Van ‘t Hoff Institute for Molecular Sciences

Annual Report 2014

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Cover: Pupils during the National Chemistry Olympiad 2014. HIMS hosted this annual event from 30 May to 6 June 2014.

June 2015

Preface

I am proud that 2014 was again an exciting year for HIMS in which we welcomed new scientific staff, produced great science and launched the Research Priority Area Sustainable chemistry with a big bang.

Three new tenure track scientists and two professors (one full time) were appointed to further strengthen the research activities of HIMS. Our researchers were successful in acquiring external funds to start new projects and produced 150 peer reviewed scientific publications, of which many in high impact journals, and 20 PhD theses of which one with cum laude by Dr. Ivan Kryven. Prof.dr.ir. Peter Schoenmakers received the prestigious Knox medal and was ranked 7th on the worldwide 'Analytical Sciences Power List 2013'. In collaboration with HRSMC three Nobel laureates visited Amsterdam, on the occasion of the yearly HRSMC symposium, and undergraduate students had the chance to interview these scientific hero's. HIMS hosted the National Chemistry Olympiad 2014, which was a great success. The spin-off company Plantics was erected, exploring the commercial potential of the new bio-plastic that was invented at HIMS.

In October we organised our first annual Industry Day, which was attended by many companies, to discuss science, meet our researchers and to show our infrastructure. The scientific advisory board gathered in December, giving a concise feedback on how the points raised in the midterm evaluation (2014) were addressed. In general, the board was very positive about the adequate response of HIMS to the recommendations in the midterm evaluation. The ceremonial ignition by Rector Magnificus Prof.dr. Dymph van den Boom of the RPA Sustainable Chemistry symbolized the boost the university gives to this already well-established area of chemistry research at the Van 't Hoff Institute of Molecular Sciences. I am delighted to see how the RPA connects scientists from all four HIMS research themes and new collaborations initiate.

Also in 2014 we further discussed the possible collaborations with the Swammerdam Institute for Life Sciences (SILS) and Free University (VU) in the area of sustainability in the context of a new virtual department. Several meetings were organised for chemists and biologists from HIMS, SILS and the VU to search for new possibilities to enhance the co-operation and synergy in 2014.

To conclude, 2014 was successful scientifically, and also in terms of valorisation, organisation of several events for science and education. These and many highlights of the institute are described in this annual report. I hope you enjoy reading.

Prof.dr. Joost Reek
Director

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1. General considerations and highlights

1.1 Key figures of HIMS in 2014

The high level of scientific output of HIMS was maintained in 2014. HIMS published 3 papers (3.3 average 2011-2013) in absolute top journals (impact factor > 15) and 17 papers (8.0 average 2011-2013) in top journals (impact factor 10-15). The total number of refereed and other professional publications, patents and book(chapter)s amounted to 217 (average 2010-2013: 190). The amount of published PhD dissertations increased substantially to 20 (from 2010 to 2013 resp. 14, 15, 9, 16).

With a total of 3.2 M€ in external funding (excluding the own matching budget of approximately 1.6 M€) the year 2014 was not as successful as former years (average 2011-2013: 5.6 M€). These funds were acquired from funding agencies such as NWO (Chemical Sciences, Vernieuwingsimpuls, FOM) and EU FP7, as well as from industry and other partners.

1.2 Personnel

In 2014 the total staff amounted to 126.8 fte. This amount is lower than the years before (136.5 in 2013 and 158.0 in 2012). The difference may be explained by a loss of temporary scientific staff (postdocs and PhD students) due to the completion of several projects and the overtaking manoeuver for promotions on the one hand and some less new projects started in 2014, as described above.

In 2014 several new staff members were appointed. Prof.dr. Garry Corthals was appointed professor of Supramolecular separations and Dr. Michelle Camenzuli started a tenure track on Enhancing analytical separations within the Sectorplan Physics and Chemistry. Within the RPA Sustainable Chemistry dr Moniek Tromp (Characterisation of first row transition metal catalysts) and dr Ning Yan (Fuel cell technology) started a tenure track and Prof.dr. Bob van der Zwaan of the Energy research Center of the Netherlands (ECN) was appointed professor by special appointment of Sustainable Energy Technology.

At the Molecular Photonics theme, Prof.dr. Sander Woutersen was appointed professor by special appointment of Molecular Spectroscopy, a chair endowed by the John van Geuns Fonds. Prof.dr. Fred Brouwer was appointed part-time group leader Nanophotochemistry at the new Advanced Research Center for Nanolithography (ARCNL), which is a collaboration of the company ASML with UvA, VU and the Foundation for Fundamental Research on Matter (FOM).

Unfortunately Dr. Anett Schallmey decided to leave our institute for a position at the technical University Braunschweig in her motherland, which left a vacancy on Biocatalysis.

Because of a revised management structure within the institute a new position of institute manager was introduced per 2014. Per 1 January 2014 Drs. Marcel Bartels was appointed on this position.

1.3 Finances

HIMS finished the year 2014 with a positive financial result of 902 k€. This result looks satisfactory, but one should note that reservations were made of 882 k€ on SNS funds and the RPA Sustainable Chemistry that were received, while not all positions where yet filled.

1.4 Highlights

1.4.1 Institutional highlights

Bioplastic furniture

Prof.dr. Gadi Rothenberg and colleagues from UvA and AUAS/HvA offered their Executive Board the very first table made of biodegradable plastic. The new thermoset plastic, made from 100% plant-based materials, was discovered by chance during trials to develop biofuel. It is made of glycerol and citric acid, and is therefore completely plant-based and biodegradable and, moreover, soluble in water. The spin-off company Plantics B.V. was launched this summer to commercialise the material.

RPA Sustainable Chemistry

An exploding hydrogen filled balloon marked the kick-off for the Research Priority Area Sustainable Chemistry on September 3rd. The ceremonial ignition by Rector Magnificus Prof.dr. Dymph van den Boom symbolized the boost the university gives to this already well-established area of chemistry research at the Van 't Hoff Institute of Molecular Sciences. The University of Amsterdam has appointed twenty-called Research Priority Areas over the entire spectrum of science. These RPA's are among the best the UvA has to offer and are internationally renowned. Van den Boom remarked that the university money was "well spent". She further appreciated the long term approach of fundamental research enabling solutions to the pressing sustainability issues. "I trust that your dedication will create opportunities".

Industry Day

On October 31st the first HIMS Industry Day was organised. Over 30 companies (from Amsterdam SMEs to multinationals) were introduced into the research themes of the institute. The programme started with a Talent lunch where PhD students and postdocs were informed about careers in industry. After a guest lecture on designing a chemical plant on planet Mars, it was time for the HIMS staff to present its expertise. First plenary, in lectures, and after that during lab tours and a poster session combined with a dinner buffet. This year's Industry Day was a success that will undoubtedly lead to new future collaborations.

20th anniversary HRSMC

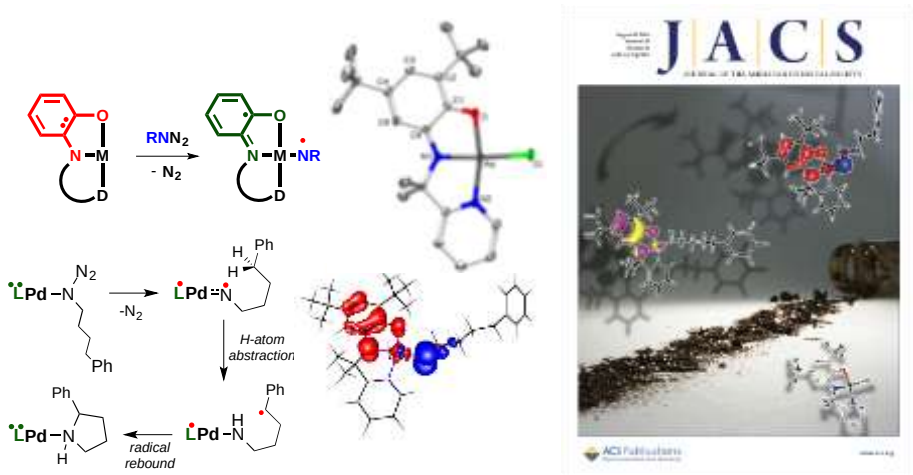
HIMS is the proud home of the Holland Research School of Molecular Chemistry (HRSMC), that celebrated its 20th anniversary in November 2014 with a festive two-day symposium. The meeting welcomed no less than three keynote lectures from Nobel laureates W.E. Moerner (2014), Arieh Warshel (2013) and Roald Hoffmann (1981). En marge of the seminar, the organisers seized the opportunity and organised a 'Chemistry Tour' where chemistry bachelor students could meet the Nobel laureates.

Students from UvA, VU University and Leiden University (the HRSMC partner universities) interviewed the laureates on their groudbreaking research, moderated by Martijn van Calmthout, science editor of the Dutch national newspaper De Volkskrant.

1.4.2 Scientific highlights

Sustainable Chemistry – Homogeneous and Supramolecular Catalysis

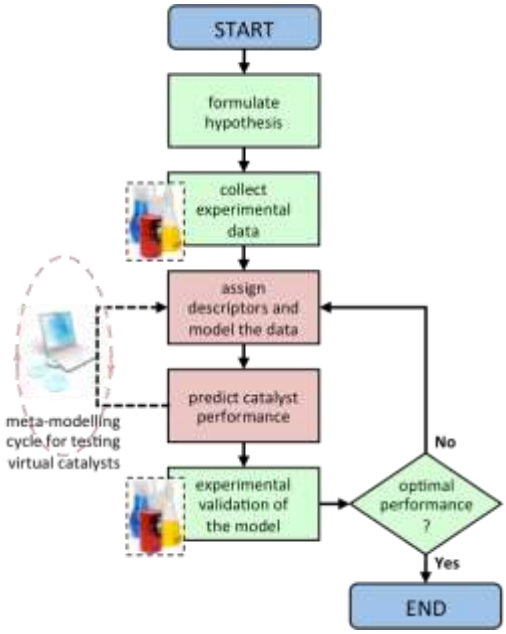
In 2014 we demonstrated the first example of selective *Ligand-to-Substrate Single Electron Transfer* (LtS SET). This novel concept, which employs the tunable redox-chemistry of redox-active ligands in combination with the well-defined coordination chemistry of redox-inert noble metal platforms, enables odd-electron reactivity with transition metal ions not disposed for such chemistry. As proof-of-principle, a crystallographically characterized Pd(II) complex bearing a novel redox-active ligand was utilized for chemoselective intramolecular C-H amination of organoazides to generate pyrrolidines. Combined kinetic, spectroscopic, crystallographic and computational data indicate a mechanism involving the initial generation of a reduced nitrene species and follow-up H-atom transfer steps, which is unprecedented for *closed-shell* Pd^{II}. This work was featured on the cover of *the Journal of the American Chemical Society* (JACS) and was also selected as *JACS Spotlight.*



Intramolecular redox-active ligand-to-substrate single electron transfer: Radical reactivity with a palladium(II) complex D.L.J. Broere, B. de Bruin, J.N.H. Reek, M. Lutz, S. Dechert, J.I. van der Vlugt* *J. Am. Chem. Soc.* **2014**, *136*, 11574-11577.

Sustainable Chemistry – Heterogeneous Catalysis and Sustainable Chemistry

In 2014, HCSC reached an important milestone in adapting the predictive modelling approach to heterogeneous catalysis. This adaptation uses the combination of descriptor models and empirical results from lab experiments and/or computations to predict the performance of sets of catalysts *in silico*. The overall result is a powerful workflow that is now used by several leading chemical companies. This long-term project was a collaboration with Avantium Technologies under the NWO-Casimir program. It has culminated in the PhD thesis of Dr. Erik-Jan Ras and in several important publications, including an open-access tutorial that teaches scientists worldwide how to apply this effective discovery workflow in their research (see figure). The simplicity of the models has caused quite some debate in academic circles, yet their effectiveness is a proven fact. These models now serve as the basis of a new consortium that has applied for large-scale European funding, with Avantium, Albemarle, Evonik, Solvay, and Janssen Pharmaceutica as partners.

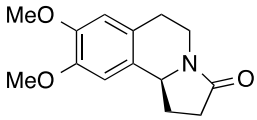


Heterogeneous catalyst discovery using 21st century tools: A tutorial. E.J. Ras and G. Rothenberg, *RSC Adv.*, **2014**, 4, 5963-5974.

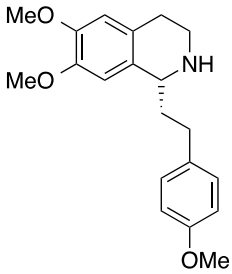
Applying topological and economical principles in catalyst design: New Alumina-Cobalt Core-Shell Catalysts. V.R. Calderone, N.R. Shiju, D. Curulla-Ferré, A. Rose, J. Thiessen, A. Jess, E. van der Roest, B.V. Wiewel and G. Rothenberg, *Top. Catal.*, **2014**, 57, 1419-1424.

Sustainable Chemistry – Synthetic Organic Chemistry

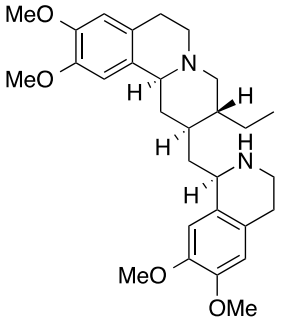
Asymmetric synthesis of bioactive products: Nature offers a rich variety of unique molecular structures that serve as models for the development of new pharmaceutical compounds. Despite tremendous efforts, the synthesis of bioactive compounds is still an extraordinary challenge owing to their chiral nature and the common finding that only one of the possible enantiomers possesses biological activity. In the field of bioactive compounds 1-substituted 1,2,3,4-tetrahydroisoquinolines such as crispine, colchietine and emitene as well as their more complicated derivatives e.g. morphine represent a particularly important class of target molecules. The development of novel synthetic strategies for the direct preparation of enantiopure 1-substituted tetrahydroisoquinolines, therefore, receives increasing attention in the literature.



(*S*)-(-)-Crispine A

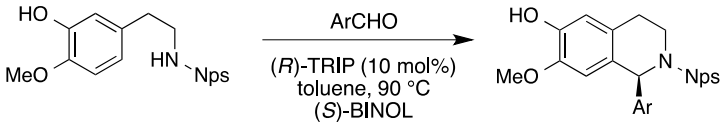


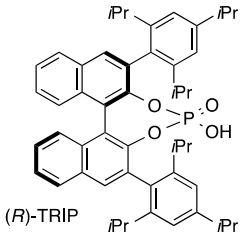
(*R*)-(+)-colchietine



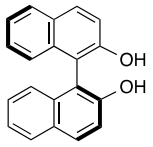
(-)-emetine

We have developed an asymmetric synthesis of 1,2,3,4-tetrahydroisoquinolines based on a sustainable organocatalytic approach starting from readily available phenylethylamines with an o-nitrophenylsulfenamide substituent on the nitrogen atom. Organocatalytic Pictet-Spengler reaction with a enantiopure BINOL phosphoric acid ((R) -TRIP) as catalalyst and (S)-BINOL as the cocatalyst results in a 1-substituted 1,2,3,4-tetrathydroisoquinoline in an enantiomer excess of up to 86%. Further purification by recrystallization gave us an enantiopure 1-substituted 1,2,3,4-tetrahydroisoquinoline suited for further transformation into natural products such as (R)-(+)-colchietine (master students Elma Mons and Würdemann, technician Martin Wanner).





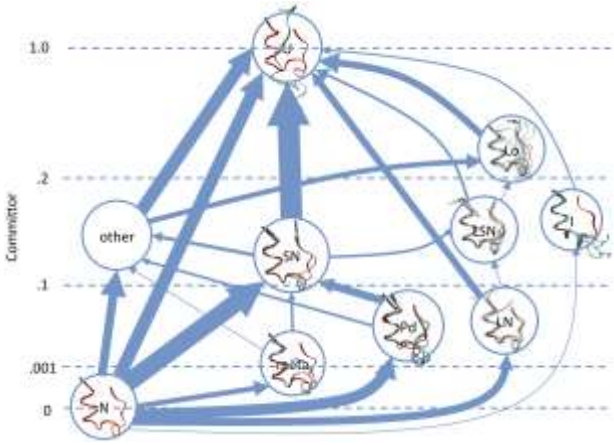
(*R*)-TRIP



(*S*)-BINOL

Computational Chemistry – Biomolecular and Molecular Simulation

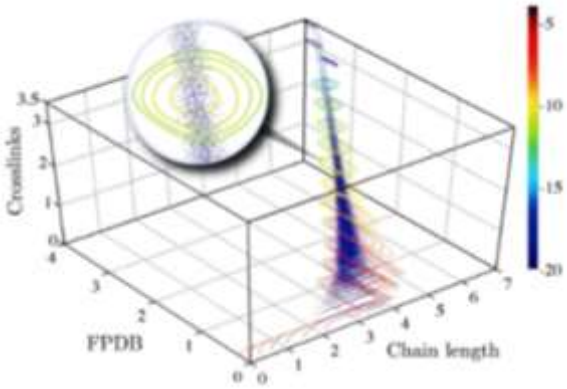
The folding of proteins is difficult to model using all atom Molecular Dynamics due to the long time scales involved in the process, caused by high free energy barriers. In our group we have developed novel multiscale modeling methodology, which enhances the sampling of such high free energy barriers. Dr. Weina Du has conducted large-scale simulation study on the folding of the miniprotein Trp cage and established for the first time the entire equilibrium kinetic folding network, including all rates. This is a milestone in the community, as previously this could only be done by brute force computations. Comparison with experiments showed the validity of the results, and adds novel insight in the complex folding process.



This research opens up the possibility to study large conformational changes in complex proteins including ligand binding, and is thus of fundamental importance. The work was published in the Journal of Chemical Physics (Du and Bolhuis, J. Chem. Phys. 140 195102 (2014)).

Computational Polymer Chemistry & Science for Arts

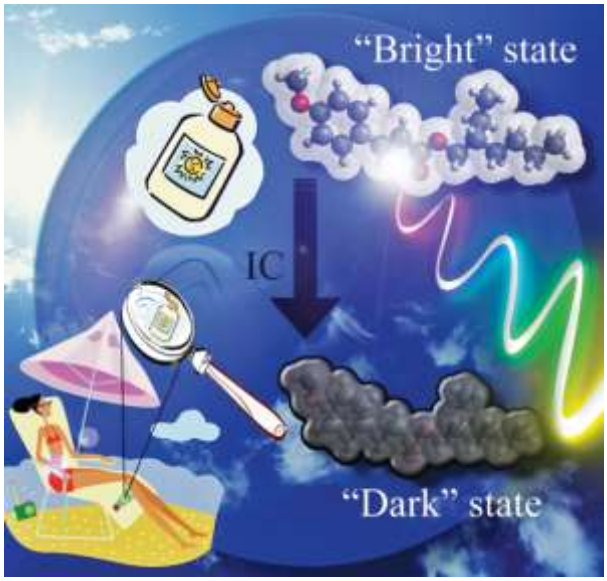
Topology evolution in macromolecular networks. Modelling stochastic molecular networks such as polymers is quite a challenge since they are complex, flowing and changing systems. While a classical molecular dynamics approach works fine for simple networks with a repetitive pattern, it often collapses with stochastic networks because of the inability of modelling in a reasonable time. Dr. Ivan Kryven has found a solution for this. He developed a mathematical toolbox for the study of evolving molecular networks expanding on any spatial or time scale.



Kryven obtained his PhD cum laude for his dissertation in which he views the assembly of molecular networks (the polymerization) from a perspective of evolving graph topology. His mathematical approach with continuously evolving distributions facilitates the description of the randomly fluctuating polymerization process that takes the molecular network from a very simple topology to a complicated interconnected structure. A remarkable result of Kryven's research is that the bigger molecular network, the more its properties are encoded by the graph representation rather than by the underlying chemistry. This means that the material properties can be explained by as simple structures as the collections of dots and their interconnecting sticks.

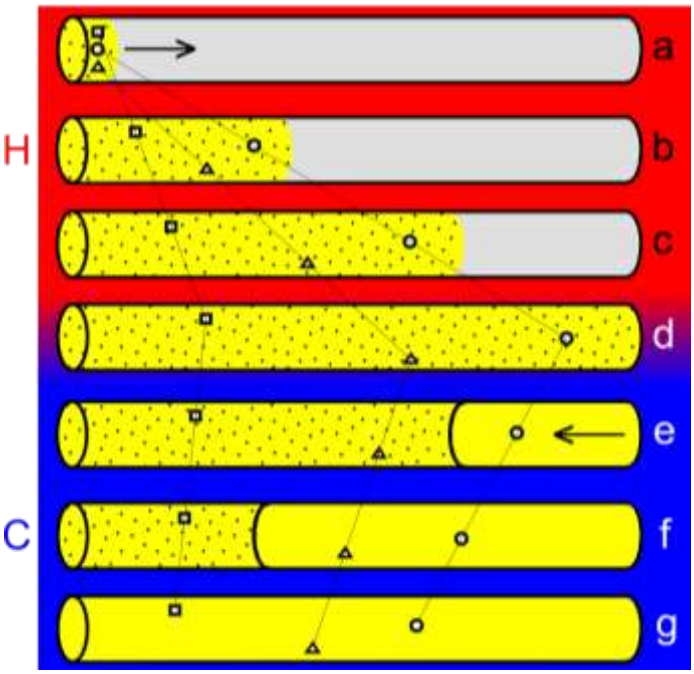
Molecular Photonics

Sunscreens at work Sunscreens are aimed at providing protection from solar UV radiation. The basic idea behind such agents is that they absorb harmful light by electronic absorption, and then rapidly dissipate this electronic energy into harmless heat. Nevertheless, by now several studies have found that light absorption by these agents may lead to adverse effects as well. We have applied high-resolution spectroscopic methods to one of the most commonly used UV-B sunscreen chromophores to study the excited-state dynamics that determine the delicate balance between favourable and adverse effects. In contrast to common belief, we find that excitation to the "bright" ππ* state does not directly lead to repopulation of the electronic ground state. Instead, internal conversion to another electronically excited state identified as the "dark" nπ* state is a major decay pathway that impedes fast energy dissipation. Microsolvation studies of sunscreen chromophores with water demonstrate that under such conditions, this bottleneck is no longer present. These observations could be a first step toward the development of sunscreens with improved photochemical properties. The article on this work received quite some attention from the scientific (Nature Chemistry) as well as the popular (see, for example, Chemistry and Engineering News) media.



Analytical Chemistry

Comprehensive two-dimensional liquid chromato-graphy is a fantastic technique in terms of peak capacity (one to two orders of magnitude higher peak capacity than one-dimensional LC in the same time) and in terms of selectivity (two "orthogonal" separation mechanisms), possibly augmented with (high-resolution) mass spectrometry. However, the compatibility of the two dimensions and the unfavourable trade-off between second-dimension band broadening and analyte dilution are serious obstacles. These can be overcome by active modulation. Anna Baglai has pioneered stationary-phase-assisted modulation (SPAM), which was subsequently applied by Rudy Vonk and Andrea Gargano for proteomics applications, in collaboration with Leo de Kong (SILS).



Henrik Cornellisson van der Ven invented in-column focusing (see figure), which uses a combination of temperature-assisted modulation and SPAM. A patent has been applied for.

1.4.3 Prizes and honours

Prof.dr.ir. Peter Schoenmakers was twice recognised as world-class in analytical sciences. Early January the

'Analytical Sciences Power List 2013' published by The Analytical Scientist magazine placed Schoenmakers at an honourable seventh place. In a European perspective he was even ranked third. The power list is a ranking of the 100 'most influential people in the analytical sciences'. The list not only measures influence, but also indicates 'who are shaping the most used and innovative techniques today'.
Only a few weeks later, Schoenmakers received the prestigious Knox medal recognising his innovation and influential work in the field of Separation Science. The medal is infrequently awarded by the Separation Science Group of the Analytical Division of the Royal Society of Chemistry (England).

Dr. René Williams and colleagues from the Marie Curie Research and Training Network UNI-NANOCUPS received the "Molecules" Best Paper Award 2014. Their paper, "Cationic Heteroleptic Cyclometalated Iridium III Complexes Containing Phenyl-Triazole and Triazole-Pyridine Clicked Ligands" received the 1st prize in the category "Articles".

Master student Rolf Beerthuis won the 'best poster' award at the Royal Dutch Society of Engineers (KIVI) symposium 'Engineering for a Sustainable Future'. Rolf Beerthuis is a master student in the Heterogeneous Catalysis and Sustainable Chemistry group. Later this year Beerthuis obtained his MSc degree cum laude and did a two-month research project at Fudan University - one of the top 5 universities in China.

