Art, which offers the opportunity for HIMS to further investigate migration phenomena in paint layers. It is intended to propose a project at HIMS, in which former PhD students from the earlier NWO-projects are cooperating with HIMS Staff: Prof. Iedema (supervision), Prof. Elsevier, Prof. Schoenmakers, Prof. Norman Tennent (Conservation Scientist at the UvA Humanities Faculty, zero appointment at HIMS), together with various museums.

- Presentation Piet Iedema at Sabic: End Report TIPb-Project, April 21, 2010, "Reactive Modification of Polypropylene and Polyethylene homo- and copolymers".
- Presentation Piet Iedema at Marie Curie ITN 'NANOPOLY' Consortium meeting, Porto, October 7, 2010, "Prediction of Branched Polymer Structures by conditional Monte Carlo simulation".
- Presentation Piet Iedema at Marie Curie ITN 'NANOPOLY' Consortium meeting, Porto, October 7, 2010, "Hybrid Deterministic/MC approach of Polymer Modification with Scission and Branching".
- Presentation Nazila Yaghini at DPI Cluster Meeting Polyolefins, Schiphol, November 2-3, 2010 "Prediction of Branched Polymer Structures by conditional Monte Carlo simulation".
- Presentation Ivan Kryven at DPI Cluster Meeting Polyolefins, Schiphol, November 2-3, 2010, "Hybrid Deterministic/MC approach of Polymer Modification with Scission and Branching".



Highlights 2010

Modification of Polyethylene leading to branched architectures

The reactive modification is initiated by peroxides and leads to a series of chain scission and branching reactions. The reactive sites at chain backbones are primary, secondary and tertiary radical sites and vinyl and vinylidene groups (shaded ovals). A kinetic model describes the creation of these and their transition (rectangles) to various "end" points: crosslinks, addition points, etc. A Monte Carlo sampling scheme combines linear chain elements with these connection points to branched architectures (centre).

3 Strategy, activities and results

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

An overview of the HIMS activities, objectives and results for the period 2010-2012, as defined in the FNWI-UvA/CvB agreement (convenant) 2010-2012, are given in the following table.

	<i>Activities</i>	<i>Objectives and results</i>
2010	a. recruitment of outside and guest PhD students b. improve the efficiency of the doctoral research path through better control and guidance c. develop policies for appointing of 1-6 endowed (part-time) professors d. discussions with education- and teaching directors, from within and outside the faculty, about a greater HIMS share in teaching tasks e. agree with the colleagues of the VU for the three HIMS key-areas on the creation of Centers of Expertise (according ACMM) f. new research initiatives with the VU, including in the new field of renewable energy (including Physics UvA and VU) g. New research initiatives in the field of forensic- and - art sciences with various partners, based on such new NWO (early 2010) and EU programs	Ad a. 1-3 additional PhD Ad b. develop and formulate policies Ad c. preparation and appointment of 1-2 new (preferably endowed) part-time professors Ad d. agree on the share in the 2010-2011 curricula Ad e. agree and formulate together with the VU colleagues for CoE <i>Synthesis & Catalysis</i> and CoE <i>Analysis and Spectroscopy</i> Ad f. prepare and submit new research initiatives together with VU colleagues Ad g. prepare and submit projects in NWO- and EU programs together with various relevant partners
2011	a. see 2010 b. see 2010 c. see 2010 d. increase contribution to develop /update / implement teaching modules. e. see 2010 f. see 2010 g. see 2010	Ad a. see 2010 Ad b. efficiency 5% better. Ad c. appointment of 1-2 new (preferably endowed) part-time professors Ad d. 5% increase in the share of HIMS in various courses together Ad e. opening CoE <i>Synthesis & Catalysis</i> and opening CoE <i>Analysis and Spectroscopy</i> Ad f. 1-2 new joint research projects. Ad g. 1-2 new joint research projects.
2012	a-g. Evaluation of activities and achievement of objectives and results and realize possible extensions	Ad a. 2-5 additional PhD students in 2010-2012 Ad b. 10% efficiency improvement in plan period 2010-2012 Ad c. 3-6 (preferably endowed) part-time professors appointed in 2010-2012 Ad d. 5-10% increase of the HIMS share in various special courses in the plan period Ad e. new projects submitted with the VU colleagues in the context of the CoE Ad f. 2-4 new joint research projects. Ad g. 2-4 new joint research projects.

Realisation of activities

Recruitment of outside and guest PhD students (activity a)

The institute has four external PhD candidates (buitenpromovendi) appointed in 2010, two PhD students in the group of Prof. Huib Bakker (FOM Amolf) and 2 PhD students in the group of Prof. Jos Oomens (FOM Rijnhuizen). Their PhD defences are expected in 2014-2015. New appointments of external candidates are expected in the groups of Prof. Schoenmakers, Prof. Kleijn and Prof. Buma and Dr. Zhang. Appointments from the Chinese Academy of Sciences are difficult because of the necessary grants for the final year of their study at the UvA. In 2010 three external PhD candidates obtained their doctorate degree, a PhD with Prof. Schoenmakers (Lurie) and two PhD's with Prof. H. Bakker (Timmer and Tielrooy). Lurie is the first PhD candidate that obtained a doctorate degree at the UvA in Forensic Sciences.

