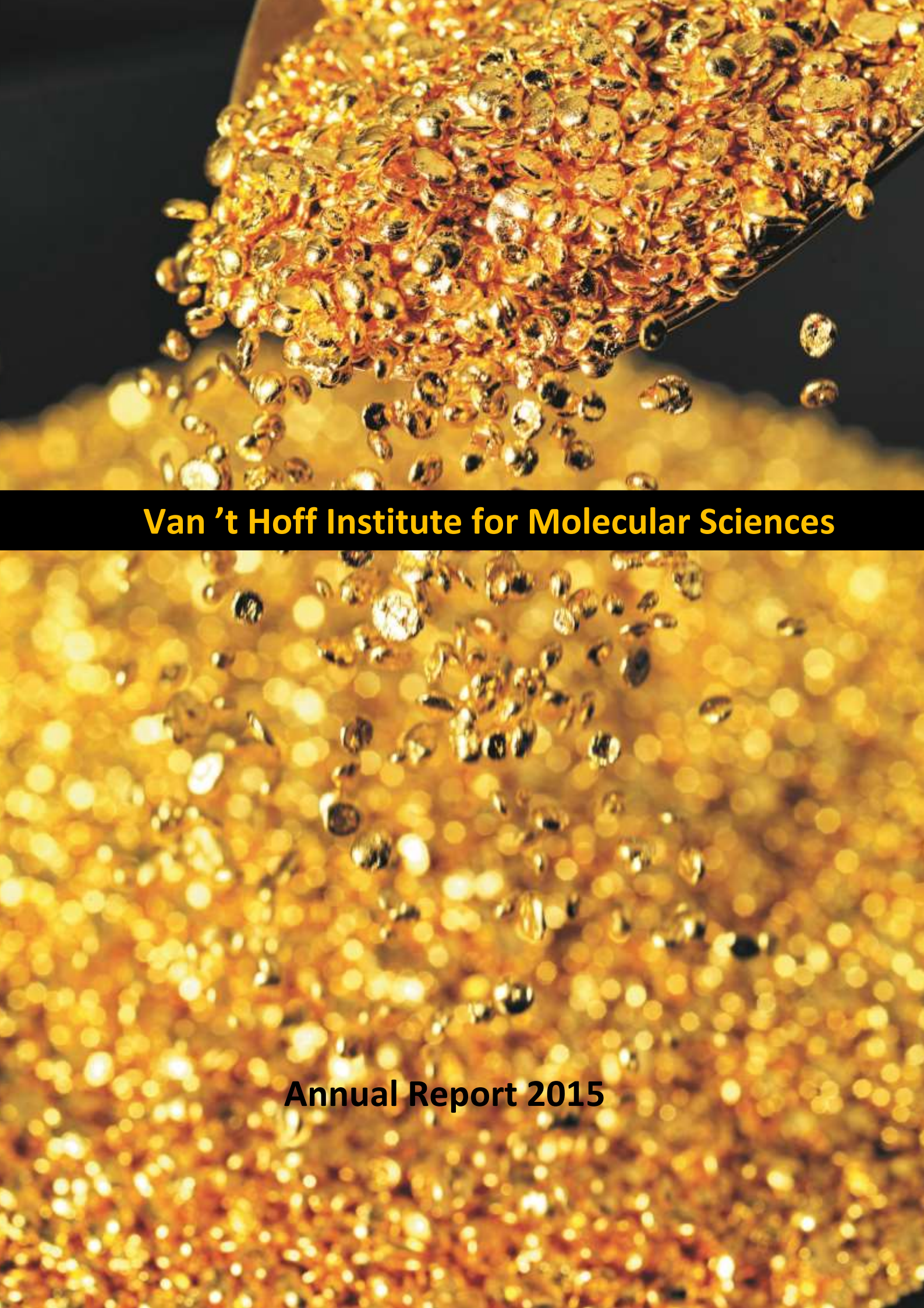

Van ’t Hoff Institute for Molecular Sciences

Annual Report 2015

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G.J.J. Zonneveld - de Boer, drs. H. Ikink, drs M.J. Bartels

Cover:
HIMS goes for Gold: A new catalyst invented by researchers from HIMS is now being implemented in the precious metals industry by Germany's oldest gold-processing company, Heimerle + Meule. The catalytic process invented at the UvA removes >99.9% of the cyanide from the process wastewater within minutes. The new process is cheaper and more efficient, with a wide spectrum of applications across the metals industry sector.

June 2016

Preface

I am proud to report that 2015 was an exceptional year for HIMS, in which we welcomed new scientific staff, were able to acquire a record number of new projects and underpinned our international position with appealing publications in renowned scientific papers.

HIMS welcomed three professors of which two were new to HIMS and the third saw his longtime senior research position rewarded with a full professorate. Furthermore, two new young tenure track scientists were appointed who chose HIMS as the ideal place to perform research for which they acquired prestigious NWO and ERC grants.

As a whole HIMS has been very successful in establishing new research. A record of 28 new projects were acquired with a total funding of 12 million euros granted by EU, NWO and Topsector Chemistry. 20 projects were inspired by future applications and 14 of these projects have already companies participating and co-financing them. In 2015 two new patent applications were filed, in collaboration with research consortia or companies. For a total of 11 HIMS research projects promising valorisation opportunities were established. The spin-off company Plantics, that commercializes a new bio-plastic invented at HIMS, started production on ton scale at its new facility in the Amsterdam harbour area.