1.4.4 Grants

Title	**Catalytic Processes for Innovative Technology Application (CAPITA)**
Applicants	Dr. Raveendran Shiju, prof.dr. Gadi Rothenberg
Partners	University of Castilla-La-Mancha (Spain), the Technological Educational Institute of Sterea Ellada (Greece), the Chemical Process Engineering Research Institute (Greece) and three companies: Hellenic Petroleum Renewables (Greece), GRAPHENANO (Spain), and Delft Solid Solutions
Grant from	FP7 ERA-Net
Amount	k€ 250

Title	**Cu-promoted Epimerization-free C-terminal Peptide Elongation enzymes with long redox chains**
Applicant	Dr. Jan van Maarseveen
Grant from	NWO Chemical Sciences (ECHO)
Amount	k€ 260

Title	**In touch with fluorescent probe molecules: microscopic visualization of contacts and friction**
Applicants	Prof.dr. Fred Brouwer, prof.dr. Daniël Bonn (Institute of Physics)
Grant from	NWO Chemical Sciences (ECHO)
Amount	k€ 260

Title	**Degradative enzymes in a synthetic context: Etherase-catalysis for the sustainable synthesis of enantiomerically pure beta-ketoethers and beta-ketosulfides**
Applicant	Dr. Anett Schallmey
Grant from	NWO Chemical Sciences (ECHO-Stip)
Amount	k€ 260
	This grant should probably be returned to NWO since the principal investigator left the institute.

Title	**The European Upconversion Network: from the design of photon-upconverting nanomaterials to (biomedical) applications**
Applicant	Dr. Hong Zhang
Partners	Consortium of 29 principal investigators from 12 European countries
Grant from	European Cooperation in Science and Technology (COST)
Amount	Budget for meetings, seminars and schools

Title	**Catalytic biomass conversion**
Applicant	Prof.dr. Gadi Rothenberg
Partners	Prof. Hualong Xu (Fudan University, China), Huayi Chemical, Shanghai
Grant from	Chinese academy, China
Amount	Possibility for exchanging students, lecturers and researchers, enabling the partners to benefit from each other's expertise and culture

Title	**Glass transition and crystallisation of active colloidal swimmers**
Applicant	Dr. Ran Ni
Grant from	NWO Veni
Amount	k€ 250

Title	**Probing the electrochemical reaction dynamics in solar water splitting cells**
Applicant	Dr. Bernd Ensing
Grant from	FOM CSER
Amount	k€ 40 + 1 PhD student

Title	**Realistic Modeling of Catalytic Water Oxidation**
Applicant	Prof.dr. Evert Jan Meijer
Grant from	FOM CSER
Amount	k€ 40 + 1 PhD student

Title	**Realistic Modeling of Catalytic Water Oxidation**
Applicants	Prof.dr. Koop Lammertsma (VU), prof.dr. Wybren Jan Buma, prof.dr. Matthias Bickelhaupt (VU)
Grant from	FOM CSER
Amount	k€ 40 + 1 PhD student

Title	**Development of a Vibrational Optical Activity analysis toolbox**
Applicants	Prof.dr. Wybren Jan Buma, prof.dr. Lucas Visscher (VU)
Partners	The companies Scientific Computing & Modelling (NL) and BioTools (USA)
Grant from	Fund New Chemical Innovations (NCI)
Amount	k€ 1,100

Title	**Start-up investment for chair Supramolecular separations**
Applicants	Prof.dr. Joost Reek, prof.dr. Peter Schoenmakers
Grant from	UvA-VU profileringsmiddelen
Amount	k€ 200

Title	**Amsterdam Solar Energy Research Initiative (SOLARDAM)**
Applicants	Prof.dr. Roberta Croce (VU), prof.dr. Tom Gregorkiewicz (IoP), prof.dr. Rienk van Grondelle (VU), prof.dr. Albert Polman (AMOLF, IoP), prof.dr. Joost Reek, Wim Sinke (ECN, IoP), prof.dr. Lucas Visscher (VU).
Grant from	UvA-VU AAA fund 2014
Amount	k€ 1,000 (of which approx. ¼ for HIMS)

Title	**Revolution in chemical synthesis via programmable C-H activation**
Applicant	Dr. Paweł Dydio
Grant from	NWO Rubicon
Amount	24 month postdoc position at University of California, Berkeley

Two projects directly paid by Industry were started in 2014:

Dr. Anett Schallmey developed a novel biocatalytic route towards the synthesis of a promising drug candidate for application in women's health and oncology with Pantarhei Bioscience BV, based in Zeist.

Dr. Moniek Tromp started a research project with TU Munich and BMW on the development of operando X-ray absorption and scattering electrochemical cells and subsequent studies of high voltage cathode materials.

1.4.5 Dissertations

14-01-2014: Erik Ras, Descriptors for solid catalysts: 21st century discovery tools, promotor: Gadi Rothenberg
07-02-2014: Sietse van der Post, Love and fear of water: Water dynamics around charged and apolar solutes, promotor: Huib Bakker
10-04-2014: Eveline Jansen, Transition Metal Catalysts for the Conversion of Biomass Inspired Substrates, promotors: Kees Elsevier, Bas de Bruin
29-04-2014: Frédéric Terrade, Nature inspired catalytic systems using sulfonamido-phosphorus based complexes, promotor: Joost Reek
06-05-2014: Rianne 't Hoen, Deuterium retention in radiation damaged tungsten exposed to high-flux plasmas, promotor: Aart Kleijn
09-05-2014: Adriana Huerta Viga, Coupled Vibrations in Peptides and Proteins, promotor: Sander Woutersen
04-06-2014: Evert Koopman, Simple numerical techniques for mesoscale polymers, (co)promotors: Peter Bolhuis and Christoffer Lowe
13-06-2014: Weina Du, Advanced path sampling of the kinetic network of small proteins, promotor: Peter Bolhuis
25-06-2014: Hanneke Brust, Chemical profiling of explosives, promotors Peter Schoenmakers, Arian van Asten
05-09-2014 Lizhe Zhu, Molecular simulations of receptor proteins, promotor Peter Bolhuis
18-09-2014 Zea Strasberger, Converting Lignin to Aromatics; Step by Step, (co)promotors Gadi Rothenberg and Stefania Grecea
30-09-2014 Arjen Breman, Novel Cinchona Derived Organocatalysts: New Asymmetric Transformations and Catalysis, (co)promotors Henk Hiemstra and Steen Ingemann
01-10-2014 Murat Kılıç, Molecular Simulations in Electrochemistry: Electron and Proton Transfer Reactions Mediated by Flavins in Different Molecular Environments, (co)promotors Evert Jan Meijer and Bernd Ensing
21-10-2014 Yasemin Gümrükçü, Direct Activation of Allylic Alcohols in Palladium Catalyzed Coupling Reactions, promotor Joost Reek
21-10-2014 Ruben Drost, The Pd-Catalyzed Semihydrogenation of Alkynes to Z-alkenes: Catalyst Systems and the Type of Active Species, promotor Kees Elsevier
22-10-2014 Ngoc A Dang, Towards a new approach for fast diagnosis of tuberculosis using gas chromatography-mass spectrometry, promotors Hans-Gerd Janssen en Peter Schoenmakers
25-11-2014 Eric Tan, Structural dynamics of isolated biological and synthetic photoswitches, promotors Wybren Jan Buma, Jos Oomens
12-12-2014 Ivan Kryven, Topology evolution in macromolecular networks, promotor Piet Iedema
16-12-2014 Kai Liu, Functionalized Upconversion Nanoparticles for Cancer Imaging and Therapy, promotors Wybren Jan Buma, X.G. Kong
17-12-2014 Pierre Boulens, Regulation of cholesterol metabolism: An IDOL-dependent pathway to degrade the LDL-receptor, promotor Joost Reek

2. Research

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

2.1 Sustainable chemistry

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

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

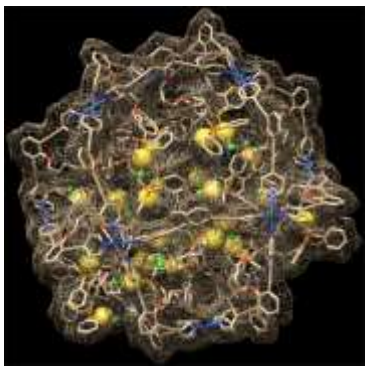
Group	Homogeneous and Supramolecular Catalysis		
Groupleader	Prof.dr. J.N.H. Reek		
Academic staff	Prof.dr. B. de Bruin Prof.dr. B. van der Zwaan (BHL) Dr. J.I. van der Vlugt Dr. M. Tromp (TT)		
Support staff	F. Ait El Maate A.M. van der Burg E. Duin-Berteling C. Mahabiersing Z. Abiri		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. R.J. Detz Dr. W.I. Dzik (VENI) Dr. R. Gramage Doria Dr. P. Gualco Dr. P. Li Dr. A.E. Pascui Dr. S. Raoufmoghaddam Dr. Q. Wang Dr. X. Wang	1-9-2013 1-11-2013 1-5-2012 1-6-2013 1-7-2013 1-1-2014 1-2-2014 1-1-2014 1-5-2014	1-1-2016 1-11-2016 1-5-2014 1-9-2014 1-1-2015 1-7-2015 1-2-2016 1-12-2015 1-5-2016

PhD students	Drs. R. Becker	1-3-2012	1-3-2016
	Drs. S.Y. de Boer	15-8-2011	15-8-2015
	Drs. B. van den Bosch	1-5-2010	1-8-2014
	Drs. D.L.J. Broere	15-5-2012	15-5-2016
	Drs. A. Chirila	1-9-2012	1-9-2016
	Drs. J.J.M. Daubignard	1-1-2011	1-1-2016
	Drs. M. Goswami	1-8-2013	1-8-2017
	Drs. C. te Grotenhuis	1-8-2013	1-8-2017
	Drs. Y. Gumrukcu	1-11-2013	1-11-2014
	Drs. A.C.H. Jans	15-3-2014	15-9-2015
	Drs. L.S. Jongbloed	15-2-2012	15-2-2016
	Drs. L.J. Jongkind	1-9-2014	1-9-2018
	Drs. J.M. Koelewijn	1-2-2011	1-2-2016
	Drs. P.F. Kuijpers	1-10-2012	1-10-2016
	Drs. S.H.A.M. Leenders	1-10-2011	1-10-2015
	Drs. S.S. Nurttila	1-6-2014	1-6-2018
	Drs. S. Oldenhof	1-10-2010	1-3-2015
	Drs. C. Rebreyend	1-8-2013	1-8-2017
	Drs. E.C.F. Schippers	1-11-2013	1-11-2017
	Drs. V. Sinha	1-9-2014	1-9-2018
	Drs. V. Subbiah	1-1-2015	1-1-2016
	Drs. Z. Tang	1-1-2011	1-7-2015
	Drs. V. Vreeken	1-5-2012	1-5-2016
	Drs. F.F. van de Watering	1-11-2012	1-11-2016
	Drs. Zaffaroni	1-12-2012	1-12-2016
MSc Students	L.A. Grobe	11-2-2014	11-7-2014
	L.L. Metz	1-2-2014	28-6-2014
	R. van Heck	1-11-2013	1-6-2014
	R. Kox	1-11-2013	1-6-2014
	D. Zant	1-9-2013	1-6-2014
	C.L.M. Baij	1-11-2013	1-6-2014
	D. den Boer	1-10-2013	1-7-2014
	W. Bohmer	1-11-2013	1-6-2014

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

Research highlights per staff member

Name: Prof.dr. J.N.H. Reek
We continued our research in the area of catalyst control by substrate orientation. We have further extended the chemistry based on the DIMPhos scaffold, and demonstrated that we can perform hydroformylation of styrene derivatives with unprecedented selectivity, which can easily be optimized to synthetic relevant conditions (*Nature Prot*, **2014**). The reaction proceeds by first binding of the substrate in the pocket, after which the reaction proceeds, which is established by detailed kinetics that show that the reaction operates via substrate and product inhibition. Yet the overall reaction rate is very because of the preorganization effect (*JACS* **2014**).



In the area of catalysis in confined space we developed a self-assembly strategy to prepare nano-sized molecular spheres with up to 24 metal complexes inside, which results in an extremely high *local catalyst concentration.* This local catalyst concentration can be controlled between 0.05 and 1.1M by just mixing the various bifunctional building blocks in different ratio's, whereas the average catalyst concentration in solution can be kept identical and at the usual mM range. This allows for the first time to thoroughly investigate reactivity at catalyst concentration at M levels, a dimension under-explored in homogeneous catalysis. The high local catalyst concentration turned out to be critical to generate an active system from *a priori* inactive AuCl- complex. The high concentration facilitates novel reaction pathways via multinuclear intermediate, which for the gold complexes is supported by UV-vis experiments. (*ACIE* **2014**) .

R. Gramage-Doria, J. Hessels, S. H. A. M. Leenders, O. Tröppner, M. Dürr, I. Ivanović-Burmazović, J.N.H. Reek,* "Gold(I) catalysis at extreme concentrations inside self-assembled nanospheres" *Angew. Chem., Int. Ed.,* **2014,** *52,* 13380–13384. **highlighted in C2W**

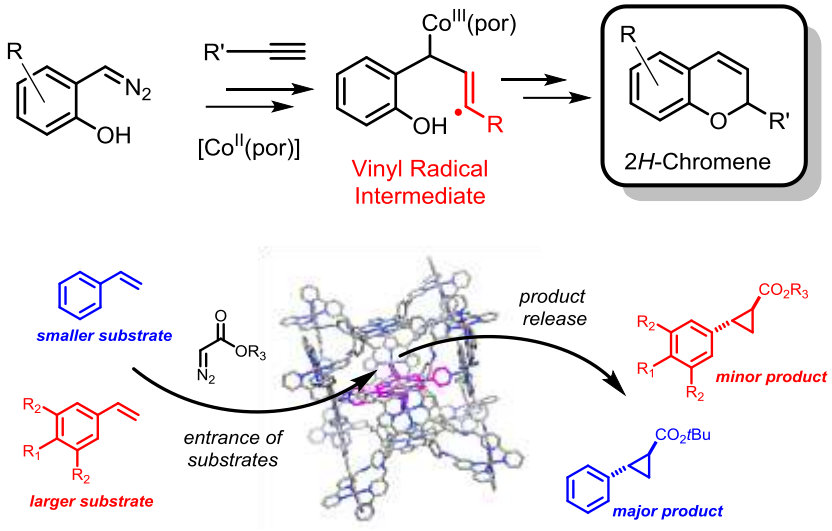
P. Dydio, R.J. Detz, B. de Bruin, J.N.H. Reek* "Beyond Classical Reactivity Patterns: Hydroformylation of Vinyl and Allyl Arenes to Valuable beta- and gamma-Aldehyde Intermediates Using Supramolecular Catalysis" *J. Am. Chem. Soc,* **2014,** *136*(23), 8418-8429.

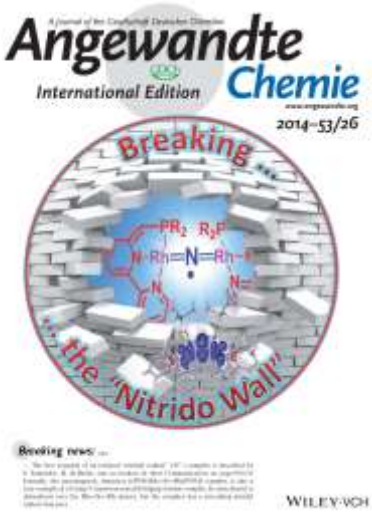
P. Dydio, J.N.H. Reek* "Scalable and chromatography-free synthesis of 2-(2-formylalkyl) arenecarboxylic acid derivatives through the supramolecularly controlled hydroformylation of vinylarene-2-carboxylic acids" *Nature Protocols,* **2014,** *9*(5), 1183-1191.

Name: Prof.dr. B. de Bruin

In the field of metallo-radical chemistry several interesting discoveries were made. The group reported a novel metallo-radical mediated one-pot catalytic process for the synthesis of 2*H*-chromenes (*JACS*, **2014**). This method provides a convenient protocol for the synthesis of these pharmaceutically relevant substructures from easily accessible starting compounds, avoiding multiple synthetic steps and elaborate work-up procedures.

A novel caged catalysts was developed that enables size-selective radical-type cyclopropanation reactions (*Chem. Eur. J.* **2014**). Achieving size-selectivity in homogeneous catalysis is a rarity, but with encapsulated catalysts this is possible, taking advantage of the limited pore-sizes providing a barrier for larger substrates.





The group further reported the very first isolated example of a 'nitridyl radical' ($N^{\bullet 2-}$) complex (*Angew. Chem. Int Ed.* **2014**). This complex is highly unusual. It is formed by photolysis of a diamagnetic Rh^{I}-azido complex, producing the paramagnetic nitridyl-radical complex with very unusual spectroscopic properties. Metal-nitrogen multiple bonding is destabilized for late transition metals, which makes the fact that this this complex was isolated using rhodium particularly striking ('breaking

the nitrido-wall'). The complex is still reactive, and can be activated with carbon monoxide to undergo radical-type N-N couple leading to N_2 formation with reduction of the metal centers (from formally Rh^{IV} to Rh^{I}).

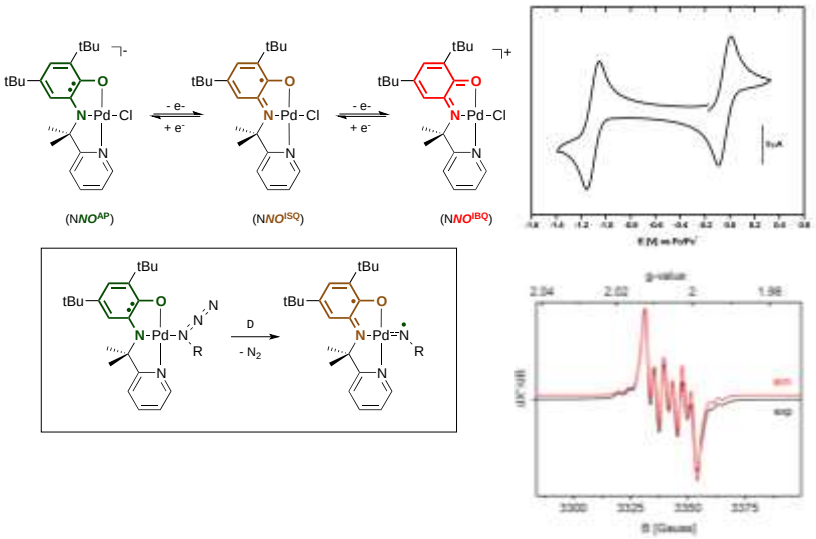
1. An Isolated 'Nitridyl-Radical' Bridged {Rh-N•-Rh} Complex. Gloaguen, Y.; Rebreyend, C.; Lutz, M.; Kumar, P.; Huber, M.; van der Vlugt, J.I.; Schneider, S.*; de Bruin, B.*; *Angew. Chem. Int. Ed.*, **2014**, *53*, 6814-6818. ***'Hot Paper'. Inside Front Cover.***

2. Encapsulated Cobalt–Porphyrin as Catalyst for Size-Selective Radical-type Cyclopropanation Reactions. Otte, M.; Kuijpers, P.F.; Troeppner, O.; Ivanović-Burmazović, I.; Reek, J.N.H.; de Bruin, B.*; *Chem. Eur. J.*, **2014**, *20*, 4880–4884.

3. A Metalloradical Approach to 2H-Chromenes. Paul, N.D.; Mandal, S. Otte, M. Cui. X. Zhang, X.P.; de Bruin, B.*, *J. Am. Chem. Soc.*, **2014**, *136*, 1090–1096.

Name: dr.ir. J.I. van der Vlugt

Within the context of ongoing research using the cooperative action of metals and ligands for substrate activation, the heterolytic cleavage of dihydrogen using mononuclear Ru-complexes was reported (*EurJIC* **2014**), as an invited contribution to a themed issue on Advances in Phosphorus Chemistry. A well-received review on the design, application and spectroscopic investigation of hybrid diphosphorus ligands for asymmetric hydroformylation was published (*Coord.Chem.Rev.* **2014**). In an extension of the group's main interest in developing novel reactive ligand concepts to invoke selective substrate activation and bond functionalization, we reported on the innovative strategy to induce single electron transfer from a redox-active ligand to a substrate, as highly promising, versatile and tunable alternative to metalloradical catalysis (*JACS* **2014**).



1. Synthesis, coordination chemistry and cooperative activation of H_2 with ruthenium complexes of proton-responsive METAMORPhos ligands F.G. Terrade, M. Lutz, J.I. van der Vlugt,***** J.N.H. Reek* *Eur. J. Inorg. Chem.* **2014**, 1826-1835.

2 Hybrid diphosphorus ligands in Rh catalyzed asymmetric hydroformylation
S.H. Chikkali,* J.I. van der Vlugt,***** J.N.H. Reek* *Coord. Chem. Rev.* **2014**, *262*, 1-15.

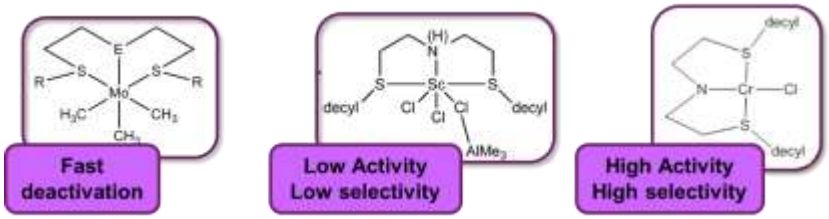
3. Intramolecular redox-active ligand-to-substrate single electron transfer: Radical reactivity with a palladium(II) complex D.L.J. Broere, B. de Bruin, J.N.H. Reek, M. Lutz, S. Dechert, J.I. van der Vlugt***** *J. Am. Chem. Soc.* **2014**, *136*, 11574-11577.

Name: Dr. Moniek Tromp

Moniek Tromp started at the HIMS on the 1st of September 2014. Her group moves from the Technical University Munich, Germany, in January 2015.

New developments in the field of X-ray absorption and X-ray emission spectroscopy for applications in the field of homogeneous and heterogeneous catalysis were pursued. Resonant inelastic x-ray absorption scattering (RIXS) enables direct imaging of electronic transitions in the d-band of supported nanoparticle Pt

catalysts in real time and in realistic environmental conditions (*ChemPhysChem* **2014**). RIXS will uniquely offer the possibility to account for support interaction, adsorbate coverage, cluster size, and changes in compressive or tensile strain within a catalyst in the process of chemical reaction, on the electronic state of the catalyst, revealing important insights in catalyst performance.



The activation mechanisms of industrially important homogeneous catalysts for the selective oligomerisation of ethane were investigated by time-resolved spectroscopy (*PhilTransRSocA***2014**), providing important insights in the genesis of the catalytic cycle and their overall performance. A combination of Cr K-edge XAS, EPR, and UV–visible spectroscopy, with novel rapid freeze-quench procedures, allowed the identification and characterization of a 4-coordinate Cr(II) intermediate (*ACSCatal***2014**).

Effects of Adsorbate Coverage and Bond Length Disorder on the d-Band Center in Carbon Supported Pt Catalysts M. W. Small, J. Kas, K. O. Kvashnina, J. J. Rehr*, R. G. Nuzzo*, M. Tromp*, A. I. Frenkel*, *Chem. Phys. Chem.* **2014**, *8*, 1569–1572.
Catalysis seen in Action M. Tromp*, *Phil. Trans. R. Soc. A* **2015**, *373*, 20130152.
On the activation of [CrCl3{R-SN(H)S}] catalysts for selective trimerisation of ethene: a freeze-quench Cr K-edge XAFS study S. A. Bartlett, J. Moulin, M. Tromp*, G. Reid, A. J. Dent, G. Cibin, D. S. McGuinness, J. Evans*, *ACS Catal.* **2014**, 4, 4201–4204.

Other activities

Prof.dr. J.N.H. Reek
Collaboration with several groups from the BIOSOLARCELLS network, and the EU network on solar fuel. Collaboration with Prof Gascon TU Delft, Prof Ivanovic-Burmazovic Univeristy Erlangen, Prof Kroutil University Gratz,Prof Ribas Universitat de Girona.
Director HIMS institute (122 FTE)
Scientific director InCatT
Director of research priority area Sustainable Chemistry UvA
Management team NRSCC
Advisory Board Eur. J. Inorg Chem.
Chair of NWO work-group Coordination and Catalysis
Board member KNCV (research)
Management team BioSolarCell (Dutch artificial leaf program)
Chair UOC UvA
Member of the World economic forum
Steering committee Co van Ledden Hulsebosch Center
Member of the Royal Holland Society of Sciences and Humanities (KHMW)

Prof.dr. B. de Bruin
Collaboration with several groups in the EU CARISMA and ECOSTBIO COST networks. Collaboration with Prof. Wybren Jan Buma (HIMS), Prof. Sander Woutersen (HIMS), Prof. Kees Elsevier (HIMS), Prof. Sven Schneider (Göttingen), Prof. X. Peter Zhang (South Florida), Prof. Hansjörg Grützmacher (ETH), Prof. Wolfgang Kaim (Stuttgart), Prof. Robert Wolf (Regensburg), Prof. Xuefeng Fu (Beijing), Prof. Ciriano & Dr. Tejel (Zaragoza), Prof. Ivana Ivanovic-Burmazovic (Erlangen).