Improve the efficiency of the doctoral research path through better control and guidance (activity b)

The institute has introduced a financial arrangement for PhD candidates to facilitate the promotion efficiency. If their thesis is completed and approved by the doctoral committee in time, the PhD candidates will receive a financial contribution from the institute for the printing costs of their thesis, namely Euro 2000 for completion within 4 years and 1 month or 500 euro for completion within five years. New policies to promote the efficiency of the doctoral research path, is subject of further discussions with the staff members. The Director will establish a mentor system. A point of consideration is to put more pressure on PhD candidates through the linking of permission for conference visits with the realization in time of a scientific publication (preferably one publication per year).

Develop policies for appointing of 1-6 endowed (part-time) professors (activity c)

Appointments of special (endowed and part-time) professors are important for HIMS to further strengthen the level of the Institute. The institute intends to create two part-time appointments in the field of Forensic Sciences (both 0.2 FTE), namely Dr. A. van Asten (NFI) in the group Schoenmakers and Dr. M. Aalders (AMC) in the group Buma / Brouwer. The succession of Prof. Schoemaker (DSM) Fine Chemicals Industrial Chair through the Stichting Beta-Plus (group Hiemstra), is ongoing. Also ongoing are new explorations in groups Reek and Bolhuis. New appointments will follow in the coming years. An option is an exchange of part-time professorships to connect with the VU.

A greater HIMS share in teaching tasks (activity d)

Prof. Klein teaches in the new Master's program on Advanced Matter Physics and Energy, a joint Master with the VU. The ambition of the Institute to participate in the third year of the Amsterdam University College (sustainability module) has not yet been realized yet. HIMS is in discussion with SILS about taking over the teaching tasks in biochemistry (especially in the bachelor chemistry) and possibly also a part of teaching tasks for the first year psychobiology students. Furthermore, the institute in consultation on the contribution of the HIMS staff in teaching in both Forensic Science - and Art Sciences.

The creation of Centers of Expertise (according ACMM) (activity e)

The institute is in consultation with Prof. Visscher of VU on future collaboration in Center(s) of Excellence (CoE), as is already realized in the field of Multiscale Modeling. The plan is to link three CoE's to the research priorities of HIMS (and the VU). This concerns sustainable Chemistry, including Energy (a combination of mainly Synthesis and Catalysis groups), Analysis and Spectroscopy (linked to or TI-COAST² and the LaserLab Amsterdam) and Multiscale Modeling, existing collaboration in the Amsterdam Center for Multiscale Modeling (ACMM)³.

² TI-COAST (Comprehensive Analytical Science and Technology) is a nationwide research and education initiative directed by NWO and the Regiegroep Chemie, which aims to generate breakthroughs and to cluster new techniques in analytical chemistry and spectroscopy by using information technology and nanotechnology. HIMS houses the headquarters of TI-COAST.

³ The Scientific advisory Board (SAC) of HIMS has advised in 2010 not to pursue multiple CoE's, but to combine all activities into one institution together with the VU.

New research initiatives with the VU (activity f)

Investment applications in the context of sectorplans (NWO-BAZIS programme) were realized and coordinated with our VU colleagues. New applications will follow for the 2011 round. HIMS groups work on joint research initiatives with the VU (eg Computational from ACMM, Analysis from TI-COAST and Photonics from the LaserLab Amsterdam and TI-COAST).

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

Various applications with HIMS participation were prepared for the new NWO Forensic Sciences and Art Sciences programmes, and also for EU / FS programmes. Where possible, collaboration with partners in the application field, including the Netherlands Forensic Institute (NFI), Institute Collection Netherlands (ICN) and the Rijksmuseum, were realized. Besides the former Director of HIMS (Dr. Zsom), several HIMS professors have contributed to the new NWO programmes for Forensic Sciences (Prof. Schoenmakers) and Art Sciences (Prof. Iedema).



Forensic Sciences



Science4Arts

4 Dissemination of knowledge, valorisation, promotional activities

Valorisation of know-how is of increasing importance, as evidenced by the two HIMS spin-off companies, *InCatT* (Prof. Reek c.s.) established in 2009 and *YellowDiesel* (Prof. Rothenberg c.s.) established in 2008. Both companies were realized under the umbrella of the UvA Holding. In order to protect our intellectual property, HIMS follows an active patenting policy, on most occasions directly with our industrial partners. The institute has applied for several patents, while some new projects are promising. Patent Applications of 2010:

- Jellema, E. , Jongerius, A.L. Fransen, N.G.M. de Bruin (Catalysis), B. DPI-UvA patent application: DPI10005 EP-P0 Functionalized materials by catalyzed carbene copolymerization (DPI Invention Award 2010 awarded to De Bruin for this patent)
- Marras, F, Wang J., Coppens, M-O, Reek (catalysis), JNH, EP14732, Mesoporous diphosphine-transition metal complexes for hydroformylation
- Improvements on CLIPS-technology, P. Timmerman, L. E. M. Smeenk, N. Dailly, J. H. van Maarseveen (Bio-Molecular Synthesis), EP 10188743.8, filing date 25-10-2011

In the future out-licensed patents could be important for HIMS as source of income.