Coordinator Science for Energy & Sustanability Master Track
Chair of the Editorial Board of the Wiley journal *European Journal of Inorganic Chemitry (society journal)*

Editorial Advisory Board *Organometallics* (ACS society journal).
Chair & co-organiser of the NIOK/HRSMC AMOCC-2014 PhD course (Advanced Metal-Organic Chemistry & Catalysis.
Guest editor *ChemComm* (RSC) Special Web Themed Issue 2014 on Redox Active Ligands
Member of the NWO-CW VIDI selection committee 2014.
Member of the Chemistry Education Committee (Onderwijscommissie Scheikunde, OCS). Chair of UvA side of the committee since 2012.
Member of the selection committee DPI Golden Thesis Award 2014.
Member NIOK Roadmap Catalysis writing team.
Member of the NIOK onderwijscommissie.

Dr.ir. J.I. van der Vlugt
Collaboration with several (inter)national groups, including prof. Woutersen & Elsevier (UvA), prof. Browne (RUG), prof. Gascon (TUD), prof. Kamer (St. Andrews, UK), prof. Peruzzini & Dr. Caporali (CNR, Florence), prof. Hey-Hawkins (Leipzig, Germany).
Member of the Advisory Board of the Technology Center at Science Park Amsterdam.
Co-organiser of the NIOK/HRSMC AMOCC-2014 PhD course (Advanced Metal-Organic Chemistry & Catalysis.
Member of EU COST CARISMA network.
Advisor, National Chemistry Olympiad, University of Amsterdam, May 30 – Jun 5, 2014.

Dr. M. Tromp
International collaborations include Dr. P. Glatzel (ESRF, Grenoble, France), Prof. J. J. Rehr (University of Washington, Seattle, USA), Prof. F. M. F. de Groot (UU), Prof. A. Frenkel (Yeshiva University, New York, USA), Prof. R. Nuzzo (University of Illinois, Urbana, USA), Profs. J. Evans, G. Reid (University of Southampton, United Kingdom), Profs. H. Gasteiger, T. Nilges, J. Lercher (Chemistry, TUM, Munich, Germany), Prof. B. Sels (University of Leuven, Belgium), Profs. C. Coperet, J. A. van Bokhoven, M. Nachtegaal (ETH, Zurich, Switzerland), Prof. C. Majed (EPFL, Lausanne, Switzerland).
Visiting Professor University of Southampton (UK)
Visiting Scientist Diamond Light Source (UK)
(Guest) Professor Technical University Munich (Germany)
Chair of the Swiss Light Source Peer Review Panel (Switzerland)
Member of the Scientific Advisory Committee of the SOLEIL synchrotron (France)
Member of BMW Diesel IAS-TUM focus group on 'Electrochemical Interfaces in Batteries' (Germany)
Member of the European Synchrotron User Organisation
Member of the international user committee of the ANKA research facility (Germany)
Member of the MAX Laboratory (Lund, Sweden) Program Advisory Committee
IWT panel member (Belgium)

Dissertations
10-04-2014: Eveline Jansen, Transition Metal Catalysts for the Conversion of Biomass Inspired Substrates, promotors: Kees Elsevier, Bas de Bruin
29-04-2014: Frédéric Terrade, Nature inspired catalytic systems using sulfonamido-phosphorus based complexes, promotor: Joost Reek
21-10-2014: Yasemin Gümrükçü, Direct Activation of Allylic Alcohols in Palladium Catalyzed Coupling Reactions, promotors Joost Reek, Bas de Bruin
17-12-2014: Pierre Boulens, Sulphonamido-Phosphorus Nickel Complexes for the Selective Oligomerisation of Olefins, promotor Joost Reek
21-10-2014: Ruben Drost, The Pd-Catalyzed Semihydrogenation of Alkynes to Z-alkenes: Catalyst Systems and the Type of Active Species, promotors: Kees Elsevier, Bas de Bruin

Grants and prizes
UvA AAA program, 1 MEuro for SOLARDAM research program, together with the VU and AMOLF.

FOM-NWO-Shell Grant (PI, Sept. 2014- Sept. 2019; 1 PhD student, 4 yr, €240.000,-). Title: Mechanistic Insights in Catalytic Energy Conversion Processes.

Invited lectures Prof.dr. J.N.H. Reek

- Invited lecture at the Inorganic chemistry symposium at the ACS, "Supramolecular strategies in transition metal catalysis" Dallas, march 2014
- Invited lecture at the ICPPP 2014, "Self-assembled transition metal catalysts using template-ligands and porphyrin building blocks" Istanbul, June 2014
- Invited lecture at bilateral symposium on solar fuel (with Korea), "Towards solar to fuel devices based on molecular components" Amsterdam, July 2014,
- Invited lecture at the 13th CSCB Annual Symposium, "Supramolecular strategies in transition metal catalysis" Dublin, Ireland, December 2014.

Invited lectures Prof. dr. B. de Bruin

- Seminar at the University of Hualva (Homogeneous Catalysis department). Jan. 28, 2014. Host: Prof. Pedro J. Pérez. October 22-24, 2014, Title: New Catalytic Reactions with Carbene Radicals.
- 5th European Chemistry Conference (ECC5) organized by EuCheMS, Istanbul (Turkey), Aug. 31-Sept. 4, 2014, Title: New Catalytic Reactions with Carbene Radicals. Keynote Lecture.
- Invited lecture at symposium "Electronic Structure Contributions to Physical Properties and Reactivity in Transition Metal Chemistry" at the 248th National ACS Meeting in San Francisco, Aug. 10-14, 2014. Title: New Catalytic Reactions with Carbene Radicals.
- 19th International Symposium on Homogenous Catalysis (ISHC-XIX), Ottawa, July 6-11, 2014, Title: New Catalytic Reactions with Carbene Radicals. Keynote Lecture
- International Conference on Porphyrins and Phthalocyanines (ICPP-8), Istanbul (Turkey), July 22-27, 2014. Title: New Catalytic Reactions with Carbene Radicals.
- ACMM (Advanced Center for Multiscale Modeling) Symposium. Febr. 7, 2014. Free University of Amsterdam (VU). Title: Catalytic Radical-type Transformations; New Catalytic Reactions with 'Carbene Radicals'.
- Seminar at the University of Mainz (Inorganic Chemistry department). Jan. 28, 2014. Host: Prof. Heinze. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Ligand Radicals'.

(Invited) Lectures Dr.ir. J.I. van der Vlugt

- Lecturer at the introductory course preceeding the AMOCC-2014 course (Jun 2014).
- Fusion Conference Small Molecule Activation, Chicago, USA (July 2014), Organometallic Cooperative Ligands: Avenues for Bifunctional Bond Activation and Catalysis
- 1st Next Generation Chemistry @ NL Symposium, Eindhoven, the Netherlands (Oct 2014), Organometallic Catalysis in 2014: Reactive & Cooperative Ligands
- 2nd International Conference on C-H Activation, Rennes, France (July 2014), Organometallic Cooperative Ligands: Avenues for Bifunctional Bond Activation and Catalysis
- 5th EuChemS European Chemistry Symposium, Istanbul, Turkey (Sep 2014), Single-Electron Reactivity on Late Transition Metals Mediated by Redox-Active Ligands

(Invited) Lectures Dr. M. Tromp

- M. Tromp, 'Probing Dynamic Species in Catalysis: Selective Polymerisation', Invited lecture, FP7-project MAO-Robots Meeting, Tutzing, June 2014.
- M. Tromp, 'Early Transition Metal CatalystsCharacterisation and Development, Kick-off Symposium SusChem UvA RPA, Amsterdam, September 2014.
- M. Tromp, 'Advanced Spectroscopic Techniques Probing Materials and Mechanisms', Invited lecture, Konstanz University, Germany, December 2014.

Outreach
Joost Reek On TV in the programme “Met de Kennis van nu”: In 2014 there was a short (7 min) documentary on public TV, the topic was the artificial leaf, and it was shot in our labs

Moniek Tromp in article by S. Knols, ‘Brain gain: from Munich to Amsterdam’, Elements: Annual Magazine NWO Chemical Sciences 2014, page 31.

Contribution to RPA Sustainable Chemistry
Most of the work that has been done in the HOMKAT group is related to the challenges formulated in the RPA sustainable chemistry. New reactivity with first row metal complexes has been discovered, and new selective catalytic processes have been developed. In the area of catalysis for solar to fuel devices new discoveries have been made. In collaboration with the molecular photonics group (Wouterse), we have studied a new hydrogenase mimic, that gives reversible monoreduction, but is inactive in proton reduction. Time resolved IR shows that the bridging ligand is mainly reduced (*Inorg Chem*). In another collaboration with the molecular photonics group (Brouwer) we have established a system homogeneous system for light driven water oxidation. Importantly, the chromophore is metallo-porphyrin, which has a much longer life time under the conditions used compared to the frequently used Ruthenium complex (*Energy & Environmental Science*).

Group	Heterogeneous Catalysis and Sustainable Chemistry		
Group leader	Prof.dr. G. Rothenberg		
Academic staff	Dr. S. Grecea Dr. N.R. Shiju Dr. N. Yan (> 1-8-2014)		
Support staff	Ing. P.F. Collignon Ing. N.J. Geels		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. A.H. Alberts Dr. M.J. Louwerse Dr. N. Madaan Jaso Dr. A.G. Maldonato Soto Dr. M.C. Mittelmeijer-Hazeleger Dr. P.L.K. Prinsen Dr. E.V. Ramos Fernandez Dr. E.G.K. Solomon Raja Drs. A.L. Dantas Ramos	1-1-2014 1-10-2012 1-12-2012 1-10-2012 1-5-1966 1-2-2014 1-3-2012 1-7-2014 1-3-2013	1-1-2015 1-10-2014 1-12-2014 1-10-2014 1-5-2016 1-2-2016 1-3-2014 30-6-2016 1-3-2014
PhD students	Drs. B. Coskuner Drs. Y. Gao Drs. E.J. Ras Drs. V. Santacroce Drs. Z.I. Strassberger	1-4-2013 1-9-2014 1-1-2010 15-9-2014 18-1-2010	1-4-2014 1-9-2018 1-1-2014 15-3-2015 18-01-2014
MSc students	H.A.A. Andriessen R. Beerthuis C. Hernandez-Mejia R. de Boer C. Pagis		

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

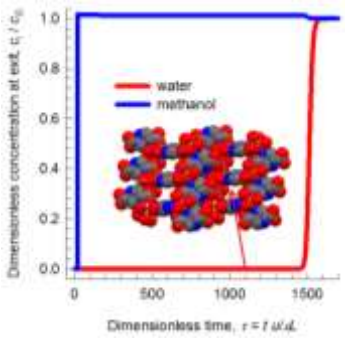
Research highlights per staff member

Dr. Raveendran Shiju
We continued our work on developing heterogeneous catalysts for converting biomass derived platform chemicals to other value-added chemicals. These conversions include dehydration, hydrogenation and oxidation reactions. Examples are conversion of furfuryl alcohol to butyl levulinate and oxidative dehydrogenation of ethyl lactate to ethyl pyruvate (see references below). The former work was a collaboration with Dr. Mario Pagliaro (Istituto per lo Studio dei Materiali Nanostrutturati, CNR). These studies revealed the importance of several structural and treatment variables on the catalytic performance and stability in biomass conversion reactions. Furthermore, our work on 'Novel Biorenewable Routes to Acrylic Acid' presented by Rolf Beerthuis, master student of Molecular Design, Synthesis and Catalysis was selected for the 'best poster' award by The Royal Dutch Society of Engineers (KIVI) during the Symposium 'Engineering for a Sustainable Future' held in March 2014 at the Eindhoven University of Technology. We are working also

on developing novel routes for the conversion of CO_2 to fuels/chemicals. One of the approaches is to use a thermochemical cycle, utilizing solar energy, based on metal oxide redox reactions (see ref. 3 below). Another approach is to use an electocatalytic membrane reactor for converting CO_2 to methanol, which was awarded the CAPITA grant in which our group is a part of a European consortium involving three companies.

1. Enhanced Heterogeneous Catalytic Conversion of Furfuryl Alcohol into Butyl Levulinate. P. Demma Carà, R. Ciriminna, N. R. Shiju, G. Rothenberg and M. Pagliaro, *ChemSusChem*, **2014**, 7, 835-840.
2. Titania-catalysed oxidative dehydrogenation of ethyl lactate: Effective yet selective free-radical oxidation. E.V. Ramos-Fernandez, N.J. Geels, N.R. Shiju and G. Rothenberg, *Green Chem*., **2014**, 16, 3358-3363.
3. Understanding the solar-driven reduction of CO_2 on doped Cerias. E.V. Ramos-Fernandez, N.R. Shiju and G. Rothenberg, *RSC Adv*., **2014**, 4, 16456-16463.

Dr. Stefania Grecea



Tackling water-alcohol separations. We succeeded in making a new type of porous material that can efficiently dehydrate alcohols. Thi hybrid organic-inorganic (MOF) material is not only structurally beautiful but also highly unusual. It has a stable microporous structure with hydrophilic one-dimensional channels which are just right for accommodating water molecules. Furthermore, the lanthanum ions, with their large and flexible coordination, facilitate structural re-organization without disrupting the overall framework. This makes the porous framework highly robust, allowing multiple dehydration/hydration cycles. Unlike most MOFs, it is also hydrothermally stable at high temperatures. This makes it a realistic candidate for removing small amounts of water from water-alcohol mixtures as well as wet gases.

1. Highly selective water adsorption in a lanthanum metal-organic framework. R. Plessius, R. Kromhout, A.L. Dantas Ramos, M. Ferbinteanu, M.C. Mittelmeijer-Hazeleger, R. Krishna, G. Rothenberg and S. Tanase, *Chem. Eur. J.*, **2014**, 7922-7925.
2. Metal-organic frameworks and their application in catalysis. A.L. Dantas Ramos, S. Tanase, G. Rothenberg *Quim. Nova*, **2014**, *37*, 123-133. Featured on the issue cover.
3. The pros and cons of lignin valorisation in an integrated biorefinery. Z. Strassberger, S. Tanase, G. Rothenberg *RSC Advances*, **2014**, *4*, 25310-25318.

Other activities

In 2014, the group has strengthened its international and industrial collaborations, especially with Fudan University in Shanghai (one of the top-5 universities in China), as with the Shanghai Hauyi Acrylic Acid Company (one of the largest chemical manufacturers in the Shanghai area). A joint project was initiated, funded by the Chinese Government, and the first MSc exchange student visited Fudan for a two-month research project. Further, a new spin-off company, Plantics BV, was started based on the invention of the biodegradable plastic. The company is run by Mr. Helias Andriessen, a graduate MSc from the group, and Dr. Albert Alberts, a senior researcher. For more information see **www.plantics.com**
We also joined the HRSMC.

Dissertations

14-01-2014: Erik-Jan Ras, Descriptors for solid catalysts: 21st century discovery tools, promotor: Gadi Rothenberg

18-09-2014 Zea Strasberger, Converting Lignin to Aromatics: Step by Step, (co)promotors Gadi Rothenberg and Stefania Grecea

Grants and prizes

European research project CAPITA (Catalytic Processes for Innovative Technology Application) for the catalytic synthesis of methanol from carbon dioxide. €250,000.

Multifunctional microporous materials, CSC fellowship awarded to Ms. Yuan Gao.
Royal Dutch Society of Engineers (KIVI) best poster award to Rolf Beerthuis.

Invited lectures

- G. Rothenberg: A new type of plastic made from plants. CatchBIo symposium, Felix Meritis, Amsterdam, March 2014 (plenary lecture).
- G. Rothenberg: New core-shell alumina/cobalt Fischer-Tropsch catalysts. XXVth ORCS conference on Catalysis of Organic Reactions, Tucson, March 2014 (invited lecture).
- G. Rothenberg: A new type of plastic made from plants. University of California, Berkeley, March 2014 (invited lecture).
- G. Rothenberg: A new type of plastic made from plants. Universtiy of California, San Diego, March 2014 (invited lecture).
- G. Rothenberg: A new type of plastic made from plants. Weizmann Institute of Science, April 2014 (invited lecture).
- G. Rothenberg: Heterogeneous catalysis and sustainable chemistry in Amsterdam. AkzoNobel R&D, Deventer, June 2014 (invited lecture).
- G. Rothenberg: New catalytic routes from biomass to chemicals. Agricultural Research Organisation (Volcani Center), Israel, October 2014 (invited lecture).
- G. Rothenberg: Finding tomorrow's catalysts today: A step change in catalyst discovery. KNCV catalysis symposium, Amsterdam, November 2014 (invited lecture).
- G. Rothenberg: A catalytic toolbox for practical biomass conversion. FC2 Green Chemistry conference, Shanghai, November 2014 (plenary lecture).
- N. R. Shiju: Topics in European Catalysis- a view from Amsterdam. 2nd CAPITA meeting on European Catalysis, Brussels, February 2014 (invited lecture).
- N. R. Shiju: Reducible oxides and heterogeneous catalysis. COST Action CM1104, working group 3 meeting, Prague, May 2014 (invited lecture).
- N. R. Shiju: Catalysis in action: from nylon to paracetamol. University of Huddersfield, July 2014 (invited lecture).

Outreach

S. Grecea: Coordination of practical lab in the National Chemistry Olympiad, UvA, May 30 - June 6, 2014.

Contribution to RPA Sustainable Chemistry

2014 was an exciting year for the RPA sustainable chemistry activities in HCSC. It marked the start of the actual research at the RPA, and the building of the Fuel Cells team and planning and design of the first high-temperature experimental fuel cell in the lab.
Further, work continued on the group's initiatives for converting biomass to high-value chemicals, with collaborations with the Photonics group on nanomaterials and with the Computational Chemistry Group on molecular separations. Outside the UvA, we initiated projects with Prof. Tasiopoulos (Cyprus University) and Dr. M. Manos (Ioanina University) on MOFs for water-alcohol separations and with Prof. Bouwman (UL) on MOFs for temperature sensing.

We also initiated research collaborations with Prof. T. Ishihara (Kyushu University, Japan) on ethane activation, Prof. B. Viswanathan and Prof. Krishnamurthy (the National Centre for Catalysis Research-IIT Madras, India) on photocatalytic activation of CO_2, and Dr. A. Panda (Centurion Institute of Technology , Orisa, India) on waste plastics to fuel.

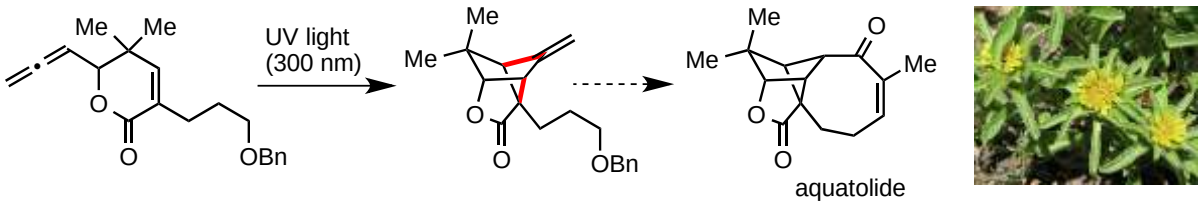
Group	Synthetic Organic Chemistry		
Group leader	Prof. dr. H. Hiemstra		
Academic staff	Prof. dr. P. Timmerman (BHL) Dr. S. Ingemann Jørgensen Dr. J.H. van Maarseveen		
Support staff	R. Klein Nijenhuis M.J. Wanner E. Zuidinga		
Temporary staff		Start date	(foreseen) end date
Postdoc	Dr. R. Renirie	1-9-2014	1-1-2015
PhD students	Drs. A.C. Breman	1-11-2013	1-11-2014
	Drs. S. Popović	1-2-2010	1-6-2015
	Drs. G.J.J. Richelle	1-11-2013	1-11-2017
	Drs. L. Steemers	1-9-2012	1-9-2016
	Drs. D.E. Streefkerk	1-6-2014	1-6-2018
	S. Žari MSc. (Tallinn, Estonia)	1-11-2014	1-4-2015
	A. Ruiz-Olalla MSc (San Seb., Sp.)	16-4-2014	1-10-2014
Stagiair	J. Streefkerk MSc.	1-9-2013	1-5-2014
MSc students	J.M. Saya	1-9-2013	1-9-2014
	M. Würdemann	1-10-2013	1-7-2014
	J.I. Scott (Erasmus, Edinburgh)	1-10-2013	1-7-2014
	C.E. Wilson (Erasmus, Edinburgh)	1-10-2013	1-7-2014
	M. Esgulian (Erasmus, Grenoble)	1-3-2014	1-8-2014
	D.E. Streefkerk	1-9-2013	1-5-2014
	N. Kyriacou	1-11-2013	1-11-2014
	K. Vos	1-9-2014	1-7-2015
	M.L. Corrado	1-9-2014	1-7-2015
	M. Acquesta	1-9-2014	1-7-2015

Mission of the group:

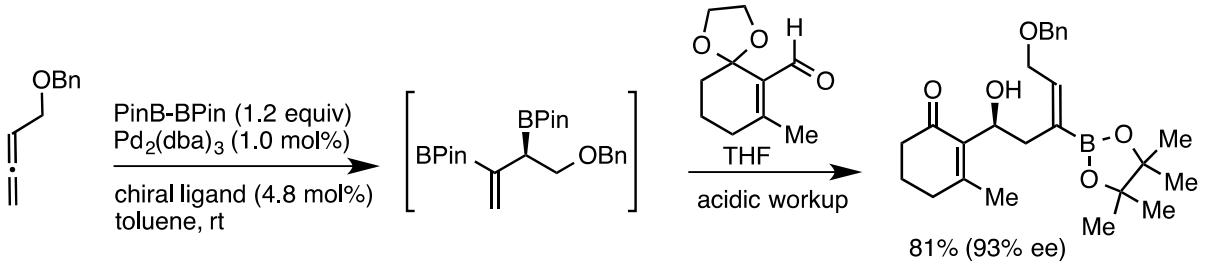
The research in the Synthetic Organic Chemistry group is directed at the development of efficient and selective, diversity-oriented synthetic methodology, in particular organocatalytic procedures, and target-oriented preparation of molecules of relevance in chemistry, biology and medicine. The main target molecules are novel enantiopure organocatalysts, indole and tetrahydro-isoquinoline alkaloids, small cyclic peptides and model systems for lasso peptides and 4-membered ring-containing terpenes, like aquatolide and solanoeclepin A, the hatching agent of potato cyst nematodes.