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

Bio-Molecular Synthesis

In autumn 2010 Prof. Henk Hiemstra was elected Novartis Lecturer Central Europe.

Dr. Jan van Maarseveen was elected by the ACD as best chemistry teacher 2009-2010.

A patent application "*Improvements on CLIPS-technology*" was filed by P. Timmerman, L. E. M. Smeenk, N. Dailly and J. H. van Maarseveen (EP 10188743.8, filing date 25-10-2011)

Dr. T. van Herk received on May 28, 2010 the prestigious "*Martinus van Marum prijs*" for Biotechnology of the Koninklijke Hollandsche Maatschappij der Wetenschappen on biotechnology for her PhD thesis "*Bacterial class A acid phosphatases as versatile tools in organic synthesis*".

More details, see chapter 2.1.

Catalysis

The group Elsevier had a very fruitful year, especially regarding the ongoing NWO-NSC-project with the National Taiwan University at Taipei. Several joint papers came out and the whole group attended the international conference on Organometallic chemistry that was held in Taipei in summer. Prof. Kees Elsevier gave an invited lecture and all other group members presented well-received posters.

Dr. Raveendran Shiju & Prof. Gadi Rothenberg received the 1st prize in the 'Nieuwe Ideeën Prijsvraag 2010' from the Science Park Amsterdam for their invention 'A new catalyst for making nylons'. The catalyst has also been patented by the University of Amsterdam.

Prof. Joost Reek was highlighted in *Angewandte Chemie* because he published his 10th article since 2000 in this prestigious journal. The group Homogeneous and Supramolecular Catalysis (Reek/De Bruin/Van der Vlugt) was also highlighted in *Nature Chemistry* for following publications in *Angewandte Chemie* and *JACS* in 2010.

Prof. Joost Reek presented a NEMO lecture with the title '*Hoe wordt vuurwerk gemaakt?*' for an audience of young kids (also published in *NRC handelsblad*). Dr. B.de Bruin was present at the NEMO Klokhuis vragendag in November 2010, where he presented the lecture "*Hoe werkt de motor van een auto?*".

Prof. Joost Reek presented at the E-Dee, organized by UvA, VU and ECN, the lecture "Catalysis for green energy application".

An article of Prof. G. Rotheberg c.s. featured on the cover of *Journal of Materials Chemistry*, as well as in a press release of the FNWI.

More details, see chapter 2.2.

Computational Chemistry

The research of Dr. Jocelyne Vreede (Veni laureate) was highlighted on the FNWI website and the WiF Best Publication Prize 2010 was also awarded to her.

The Computational groups organized several conferences/schools. To mention here are the three organized in Amsterdam, the Winterschool MolSim 2010 (Meijer, Ensing, Dubbeldam), the ACMM Spring and Fall symposia (Bolhuis) and Amsterdam Photoreceptor Meeting (Ensing, Vreede Amsterdam). More details, see chapter 2.3.

Macromolecular and Biosystems Analysis

COAST (Comprehensive Analytical Science and Technology) was officially launched on November 1st, 2010. This national initiative on strengthening the foundations of analytical science took many years of preparation by a number of people, including Peter Schoenmakers and Hans-Gerd Janssen. COAST has elected Science Park Amsterdam as its headquarters and Peter Schoenmakers is its Education Director.

Ira Saul Lurie received his doctoral degree for his thesis on '*Ultra High Performance Liquid Chromatography of Seized Drugs*', the first UvA thesis on a forensic subject.

More details, see chapter 2.4.

Molecular Photonics

A large part of the key publications of the Molecular Photonics theme has attracted the attention of the popular press, leading to articles and commentaries in popular journals and on the web. Promotional activities included radio interviews with Sander Woutersen (Noorderlicht, April 12 and June 17, 2010), contributions to popular scientific journals (e.g. Nederlands Tijdschrift voor Natuurkunde 2010, 76, 350-355), and popular lectures (PAC Symposium "*Chemistry makes Sense*").

Prof. Jos Oomens and Prof. Wybren Jan Buma are part of the NWO Astrochemistry Programme approved in 2010.

The Molecular Photonics group is a full partner now in LaserLab Amsterdam of the Vrije Universiteit Amsterdam, an important European facility (part of Laser Lab Europe).

More details, see chapter 2.5.

Conservation and Restoration of Art objects

Prof. Iedema contributed to the NWO programme, Science4, a new research activity in the area of Conservation and Restoration of Art objects. It is intended to propose a project at HIMS together with various museums, in which former PhD students from the earlier NWO-projects are cooperating with the HIMS staff-members Prof. Iedema (supervision), Prof. Elsevier, Prof. Schoenmakers, Prof. Norman Tennent (Conservation Scientist at the UvA Humanities Faculty, also part-time appointment at HIMS).