Research highlights

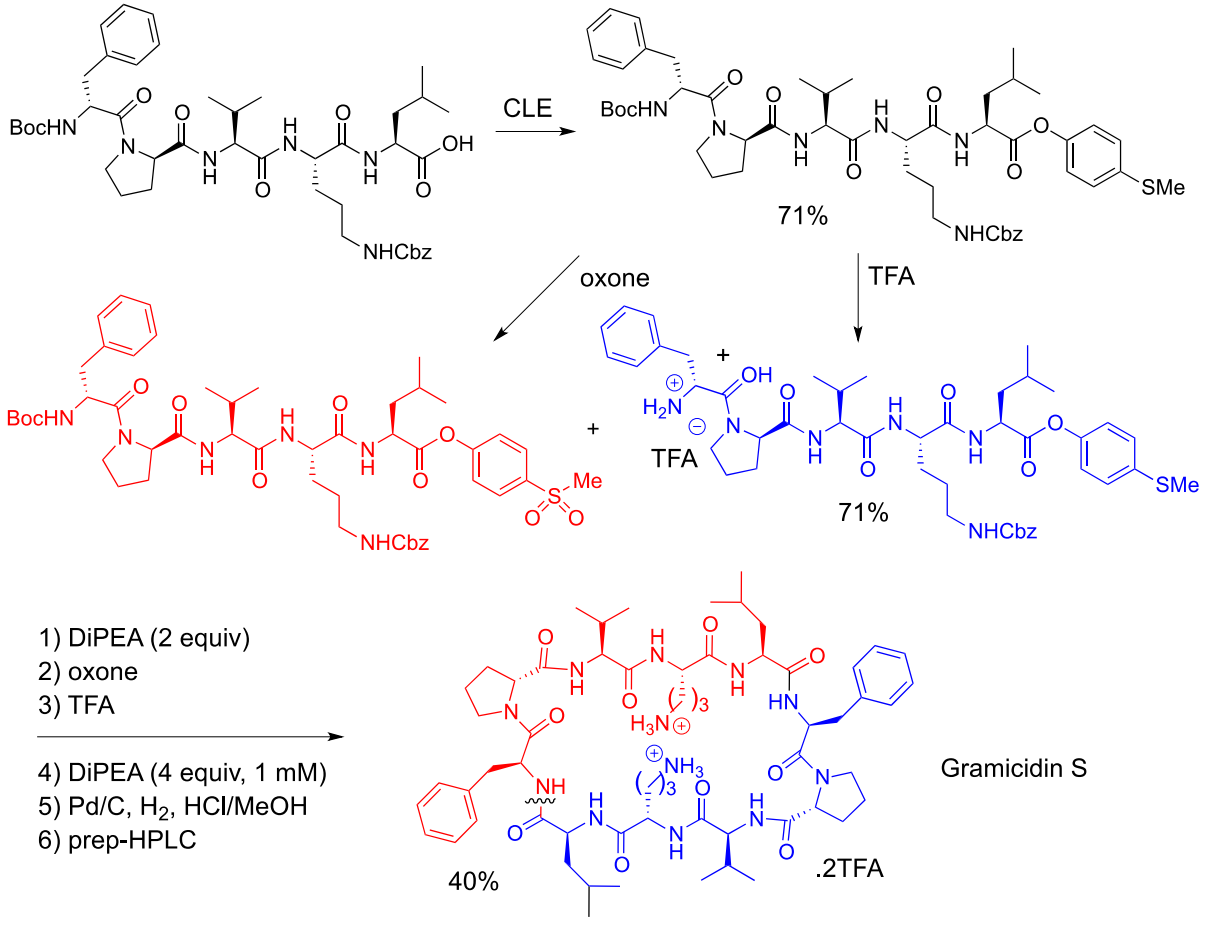
Total synthesis of aquatolide. The sesquiterpene lactone aquatolide (from *Asteriscus aquaticus*, a Mediterranian plant) was synthesized in the laboratory for the first time (master student Jordy Saya). The key step was the intramolecular [2+2]-photocycloaddition providing the four-membered ring in a tricyclic arrangement. The eight-membered ring was closed by way of a Mukaiyama aldol reaction.



Asymmetric catalysis in solanoeclepin A synthesis. In our synthetic approach to solanoeclepin A (hatching agent of potato cyst nematodes) the substrate for the crucial intramolecular [2+2]-photocycloaddition was prepared in a few steps in high yield and enantioselectivity by using chiral palladium-catalysed diborylation of an allene and subsequent stereoselective aldehyde addition (technician Roel Kleinijenhuis).



Synthesis of the antibiotic gramicidin S. Peptide cyclization inevitably requires activation of the C-terminus. By C-activation using the Cu(II)-catalyzed Chan-Lam-Evans (CLE) reaction, subsequent fragment coupling, and cyclization the stereoselective synthesis of the cyclic C2-symmetric decapeptide gramicidin S was accomplished (PhD work of Stanimir Popovic).



Key publications

- Mons, E.; Wanner, M. J.; Ingemann, S.; van Maarseveen, J. H.; Hiemstra, H., Organocatalytic enantioselective Pictet-Spengler reactions for the synthesis of 1-substituted 1,2,3,4-tetrahydroisoquinolines. *J. Org. Chem.* **2014**, *79*, 7380-7390
- Breman, A. C.; Ruiz-Olalla, A.; van Maarseveen, J. H.; Ingemann, S.; Hiemstra, H., Synthesis of quinuclidines by intramolecular silver-catalysed amine additions to alkynes. *Eur. J. Org. Chem.* **2014**, 7413-7425
- Tan, E. M. M.; Amirjalayer, S.; Mazzella, P.; Bakker, B.H.; van Maarseveen, J.H.; Bieräugel, H.; Buma, W.J., Molecular Beam and ab Initio Studies of Photoactive Yellow Protein Chromophores: Influence of the Thioester Functionality and Single Bond Rotation. *J. Phys. Chem. B* **2014**, *118*, 12395-12403
- Wallbecher, R.; Depré, L.; Verdurmen, W.P.R.; Bovée-Geurts, P.H.; van Duinkerken, R.H.; Zekveld, M.J.; Timmerman, P.; Brock, R., Exploration of the Design Principles of a Cell-Penetrating Bicyclic Peptide Scaffold. *Bioconjugate Chem.* **2014**, *25*, 955-964.

Other activities

Prof.dr. H. Hiemstra

- Elected Member of the Royal Holland Society of Sciences (KHMW)
- Member of the International Advisory Board of the Organic division of the Czech Chemical Society
- Member of the Programme Committee of the 27th European Colloquium on Heterocyclic Chemistry, Amsterdam, July 2016
- Member of the Editorial Board of Molecules (Open Access Organic Chemistry Journal)
- Chairman of the Examination Committee master Chemistry and bachelor Scheikunde, UvA

Prof.dr. P. Timmerman

- Member of the scientific advisory board of the yearly TIDES-meeting organized in the US.

Dr. J. H. van Maarseveen

- Member of the Board of the NWO-CW study group Design & Synthesis.
- Expert member, Panel W&T4 Fonds Wetenschappelijk Onderzoek, Flanders, Belgium
- Member of the International Advisory Board European Journal of Organic Chemistry

Dr. S. Ingemann

- Member of The European Chemistry Thematic Network (on behalf of the Faculty of Science)
- Coordinator of the Master Chemistry Track: Molecular Design, Synthesis and Catalysis
- Head of the Structure Analysis group at HIMS comprising the instrumental methods: MS, NMR, X-Ray and EPR

Dissertations

30-09-2014: Arjen Breman, Novel Cinchona Derived Organocatalysts: New Asymmetric Transformations and Catalysis, (co)promotors Henk Hiemstra and Steen Ingemann

Invited lectures

Prof.dr. H. Hiemstra

- "Asymmetric Organocatalysis and Alkaloids", Plenary lecture at the Zing Conference on Asymmetric Synthesis, Nerja, Spain, February 27th, 2014.
- "Synthetic studies towards cyclobutane-containing natural products", Plenary lecture at the Twelfth Anglo-Norman Organic Chemistry Colloquium, Norwich, UK, July 1st, 2014.

Prof. dr. P. Timmerman

- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Site-visit at Roche Pharmaceuticals, Basel/Switzerland, January 16th, 2014.
- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Site-visit at Novartis, Basel/Switzerland, January 17th, 2014.

- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Invited lecture at 9th Status Seminar Chemical Biology, DECHEMA, Frankfurt/Germany, January 22nd, 2014.
- "2-CLIPS Peptides for Affinity Chromatography Applications", Invited lecture at ISPT Cluster Meeting, Amersfoort, January 23rd, 2014.
- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Invited lecture at Belgium Peptide Symposium, Gent/Belgium, February 11th, 2014 (cancelled because of heart problems).
- "2-CLIPS Peptides: Discovery & Optimization of a Novel Class of Biopharmaceuticals", Lecture at Peptide Congress, London/UK, April 3rd, 2014.
- "2-CLIPS Peptides: Discovery & Optimization of a Novel Class of Biopharmaceuticals", Lecture at 9th Annual Drug Discovery Chemistry Meeting, San Diego/US, April 24th, 2014.
- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Invited lecture at FTNLS Symposium "Applying Chemical Tools to Study Biology", Antwerp/Belgium, June 12th, 2014.
- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Invited lecture at 50th International Symposium on Medicinal Chemistry "Interfacing Chemical Biology and Drug Discovery", Rouen/France, July 2nd, 2014.
- "2-CLIPS Peptides: A Novel Class of Biopharmaceuticals", Invited lecture at MipTech Conference 2014, Basel/Switzerland, September 23rd, 2014.

Dr. J. H. van Maarseveen

- "Enantioselective Synthesis of Natural and Biologically Active Tetrahydroisoquinolines via Organocatalytic Pictet-Spengler Reactions", COST ORCA, Palermo, Italy, May 9th 2014.
- "C-Terminal peptide activation: learning lessons from Nature", HRSMC Lustrum Symposium, KNAW, Amsterdam, November 21st 2014.

Dr. S. Ingemann

- "Novel Cinchona alkaloid derivatives as organocatalysts for asymmetric synthesis", 20th
- IUPAC International Conference on Organic Synthesis, Budapest, Hungary, 29 June – 4 July 2014.

Outreach

Dr. J. H. van Maarseveen

- "*Hoe heet is sambal?,* NEMO Wakker Worden lecture, January 19th 2014
- Universiteit van Nederland, ClubAIR Amsterdam, recording five Webcolleges on general chemistry (see: www.universiteitvannederland.nl). January 21st 2014
- *Zoet, zoeter, zoetst! Welk zoetje is het lekkerst?,* VARA Kassa (television) (see: http://kassa.vara.nl/tv/afspeelpagina/fragment/zoet-zoeter-zoetst-welk-zoetje-is-het-lekkerst/speel/1/), March 8th 2014
- *Raakt water nooit op?,* Science Museum NEMO, April 6th 2014
- *Breaking Bad effect?,* VARA De Wereld draait door (television), (see: http://dewereldraaitdoor.vara.nl/Gastendetail.2291.0.html?tx_ttnews[tt_news]=34652&cHash=72d9c7b43a6857222f4ed589b967893d), April 29th 2014
- *Van de Oerknal naar het Leven,* Leidenhoven College, Amsterdam, May 15th 2014
- *Organische Chemie*. Cursus voor Scheikunde Olympiade. Science Park, May 2014.
- *Het ontstaan van het leven (ofwel hoe werd chemie biologie?)*, Intreeweek, Gapen bij de Apen, Artis, August 29th 2014.
- *Climate and Molecules*, AMPA symposium, Science Park Amsterdam, September 16th 2014.
- *Is de goedkoopste vitamine C pil ook goed?* AVROTROS Radar (television), (see: http://www.radartv.nl/uitzending/archief/detail/aflevering/03-11-2014/vitamine-c-of-vitamine-EUR/), November 3rd 2014.
- *Recente highlights uit de Organische Chemie en nieuws vanuit het front.* Rotterdamsche Chemische Kring. Hogeschool Rotterdam, December 8th 2014.

Dr. S. Ingemann

- Member of local organizing committee of the Chemistry Olympiad, University of Amsterdam, June 2014 and also lectures in general, physical and inorganic chemistry during the Olympiad.

Contribution to RPA Sustainable Chemistry

- Development of new organocatalytic procedures for the production of bioactive compounds
- Cooperation with the Reek group on several (student) projects in catalysis

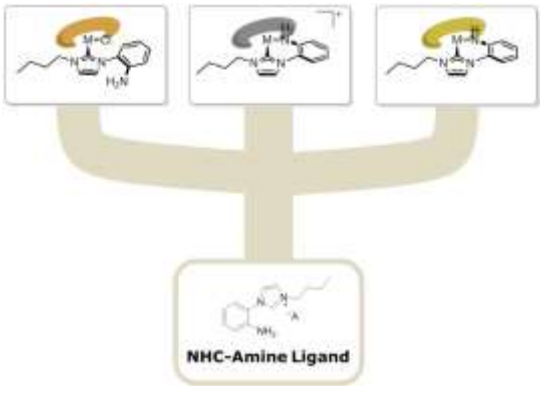
Group	Molecular Inorganic Chemistry		
Groupleader	Prof.dr. C.J. Elsevier		
Support staff	J.M. Ernsting D.S. Tromp		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. T.J. Korstanje	15-8-2013	1-10-2015
PhD students	Drs. R.M. Drost	1-4-2010	1-10-2014
	Drs. E. Jansen	1-10-2013	1-5-2014
	Drs. S.N. Sluijter	1-6-2011	1-6-2015
	Drs. A. Volpe (guest)	1-1-2014	1-6-2014

Mission of the group:

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

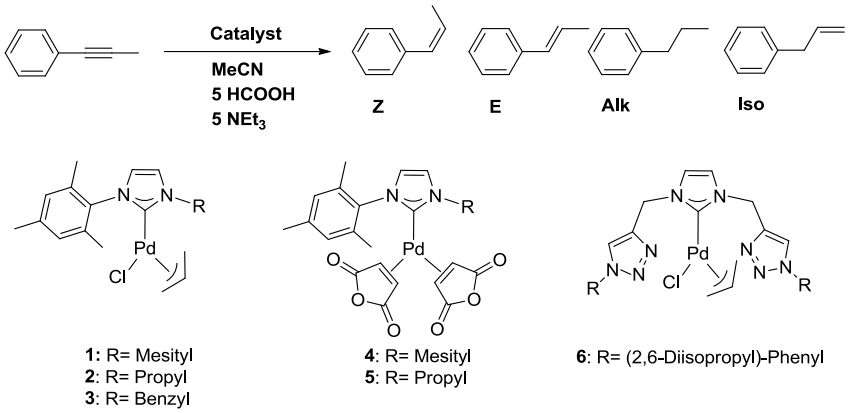
Group high light 2014

Currently, we focus on important hydrogenation and alkylation reactions involving transition-metal-poly-phosphine, N-heterocyclic carbene (NHC) and heteroditopic bis-carbene complexes. The development of a novel set of complexes bearing an NHC-amine ligand (C^{NHC}-NH2) is described. M(cod) complexes (M = Ir, Rh) and a Ru complex have been synthesized in which three different coordination modes of the ligand were established: monodentate, neutral bidentate, and anionic bidentate. The anionic bidentate coordination mode of the anionic C^{NHC}-NH^- ligand arises from deprotonation of the amine moiety of the neutral C^{NHC}-NH2 ligand. Ligand deprotonation proved to be reversible for the Rh and Ir complexes, as was shown by subsequent treatment of the complexes with base and acid. The structural parameters of these differently coordinated ligands were examined, and it was shown that the conjugation of the aniline ring plays a major role in determining the ligand properties. Structural parameters derived from DFT calculations confirm delocalization of the anionic charge over the ligand framework, as is clear from a comparison of the (hypothetical) neutral bidentate complexes $[M(cod)(\kappa^2C,N\text{-}\{C^{NHC}\text{-}NH_2\})]^+$ with those of the (synthesized) monoanionic complexes $[M(cod)(\kappa^2C,N\text{-}\{C^{NH}C\text{-}NH\})]$ (M = Rh, Ir). A similar trend in the structure and bond lengths of the aniline rings was found in the solid-state structure of the novel dimeric complex $[(Ru(\kappa^2C,N\text{-}\{C^{NHC}\text{-}NH\})(\kappa^2C,N\text{-}\{C^{NHC}\text{-}NH_2\})Cl)_2(\mu\text{-}Cl)](PF_6)$.



The octahedral d^5 ruthenium(III) centers in this complex both contain a neutral bidentate C^{NHC}-NH_2 ligand as well as an anionic bidentate C^{NHC}-NH^- ligand. Quite remarkably, the complex is diamagnetic, arising from antiferromagnetic coupling of the two low-spin ruthenium(III) centers over the chloride linker. DFT calculations indeed confirm that the open-shell singlet electronic structure is most stable.

Furthermore, a convenient and easy to use protocol for the Z-selective transfer semi-hydrogenation of alkynes was developed, using ammonium formate as the hydrogen source and the easily prepared and commercially available, highly stable complex $PdCl(\eta^3\text{-}C_3H_5)$ (IMes) (**1**) as the (pre)catalyst. Combined with triphenyl posphine as an additive ligand, this system provides a robust catalytic synthetic method that shows little to no over-reduction or isomerization after full substrate conversion. The system allows the direct use of solvents and reagents, as received from the supplier without drying or purification, thus providing a practical method for semi-hydrogenation of a broad range of alkynes. The mechanism behind these high and enhanced selectivities was determined through a combined set of kinetic experiments.



Other activities

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

Collaboration with dr. B. Milani (Trieste) concerning co-polymerization and development of molecular catalysts.

Dissertations

10-04-2014: Eveline Jansen, Transition Metal Catalysts for the Conversion of Biomass Inspired Substrates, promotors: Kees Elsevier, Bas de Bruin

21-10-2014 Ruben Drost, The Pd-Catalyzed Semihydrogenation of Alkynes to Z-alkenes: Catalyst Systems and the Type of Active Species, promotors Kees Elsevier, Bas de BRuin

Group:	Biocatalysis and Bio-organic Chemistry		
Group leader:	Dr. A. Schallmey (until 30-09-2014)		
Academic staff:	Prof. dr. R. Wever (Emeritus)		
Support staff:	A.F. Hartog		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. M.P. Bracco Garcia	01-03-2014	14-11-2014
PhD students:	-		
MSc students:	Suzanne Flaton	01-07-2014	31-10-2014

Mission of the group:
The Biocatalysis group focuses on the use and development of biocatalysts in synthetic organic chemistry as a "green" alternative for existing chemical procedures with a special focus on oxygen insertion and sulfation reactions as well as biomass utilization. Our research also involves the identification of novel enzyme activities as well as the optimization of biocatalyst characteristics by protein engineering. With this, it fits perfectly in the Research Priority Area “Sustainable Chemistry” at UvA.

Research results per sub project
Title: Biocatalytic sugar sulfation
Researchers: A.F. Hartog
The arylsulfotransferase AST from *Desulfitobacterium hafniense* was earlier shown to sulfate a number of phenolic and aliphatic compounds using *p*-nitrophenylsulfate as sulfate donor. We now could show that also sugars are accepted as substrates broadening the biocatalytic applicability of this enzyme. Sulfated sugars are required for the synthesis of sulfated oligo- and polysaccharides which are important for various medical applications.

Title: Steroid hydroxylation by CYP154C5
Researchers: M.P. Bracco Garcia
Using the bacterial cytochrome P450 monooxygenase CYP154C5, various steroids can be hydroxylated with exclusive formation of the 16□-hydroxylated products. In a protein and substrate engineering approach we now could show that the regioselectivity of CYP154C5 can be also altered giving, e.g., 15□-hydroxylated steroids. Furthermore, the crystal structure of that enzyme was solved in collaboration with Dr. Kurt Hoffmann from the Fraunhofer Institute IME in Aachen, Germany.

Other activities
A research project, financed by Pantarhei Bioscience, was started on the biocatalytic synthesis of an important steroidal API. Additionally, a collaboration with Dr. Hein Wijma and Prof. Dr. Dick Janssen (Groningen Biomolecular Sciences and Biotechnology Institute, Rijksuniversiteit Groningen) was established on the computational analysis of changes in CYP154C5’s regioselectivity in steroid hydroxylation upon mutagenesis of the enzyme active site.
Furthermore, a collaboration with Prof. Dr. Peter Schoenmakers (Analytical Chemistry, HIMS) was initialized regarding the development of analytical technology for lignin analyses and degradation products thereof. This collaboration is based on the COAST project proposal “MAnIAC”.

Key publications per academic staff member

- Schallmey, M., Koopmeiners, J., Wells, E., Wardenga, R., Schallmey, A. (2014) Expanding the halohydrin dehalogenase enzyme family: Identification of novel enzymes by database mining. Appl. Environ. Microbiol., 80, 7303–7315.
- Herzog, K., Bracco, P., Onoda, A., Hayashi, T., Hoffmann, K., Schallmey, A. (2014) Enzyme-substrate complex structures of CYP154C5 shed light on its mode of highly selective steroid hydroxylation. Acta Cryst., D70, 2875-2889.

- Picart, P., Müller, C., Mottweiler, J., Wiermans, L., Bolm, C., Dominguez de Maria, P., Schallmey, A. (2014) From gene towards selective biomass valorization: Novel bacterial beta-etherases with catalytic activity on lignin-like polymers, ChemSusChem, 7, 3164–3171.

Grants and prizes

CW-ECHO-STIP grant (NWO) on bacterial □-etherases for lignin degradation;
EID (European Industrial Doctorate) grant (EU funding) on Biocascades for aminoalcohol synthesis

Invited lectures

- Biocat, Hamburg, Germany, 31-8 until 04-09-2014
- Active Enzyme Molecule, Toyama, Japan, 17 until 19-12-2014

2.2 Computational Chemistry

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

Group	Biomolecular and Molecular Simulation		
Groupleaders	Prof.dr. P.G. Bolhuis Prof.dr. E.J. Meijer		
Academic staff	Prof.dr. R. Krishna (em.) Dr. D. Dubbeldam Dr. B. Ensing Dr. C.P. Lowe Dr. J. Vreede		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. A.J. Cruz Cabeza (VIDI) Dr. R. Ni (VENI) Dr. D. Sun Dr. D.W.H. Swenson Dr. T.A. Wassenaar	1-11-2011 1-9-2014 21-10-2013 1-1-2012 1-3-2014	22-2-2015 1-9-2017 21-10-2015 1-7-2015 1-8-2015
PhD students	Drs. Z.F. Brotzakis Drs. N.C. Burtch Drs. K. De Wispelaere Drs. G. Diaz Leines Drs. W. Du Drs. J. Heinen Drs. W. H. Homsi Brandeburgo Drs. M. Kilic Drs. A. Kumar Drs. J.A. Luiken Drs. A. Newton Drs. M. Nowosielski Drs. K. Singhal Drs. A. Torres Knoop Drs. A. Vijaykumar Drs. E. van Mastbergen	1-9-2012 1-6-2014 1-9-2013 1-5-2013 1-11-2013 1-9-2014 15-1-2011 1-3-2013 1-9-2010 1-10-2010 15-4-2012 15-4-2011 15-5-2010 1-3-2012 1-6-201316- 6-2014	1-9-2016 1-9-2014 1-3-2014 1-5-2014 20-6-2014 1-9-2018 15-7-2015 1-3-2014 1-5-2015 1-10-2015 15-4-2016 15-4-2015 15-5-2015 1-3-2016 1-6-2017 1-9-2015
MSc Students BSc Students	Eva van Mastbergen Mascha Gehre Jurn Heinen Samia Ouhajji Karin de Groot Margo van der Pijl Eva Bontje	1-1-2014 1-2-2014 1-11-2013 1-3-2014	15-6-2014 31-1-2014 1-7-2014 1-7-2014

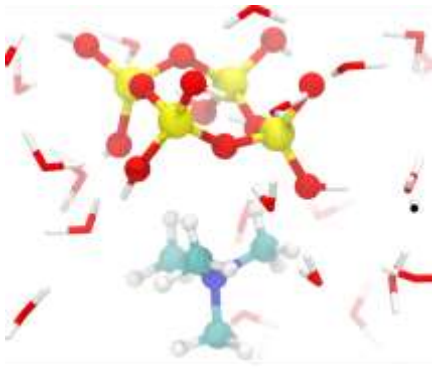
Mission of the group:

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

Research high lights per staff member

Prof.dr. Evert Jan Meijer

Proton transfer and mobility plays an important role in a large variety of (bio)chemical processes. Using ab initio molecular dynamics (AIMD) methodology we addressed the early stage of zeolite formation, that involves the oligomerization of silicate species in aqueous solution. The mechanism involves a proton-transfer mediated dehydration step. We addressed the effect of a structure directing counterion (TMA+) on the formation of small linear and ring structures. Our study provided evidence that the experimentally observed formation of D4R.8TMA crystals is controlled by the single 4-ring formation step.



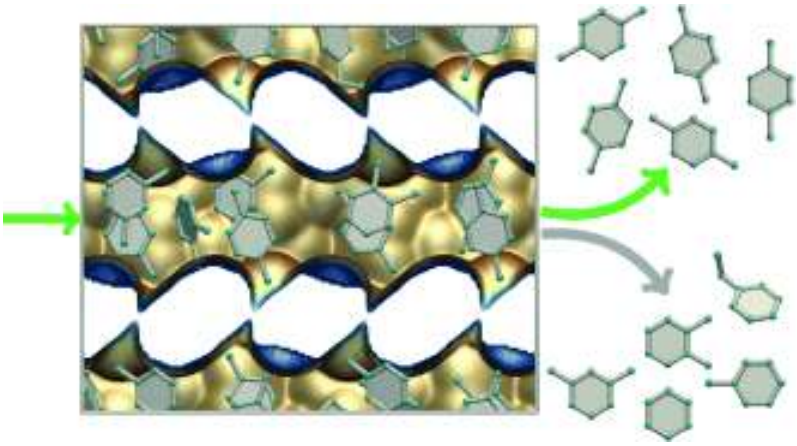
TMA. 4-ring silicate

Key publications

1. *The role of a structure directing agent tetramethylamonium template in the initial step of silicate oligomerization in aqueous solution*, Thuat T. Trinh, Khanh-Quang Tran, Xue-Qing Zhang, Rutger A. van Santen, Evert Jan Meijer Phys. Chem. Chem. Phys. (submitted).
2. *Exploring new frontiers in modeling complex zeolite-catalyzed reactions using advanced molecular dynamics techniques.* Kristof De Wispelaere, Bernd Ensing, An Ghysels, Evert Jan Meijer, Veronique Van Speybroeck, Chem.-Eur. J. (in press)

Dr. David Dubbeldam

The separation of xylene isomers is of great importance in the petrochemical industries. This separation can be achieved by selective adsorption in ordered crystalline nanoporous materials such as zeolites like Ba-X by exploiting subtle differences on molecular configurations. In Ref. (Torres-Knoop et al., Angewandte Chemie, 53, 7774,2014) we compared the performance of Ba-X with the predicted performance of many metal-organic frameworks (MOFs). A particularly promising structure was MAF-X8 that showed equivalent selectivity as Ba-X but, importantly, at a much higher pore loading. Higher adsorption capacities are desirable because they result in lower frequencies of the adsorption/desorption cycles and significant energy savings.

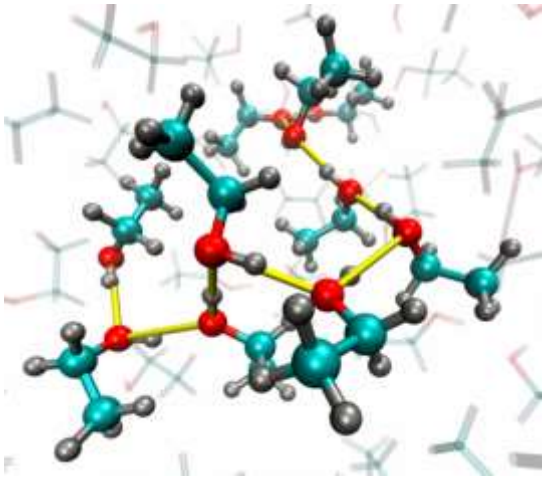


Key publications

1. R. Bueno-Perez, A. Martin-Calvo, P. Gomez-Alvarez, J.J. Gutierrez-Sevillano, P.J. Merkling, T.J.H. Vlugt, T. van Erp, D. Dubbeldam, and S. Calero. Enantioselective adsorption of ibuprofen and lysine in metal- organic frameworks. *Chem. Commun.*, 50:10849–10852, 2014.
2. Ariana Torres-Knoop, Rajamani Krishna, and David Dubbeldam. Separating xylene isomers by commensurate stacking of p-xylene within channels of MAF-X8. *Angew. Chem. Int. Ed.*, 53(30):7774–7778, 2014.
3. Ariana Torres-Knoop, Sayee Prasaad Balaji, Thijs Vlugt, and David Dubbeldam. A comparison of advanced Monte Carlo methods for open systems: CFCMC vs. CBMC. *J. Chem. Theory and Computat.*, 10(3):942–952, 2014.

Dr. Bernd Ensing

In school we learn that molecules in a liquid are randomly arranged. But is that completely correct? Based on computer simulations it has been thought for many years that the molecules in many liquids are locally ordered, especially if the molecules have a strong interaction with each other as is the case for water or alcohol. In a collaborative effort with the HIMS photonics group, we have shown that this idea is correct: in alcohol there is local orientational order. This means that nearby molecules are ordered at a fairly well-defined angle with respect to each other, although there is no long-distance ordering like in a crystal.



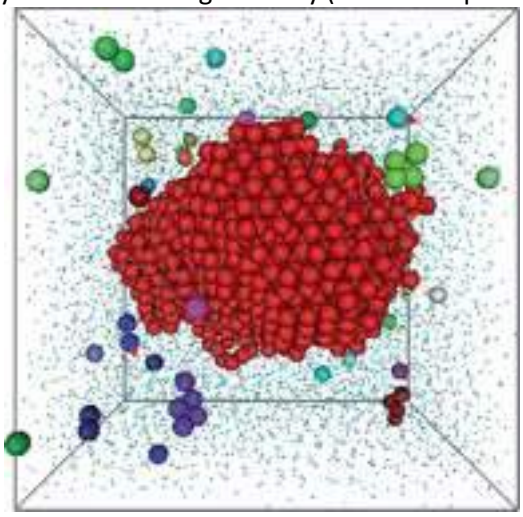
From: *Phys.org about our paper with the Woutersen group on the orientational order in liquids [Phys. Rev. Lett. 113, 207801 (2014)]. The Volkskrant (Dutch Newspaper) reported our findings on 15 November. Our work was also highlighted on the websites of FOM and HIMS (in Dutch).*

Key publications

1. Local orientational ordering in liquids revealed by resonant vibrational energy transfer.
   Matthijs R. Panman, Daniel J. Shaw, Bernd Ensing, and Sander Woutersen
   Phys. Rev. Lett. **113** (2014), 207801
2. Acidity constants of lumiflavin from first principles molecular dynamics simulations.
   Murat Kılıç and Bernd Ensing *Phys. Chem. Chem. Phys.* **16** (2014), 18993 - 19000
3. Interaction of H_2 with a double walled armchair nanotube by first principles calculations.
   Francesca Costanzo, Bernd Ensing, Roberto Scipioni, Francesco Ancilotto, and Pier Luigi Silvestrelli *J. Phys. Chem. C* **118** (2014), 15816 - 15824

Prof.dr. Peter Bolhuis

Crystallization and vitrification are two different routes to form a solid. Normally these two processes suppress each other, with the glass transition preventing crystallization at high density (or low temperature). This is even true for systems of colloidal hard spheres, which are commonly used as building blocks for novel functional materials with potential applications, e.g. photonic crystals. By performing Brownian dynamics simulations of glassy systems consisting of mixtures of active and passive hard spheres, we show that the crystallization of such hard-sphere glasses can be dramatically promoted by doping the system with small amounts of active particles. Surprisingly, even hard-sphere glasses of packing fraction up to $\varphi = 0.635$ crystallize, which is around 0.5% below the random close packing at φ 0.64. Our results suggest a novel way of fabricating crystalline materials from (colloidal) glasses. This is particularly important for materials that get easily kinetically trapped in glassy states, and the crystal nucleation hardly occurs.



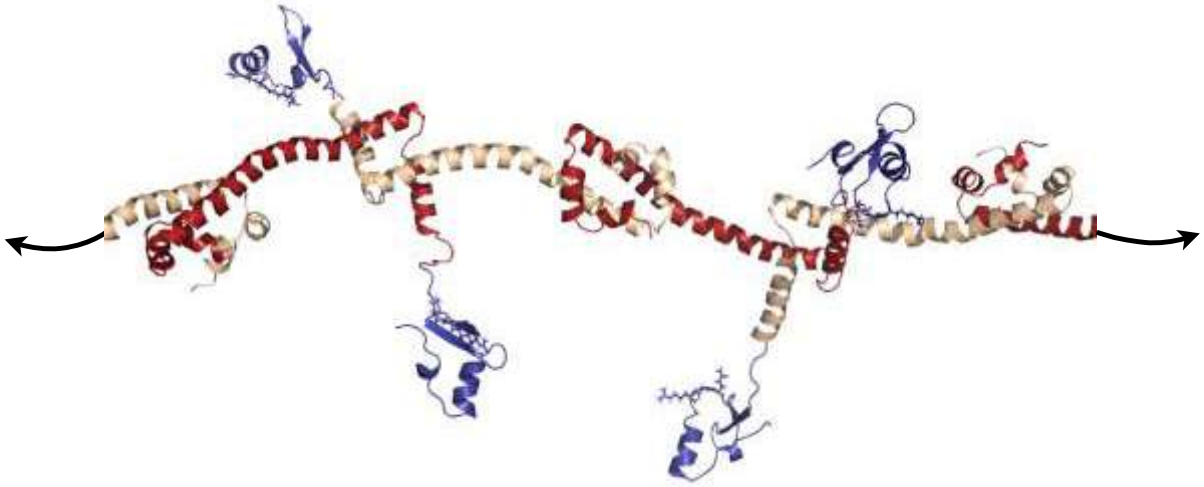
Key publications:

1. A replica exchange transition interface sampling method with multiple interface sets for investigating networks of rare events
   David W. H. Swenson and Peter G. Bolhuis, J. Chem. Phys. 141 044101 (2014)

2. Sampling the equilibrium kinetic network of Trp-cage in explicit solvent
   Weina Du and Peter G. Bolhuis, J. Chem. Phys. 140 195102 (2014)
3. Crystallizing hard-sphere glasses by doping with active particles
   Ran Ni, Martien Cohen Stuart, Marjolein Dijkstra, and Peter G. Bolhuis, Soft Matter 10 6609-6613 (2014)

Dr. Jocelyne Vreede

The DNA bridging protein H-NS (histone-like nucleoid structuring protein) forms filaments along strands of duplex DNA and plays an important role in regulating gene expression in enterobacteria. Using the currently available structural data we constructed a model of an H-NS filament as well as several structural models for H-NS homologues from different organisms. These models will facilitate a better understanding of the mechanisms underlying the function of H-NS [4].

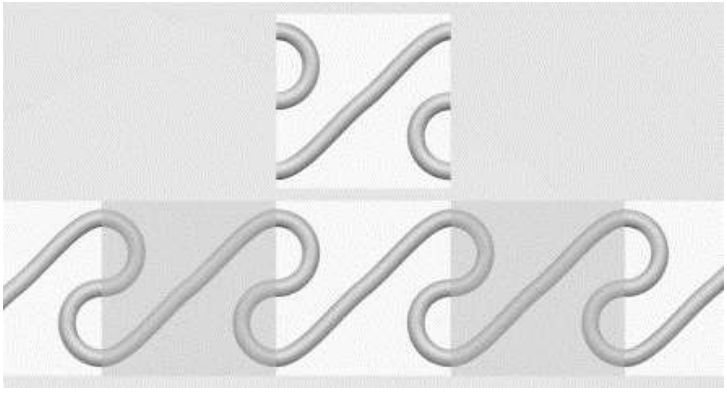


Key publications

1. *Multiscale approach to the determination of the photoactive yellow protein signaling state ensemble.* A Rohrdanz M, Zheng W, Lambeth B, Vreede J, Clementi C. PLoS Comput Biol. 2014;10:e1003797.
2. *Solvent-Exposed Salt Bridges Influence the Kinetics of α-Helix Folding and Unfolding.* Meuzelaar H, Tros M, Huerta-Viga A, van Dijk CN, Vreede J, Woutersen S. J Phys Chem Lett. 2014;5:900.
3. *Genomic looping: a key principle of chromatin organization.* van der Valk RA, Vreede J, Crémazy F, Dame RT. J Mol Microbiol Biotechnol. 2014;24:344

Dr. Christopher Lowe

The problem of detecting a percolating structure in an off-lattice model polymer system with periodic boundary conditions is hard. Physically, with increasing polymer density, the point at which percolation first occurs is the gel point. A connected structure spans all space and the system becomes solid-like. This problem is similar to that of finding connected paths in lattice bond percolation and site percolation models. Algorithms that detect these structures in finite systems will not always yield the correct answer for a system that is periodically repeated in space. Koopman [1] developed an algorithm that detects clusters that connect to themselves over an arbitrary number of periodic replicas. Because of the periodic replication this means that they are connected over all space. For system sizes that are typically tractable in simulations a relatively minor



proportion of configurations are misclassified for a lattice model. However, the fraction that is misclassified is significant for the polymer system. Misclassified configurations when included in the calculation of ensemble averages will include configurations with spurious physical properties, which are corrected by the novel algorithm.

Key publications

1. *An algorithm for detecting percolating structures in periodic systems - Application to polymer networks*
   E. A. Koopman, C.P. Lowe, J. Comp. Phys. 274, 758-769 (2014)

Other activities

- David Dubbeldam received his Basiskwalificatie Onderwijs on 7 April 2014
- Bernd Ensing organized the Graduate Winterschool on Theoretical Chemistry and Spectroscopy, December 8-12, Han-sur-Lesse, Belgium
- Jocelyne Vreede organized the ACMM symposium on Multiscale Modeling of Biomolecular Systems Friday 28 November 2014
- Peter Bolhuis became director of the Dutch CECAM node.
- Evert Jan Meijer, Bernd Ensing, David Dubbeldam organized the Graduate winterschool on Understanding Molecular Simulation, January 6-17, 2014; Amsterdam.

Dissertations

04-06-2014: Evert Koopman, Simple numerical techniques for mesoscale polymers, (co)promotors: Peter Bolhuis and Christopher Lowe
13-06-2014: Weina Du, Advanced path sampling of the kinetic network of small proteins, promotor:Peter Bolhuis
05-09-2014 Lizhe Zhu, Molecular simulations of receptor proteins, promotor Peter Bolhuis
01-10-2014 Murat Kılıç, Molecular Simulations in Electrochemistry: Electron and Proton Transfer Reactions Mediated by Flavins in Different Molecular Environments, (co)promotors Evert Jan Meijer and Bernd Ensing

Grants and prizes

Grants:
- NWO/FOM/Shell CSER (Computational sciences for energy research) grant on “Simulating charge transfer dynamics in complex environments” for 1 PhD student + equipment.
- NWO/FOM/Shell CSER (Computational sciences for energy research) grant on “Realistic Modeling of Catalytic Water Oxidation” for 1 PhD student + equipment.

Invited lectures

Evert Jan Meijer

1. Modeling of Chemical Reactions in Solution. February 7, 2014. Colloquium at ENS-Paris, Paris, France.
2. 51th Clay Minerals Society Annual Meeting. May 17-21, 2014. Texas A&M University, College Station, US.
3. ICTAC-15, June 30 - July 4, 2014. London, UK.
4. 5th Annual Global Congress of Catalysis, September 21-23, 2014. Qingdao, China.
5. Molecular Simulation of the Initial Stages of Silicate Growth, September 24, 2014. Colloquium at Nanjing University, Nanjing, China.
6. Ab Initio Modeling of Complex Chemical Processes, Beijing Computational Science Research Center, September 26, 2014. Beijing, China.
7. WATOC-2014, October 5-10, 2014, Santiago, Chile.

David Dubbeldam

1. Understanding zeolite catalysis of selective hydroisomerization and hydrocracking, 7 July 2014, Shell

Bernd Ensing

1. CECAM workshop “Long time dynamics from short time simulations”, March 12 – 14, 2014, Lugano, Switzerland
2. Conference on "Recent Advances in Modeling Rare Events: Methods and Applications" May 29 – June 1, 2014, Kerala, India.
3. Atomistic Scale Modelling of Materials”, CCMX Summer School, September 1–3, 2014, Lausanne, Switzerland
4. CECAM workshop “Advanced modeling to investigate biomolecules, November 20–21, 2014, Genova, Italy
5. Conference “Extended Molecular Dynamics and Enhanced Sampling: Nose Dynamics 30 Years”, November 10–11, 2014, at Keio University, Yokohama, Japan

Peter Bolhuis

1. Aggregation of peptides at multiple levels, 15 January 2014, ICMS, TuE, Eindhoven
2. CECAM workshop “Long time dynamics from short time simulations”, March 12 – 14, 2014, Lugano, Switzerland
3. Conference on "Recent Advances in Modeling Rare Events: Methods and Applications" May 29 – June 1, 2014, Kerala, India.
4. “Binding free energy and kinetics: computation meets experiments" workshop, June 10-12 2014, - Genoa - Italy
5. “Searching for Reaction Coordinates" workshop July 11-14, 2014, Telluride Colorado,
6. Scale Bridging Techniques in Molecular Simulation, workshop 25-27 August, Berlin
7. David Chandler 70th birthday symposium, 17-18 October 2014, MIT, Cambridge, Massachusetts
8. “Aggregation and Clustering of Molecules” workshop, 30-31 october Royal Danish Academy of Sciences Copenhagen, Denmark
9. “Bridging time and length scales in complex molecular systems “ physics colloquium, 11 December 2014, Rijksuniversiteit Groningen, Groningen

Jocelyne Vreede

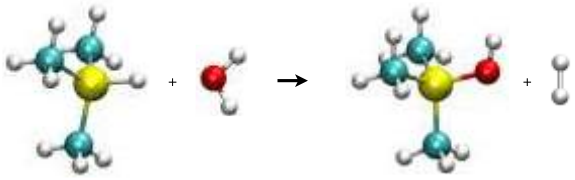
1. Lecture at Max Planck Institute for Colloids and Interfaces, Berlin
2. Biophysical Society meeting on Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery: Bridging Experiments and Computations, Istanbul

Outreach

- Kinderlezing door Bernd Ensing, UvA Open Dag, October 4, 2014, Amsterdam
- Wakker Worden Kinderlezing door Jocelyne Vreede, 16 maart 2014, NEMO Amsterdam
- Deelname Jocelyne Vreede aan Klokhuis Vragendag, 17 mei 2014, NEMO Amsterdam

Contribution to RPA Sustainable Chemistry

- Ensing has started a research line on unraveling and improving the water splitting reaction with silanes on silver and silver oxide nanoparticles in collaboration with the Dr. N. R. Shiju of the heterogeneous catalysis group.



- The group will coordinate a (RPA-SC funded, initially 1-year) postdoc project with a computational focus involving other HIMS groups.
- The research projects granted in 2014 by the FOM/SHELL CSER program will address topics in the field of energy research that have overlap with the focus of RPA-SC.

Group	Computational Polymer Chemistry & Science for Arts		
Groupleader	Prof.dr. P.D. Iedema		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. K. Keune Dr. A. van Loon Dr. I. Kryven	1-8-2012 1-8-2012 1-3-2015	1-8-2016 1-8-2016 31-12-2015
PhD students	Drs. J.J.Hermans Vacancy (Bergman)	1-2-2013	1-2-2017

Mission of the group:

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

Research high lights per staff member

Dr. Katrien Keune and Dr. Annelies van Loon

PAinT Project

In the first stage of the PAinT project, all paintings case studies have been carefully investigated in collaboration with the museum partners. Conservation questions have been addressed via analytical studies of paint samples and model systems. One prominent conservation issue that was targeted is metal-soap related degradation phenomena in oil paintings. Three examples of these defects in the case studies are: concentric rings in Couple with Clouds in their Heads by Dalí (1936, Boijmans van Beuningen, Rotterdam), raised paint and the tunnels inside the paint layers of the Evolution by Mondrian (c.1911, Gemeentemuseum the Hague), and a white haze on the surface of Rembrandt's Homer (1663, Mauritshuis, the Hague).

PAinT research has demonstrated that in the Couple, the zinc white pigment has reacted away due to acids derived from the oil as well as from the wooden frame. This has resulted in a thick transparent surface layer rich in zinc carboxylate salts.

The tunnels (areas where the paint has lifted off underlying layers in the form of long channels) in the Evolution manifested themselves in areas where the paint was also rich in zinc white. Our research demonstrated that the zinc white has formed zinc carboxylates (soaps), which have accumulated at the interface between paint layers, resulting in delamination and flaking of the paint.

Synchrotron-based FTIR, XRF, XANES and XRD studies (at Synchrotron Soleil, Paris) on paint samples from Rembrandt's Homer and related paint samples provided improved insight into the lead soap formation and associated migration and crystallization that caused a white haze on the painting's surface. Lead inside lower paint layers reacted with the oil binder and formed lead soaps. These were present as amorphous species inside the paint. The solubilized lead then travelled through the layered paint system and formed new complex salts on its surface, after reaction with atmospheric compounds.

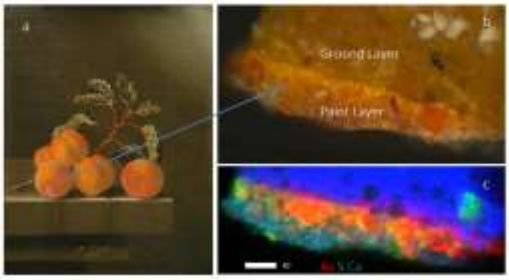


Figure 1: a) Adriaen Coorte, *Still Life with Five Apricots,* Mauritshuis; b) Paint cross-section from the region indicated, c) Composite elemental map– red = As, green = S, and blue = Ca (micro-XRF data, SSRL).

Similar synchrotron-based techniques (at ESRF, Grenoble and at SSRL, USA) were used to identify new degradation products of the red/orange pigment realgar (As4S4) in Still Life with Five Apricots, a painting by Coorte (1704, Mauritshuis). Realgar is known to photo-oxidize via various intermediate phases and via pararealgar into arsenic trioxide (As2O3). Our measurements showed that besides the presence of arsenic trioxide also calcium and iron-containing arsenates (As5+) were formed as degradation products. The presence of these degradation products throughout the whole multi-layered paint system, demonstrated that arsenic migrated through the system via water transport.

- Hermans, J.J., Keune, K., van Loon, A., Corkery, R.W., Iedema, P.D. (2014). The molecular structure of three types of long-chain zinc(II)alkanoates for the study of oil paint degradation. Polyhedron, 81, 335–340.
- Hermans, J. J., Keune, K., van Loon, A., Stols-Witlox, M. J. N., Corkery, R. W., & Iedema, P. D. (2014). The synthesis of new types of lead and zinc soaps: A source of information for the study of oil paint degradation. In J. Bridgland (Ed.), ICOM-CC 17th Triennial Conference Preprints, Melbourne, 15-19 September 2014 (p. art. 1603). Paris: International Council of Museums.
- Iedema, P.D., Hermans, J. J., Keune, K., van Loon, A., Stols-Witlox, M. J. N., P. D. (2014). Mathematical Modeling of Mature Oil Paints. In J. Bridgland (Ed.), ICOM-CC 17th Triennial Conference Preprints, Melbourne, 15-19 September 2014 (p. art. 1604). Paris: International Council of Museums.
- K.J. van den Berg, K. Keune, S. de Groot, H. van Keulen, I. D. van der Werf and A. Burnstock (2014). 'Analysis of binding media in Tudor paintings'. In J. Bridgland (Ed.), ICOM-CC 17th Triennial Conference Preprints, Melbourne, 15-19 September 2014. Paris: International Council of Museums.
- Petria Noble, Annelies van Loon, Geert van der Snickt, Koen Janssens, Matthias Alfeld, Joris Dik, 2014, 'The development of new imaging techniques for the study and interpretation of late Rembrandt paintings', in *Preprints ICOM Committee for Conservation 17th Triennial Meeting, Melbourne, 15-19 September 2014*.
- Keune, K. and Boéve-Jones, G. (2014), 'Its surreal: zinc-oxide degradation and misperceptions in Salvador Dalí's Couple with Clouds in their Heads, 1936', In: Issues in Contemporary Oil Paints (ICOP), Proceedings from the Symposium, 28 and 29 March 2013, Amersfoort, The Netherlands, eds. K.J. van den Berg, A. Burnstock, A. de Tagle, M. de Keijzer, G. Heydenreich, J. Krueger and T. Learner, Springer, p. 283-294.

Prof.dr. Piet Iedema

Chemical synthesis of metal soaps in the laboratory

The formation of zinc palmitate and zinc stearate in ZnO-containing oil paints is an important problem for painting conservators. Besides causing the loss of pigment, the zinc alkanoates ($Zn(Cn)_2$, Cn = $CH_3(CH_2)n-2COO-$) are known to cause increased transparency that alters the appearance of the painting and their growing aggregates often weaken the entire paint layer, causing craquelures and paint flaking. To improve our understanding of such degradation processes, we investigated the exact structure and likely compositions of zinc alkanoates formed in oil paint systems. It was found that in the presence of Na^+ and K^+ ions, mixed metal soaps form in linseed oil. The molecular structure of $ZnNa_2(Cn)_4$ and $ZnK_2(Cn)_4$ complexes was elucidated by using a newly developed method that combines FTIR spectroscopy and powder-XRD, and comparing crystal spacings of homologous series of zinc soap complexes with published single-crystal data.

This work provides a method for structural analysis of layered structures that do not form crystals suitable for single-crystal XRD, and highlights the potentially large variation in metal soap structures formed in oil paint systems.

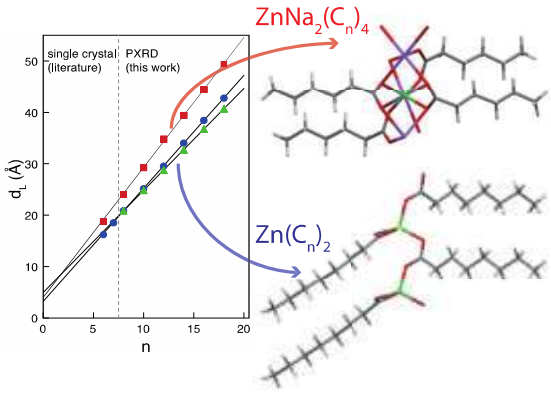


Figure 1. Structures of zinc alkanoates and crystal spacings versus alkane length from XRD.

- Yaghini, N., Iedema, P.D. (2014). Molecular Weight and Branching Distribution Modeling in Radical Polymerization with Transfer to Polymer and Scission Under Gel Conditions and Allowing for Multiradicals. Macromolecules, 47, 4851−4863
- Kryven, I., Iedema, P.D. (2014). Transition into the gel regime for crosslinking polymerization in a batch reactor. Polymer, 55, 3475-3489.
- Kryven, I., Iedema, P.D. (2014). Topology change by polymer modification. Macromol. Theory Simul., 23, 7-14.