More details, see chapter 2.6.

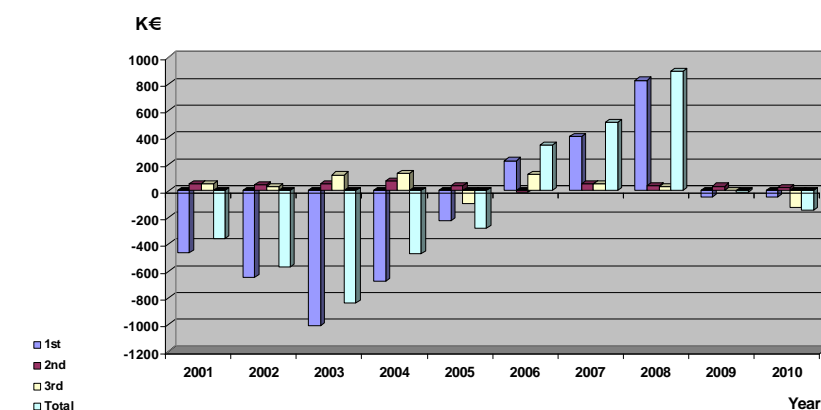
5 Management and finances

Since 2006, the year of introduction of the new (integral costs) allocation model of the university board, the financial position of HIMS has much improved, reflecting the foreseen effect of the reorganization of the chemistry department that took place in the years 2002-2004, as illustrated by the graph below. The integral results (all funding sources) obtained in 2009 (-12 k€) and 2010 (-147 k€) are appreciably lower than obtained in 2008 (+899 k€). Nevertheless, this result is satisfactory, knowing that HIMS is confronted with a budget reduction of the structural university budgets (1st moneystream/ 1^e geldstroom) of 10% (1 M€) for the years 2009-2012. This reduction forced the institute not to fulfil all vacancies in the 1st moneystream, therefore less was spent on salary costs in the years 2009 and 2010.

Again, HIMS was successful in 2010 with external funds: a total of 5,00 M€ external funds (6,56 M€, including 2,70 M€ NRSC-C, in 2009) was acquired from subsidiaries such as NWO (1 Vidi, 1 TOP and 2 ECHO grants), EU, NanoNext (FES), Towards Biosolar (FES), NFI, etc.

A general overview of HIMS results in the current decade is presented in the diagram below.

HIMS result 2001 – 2010 (all funding sources; k€)



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

More specifically, actual numbers of 2010 and 2009 are given in the subsequent tables.

HIMS resources and results 2010 (€)

2010	1 st structural	1 st others	1 st total	2 nd	3 rd	total
Total benefits/budget	5926	471	6397	3482	4929	14809
Personnel costs	-3512	-293	-3805	-1470	-1475	-6750
Other costs	-2435	-203	-2638	-1988	-3580	-8206
Total costs	-5947	-496	-6443	-3458	-5055	-14956

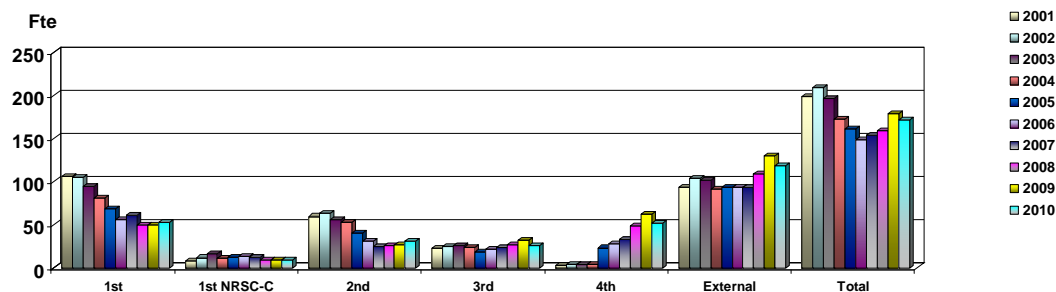
For more details, see chapter 7,3

HIMS resources and results 2009 (€)

2009	1 st structural	1 st others	1 st	2 nd	3 rd	total
Total benefits/budget	6557	538	7096	3750	3699	14544
Personnel costs	-3729	-261	-3990	-1661	-1296	-6947
Other costs	-2559	-178	-2737	-2055	-2817	-7609
Total costs	-6288	-439	-6727	-3716	-4113	14556
Result 2009	-144	99	-46	34	0	-12

The 2nd and 3rd moneystream together (including matching) increased in 2010 with +962 k€ as compared with the previous year. Personnel costs decreased 197 k€. The other costs increased with 597 k€ because of higher prices for basic facilities.

The graph below shows the personnel development of HIMS 2001-2010 per funding source.