Other activities

Katrien Keune Reviewer for:

- Journal 'Studies in Conservation',
- Project proposal for NU-ACCESS Center (Notherwestern University/ Art Institute of Chicago Center for Scientific Studies in the Arts

Dissertations

12-12-2014 Ivan Kryven, Topology evolution in macromolecular networks (Cum Laude), promotor Piet Iedema

Invited lectures

- Keune, K., '500 years of history in paint layer', TEDx Amstedam, 28 november 2014 (invited lecture)
- Keune, K., 'Paintings in the Laboratory in 2040?', Lunchmeeting Cultural Heritage Agency of The Netherlands, 4 november 2014 (invited lecture)
- Keune, K., 'Paintings in the Laboratory in 2040?', symposium 'Tribute to Karin Groen', Ateliergebouw, Amsterdam, 1 September 2014 (invited lecture)
- Keune, K. Studying the Mobility of Oil Paint Constituents in Paintings, Gordon Research Conference, "Scientific Methods in Cultural Heritage Research: Challenges and Complexity in Characterization and Conservation, July 27 - August 1, 2014, Sunday River Resort, Newry, ME (invited lecture)
- Keune, K. How to study a pigment that has disappeared?, UvA Alumni meeting in New York, 9 April 2014 (invited lecture)
- Keune, K. 'PAinT project: Studying Paint Alteration in Time', Science4Art meeting (NWO), 6 march 2014 (invited lecture)
- Keune, K., 'Synchrotron studies on degraded arsenic-containing pigments', Workshop TI-COAST students, 28 February 2014, Amsterdam (invited lecture).

Outreach

- The importance of previous analytical work on the mechanism of darkening of red vermilion pigment by Keune was stated in *Nature* by D. Castelvecchi dd. October 4, 2013.
- Research work on Vermillion behaviour in paintings by Dr. Keune has been used for examination 2014 of Dutch High school (VWO eindexamen). See pages 6-8 in http://www2.cito.nl/vo/ex2014/VW-1028-a-14-1-o.pdf.

Other:

- Member of the examination board of the UvA/Conservation and Restoration Program

2.3 Molecular Photonics

Groups:	Molecular Spectroscopy; Spectroscopy and Photonic materials; Time Resolved Vibrational Spectroscopy		
Group leaders:	Prof.dr. A.M. Brouwer [1],[2] Prof.dr. W.J. Buma[1]		
Academic staff:	Prof.dr. M.C.G. Aalders (BHGL) Prof.dr. H.J. Bakker (BHGL) Prof.dr. J. Oomens (BHGL) Dr. R.M. Williams[1] Prof.dr. S. Woutersen (BHGL) [1] Dr. H. Zhang[1]		
Support staff:	Drs. ing. M.F. Hilbers Ing. P.P. Reinders Drs. H.J. Sanders		
Temporary staff		Start date	(Foreseen) end date
Visiting scholars:	- -		
Postdocs:	Dr. M.R. Panman	01-04-2013	30-06-2014
PhD students:	H.C. Chen, MSc. Y. Ding, MSc. T.S. Kumpulainen, MSc. Drs. K. Liu E. Maltseva, MSc. Drs. H. Meuzelaar Drs. S.J. Roeters E.M.M. Tan, MSc. Drs. T.H. van der Loop M. Raeisolsadati Ouskoui B.M. Rocha Martins MSc. Drs. B.H. Strudwick Drs. F. Wu Y.Zhang MSc. D. Zheng MSc. T. Suhina (guest, IoP)	01-09-2011 01-02-2013 01-10-2010 15-03-2014 01-08-2012 01-10-2010 15-10-2011 01-04-2010 01-03-2010 01-11-2012 01-11-2014 01-08-2014 01-03-2014 01-11-2014 01-09-2014 01-09-2012	31-08-2015 01-03-2015 31-03-2015 31-12-2014 31-07-2016 30-09-2015 14-10-2016 31-03-2015 31-01-2015 30-09-2015 31-10-2018 31-01-2016 31-12-2014 31-10-2018 31-08-2018 01-09-2016
MSc + BSc students:	J. Bruijn J.B. Brummel D. den Uyl G. Torday C.M.P. Talavera Ormeno (guest) F. Veenstra (HBO) J.P Oudsen D. van Manen	25-02-2013 11-02-2014 01-09-2013 09-04-2013 01-09-2014 01-10-2014 18-08-2014 01-09-2014	25-02-2014 11-07-2014 01-06-2014 31-05-2014 31-01-2015 01-07-2015 24-02-2015 08-12-2014

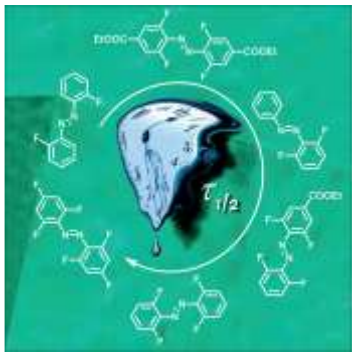
[1] These staff members participate in the RPA Sustainable Chemistry.

[2] Per July 2014 professor Brouwer is part time group leader Nanophotochemistry at the Advanced Research Center for Nanolithography (ARCNL).

Mission of the group

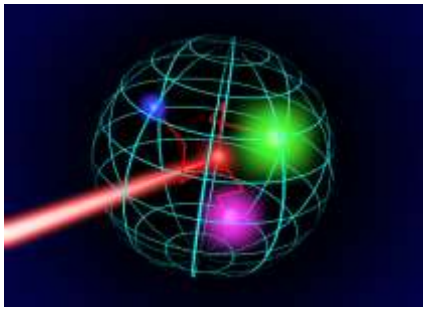
The Molecular Photonics group aims to advance the fundamental knowledge of the dynamics of excited states in molecules and nano-sized objects, and to contribute with its expertise to applications of the photosciences. Light-induced chemical conversions play a key role in many technological and biological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

Research high lights



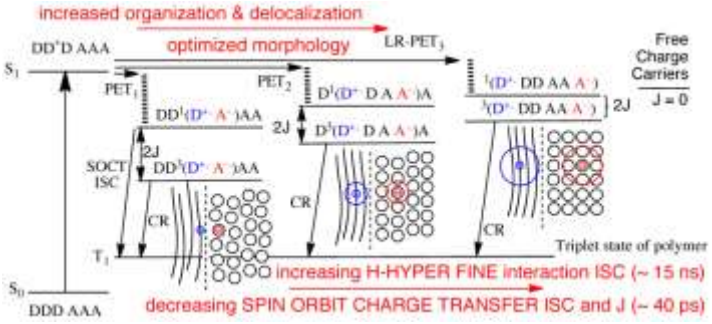
Azobenzene photoswitches The collaboration with the group of Stefan Hecht and David Bléger in Berlin led to a full paper in Chem. Eur. J., in which the recently discovered effects of fluorine substitution on the properties of azobenzene photoswitches were further explored. The unusual ability for an azobenzene to switch in both directions E-Z and Z-E with visible light was found to be a general property for a wider range of derivatives and was quantified in detail. The most remarkable finding is the exceptionally long thermal lifetime of the unstable Z-isomer of hexafluoroazobenzene, 95 hours at 60°C.

Vibrational circular dichroism Vibrational circular dichroism (VCD), the circular dichroism associated with vibrational transitions, has emerged as a powerful tool for absolute-structure determination, but its application still is severely impeded by small signal intensities and by spectral congestion. We have developed new methods to realize signal enhancements of more than two orders of magnitude by coupling the vibrational manifold with electronically excited states. We find that this enhancement factor is strongly dependent on the mode and on the distance between the oscillator and the chromophore providing the electronically excited states. We have shown that these properties can be used to design a local VCD amplifier that can be switched ON and OFF electrochemically. By subtracting the VCD spectra obtained when the amplifier is in the ON and OFF states, the VCD of the local environment of the amplifier can be separated from the total VCD spectrum. Switchable local VCD amplification thus makes it possible to avoid congestion and to "zoom in" on a specific part of a chiral molecule.



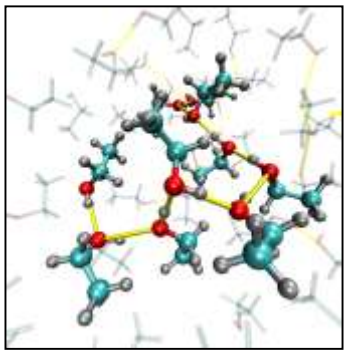
Biophotonic nanomaterials We have designed and optimized functional biophotonic nanomaterials, focusing on two sorts of novel nanomaterials. (1) *Luminescence upconversion nanomaterials*: besides optimization of FRET based upconversion nanoplatforms for diagnosis and therapy of cancers, we explore various excitation methods and/or nanohosts to get the upconversion efficiency higher than for current systems based on $NaYF_4$. (2) *Carbon based quantum dots*: we have studied experimentally and theoretically the origin of the luminescence and the mechanism of color tuning. We have demonstrated that this sort of material can form "luminescence nano-bombs" triggered by water and have demonstrated its application in water printing, anti-fake printing and forensics.

Organic photovoltaic materials A new model for triplet state formation by charge recombination, an important loss channel in organic photovoltaic materials is proposed. This model is based purely on information from previous literature and comes from the combination of studies on molecular electron donor-acceptor systems in solution, but has so-far not be connected to the solid state physics of organic photovoltaic materials. Nanoscale morphology not only influences interfacial area and conduction of holes and electrons, also the mechanism of Inter System Crossing (ISC) can be influenced. Next to the slower proton hyperfine interactions (H-HFI), also faster ISC in which the orbital angular momentum is changed during direct charge recombination from the singlet charge transfer state can be the mode of operation (SOCT-ISC). The nature of the charge transfer state (compact [with a large exchange integral, J] or resulting from long-range photoinduced electron transfer, LR-PET, with a small J), which is influenced by the nanoscale morphology, thereby dictates the ISC mechanism.



Spin Orbit Charge Transfer Inter System Crossing is faster in compact CT states with a large J (left). Optimized morphology enables long range electron transfer leading to CT states with a small J which inter system cross slower via proton hyper fine interactions (right).

Orientational order in liquids It is commonly believed that liquids are completely disordered, but simulations suggest that in some liquids local ordering occurs, in which the bonds of neighboring molecules are preferentially at a specific angle with respect to each other. This local orientational order is a hot topic in condensed-matter research (it is believed to be the main cause of the anomalous properties of water), but to date has been difficult to observe. We have developed an experimental method for directly observing orientational order in liquids, and have demonstrated the existence of this phenomenon in ethanol and N-methylacetamide. We could even determine the average nearest-neighbor angle, which was found to be very different in these two liquids. The theoretical analysis was done in close cooperation with the Computational Chemistry group, and has resulted in a joint publication in Physical Review Letters.



Key publications

1. Domingos, S.R.; Huerta-Viga, A.; Baij, L.; Dunnebier, D.; Finger, M.; Walters, A.J.C.; Nafie, L.W.; de Bruin, B.; Buma, W.J.; S. Woutersen, Amplified vibrational circular dichroism as a probe of local biomolecular structure. *J. Am. Chem. Soc.* **2014**, *136*, 3530-3535.
2. Domingos, S.R.; Sanders H.J.; Hartl, F.; Buma, W.J.; Woutersen, S., Switchable amplification of vibrational circular dichroism as a probe of local chiral structure. *Angew. Chem. Int. Ed.* **2014**, *53*, 14042-14045.
3. Gao, J.H.; Berden, G.; Oomens, J., Laboratory infrared spectroscopy of gaseous negatively chanrged polyaromatic hydrocarbons. *Astrophys. J.* **2014**, *787*, 170.
4. Knie, C.; Utecht, M.; Zhao, F.; Kulla, H.; Kovalenko, S.; Brouwer, A. M.; Saalfrank, P.; Hecht, S.; Bléger, D. Ortho-Fluoroazobenzenes: Visible Light Switches with Very Long-Lived Z Isomers. *Chem. Eur. J.* **2014**, *20*, 16492–16501.
5. Li, P.; Amirjalayer, S.; Hartl, F.; Lutz, M.; de Bruin, B.; Becker, R.; Woutersen, S.; Reek, J.N.H., Direct Probing of Photoinduced Electron Transfer in a Self-Assembled Biomimetic [2Fe2S]-Hydrogenase Complex Using Ultrafast Vibrational Spectroscopy. *Inorg. Chem.* **2014**, *53*, 5373-5383

6. Lou, Q.; Qu, S.; Jing, P.; Ji, W.; Li, D.; Cao, J.; Zhang, H.; Liu, L.; Zhao, J.; Shen, D. Water-triggered luminescent “nano-bombs” based on supra-(carbon nanodots) *Adv. Mater.* DOI: 10.1002/adma.201403635.
7. Meuzelaar, H.; Tros, M.; Huerta-Viga, A.; Van Dijk, C.N.; Vreede, J.; Woutersen, S. Solvent-Exposed Salt Bridges Influence the Kinetics of α-Helix Folding and Unfolding. *J. Phys. Chem. Lett.* **2014**, *5*, 900-904.
8. Morsa, D.; Gabelica, V.; Rosu, F.; Oomens, J.; De Pauw, E., Dissociation Pathways of Benzylpyridinium "Thermometer" Ions Depend on the Activation Regime: An IRMPD Spectroscopy Study. *J. Phys. Chem. Lett.* **2014**, *5*, 3787-3791.
9. Panman, M.R.; Shaw, D.J.; Ensing, B.; Woutersen, S., Local Orientational Order in Liquids Revealed by Resonant Vibrational Energy Transfer, *Phys. Rev. Lett.* **2014**, *113*, 207801.
10. Siekierzycka, J. R.; Hippius, C.; Würthner, F.; Williams, R. M.; Brouwer, A. M. A Multi-Property Fluorescent Probe for the Investigation of Polymer Dynamics Near the Glass Transition. *Cent. Eur. J. Chem.* **2014**, *12*, 937–952.
11. Tan, E.M.M.; Hilbers, M.; Buma, W.J., Excited-state dynamics of isolated and microsolvated cinnamate-based UV-B sunscreens”, *J. Phys. Chem. Lett.* **2014**, *5*, 2464-2468.
12. Tan, E.M.M.; Amirjalayer, S.; Mazzella, P.; Bakker, B.H.; van Maarseveen, J.H.; Bieraugel, H.; Buma, W.J., Molecular beam and ab initio studies of Photoactive Yellow Protein chromophores: the influence of the thioester functionality and single bond rotation. *J. Phys. Chem. B* **2014**, *118*, 12395-12403.
13. Tu, L.; Liu, X.; Wu, F.; Zhang, H. Excitation energy migration dynamics in upconversion nanomaterials. *Chem. Soc. Rev*. DOI:10.1039/c4cs00168k.
14. Vachon, J.; Carroll, G. T.; Pollard, M. M.; Mes, E. M.; Brouwer, A. M.; Feringa, B. L. An Ultrafast Surface-Bound Photo-Active Molecular Motor. *Photochem. Photobiol. Sci.* **2014**, *13*, 241–246.
15. Xia, L.; Kong, X.; L. Xiaomin, Tu, L.; Zhang, Y.; Chang, Y.; Liu, K.; Shen, D.; Zhao, H.; Zhang, H. An upconversion nanoparticle-zinc phthalocyanine based nano-photosensitizer for photodynamic therapy. *Biomaterials* **2014**, *35*, 4146-4156.

Other activities

Prof.dr. A.M. Brouwer

- Collaborations with J. Qian (Shanghai, China), T. Ogoshi (Kanazawa, Japan), J. Abe (Kanagawa, Japan), S. Bonnet (Leiden), T. Gacoin (Ecole Polytechnique, Palaiseau, F), D. Bonn (IoP, UvA).
- Member of the Review Group of the project “Application of Cooperative-Excitation into Innovative Molecular Systems with High-Order Photofunctions”, MEXT, Japan, 2014-2018.
- Member of the Permanent Steering Committee of the Biannual Conference on Methods and Applications of Fluorescence: Spectroscopy, Imaging & Probes (MAF:SIP)
- Member of IUPAC Sub-commission on Photochemistry
- Co-organizer of EPA/HRSMC Summer Schools on Photochemistry 1998, 2003, 2008, 2012
- Member of international organizing committee IUPAC Symposium on Photochemistry, Bordeaux, 2014.
- Chair IUPAC project Measurement of Photoluminescence Quantum Yields
- Member of the board of the Study Group Structure and Reactivity (Chemical Sciences, Netherlands Science Foundation)
- Member of board of Works Council of Faculty of Science, University of Amsterdam

Prof.dr. W.J. Buma

- Collaborations with R. Waters (API (UvA), SRON), T. Gregorkiewicz (IoP (UvA)), J. Oomens, J. Bakker, A.M. Rijs (all RU), L. Visscher, M. Bickelhaupt and K. Lammertsma (all VU), W. Brown (RUG), S. Amirjalayer (University of Münster), S. Meech (University of East Anglia), M. Pryce (University of Dublin), F. Zerbetto (University of Bologna).
- Scientific Director Graduate School “Holland Research School of Molecular Chemistry” (HRSMC).
- Programme manager “Analytical Chemistry and Spectroscopy” of LaserLab Amsterdam (partner of LaserLab Europe).
- Member Management team Institute QuantiVision (Innovative Medical Devices Initiative initiated by ZonMW).
- Member Senate of the University of Amsterdam.

- Member and secretary Board Stichting Bèta Plus.
- Chairman John van Geuns Fonds foundation.

Dr. R.M. Williams

- Collaborations with Prof. Pietrick Hudhomme (Angers, France) on fulleropyrrolidine-perylenemonoimide dyads, Dr. Stephanie Leroy-Lhez (Limoges, France) on photoactive porphyrines for medical applications, Prof. Joost Reek on water-oxidation (within biosolar fuels).
- Member of the Board of Examiners of the Forensic Science Master.
- Member of the FNWI library committee.
- Member of the Editorial Advisory Board of "The Open Inorganic Chemistry Journal".
- Member of the Editorial Advisory Board of "The Scientific World Journal".

Dr. H. Zhang

- Professor at Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences
- Chair Professor at Northeast Normal University
- Member of academic committee, Centre for Advanced Optoelectronic Functional Materials Research, Key Laboratory for UV Light-Emitting Materials and Technology of the Ministry of Education, Northeast Normal University
- Managing editor of Journal of Rare Earth
- Chair of advisory committee of the First International Symposium of Micro-Nanosystem Luminescence and Their Optoelectronic Properties (ISMLOP2014), July 24-25, 2014, Changchun, China
- Member of advisory committee of Luminescence Properties of Doped Nanomaterials of China, August 11-15, 2014, Harbin, China
- Close collaboration with LUMC (Prof. Löwik), AMC (Profs. Van Leeuwen and Aalders), University of Rome "Tor Vergata" (Profs. Casaboni and Prosposito), Chinese Academy of Sciences (Prof. H.J. Zhang).

Prof.dr. S. Woutersen

- Member of the scientific advisory board of the Max Planck Institute for Polymer Research (Mainz).
- Member of the organizing committee of the *European Conference on the Spectroscopy of Biological Molecules.*

Dissertations

- Sietse van der Post (07-02-2014), Love and fear of water: Water dynamics around charged and apolar solutes. Promotor: prof. dr. H.J. Bakker
- Adriana Huerta Viga (09-05-2014), Coupled Vibrations in Peptides and Proteins. Promotor prof. dr. Sander Woutersen
- Eric Tan (25-11-2014), Structural dynamics of isolated biological and synthetic photoswitches. Promotors prof. dr. Wybren Jan Buma, prof. dr. Jos Oomens
- Kai Liu (16-12-2014), Functionalized Upconversion Nanoparticles for Cancer Imaging and Therapy. Promotors prof. dr. Wybren Jan Buma, prof. dr. X.G. Kong

Grants and prizes

Prof.dr. A.M. Brouwer

- "*In touch with fluorescent probe molecules: microscopic visualization of contacts and friction*", NWO-CW ECHO grant together with D. Bonn (IoP, UvA) (260 kEuro)

Prof.dr. W.J. Buma

- "Solar energy conversion – breaking the 700 nm absorption barrier", Shell-NWO/FOM call Computational Sciences for Energy Research (CSER) together with K. Lammertsma (VU) and F.M. Bickelhaupt (VU) (280 kEuro).
- "Development of a Vibrational Optical Activity analysis toolbox", NWO-NCI TA program (together with L.Visscher (VU), SCM, and BioTools, (1147 kEuro)

Dr. R.M. Williams

- "Molecules Best Paper Award 2014": René M. Williams (and Pablo Contreras-Carballada, Marco Felici, Jan M.M. Smits, Roeland J.M. Nolte, Martin C. Feiters ,Luisa De Cola).

Dr. H. Zhang

- "The European Upconversion Network: From the Design of Photon-upconverting Nanomaterials to (Biomedical) Applications", European COST project CM1403.
- "Key problem in constructing upconversion nanophotosensitizers", Natural Science Foundation of China (1-1-2015 till 31-12-2018) (120 kEuro).
- "Energy transfer dynamics in upconversion nanomaterials and carbon dots", Innovation program of State Key Laboratory of Luminescence and Application of China (1-1-2014 till 1-1-2018) (1500 kEuro).

Prof.dr. S. Woutersen

- "Unraveling the mechanism of Fe-based photo-catalytic complexes for solar hydrogen production", LaserLab Europe proposal with G. Knor (Univ. of Linz).

Invited lectures

Prof.dr. A.M. Brouwer

- "*Fluorescent probes for contact*", 1st International Caparica Conference on Chromogenic and Emissive Materials, Caparica, Portugal, September 8-10, 2014.
- "*Looking into materials with fluorescence micro-spectroscopy*", Symposium in honor of Pierre Audebert, Cachan, France, October 20, 2014.
- "*Dynamics of rotaxane-based molecular shuttles*", Workshop "Optical manipulation of nano-objects: from light driven molecular motors to nanoscale optical tweezers", Saclay, France, December 15, 2014.

Prof.dr. W.J. Buma

- "*High-resolution molecular beam spectroscopy of PAHs in the 3 µm region: theory meets experiment … or not?*", 3rd bilateral meeting between The Dutch Astrochemistry Network (DAN) and NASA Ames Space Science and Astrobiology Division, May 27-29, 2014, Mountain View (CA), USA
- "*Vibronic Circular Dichroism*", Fourth International Conference on Vibrational Optical Activity (VOA-4), Hebei University, Baoding, China, October 26-29, 2014.

Dr. R.M. Williams

- "*Triplet states in organic photovoltaic materials*", Limoges, France, July 2, 2014.

Dr. H. Zhang

- Cardiac growth & regeneration - visualizing the future, June 22-26, 2014, Viterbo, Italy.
- First International Symposium of Micro-Nanosystem Luminescence and Their Optoelectronic Properties (ISMLOP2014), July 24-25, 2014, Changchun, China.
- Luminescence Properties of Doped Nanomaterials of China, August 11-15, 2014, Harbin, China.

Prof.dr. S. Woutersen

- *"New light on molecular machines, protein folding, and chirality",* seminar at the University of Glasgow, March 6, 2014.
- *"Real-time observation of photo-induced electron transfer in a ZnTPP·Fe2S2 supramolecular complex provides insight into its photocatalytic properties",* Int. Conf. Porph. Phtalocyan., Istanbul, June 22-27, 2014.
- *"Local orientational order and liquid-liquid transitions in H-bonded liquids",* Gordon Research Conference on Vibrational Spectroscopy, Biddeford (ME), August 3-8, 2014.

Outreach

Prof.dr. A.M. Brouwer

- Lectures Instrumental Analysis in National Chemistry Olympiad, UvA, June 2, 2014.

Prof.dr. S. Woutersen

- *"Zelf Moleculaire Machines maken",* SPUI25 colloquium together with Charles Hupperts, November 5, 2014.

Contribution to RPA Sustainable Chemistry

- Water splitting by NIR light employing upconversion nanoparticles.
- Collaboration with Reek group on photochemical water oxidation.
- Collaboration with Pryce and Long group at Dublin University (financed via LaserLab Amsterdam) on photocatalytic reduction of CO_2.
- Collaboration with Reek group on photochemical hydrogen generation.
- Collaboration with Knor group (University of Linz) on photochemical hydrogen generation (financed via LaserLab Amsterdam).

2.4 Analytical Chemistry

Group	Analytical Chemistry		
Group leader	Prof.dr.ir. P.J. Schoenmakers		
Academic staff	Prof.dr. G.L.Corthals (per 01-05-2014) Prof.dr.ir. J.G.M. Janssen (part-time professor) Prof.dr. A.C. van Asten (part-time professor) Prof.dr. S. van der Wal (em. part-time professor) Dr. W. Th. Kok Dr. G.I. Vivó Truyols Dr. M. Camenzuli (per 01-03-2014)		
Support staff	T. Aalbers P. Aarnoutse P.G.Verschuren		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. M. Camenzuli	1-3-2013	1-3-2014
	Dr. A.F.G. Gargano	1-9-2013	1-2-2016
	Dr. S. Pous Torres	1-4-2013	1-4-2014
PhD students	L.D.J. Bos	1-3-2012	1-11-2014
	G.M.H. Brust, MSc	1-11-2013	1-7-2014
	H. Cornelisson van de Ven, MSc	1-10-2012	1-10-2016
	E. Davydova, MSc	1-6-2011	1-10-2015
	J. Králová, MSc	1-8-2011	1-8-2015
	M. Marioli, MSc	1-8-2011	1-8-2015
	A.D. Ngoc, MSc	1-6-2014	1-10-2014
	A.A.S. Sampat, MSc	1-2-2012	1-2-2016
	R.J. Vonk, MSc	1-4-2011	1-4-2015
	M. Woldegebriel, MSc	1-4-2013	1-4-2017
	M.Pacheco Bothelho Mourao, MSc	1-9-2013	1-7-2016
	A.A. Baglai	1-10-2012	1-10-2016
	A. Barcaru	1-4-2013	1-4-2017

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

Research highlights per staff member

Prof.dr. Arian van Asten
The forensic-science activities within HIMS are coordinated by Arian van Asten through the Co van Ledden Hulsebosch Center (CLHC), the Amsterdam Center for Forensic Science and Medicine. This centre was formally opened in 2013 and it continued to flourish in 2014. A detailed description of the activities can be found in the Annual Report of the CLHC.
An important highlight for HIMS was the promotion of Hanneke Brust on a thesis entitled *Chemical profiling of explosives*. This was the first promotion to result from the intensive collaboration between HIMS and the NFI. One peer-reviewed paper on this work was published in 2014, while several other papers were submitted for publication in 2015.

- H. Brust, A. van Asten, M. Koeberg, J. Dalmolen, A. van der Heijden and P.J. Schoenmakers,
- Accurate quantitation of pentaerythritol tetranitrate and its degradation products using liquid chromatography-atmospheric pressure chemical ionization-mass spectrometry *J.Chromatogr.A* **1338** (2014) 111-116.

Dr. Michelle Camenzuli

The year 2014 was the first (partial) year of Michelle Camenzuli's tenure-track position. As such, the focus was on laying the foundations for future research. Key highlights include the development on a new metric for orthogonality in multidimensional chromatography. This work was published in Analytical Chimica Acta; a peer-review journal with an impact factor of 4.517. Camenzuli also gave a lecture on this new metric at the HPLC2015 conference in New Orleans. This conference is regarded as the most prestigious conference series in the field of separation science. In addition she hosted a one-day workshop on the optimization of two-dimensional liquid chromatography for an audience from academia and industry which was well received. She was invited to contribute a review on her research in active flow technology for the LCGC Europe magazine, which was given the front cover of the February 2015 issue. Camenzuli also complete a three-month secondment at DSM Resolve in Geleen where she focused on investigating the instrumental mass spectrometry parameters affecting ionisation of polyacrylamides in electrospray. This secondment increased her experience and knowledge of mass spectrometry, which is a crucial asset for her future work with Prof. Corthals.

- M. Camenzuli and P.J. Schoenmakers, A new measure of orthogonality for multi-dimensional chromatography, *Anal.Chim.Acta* **838** (2014) 93-101.

Prof.dr. Garry Corthals

Still within the first year at the UvA Corthals is building his lab and scientific network in the Netherlands. As no pre-existing lab or people existed for this Chair most activity has been on organising and building the laboratory, research group and the overall scientific infrastructure. The emphasis of the group in Amsterdam will be development and application of technological and analytical methods in life sciences that on MS and proteome-based molecular analyses. The focus of the group is listed in the UvA webpage and extends to many fields from health and disease, to forensics and in biotechnology and agriculture research. Additionally the group now supports and is starting activities in art conservation science. In December the lab concluded the installation of a state-of-the-art mass spectrometer to conduct measurements of proteins and proteomes and the started the process of hiring new postdoctoral personnel. Overall the group has published 6 articles in 2014 with an IF's >5, and additional 6 are in review. Corthals has stepped down as head of the EuPA New Developments committee, and serves in its committee, and is now head of HUPO Education and Training. In 2014 Corthals organised two large international conferences in March on Quantitative Proteomics (Turku, Finland) and in October on Imaging MS (Turkey, Antalya), a Summer School in Mass Spectrometry in Biotechnology and Medicine (Dubrovnik, Croatia) and a COST Workshop in Imaging MS and Tissue Analysis (Turku, Finland). He was an opponent of 1 PhD student (Helsinki, Finland) and invited speaker at more than 10 conferences.

- Kannaste, O., Suomi, T., Salmi, J., Uusipaikka, E., Nevalainen, O., Corthals, G.L., Cross-correlation of spectral count ranking to validate quantitative proteome measurements, *J. Proteome Res.* **13** (2014) 1957-1968.
- Vehmas, A.P., Muth-Pawlak, D., Huhtinen, K., Saloniemi-Heinonen, T., Jaakkola, K., Laajala, T.D., Kaprio, H., Suvitie, P.A., Aittokallio, T., Siitari, H., Perheentupa, A., Poutanen, M., Corthals, G.L., Ovarian endometriosis signatures established through discovery and directed mass spectrometry analysis, *J. Proteome Res.* **13** (2014) 4983-4994.
- McDonnell, L.A., Walch, A., Stoeckli, M., Corthals, G.L., MSiMass list: A public database of identifications for protein MALDI MS imaging, *J. Proteome Res.* **13** (2014) 1138-1142.

Prof.dr. Hans-Gerd (J.G.M.) Janssen

Mid 2014 Prof. Janssen's second 5-year term as extra-ordinary professor Biomacromolecular Separations ended. All parties involved (Unilever, UvA and Prof. Janssen) were positive on the results achieved in research and education in the past two periods and agreed that continuation would again be to the benefit of all involved [continuation was effected in 2015]. A key highlight of the work in 2014 was the development and application of a new model for diagnosis of tuberculosis based on the presence or absence of 20 easily measurable, low-molecular-weight markers in sputum. This opens new ways for small, bed-side equipment for disease detection. Instrumentation was being developed in a partnership with ATAS GL and Q-Micro. This work was largely done by Dr. Ngoc A Dang who successfully defended her PhD thesis in October 2014.

In addition to the PhD students working at the UvA Prof. Janssen also supervises two industrial PhD students at Unilever Shanghai, China. Janssen presented lectures at many national and international meetings, including the Symposium on Hyphenated Techniques in Chromatography (Bruges, Belgium), the prestigious Symposium on Capillary Chromatography (Riva del Garda, Italy), the Nordics meeting on Comprehensive Chromatography (Copenhagen, Denmark) and the Supercritical-Fluid Chromatography users day of Waters Instruments (Basel, Switzerland). He published 8 papers, some in influential analytical journals (Anal. Bioanal. Chem, J. Chromatogr. A) other ones in high-distribution (peer-reviewed) journals as LC-GC Europe and LC-GC North America.

- D. Peroni and H.-G. Janssen, Comprehensive two-dimensional gas chromatography under high outlet pressure conditions: a new approach to correct the flow-mismatch issue in the two dimensions, J. Chromatogr. A., Journal of Chromatography A, 1332 (2014) 57–63.
- L. D. J. Bos, I. Martin-Loeches, J. B. Kastelijn, G. Gili, M. Espasa, P. Povoa, A. H. J. Kolk, H.-G. Janssen, P. J. Sterk, A. Artigas, M. J. Schultz, The volatile metabolic fingerprint of ventilator associated pneumonia, Intensive Care Med, DOI 10.1007/s00134-014-3260-5
- H.-G. Janssen, Advances in Food Analysis, LCGC North America, Volume 32, number S5, May 2014, page 8, also published in LCGC Europe, September 2014.

prof.dr. Peter Schoenmakers

Emphasis in 2014 was on the HYPERformance LC project, which is a large consortium of eight industrial partners and two universities (UvA and RU Groningen). PhD students and postdocs spent time in industry ("secondments"). Anna Baglai investigated possible benefits of modulated LC-MS (so-called "one-and-a-half-dimensional LC") for food-science applications together with RIKILT (Wageningen, Dr. Hans Mol). Henrik Cornelisson van de Ven wrote a patent application on a smart way to focus analytes and change solvents after a (first-dimension) HPLC separation.

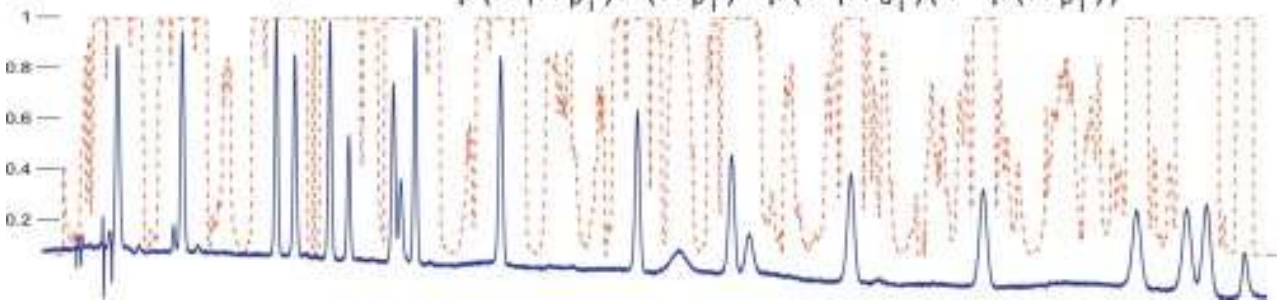
Peter Schoenmakers and Petra Aarnoutse published a feature (cover-page) article in Analytical Chemistry on multi-dimensional separations of polymers. The cover picture was taken by Petra Aarnoutse in SP Amsterdam.

- Chojnacka, J.G.M. Janssen and P.J. Schoenmakers, Detailed study of polystyrene solubility using pyrolysis-gas chromatography-mass spectrometry and combination with size-exclusion chromatography, *Anal.Bioanal.Chem.* **406** (2014) 459-465.
- P.J. Schoenmakers and P.J. Aarnoutse, Multi-dimensional separations of polymers, *Anal.Chem.* **86** (2014) 6172-6179.
- R.J. Vonk, A. Vaast, S. Eeltink and P.J. Schoenmakers, Titanium-scaffolded organic-monolithic stationary phases for ultra-high-pressure liquid chromatography, *J.Chromatogr.A* **1359** (2014) 162-169.

Dr. Gabriel Vivó Truyols

The 3 PhDs under Gabriel's supervision have been progressing. Martin Lopatka finished his work package on probabilistic peak detection, and the paper was published. Martin presented his work at an oral presentation at the prestigious CAC symposium Richmond (Virgina, US). Additionally, Martin did an internship at the laboratory of prof. Sigman at University of Central Florida, in the area of classification of flame accelerants. The idea of the collaboration of Martin in Sigman's group was to introduce the Total Ion Spectra (opposed to the Total Ion Chromatogram) concept for the classification of flame accelerants. This collaboration resulted in an additional paper . On the other hand, Andrei Barcaru finished his work package on retention time prediction in GCxGC, and published it in Journal of chromatography A. Andrei presented his work at the GCxGC symposium in Riva del Garda (Italy). On the other hand, Andrei performed an internship at DSM, and advanced in his idea on Bayesian peak tracking on GCxGC. The paper is currently drafted and it is in correction phase. Michael Woldegebriel did an intership at the Nederlands Forensic Instituut, on developing a method for toxicology screening using Bayesian statistics

$$P(H_{p_i}|D) = \frac{p(D|H_{p_i})P(H_{p_i})}{p(D|H_{p_i})P(H_{p_i}) + p(D|H_{d_i})(1-p(H_{p_i}))}$$



Map of the probabilistic peak detection method in chromatography, later used for studies at the NFI.

Michael presented his work at the ISC symposium in Salzburg (Austria). On the other hand, he has been conducting one MSc project (R. Smits, together with Océ), and collaborated with others (J. Kostkamp, also at Océ). Also, he conducted a BSc thesis (B. Schoenmakers, together with Panalytical).

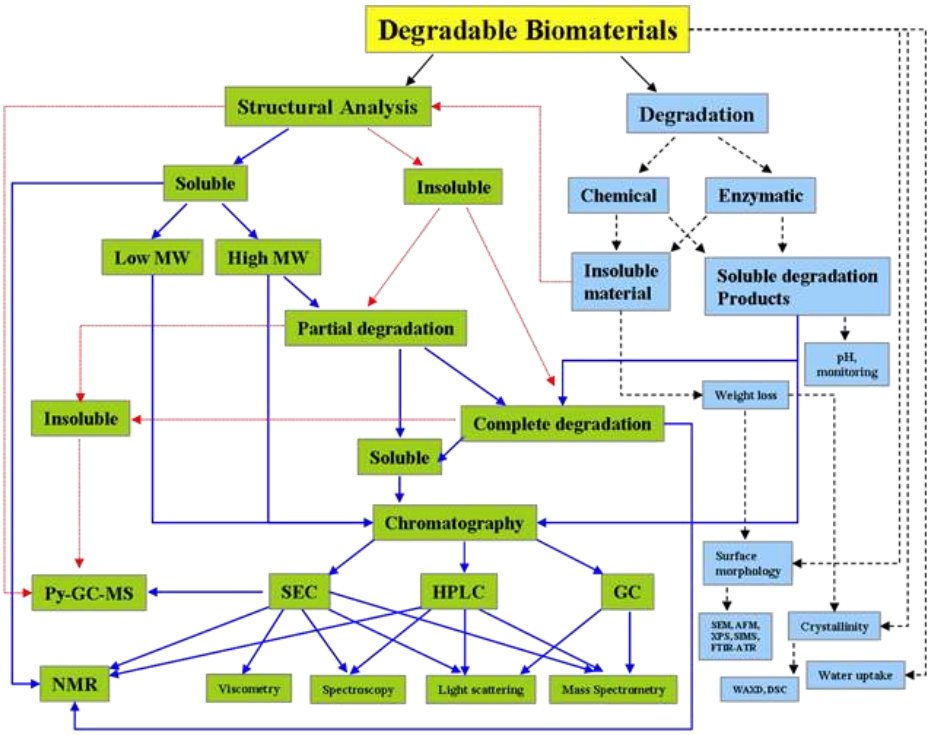
Gabriel has been invited to several symposiums in 2014. He was lecturing and giving a course at the symposium in Riva del Garda (Italy), as well at the GPC symposium (Frankfurt, Germany) and at the workshop in Metabolomics (Barcelona, Spain). This has given strength in his potential to raise money from industry.

- M. Lopatka, G. Vivó-Truyols, M. Sjerps, "Probabilistic peak detection for first-order chromatographic data", Anal. Chim. Acta, 817 (2014) 9-16.
- Barcaru, A. Anroedh-Sampat, H.-G. Janssen, G. Vivó-Truyols, "Retention time prediction in temperature-programmed, comprehensive two-dimensional gas chromatography: Modelling and error assessment", J. Chromatogr. A, 1368 (2014) 190-198.

Prof.dr. Sjoerd van der Wal

Together with former PhD student Abdul Ghaffar Sjoerd van der Wal published a key review on the analysis of synthetic-polymer biomaterials, which is summarizing many of the learnings from his two periods as part-time professor at the University of Amsterdam and putting these in a global perspective.

- Ghaffar, P.J. Schoenmakers and Sj. van der Wal, Methods for the Chemical Analysis of Degradable Synthetic Polymeric Biomaterials, *Crit.Rev.Anal.Chem.* **44** (2014) 23-40.



Other activities

The collaboration with the mass-spectrometry group of Chris de Koster (SILS) was very successful, culminating in two papers submitted together with Dr. Leo de Koning for publication in 2015. Both papers concern two-dimensional LC separations of protein digests prior to characterization by Fourier-transform ion-cyclotron-resonance MS.

Dissertations

25-06-2014: Hanneke Brust, Chemical profiling of explosives, promotors Peter Schoenmakers and Arian van Asten

22-10-2014 Ngoc A Dang, Towards a new approach for fast diagnosis of tuberculosis using gas chromatography-mass spectrometry, promotors Hans-Gerd Janssen and Peter Schoenmakers

Invited lectures

- Hyphenated Techniques in Chromatography (Bruges, Belgium, Jan 31 – Feb 1, 2014), Hans-Gerd Janssen, Peter Schoenmakers.
- HPLC2014 New Orleans, (New Orleans, LA, USA, May 11-15, 2014), Peter Schoenmakers.
- Symposium on Capillary Chromatography (Riva del Garda, Italy, May 20-23, 2014), Hans-Gerd Janssen, Peter Schoenmakers.
- Annual meeting of the Brazilian Chemical Society (Natal, Brazil, May 26-29, 2014), Peter Schoenmakers.
- International Symposium on Chromatography (Salzburg, Austria, Sep 14-18, 2014), Peter Schoenmakers.
- Nordics meeting on Comprehensive Chromatography (Copenhagen, Denmark, Nov 14, 2014) , Hans-Gerd Janssen, Peter Schoenmakers.

Patents and utilization

- Patent application prepared by H.C. van de Ven (submitted for comments to HYPERformance LC project and to NWO).
- *REMI: reflectron modulation interface for modulation in two-dimensional chromatography*

Outreach

Outreach activities are mainly conducted through the about 70 honours students that are enrolled in the COAST programs directed by Peter Schoenmakers.

3. Evaluation

After the mid-term evaluation in 2013, there was only a light assessment by the Scientific Advisory Board (WAR) of HIMS in 2014. Based upon a presentations on the follow-up of the 2013 WAR-report and a discussion with the members of the HIMS management team the WAR gave a general advice to HIMS and specifically addressed the research within the four research themes: Sustainable Chemistry, Analytical Chemistry, Molecular Photonics and Computational Chemistry. Quotes of the general conclusions of the WAR-report are given below.

The research at HIMS continues to be of high scientific quality with a large number of high impact publications. Since the midterm evaluation a number of changes have occurred: the merger with the VU (Free University of Amsterdam) will not proceed as was earlier envisaged. Still, a concentration of sustainability related chemistry research ('green') around the present location of HIMS (Science Park) and bio-chemical/medical research related to health ('red') at the 'Zuid-As' close to the VU Medical center remains a valid strategy. The concentration will give opportunities to strengthen the HIMS research, especially in the areas of Computational/Theoretical chemistry and Molecular Photonics. The proposed Virtual Interfaculty Department may not be an efficient solution as a transition towards a potential future merger with the VU. Embedding of the chair of Organic Chemistry at the VU within the Sustainability research was proposed in the midterm evaluation. Meanwhile it has become clear that this as such cannot be realized. However, it remains important to strive for incorporating of the relevant unique expertise of the VU group within the Sustainable Chemistry related research in Science Park.

In addition to a positive overall evaluation there were several more general concerns and recommendations for the Institute that will be briefly indicated below, together with the actions taken since the midterm evaluation.

There are substantial delays in the graduation of PhD students. Action has been taken to increase the awareness and commitment among staff members about the importance of finishing in time. A premium of 2000 € for finishing in time (manuscript ready within 48 mo) has been instituted. An extension of an appointment is now allowed only for valid reasons. The WAR appreciates the actions taken. It seems to be sufficient for now but the effects should be monitored closely in the coming years.

A number of positions created within the 'Sectorplan' Chemistry and Physics (SNS) were still not filled in October 2013. A sense of urgency was expressed by the WAR. In the past year, the positions have been filled and also two other tenure trackers have started. This is a positive development. Unfortunately, the Biocatalysis position is vacant again due to the choice of the newly appointed professor to move to Braunschweig, largely due to personal reasons. It is important to reconsider the profile of the Biocatalysis position and if a Biocatalysis group is necessary or if this can be addressed through collaborations with leading groups at other universities. A good embedding of the SNS position within HIMS requires a profile with strong connections to other groups within Sustainable Chemistry.

A shift of the Science for Art activity from the Computational Chemistry group to Analytical Chemistry was advised. The embedding has changed and Science for Art has now strong connections with all four groups. The opportunities for funding within this theme have been addressed, but a final decision depends on developments at NWO.

The entrepreneurship activity was found to be limited and a stronger effort was advised to stimulate students, post-docs and staff to be involved in start-up/spin-off companies and focus more on valorization of research results. A number of measures have been taken: PhD students and post-docs participate in a Bootcamp business plan, SUSCHEM has a budget for spin-off activities (funding for several post-doc years), organization of the HIMS industry day, participation in the Innovation Labs and support for entrepreneurial staff members. Also instituting a SusChem Industrial Advisory board is a worthwhile initiative. The proposed names are often the 'usual suspects' and it may be wise to think out-of-the-box in the selection of some new members for this board. The cooperation with ASML in ARCNL will add to a stronger valorization profile. The WAR appreciates the swift action and expects to see positive results in the coming years.

The research topics of the different groups within HIMS vary but do allow for a better coherence than in the past. In the new setting (joint housing in the Science Park) a stronger interaction should be promoted. Also here, appropriate action has been taken in the form of staff lunches, joint research proposals and the common 'Zwaartepunt' Sustainable Chemistry in which all four groups participate. There is an increasing number of joint publications and this should be considered as an important measure for the success of (continued) cooperation within HIMS.
The full cost model for externally and internally funded research projects makes it considerably more expensive to employ PhD students than Post-Docs. It was indicated during the midterm review that this makes it unattractive to appoint PhD students which interferes with an important task of the university as an educational institute for young researchers. There are no options to change the full cost model. In spite of undesired side effects, there is within the WAR also appreciation for the full cost model as it allows for a fair distribution of infrastructural costs involved in research.

In general, the WAR is very positive about the adequate response of HIMS to the recommendations in the midterm evaluation. Specifically, the research director and managing director, both recently appointed, have clearly taken the recommendations to heart and taken appropriate actions that seem to find support within HIMS. It is important that the effects are closely monitored and where necessary result in changing the strategy.

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

4. Valorisation

HIMS researchers explore a range from pure basic scientific inspired quests to application inspired fundamental research projects. Out of the fourteen granted research proposals (see section 1.4.4) eight projects were inspired by future utilisation of the project and five projects have already companies participating and co-financing them. On top of that two new contract research projects were started for companies.

In 2014 three new patent applications were prepared, in collaboration with research consortia or companies. it is expected that these applications will be filed in 2015. In case results of HIMS research may have future commercial value, HIMS follows an active approach to find industrial partners to collaborate with. The Technology Transfer Office supports HIMS scientists with contracts, IP affairs and advises on funding (grants). Where appropriate HIMS protects its intellectual property. Usually industrial partners, that are the potential users of the knowledge, will be involved in an early stage. Therefor the institute often does not always apply for patents itself.

Plantics BV is a new spin-off company of HIMS that was erected in 2014. Its mission is to develop and market new plant-based bioplastics invented at HIMS by prof.dr. Gadi Rothenberg and dr. Albert Alberts. The company's managing director is Helias Andriessen.

On 31 October, HIMS organised its (first) annual Industry Day. Over 30 companies (from Amsterdam SMEs to multinationals) were introduced into the research themes of the UvA chemistry research institute. The Industry Day started with a talent lunch where PhD students and postdocs were informed about careers in industry. After a guest lecture on designing a chemical plant on planet Mars, it was time for the HIMS staff to present its expertise. First plenary, in lectures, and after that during lab tours and a poster session combined with a dinner buffet. Representatives of the Netherlands Organisation for Scientific Research NWO were also present to elaborate on the NWO funding instruments for public-private cooperation.

The collaboration with the Innovation Lab Chemistry Amsterdam (ILCA) was intensified in 2014. Several companies housing in the Matrix buildings at the Science Park Amsterdam visit HIMS on a regularly base to collect NMR spectra or perform other measurements.

5. Organisation and finances

With the appointment of the new institute director prof.dr. Joost Reek at the end of 2013 the management structure of HIMS was changed. In this new system the director is both scientific director of the institute and active scientific group leader. The position of institute manager was introduced per 2014, to take care of the more hand-on management tasks. Per 1 January 2014 drs. Marcel Bartels was appointed on this position.