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

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

1st NRSC-C (Top Research School Catalysis)

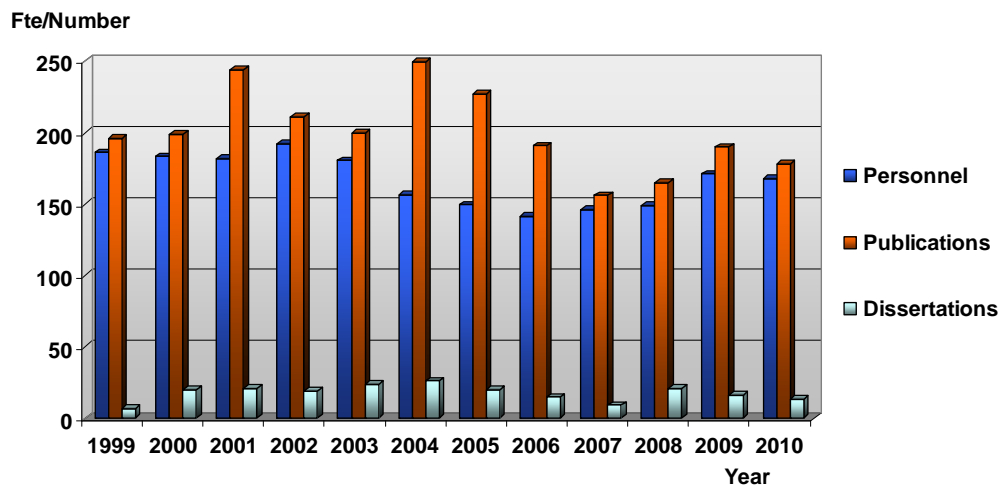
2nd Research grants (tweedegeldstroom; NWO-CW, ERC, FOM, STW, KNAW)

3rd Contract research (derdegeldstroom; EU, DPI, AGENTSCHAP.NL, FES/NanoNed, NFI, Industrial)

4th Other (vierdegeldstroom; guest PhD students & guest researchers employed elsewhere, PhD students with finished contracts/not yet graduated, etc.)

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

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



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

The increase in projects in the latter years is reflected by an increase in output (number of publications in 2009-2010 and is in the coming years also expected in the number of dissertations).

6 External evaluation

On the occasion of the 2010 assessment of research quality (that took place in September 2010; report expected in 2011), the CWTS conducted a bibliometric analysis over the period 1999-2008. The results of the three most recent bibliometric surveys for the HIMS themes and groups are shown in the table below.

Latest VSNU scores of the HIMS research themes and groups

HIMS themes & Other activities	Research group	CPP/FCSm ¹ 1991-2000	CPP/FCSm ² 2001-2007	CPP/FCSm ³ 1999-2008	
				group	theme
Bio-Molecular Synthesis	Hiemstra	1.81	1.79	2.01	1.86
	Wever	1.19	1.39	0.99	
Catalysis	Reek / Van Leeuwen	2.70	2.32	2.07	1.87
	Elsevier	2.08	1.37	1.37	
	Rothenberg	-	-	1.51	
Computational Chemistry	Krishna	3.00	1.31	1.82	2.14
	Bolhuis/Smit	2.61	1.94	2.34	
Macromolecular and Biosystems Analysis	Schoenmakers	1.64	1.29	1.26	1.26
Molecular Photonics	Buma	0.96	1.17	1.89	1.81
	Brouwer	-		1.50	
Röntgen Diffraction	Peschar / Schenk	0.64	0.79	0.80	1.02
Polymer & Process Systems	Iedema	0.53	0.99	0.98	
Reactor Dynamics	Van den Heuvel	-	-	1.50	
Total HIMS		1.51	1.58	1.81	

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

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

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

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

CPP/FCSm, the ratio of the average number of citations per publication (corrected for self-citations) CCP and the world mean field citation score FCSm is an important indicator of a publication's impact compared to the international average. 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 standard of 1.0.

Furthermore, all five HIMS themes have individual scores well above 1.0 (see table above). It should be noted that the registration in the present 2010 CWTS analysis (future perspective; publications of staff members per theme present at January 01, 2008) is quite different from the registration in the older analyses (past performance; publications of all staff members per theme present in that period).

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

Compared to the journal and field average impact levels, HIMS performs very well. With CPP/JCSm and CPP/FCSm values of 1.21 and 1.81 respectively, the HIMS researchers score higher than the average of all Dutch chemistry researchers combined (see table below).

The output is stable over the years, while the impact shows a fluctuating pattern, with high impact scores at both the initial and final blocks of the trend analysis. Since this is due to high impact papers in the early years and some high impact publications in 2007 and 2008, it shows that the younger staff has reached the high quality level of their predecessors and re-established the international position of the individual research groups.