The Policy Advise Committee (Beleidsadviesraad, BAR) containing all professorsof the institute was replaced by a management team that advices the director. The leaders of the four HIMS themes and education are represented in management team. Per 31 December 2014 the management team consists of:

Prof.dr. Joost Reek (chair)
Drs. Marcel Bartels (secretary)
Prof.dr. Peter Bolhuis (Computational Chemistry)
Prof.dr. Wybren Jan Buma (Molecular Photonics)
Prof.dr. Gadi Rothenberg (Sustainable Chemistry)
Prof.dr. Peter Schoenmakers (Analytical Chemistry)
Dr. Sape Kinderman (education)
Gerda Zonneveld (minutes)

The institute management is greatly supported by a business office (bedrijfsbureau). Ultimo 2013 the support organisation of HIMS was staffed as follows:

Operations management (bedrijfsvoering):	Gerda Zonneveld - de Boer
	Drs. Hilde Zwaan - van der Plas (HRSMC)
Supporting team:	Petra Hagen
	Renate Hippert
	Maureen Sabandar - Mumu
	Ineke Weijer (HRSMC)
Special tasks:	Erik Duin-Berteling BA (Safety)
	Paul Collignon (ICT)

In 2014 the HIMS PhD Council was founded to act as a bridge between students, PhD's and the scientific staff. The council consists of four PhD students that represent the four main research themes within the institute and one of the members is also part of the Faculty PhD Council. The council aims to improve the interaction within and between research groups of HIMS and to help in personal PhD tracks.

Members (from left to right on the picture):
Tomislav Suhina (Molecular Photonics)
Marta Pacheco Botelho Mourao (Analytical Chemistry)
Vincent Vreeken (Sustainable Chemistry)
Arthur Newton (Computational Chemistry)

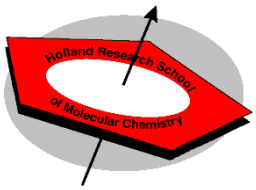
The council has undertaken the following activities in 2014:

- Contribution to the HIMS PhD-brochure
- Feedback at several MT meetings on the subject of courses, evaluations and the PhD track
- Representing the HIMS PhDs at the SILS/HIMS/VUA virtual department meetings
- Organisation of social activities for HIMS PhDs and postdocs

For 2015 the council plans to continue the started effort to represent PhDs at the management level of the department and the continue promoting cohesion of PhDs of the different research groups of the HIMS.

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

5.1.1. HRSMC



The Holland Research School of Molecular Chemistry (HRSMC) comprises research groups of the van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam (UvA); the Institute for Electrons and Molecular Structure (EMS) of the VU University (VU); and the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Leiden University (UL). The University of Amsterdam legally represents the HRSMC. Currently Prof. dr. W.J. Buma (HIMS, UvA) is the scientific director. The main targets of the HRSMC are:

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

Major activities 2014

1. The festive 20th annual symposium of the HRMSC on 20/21 November in the Trippenhuis of the Royal Dutch Academy of Arts and Sciences in Amsterdam. Besides lectures from HRSMC staff members and PhD students, there were key note lectures from Prof. Erick Carreira and Nobel laureates Prof. W. E. Moerner (2014), Prof. Arieh Warshel (2013) and Prof. Roald Hoffmann (1981). In addition, Dr. Tjøstil Vlaar gave a lecture as the winner of the annual Dick Stufkens Prijs. This prize is awarded annually to the best thesis of the HRSMC. The special programme attracted over 200 participants.
2. The HRSMC educational activities of 2014 consisted of:
   - HRSMC Course 'Photophysics, Photochemistry & Photobiology' (31 March – 11 April)
   - HRSMC/NIOK Summer School 'Advanced Metal-Organic Chemistry and Catalysis' (30 June – 4 July)

   Furthermore, the HRSMC has participated in the organization of the two weeks Course 'Molecular Simulation' (6-18 January)

   The Molecular Simulation course as well as the HRSMC Schools have by now become rather well known with the majority of the participants actually coming from abroad.

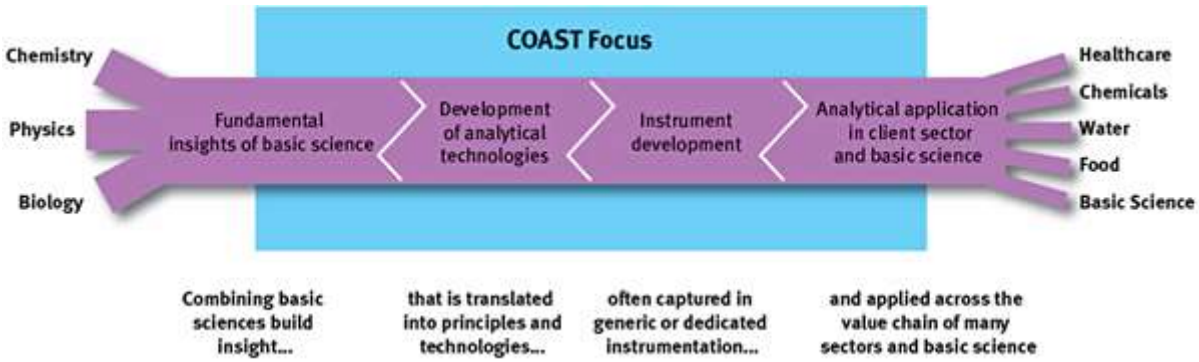
5.1.2. TI-COAST

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

COAST aims to advance Dutch excellence in its TOPsectors by providing pivotal analytical knowledge and instruments based on fundamental science and by ensuring transfer of analytical expertise between application areas. COAST realizes this by securing and improving Dutch expertise in analytical science and technologies. COAST's mission is to strengthen analytical science in the Netherlands by combining efforts in R&D, human capital and infrastructure:

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

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



In 2014 the COAST research portfolio comprised 15 public-private scientific research projects in which 34 companies (including 11 SMEs) collaborate with 19 academic groups. 17 PhD students and 13 Postdoc were employed in the research program in 2014, 13 PhD and postdoc positions were open for application. A total of 69 students were enrolled in the COAST BSc and MSc talent programs in analytical chemistry. Moreover, the first graduates of the talent programs were welcomed as employees of COAST participants. As part of the infrastructure program COAST participates in uNMR-NL, the consortium realizing the 1.2 GHz NMR facility in NL in 2017. In addition, the web facility on analytical infrastructure presents 62 rare or unique high-end facilities available in the laboratories of COAST participants for use by other COAST participants. In 2014 COAST grew to 74 participants (43 companies, 26 academic groups and 5 universities for applied sciences [hbo]).

5.1.3. Co van Ledden Hulsebosch Center

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

In 2014 a significant amount of work was undertaken to further strengthen the CLHC in terms of organizational structure, forensic science program (i.e. expanding the project portfolio and special chairs in forensic science in the participating institutes), the national and international network, CLHC awareness with the general public and contribution to the Forensic Master program within the Institute of Interdisciplinary Studies (IIS). These efforts resulted in a unique national and internationally acknowledged expertise center.

In 2014 six forensic PhD theses were defended successfully, a total of 74 peer reviewed publications appeared and 87 oral presentations were given at international and national conferences and symposia. Nine new project proposals were granted making a total of 29 ongoing forensic PhD studies involving 34 PhD students and 4 postdocs. The progress of the forensic science projects was presented by the PhD students during the 1st Forensic PhD symposium organized at Science Park in the fall of 2014.
An important building block for the forensic program in Amsterdam is the realization of special chairs for important forensic science areas. In 2014 two official appointments were realized. On July 1st Rick van Rijn (AMC/NFI) was appointed on a special chair in forensic (pediatric) radiology and on September 1st Zeno Geradts (NFI) was appointed professor in forensic data science within the Informatics Institute. With these new appointments a total of 6 special chairs in Forensic Science are currently operating within the CLHC in the area of Forensic Biology (IBED), Forensic Statistics (KdVI), Forensic Analytical Chemistry (HIMS), Forensic Biophysics (AMC), Forensic Radiology (AMC) and Forensic Data Science (IvI).

6. Facts and figures

6.1 Personnel

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

Research- and supporting staff 2014 of the HIMS themes, per employment type (fte)[a]

	SC	COMP	ACF	MOLP	Other	**Total**
Tenured staff	5,6	3,0	2,4	2,4	0,8	14,2
Non-tenured staff	15,3	5,1	2,0	0,7	1,8	24,9
PhD candidates	22,7	8,5	9,9	9,4	1,7	52,2
Total research staff	**43,6**	**16,6**	**14,3**	**12,5**	**4,3**	**91,3**
Technicians [b]	12,4	0,0	2,5	3,4	0,0	18,3
Visiting fellows [c]	0,0	0,0	0,2	0,2	0,0	0,4
Total research	**56,0**	**16,6**	**17,0**	**16,1**	**4,3**	**110,0**
Supporting staff					6,0	6,0
Total staff	**56,0**	**16,6**	**17,0**	**16,1**	**10,3**	**116,0**

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

Research- and supporting staff 2014 of HIMS and the HIMS groups, per employment type (fte)[a]

	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	Other	**Total**
Tenured staff	1,6	0,3	1,7	0,5	1,5	2,0	1,0	2,4	1,4	1,0	0,8	14,2
Non-tenured staff	0,6	0,8	8,1	0,9	4,9	4,2	0,9	2,0	0,6	0,1	1,8	24,9
PhD candidates	2,3	0,0	17,1	1,9	1,3	6,8	1,7	10,0	6,8	2,6	1,7	52,2
Total research staff	**4,5**	**1,1**	**26,9**	**3,3**	**7,7**	**13,0**	**3,6**	**14,4**	**8,8**	**3,7**	**4,3**	**91,3**
Technicians [b]	3,2	0,9	4,5	1,8	2,0	0,0	0,0	2,5	2,3	1,1	0,0	18,3
Visiting fellows [c]	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,2	0,2	0,0	0,0	0,4
Total research	**7,7**	**2,0**	**31,4**	**5,1**	**9,7**	**13,0**	**3,6**	**16,9**	**11,3**	**5,0**	**4,3**	**110,0**
Supporting staff											6,0	6,0
Total staff	**7,7**	**2,0**	**31,4**	**5,1**	**9,7**	**13,0**	**3,6**	**16,9**	**11,3**	**5,0**	**10,3**	**116,0**

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

[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.

6.2 Research

6.2.1 Research input of the HIMS themes

Research- and supporting staff 2014 of HIMS per funding type (fte)[a]

HIMS themes	SC	COMP	ACF	MOLP	Other	**Total research**	***%***	Supp. Staff	**Total staff**	***%***
Direct funding[1a]	19,3	2,5	4,5	6,2	0,5	**33,0**	***30***	4,6	37,6	***33***
Indirect funding [1b]	3,6	0,0	0,0	0,0	0,0	**3,6**	***3***	0,0	3,6	***3***
Direct[1a] + indirect[1b]	**22,9**	**2,5**	**4,5**	**6,2**	**0,5**	**36,6**	**33**	**4,6**	**41,2**	***36***
Research grants[2]	18,8	10,5	5,6	4,6	2,6	**42,1**	***38***	0,0	42,1	***36***
Contract research[3]	7,2	0,8	3,7	0,1	0,8	**12,6**	***12***	1,4	14,0	***12***
Other[4]	7,1	2,8	3,2	5,2	0,4	**18,7**	***17***	0,0	18,7	***16***
Total	**56,0**	**16,6**	**17,0**	**16,1**	**4,3**	**110,0**	***100***	**6,0**	**116,0**	***100***

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

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	**Other**	**Total research**	Supp staff	**Total staff**	**%**
Direct funding[1a]	4,4	2,0	6,2	2,2	4,5	1,6	1,0	4,5	3,6	2,6	0,5	**33,0**	4,6	**37,6**	***33***
Indirect funding[1b]	0,1	0,0	2,4	0,9	0,2	0,0	0,0	0,0	0,0	0,0	0,0	**3,6**	0,0	**3,6**	***3***
Direct[1a] + indirect[1b]	**4,5**	**2,0**	**8,6**	**3,1**	**4,7**	**1,6**	**1,0**	**4,5**	**3,6**	**2,6**	**0,5**	**36,6**	**4,6**	**41,2**	***36***
Research grants[2]	1,8	0,0	16,5	0,0	0,5	8,6	1,9	5,6	3,3	1,3	2,6	**42,1**	0,0	**42,1**	***36***
Contract research[3]	0,1	0,0	3,8	1,1	2,2	0,8	0,0	3,7	0,1	0,0	0,8	**12,6**	1,4	**14,0**	***12***
Other[4]	1,3	0,0	2,6	0,9	2,3	2,1	0,7	3,2	4,1	1,1	0,4	**18,7**	0,0	**18,7**	***16***
Total	**7,7**	**2,0**	**31,5**	**5,1**	**9,7**	**13,0**	**3,6**	**17,0**	**11,1**	**5,0**	**4,3**	**110,0**	**6,0**	**116,0**	***100***

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

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

Externally financed projects acquired in 2014 (mln €) per funding type[1]

HIMS themes	SC	COMP	MB	MOLP	Other	**Total[6]**
1st - NRSC-C [2]	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [3]	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [4]	1.10	0.25	0.79	0.91	0.00	**3.05**
3rd [5]	0.14	0.00	0.00	0.00	0.00	**0.14**
Total	**1.24**	**0.25**	**0.79**	**0.91**	**0.00**	**3.20**

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

HIMS groups	HH	RW	JR	CE	GR	PB	EJM	PS	WJB	FB	PI	Total[6]
1st - NRSC-C [2]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [3]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [4]	1.06	0.00	0.00	0.00	0.04	0.25	0.00	0.79	0.65	0.26	0.00	**3.05**
3rd [5]	0.00	0.02	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.14**
Total	**1.06**	**0.02**	**0.12**	**0.00**	**0.04**	**0.25**	**0.00**	**0.79**	**0.65**	**0.26**	**0.00**	**3.20**

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

[1] Matching contributions UvA/FNWI (total 1,63 mln € foreseen) excluded; own contributions HIMS (in kind and cash/from reserves) included
[2] NRSC-C (TOP Research School Catalysis);
[3] COF, CvB (Funds from University Board);
[4] NWO-CW, FOM, STW, KNAW, ERC
[5] EU, DPI, AGENTSCHAP.NL, NanoNext, NFI, Industry
[6] Rounding difference 0,01.

6.2.2 Research output of the HIMS themes

Research output 2014 per type of publication (source: METIS)

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint[1]	**Total**
Refereed articles	59	26	20	32	22	-9	**150**
Non-refereed articles	0	0	0	0	0		**0**
Books	0	0	0	0	0		**0**
Book chapters	1	0	1	0	0		**2**
PhD-theses	9	5	2	4	0		**20**
Conference papers	0	0	0	0	0		**0**
Patents	1	0	0	0	1		**2**
Professional publications	0	6	1	0	0		**7**
Publications general public	0	0	0	0	0		**0**
Other research output	24	5	0	6	1		**36**
Total	**94**	**42**	**24**	**42**	**24**	**-9**	**217**

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

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	PI	Joint[1]	**Total**
Refereed articles	3	0	34	4	16	2	9	10	22	20	28	4	7	-9	**150**
Non-ref. articles	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Books	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Book chapters	0	1	0	0	0	0	0	0	0	1	0	0	0		**2**
PhD-theses	1	0	3	2	2	1	3	1	0	2	4	0	1		**20**
Conference papers	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Patents	0	0	0	0	1	0	0	0	1	0	0	0	0		**2**
Prof. publications	0	0	0	0	0	0	0	0	0	1	0	0	6		**7**
Publ. general public	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Other output	9	0	8	7	0	0	3	2	1	0	0	6	0		**36**
Total	**13**	**1**	**45**	**13**	**19**	**3**	**15**	**13**	**24**	**24**	**32**	**10**	**14**	**-9**	**217**

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

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

Number of refereed articles 2014, in ranges of different impact factor Source: METIS

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint[1]	**Total**
>15	1	1	0	0	1		**3**
10-15	11	2	0	2	4	-2	**17**
5-10	18	4	4	9	5	-3	**37**
<5	29	19	16	21	12	-4	**93**
Total	**59**	**26**	**20**	**32**	**22**	-9	**150**

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

HIMS groups	HH	RW	JR	CE	GR	AK	PB	EJM	RK	PS	WJB	FB	PI	Joint[1]	**Total**
>15	0	0	1	0	0	0	0	1	1	0	0	0	0		**3**
10-15	0	0	11	0	0	0	1	1	4	0	2	0	0	-2	**17**
5-10	0	0	12	1	4	1	1	2	5	4	8	1	1	-3	**37**
<5	3	0	10	3	12	1	7	6	12	16	18	3	6	-4	**93**
Total	**3**	**0**	**34**	**4**	**16**	**2**	**9**	**10**	**22**	**20**	**28**	**4**	**7**	**-9**	**150**

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

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

6.2.3 Efficiency of the doctoral research path

The following tables show the efficiency of the doctoral research path (period of appointment 2006-2010; planned PhD defence 2010-2014).

Employed PhD-candidates

Enrolment (-)				**Success rates of graduation**							
Starting Year	**Enrolment**		**Total (M+F)**	**< 4 years**	**4 - 5 years**	**5 - 6 years**	**6 -7 years**	**>7 years**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
	M	**F**									
2006	12	4	16	1	7	4	1	0	0	3	0
2007	2	6	8	0	2	1	1	0	0	3	1
2008	4	9	13	0	6	5	0	0	0	0	2
2009	4	7	11	0	7	1	0	0	0	1	2
2010	12	4	16	0	5	0	0	0	0	10	1
Total	34	30	64	1	27	11	2	0	0	17	6
Cumulative 2006-2010											
SC	18	11	29	1	15	3	0	0	0	6	4
COMP	6	6	12	0	3	3	1	0	0	4	1
ACF	1	7	8	0	3	1	1	0	0	2	1
MOLP	7	5	12	0	5	4	0	0	0	3	0
Other	2	1	3	0	1	0	0	0	0	2	0
Total	34	30	64	1	27	11	2	0	0	17	6
%	*53*	*47*	*100*	*2*	*42*	*17*	*3*	*0*	*0*	*27*	*9*

Non-employed PhD-candidates

Enrolment (-)				Success rates of graduation							
Starting Year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	2	1	3	2	1	0	0	0	0	0	0
2007	7	1	8	4	1	0	0	0	1	2	0
2008	5	1	6	0	2	1	0	0	1	2	0
2009	5	0	5	0	2	2	0	0	0	0	1
2010	0	1	1	0	0	0	0	0	0	1	0
Total	19	4	23	6	6	3	0	0	2	5	1
Cumulative 2006-2010											
SC	2	0	2	0	0	2	0	0	0	0	0
COMP	0	0	0	0	0	0	0	0	0	0	0
ACF	6	2	8	4	0	0	0	0	0	3	1
MOLP	11	2	13	2	6	1	0	0	2	2	0
Other	0	0	0	0	0	0	0	0	0	0	0
Total	19	4	23	6	6	3	0	0	2	5	1
%	*83*	*17*	*100*	*26*	*26*	*13*	*0*	*0*	*9*	*22*	*4*

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

As can be seen from the tables, a number of PhD students have not received their doctor title within 6 years. Several delays are related to personal circumstances like a new job and/or a busy family life, or health problems. Most PhD students who discontinued their doctoral research, did so in their first year and changed their career on their own initiative. In a few cases the 4-year PhD research project was completed but the PhD student decided not to defend a PhD thesis.

Employed and Non-employed PhD-candidates

Sustainable Chemistry (SC)

Enrolment (-)				Success rates of graduation							
Starting year	Enrollment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	7	1	8	1	4	2	0	0	0	1	0
2007	0	1	1	0	0	0	0	0	0	1	0
2008	3	4	7	0	4	1	0	0	0	0	2
2009	5	4	9	0	5	2	0	0	0	1	1
2010	5	1	6	0	2	0	0	0	0	3	1
Total	20	11	31	1	15	5	0	0	0	6	4
%	*65*	*35*	*100*	*3*	*48*	*16*	*0*	*0*	*0*	*19*	*13*

Computational Chemistry (COMP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	1	1	2	0	0	1	0	0	0	1	0
2007	1	1	2	0	1	0	1	0	0	0	0
2008	1	2	3	0	1	2	0	0	0	0	0
2009	0	2	2	0	1	0	0	0	0	0	1
2010	3	0	3	0	0	0	0	0	0	3	0
Total	6	6	12	0	3	3	1	0	0	4	1
%	*50*	*50*	*100*	*0*	*25*	*25*	*8*	*0*	*0*	*33*	*8*

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

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	2	1	3	2	0	0	1	0	0	0	0
2007	3	5	8	2	0	1	0	0	0	4	1
2008	1	1	2	0	1	0	0	0	0	1	0
2009	1	1	2	0	1	0	0	0	0	0	1
2010	0	1	1	0	1	0	0	0	0	0	0
Total	7	9	16	4	3	1	1	0	0	5	2
%	*44*	*56*	*100*	*25*	*19*	*6*	*6*	*0*	*0*	*31*	*13*

Molecular Photonics (MOLP)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	3	2	5	0	4	1	0	0	0	0	0
2007	5	0	5	2	2	0	0	0	1	0	0
2008	4	3	7	0	2	3	0	0	1	1	0
2009	3	0	3	0	2	1	0	0	0	0	0
2010	3	2	5	0	1	0	0	0	0	4	0
Total	18	7	25	2	11	5	0	0	2	5	0
%	*72*	*28*	*100*	*8*	*44*	*20*	*0*	*0*	*8*	*20*	*0*

Others (group Iedema)

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	1	0	1	0	0	0	0	0	0	1	0
2007	0	0	0	0	0	0	0	0	0	0	0
2008	0	0	0	0	0	0	0	0	0	0	0
2009	0	0	0	0	0	0	0	0	0	0	0
2010	1	1	2	0	1	0	0	0	0	1	0
Total	2	1	3	0	1	0	0	0	0	2	0
%	*67*	*33*	*100*	*0*	*33*	*0*	*0*	*0*	*0*	*67*	*0*

Total HIMS

Enrolment (numbers)				Success rates of graduation							
Starting year	Enrolment		Total (M+F)	< 4 years	4 - 5 years	5 - 6 years	6 -7 years	>7 years	Outside UvA	Not yet finished	Discon-tinued
	M	F									
2006	14	5	19	3	8	4	1	0	0	3	0
2007	9	7	16	4	3	1	1	0	1	5	1
2008	9	1	19	0	8	6	0	0	1	2	2
2009	9	7	16	0	9	3	0	0	0	1	3
2010	12	5	17	0	5	0	0	0	0	11	1
Total	53	34	87	7	33	14	2	0	2	22	7
Cumulative 2006-2010											
SC	20	11	31	1	15	5	0	0	0	6	4
COMP	6	6	12	0	3	3	1	0	0	4	1
ACF	7	9	16	4	3	1	1	0	0	5	2
MOLP	18	7	25	2	11	5	0	0	2	5	0
Other	2	1	3	0	1	0	0	0	0	2	0
Total	53	34	87	7	33	14	2	0	2	22	7
%	*61*	*39*	*100*	*8*	*38*	*16*	*2*	*0*	*2*	*25*	*8*

M = male; F = Female

6.3 Finance 2014

The table below shows the HIMS financial result 2014.

HIMS result 2014 (k€)

	1st (1 structural	1st (2 Other	1st total	2nd (3	3rd (4	Total
HIMS						
Budget (fixed)	4.033		4.033			**4.033**
Budget (variable[5])	5.226		5.226	2.260	2.842	**10.328**
Other income		173	173			**173**
Matching contract research	-3.738		-3.738	2.502	1.236	**0**
Budget total	**5.521**	**173**	**5.694**	**4.762**	**4.078**	**14.534**
Percentage	**38**	**1**	**39**	***33***	**28**	***100***
Personal costs	-3.353	-28	-3.381	-1.684	-1.581	**-6.646**
Other costs (projects)	-1.127	-19	-1.146	- 611	-759	**-2.516**
Overhead (central)	839		839	-505	-334	**0**
Overhead (faculty)	-790	-11	-801	-935	- 606	**-2.342**
Overhead (institute)	1.694	11	1.705	-1.029	- 676	
Various costs	-1		-1			**-1**
Other (secundary) costs	- 2.116		-2.116		-11	**-2.127**
Costs total	**-4.854**	**-47**	**-4.901**	**-4.764**	**-3.967**	**-13.632**
Percentage	**35**	**1**	**36**	**35**	**29**	**100**
Result 2014	**667**	**126**	**793**	**-2**	**111**	**902**
Reservations[6]	833	49	882			882
Result excluding reservation	**-166**	**77**	**-89**	**-2**	**111**	**20**

[1] Direct funding (1st, eerstegeldstroom; university/direct funding,
[2] Various contibutions for HIMS, HRSMC and CLHC)
[3] Research grants (2nd, tweedegeldstroom; NWO-CW, FOM, STW, KNAW)
[4] Contract research (3rd, derdegeldstroom; EU, DPI, AGENTSCHAP.NL, FES/NanoNed, Industrial)
[5] 1e gs assigned via allocation model (incl. HRSMC, CLHC, SectorPlan, Sus.Chem)
[6] Reservations incl. SectorPlan and Sustainable Chemistry

The HIMS result for 2014 amounts to + 902k€. This result includes reservations of 882 k€ budget for appointments in the framework of the Sectorplan Natuur- en Scheikunde (SNS), Sustainable Chemistry and some other appointments. It is a reservation for costs to be made in the coming years.