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

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

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

VSNU scores of HIMS compared with the average scores of all Dutch universities ³

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

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

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

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

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

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

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

7 Facts and figures

7.1 Personnel

7.1.1 Research input

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

Research - and supporting staff 2010 of the HIMS themes, per employment type (fte)^a **source: METIS**

	BMS	CAT	COMP	MBA	MOLP	Others	Total
Tenured staff	2,1	3,5	2,6	1,5	2,5	1,0	13,2
Non-tenured staff	2,2	13,0	5,4	6,2	3,8	1,4	32,1
PhD candidates	6,6	15,2	8,9	11,4	10,9	1,3	54,4
Total research staff	10,9	31,7	16,9	19,1	17,2	3,8	99,6
Technicians ^b	4,7	10,1	0,5	2,4	3,8	2,2	23,6
Visiting fellows ^c	0,1	0,3	0,0	0,4	0,2	0,0	1,0
Supporting staff						6,8	6,8
Total staff	15,6	42,1	17,4	21,9	21,3	12,7	131,0

Research - and supporting staff 2010 of HIMS and the HIMS groups, per employment type (fte)^a
source: METIS

	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	Others	Total
Tenured staff	1,6	0,5	1,5	0,5	1,5	1,6	0,5	0,5	1,5	1,5	1,0	1,0	13,2
Non-tenured staff	1,8	0,5	8,8	0,0	4,3	3,1	0,9	1,4	6,2	2,2	1,7	1,4	32,1
PhD candidates	3,9	2,8	10,0	3,1	2,1	2,9	5,8	0,2	11,4	5,8	5,1	1,3	54,4
Total research staff	7,2	3,7	20,2	3,7	7,9	7,6	7,2	2,1	19,1	9,5	7,8	3,8	99,6
Technicians ^b	3,5	1,2	4,6	2,0	3,5	0,0	0,0	0,5	2,4	2,2	1,6	2,2	23,6
Visiting fellows ^c	0,1	0,0	0,1	0,2	0,0	0,0	0,0	0,0	0,4	0,2	0,0	0,0	1,0
Supporting staff												6,8	6,8
Total staff	10,8	4,9	24,9	5,9	11,4	7,6	7,2	2,6	21,9	11,9	9,4	12,7	131,0

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

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

^c Endowed and visiting professors.

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

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema, Van den Heuvel (discontinued 2010) and Peschar (discontinued 01-01-2011)

7.1.2. Scientific staff

Bio-Molecular Synthesis

2 research groups

Prof.dr. H. Hiemstra (rg⁴-1.1)
Synthetische Organische Chemie

Prof.dr. R. Wever (rg-1.2)
Biokatalysatoren en Bio-Anorganische Chemie

Vacancy (rg-1.1)
Industriële Fijnchemie (0.2 Fte)
(bijzonder hoogleraar Stichting Betaplus)

Prof.dr. P. Timmerman (rg-1.1)
Protein-mimetic Chemistry (0.2 Fte)
(Bijzonder hoogleraar Genootschap ter bevordering van Natuur-, Genees- en Heelkunde)

Dr. J.H. van Maarseveen, uhd (rg-1.1)
Dr. S. Ingemann Jørgensen, ud (rg-1.1)
Dr. S. Kinderman, Veni lauriate, pd (rg-1.1)

Catalysis

3 research groups

Prof.dr. J.N.H. Reek, Vici Laureate (rg-2.1)
Supra-Moleculaire Katalyse

Prof.dr. C.J. Elsevier (rg-2.2)
Coördinatie- en Organometaalchemie

Prof.dr. G. Rothenberg, Vidi Laureate (rg-2.3)
Heterogene Katalyse en Duurzame Chemie

Dr. B. de Bruin, Vidi and ERC Laureate, uhd (rg-2.1)
Dr. J.I. Van der Vlugt, Veni Laureate, ud (rg-2.1)
Dr. E. Eiser (0.1 Fte), ud (rg-2.2)
Vacancy, ud (rg-2.2)
Dr. N.R. Shiju, ud (rg-2.3)
Dr. D.G.H. Hetterscheid, Veni lauriate, pd (rg-2.1)
Dr. S. Grecea, Veni lauriate, pd (rg-2.3)

⁴ rg = research group

Computational Chemistry

2 research groups

Vacancy (rg-3.1)

Complexe Moleculaire Simulaties

Prof.dr. R. Krishna (rg-3.2)

Chemische Reaktorkunde

Prof. dr. A. Fasolino/KUN (rg-3.1)

Computatieve Fysica van de Gecondenseerde Materie (0.0 Fte)

Prof.dr. P.G. Bolhuis, Vici, Vidi and FOM Springplank Laureate (rg-3.3)

Simulaties van bio-moleculaire systemen

Dr. E.J. Meijer (rg-3.1), KNAW fellow, uhd

Dr. C.P. Lowe (rg-3.3), KNAW fellow, uhd

Dr. D. Dubbeldam (rg-3.3), Vidi laureate, ud

Dr. B. Ensing (rg-3.1), Vidi laureate, ud

Dr. J. Vreede (rg-3.3), Veni laureate, pd

Macromolecular and Biosystems Analysis / Forensic Analytical Chemistry

1 research group⁵

Prof.dr.ir. P.J. Schoenmakers (rg-4)

Analytical Chemistry including its applications in Forensic Science

Prof.dr.ir. J.G.M. Janssen/Unilever

Analytische Scheidingen van Biomacromoleculen (0.2 Fte)

(bijzonder hoogleraar Stichting Betaplus)

Prof.dr. S. van der Wal /DSM

Bioterials Analysis (0.2 Fte)

(bijzonder hoogleraar Stichting Betaplus)

Dr. W.Th. Kok, uhd

Dr. G. Vivó Truyols, ud

Molecular Photonics

1 research group

Prof.dr. W.J. Buma (rg-5)

Molecuulspectroscopie

Prof.dr. A.M. Brouwer, uhd (rg-5)

Molecuulspectroscopie (0.2 Fte)

(bijzonder hoogleraar John van Geunsfonds)

Prof.dr. H.J. Bakker/FOM-Amolf

Ultrasmalle Spectroscopie van Moleculen in de Gecondenseerde Fase (0.0 Fte)

⁵ Collaboration with De Koster and Smilde from SILS

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

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

Other activities

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

Art sciences/Polymer and Process Systems
Prof.dr. P. Iedema
Fysische Technologie

Scanning Tunneling Microscopy (STM)
Dr. J.C. van den Heuvel, uhd

Röntgen Diffraction department
Dr. R. Peschar, ud

7.2 Research

7.2.1 Research input of the HIMS themes

Research - and supporting staff 2010 of HIMS and the HIMS themes, per funding type (fte)^a source: METIS

	BMS	CAT	COMP	MBA	MOLP	Others	Total	%
Direct funding ¹	9,4	17,8	4,7	4,5	7,9	9,9	54,3	41
Research grants ²	3,0	7,2	7,1	0,8	5,4	0,0	23,5	18
Contract research ³	0,0	8,9	1,8	4,5	2,2	0,0	17,5	13
Other ⁴	3,2	8,2	3,8	12,1	5,7	2,8	35,8	27
Total	15,6	42,1	17,4	21,9	21,3	12,7	131,0	100

Research - and staff 2010 of HIMS and the HIMS groups, per funding type (fte)^a source: METIS

	HH	RW	JR	CE	GR	PB	EJ M	RK	PS	WJ B	FB	Other s	Total	%
Direct funding ¹	7,3	2,1	8,9	3,7	5,2	2,3	0,5	2,0	4,5	4,6	3,4	9,9	54,3	41
Research grants ²	2,3	0,8	5,8	0,7	0,7	3,3	3,2	0,6	0,8	3,6	1,9	0,0	23,5	18
Contract research ³	0,0	0,0	5,3	0,8	2,9	0,8	1,1	0,0	4,5	0,8	1,4	0,0	17,5	13
Other ⁴	1,2	2,0	4,8	0,7	2,7	1,3	2,5	0,0	12,1	2,9	2,8	2,8	35,8	27
Total	10,8	4,9	24,9	5,9	11,4	7,6	7,2	2,6	21,9	11,9	9,4	12,7	131,0	100

¹Direct funding (eerstegeldstroom; university/direct funding, NRSC-C/Top Research School Catalysis)

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

³Contract research (derdegeldstroom; EU, DPI, AGENTSCHAP.NL, FES/NanoNed, Industrial)

⁴Other (vierdegeldstroom; guest PhD students & guest researchers employed elsewhere, PhD students with finished contracts/not yet graduated, etc.)

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

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

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema, Van den Heuvel (discontinued 2010) and Peschar (discontinued 01-01-2011)

Externally financed projects acquired in 2010 (mln €) and HIMS themes per funding type¹

	BMS	CAT	COMP	MBA	MOLP	Others	Total
1 st - NRSC-C ²	-	-	-	-	-	-	-
1 st - Others ³	-	-	-	-	-	-	-
2 nd ⁴	0.00	1.04	1.04	0.00	0.26	0.00	2.34
3 rd ⁵	0.00	1.04	0.26	0.93	0.45	0.00	2.67
Total	0.00	2.08	1.30	0.93	0.71	0.00	5.01⁶

Externally financed projects acquired in 2010 (mln €) and HIMS themes per funding type¹

	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	Others	Total
1 st - NRSC-C ²	-	-	-	-	-	-	-	-	-	-	-	-	-
1 st - Others ³	-	-	-	-	-	-	-	-	-	-	-	-	-
2 nd ⁴	0.00	0.00	1.04	0.00	0.00	1.04	0.00	0.00	0.00	0.00	0.26	0.00	2,34
3 rd ⁵	0.00	0.00	0.81	0.00	0.23	0.26	0.00	0.00	0.93	0.21	0.24	0.00	2.67
Total	0.00	0.00	1.85	0.00	0.23	1.30	0.00	0.00	0.93	0.21	0.50	0.00	5.01⁶

¹ Matching contributions UvA/FNWI and own contributions HIMS (in kind and cash/from reserves) included

² NRSC-C (TOP Research School Catalysis); ³ COF, CvB (Funds from University Board); ⁴ NWO-CW, FOM, STW, KNAW, ERC

⁵ EU, DPI, AGENTSCHAP.NL, NanoNed, Industry

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

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema, Van den Heuvel (discontinued 2010) and Peschar (discontinued 01-01-2011)

7.2.2 Research output 2010 of the HIMS themes

Research output 2010 of HIMS, per type of publication

source: METIS

HIMS themes

	BMS	CAT	COMP	MBA	MOLP	Others	Joint ¹	Total
Refereed articles	3	54	43	17	61	0	0	178
Non-refereed articles	0	0	0	2	1	0	0	3
Books	0	0	0	0	0	0	0	0
Book chapters	0	0	3	0	0	0	0	3
PhD-theses	1	4	0	3	6	0	0	14
Patents	2	1	0	0	0	0	0	3
Professional publications	0	0	0	0	0	0	0	0
Total	6	59	46	22	68	0	0	201

HIMS groups

	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	Joint ¹	Total
Refereed articles	2	1	35	5	14	20	7	17	17	49	17	-6	178
Non-refereed articles	0	0	0	0	0	0	0	0	2	0	1	0	3
Books	0	0	0	0	0	0	0	0	0	0	0	0	0
Book chapters	0	0	0	0	0	1	2	0	0	0	0	0	3
PhD-theses	1	0	4	0	0	0	0	0	3	4	2	0	14
Patents	2	0	0	0	1	0	0	0	0	0	0	0	3
Prof. publications	0	0	0	0	0	0	0	0	0	0	0	0	0
Total	5	1	39	5	15	21	9	17	22	53	20	-6	201

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

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

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema, Van den Heuvel (discontinued 2010) and Peschar (discontinued 01-01-2011)

Number of citations 2010 of HIMS, in ranges of different impact factor **Source: METIS**

HIMS themes

	BMS	CAT	COMP	MBA	MOLP	Others	Joint ¹	Total
>15	0	3	0	0	4	0	0	7
10-15	0	6	2	1	2	0	0	11
5-10	0	9	5	2	9	0	0	25
<5	3	36	36	14	46	0	0	135
Total	3	54	43	17	61	0	0	178

HIMS groups

	HH	RW	JR	CE	GR	PB	EJM	RK	PS	WJB	FB	Others	Joint ¹	Total
>15	0	0	2	0	1	0	0	0	0	4	1	0	-1	7
10-15	0	0	5	0	1	2	0	0	1	1	1	0	0	11
5-10	0	0	6	1	2	1	1	3	2	6	3	0	0	25
<5	2	1	22	4	10	17	6	14	14	38	12	0	-5	135
Total	2	1	35	5	14	20	7	17	17	49	17	0	-6	178

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

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

Research groups: HH = group Hiemstra; RW = group Wever; JR = group Reek; CE = group Elsevier; GR = group Rothenberg; EJM = group Meijer; RK = group Krishna; PB = group Bolhuis; PS = group Schoenmakers; WJB = group Buma; FB: group Brouwer; Others: groups Iedema, Van den Heuvel (discontinued 2010) and Peschar (discontinued 01-01-2011)

7.3 Finance 2010

The table below shows the HIMS financial result 2010, excluding the teaching activities of the HIMS staff (810 k€).

HIMS result 2010 (k€)

	1 st structural	1 st others	1 st total	2 nd	3 rd	Total
HIMS						
Budget (base)	5893	751	6644	1314	3235	11193
Budget (allocation model)	3115		3115			3115
Other income	276		276	18	215	510
Matching contract research	-3358	-280	-3638	2150	1479	-9
Budget total	5926	471	6397	3482	4929	14809
<i>percentage</i>	<i>40,0</i>	<i>3,2</i>	<i>43,2</i>	<i>23,5</i>	<i>33,3</i>	<i>100</i>
Personal costs	-3512	-293	-3805	-1470	-1475	-6750
Other costs (projects)	-638	-53	-692	-331	-1662	-2684
Overhead (central)	602	50	652	-327	-325	0
Overhead (faculty)	-1050	-87	-1137	-676	-868	-2671
Overhead (institute)	1280	107	1387	-653	-734	0
Various costs	-45	-4	-49		-1	-50
Other (secondary) costs	-2584	-215	-2800			-2800
Costs total	-5947	-496	-6443	-3458	-5055	-14956
<i>percentage</i>	<i>52,0</i>	<i>4,3</i>	<i>56,4</i>	<i>21,8</i>	<i>21,9</i>	<i>100</i>
Result	-21	-25	-46	24	-126	-147

¹ Direct funding (1st, eerstegeldstroom; university/direct funding, NRSC-C/Top Research School Catalysis)

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

³ Contract research (3rd, derdegeldstroom; EU, DPI, AGENTSCHAP.NL, FES/NanoNed, Industrial)

Including the reservation for discontinuation of the röntgen diffraction activities (correction of -490 k€) the HIMS result 2010 amounts to - 637 k€.