The scientific level of HIMS research is very high, which is reflected in 221 peer reviewed scientific publications of which many in high impact journals, including two science papers. 19 PhD students successfully defended their thesis. The quality of HIMS scientists is also reflected in the prizes and honours awarded, and we are proud to have two new members installed at the Royal Netherlands Academy of Arts and Sciences. Professor Peter Schoenmakers received the Csaba Horváth Memorial award and the 20th annual CASSS award, both honourable distinctions in the field of separation science. Professor Bas de Bruin was elected Faculty Lecturer of the Year 2015 and subsequently UvA Lecturer of the Year 2015 by faculty and university student representatives. In recognition of our efforts in the field of art conservation and restoration, HIMS joined the Netherlands Institute for Conservation, Art and Science (NICAS), a nationwide initiative establishing a cohesive research program in close cooperation with and active involvement of the cultural heritage field.

The RPA Sustainable Chemistry is very active at many different levels. The valorisation possibilities have been discussed with the Industrial Advisory Board in October 2015, several scientific meetings have been organized on various topics, and the student exchange program has started. A NWO-TOP-PUNT grant has been submitted (and awarded), and the new TT staff members have started their research programs. Also the post-doc program has started, leading to joined research projects, connecting various research themes of HIMS. The research is of high level, with many scientific papers produced. A wonderful example of valorisation is that Germany's oldest gold and silver refining company is evaluating a catalyst for waste effluent treatment that was developed and patented within the RPA Sustainable Chemistry.

To conclude, 2015 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

Table of contents

1. General considerations and highlights

1.1 Key figures of HIMS in 2015

The high level of scientific output of HIMS was maintained in 2015. HIMS published 8 papers in absolute top journals (impact factor > 20) and 20 papers in top journals (impact factor 10-20). The total number of refereed and other professional publications, patents and book(chapter)s amounted to 194, of which 17 where joint publications. The amount of published PhD dissertations was 19 (from 2010 to 2014 resp. 14, 15, 9, 16, 20).

With a total of 5.8M€ in external funding (excluding the own matching budget of approximately 2,5M€) the year 2015 was as more successful than former years (average 2011-2013: 5.3M€). These funds were acquired from funding agencies as NWO/FOM (3.6M€), EU (1.8M€), as well as from industry and other partners (0.4M€).

1.2 Personnel

In 2015 the total staff amounted to 127.9 fte. In 2014 it was 126.8 fte and in 2013 136.5 fte.
This year Dr Tati Fernández-Ibáñez (Synthesic Organic Chemistry) and Dr Francesco Mutti (Biocatalysis) started their tenure track, both with a strong focus in the field of Sustainable Chemistry.
Prof. Jan van Maarseveen of the Synthetic Organic Chemistry group at HIMS was appointed professor of Bio-Inspired Organic Synthesis. He develops sustainable methods for the synthesis of biologically relevant molecules.
Prof. Maarten van Bommel, former senior scientist at the Dutch Cultural Heritage Agency, was appointed professor of Conservation Science to both the Faculty of Humanities and the Van 't Hoff Institute for Molecular Sciences. His appointment is aimed at building a bridge between art and culture studies on the one hand, and sciences on the other.
Prof. Ron Peters, science manager analytics at DSM Coating Resins, was appointed professor by special appointment of Bioterials Analysis on behalf of the Science Plus Foundation (Stichting Bèta Plus). His research will focus primarily on characterising the molecular structure of complex functional polymers.

1.3 Finances

HIMS finished the year 2015 with a negative financial result of - 44k€. This result should be corrected with the costs (120k€) that find their resources in the reservations for appointments in the framework of the Sectorplan Natuurwetenschappen, Zwaartepunt Sustainable Chemistry and some other appointments. The remaining result for 2015 is 76 k€ positive.

1.4 Highlights

1.4.1 Institutional highlights

Solar Fuel Future
As part of the UvA Research Priority Area Sustainable Chemistry and sponsored by the John van Geuns foundation HIMS hosted a successful mini-symposium on sustainability and solar fuels on 26 January 2015.

Art history, conservation and science
HIMS joined the Netherlands Institute for Conservation, Art and Science (NICAS), that was opened on 25 September 2015 in the Rijksmuseum. NICAS is a new innovative interdisciplinary research center housed in the Ateliergebouw in Amsterdam, uniting art history, conservation and science.

Industry Day
On 30 October 2015, HIMS organised its annual Industry Day. About 30 companies (from Amsterdam SMEs to multinationals) were introduced into the research themes of the UvA chemistry research institute. The Industry Day contained a talent lunch with PhD students and postdocs, active workshops and an informal poster session.

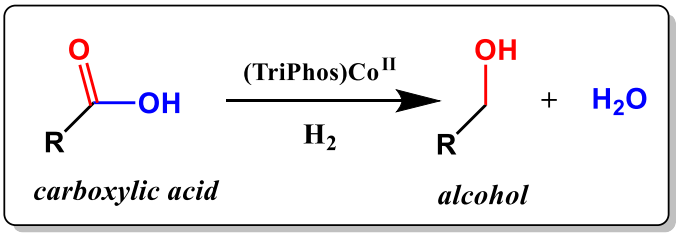
Sino-Dutch collaboration in Sustainable Chemistry
On 10 December 2015 the emeritus lecture of former HIMS director Prof. Aart Kleijn was embedded in a special Sustainable Chemistry seminar 'Amsterdam meets China', celebrating Sino-Dutch collaboration on sustainability.

CASA: Measurements matter
Prior to the inaugural speech of Prof. Garry Corthals, the UvA-VU Center for Analytical Sciences Amsterdam (CASA) organised a seminar for researchers from industry and academia, offering them a perspective into the activity and scope of analytical sciences.

New research projects
Not less than 28 research proposals of HIMS researchers where granted in 2015 (see section 1.4.4). 22 of these projects were inspired by future applications and 14 projects have already companies participating and co-financing them.

1.4.2 Scientific highlights

Homogeneous and Supramolecular Catalysis
Efficient Catalytic Reaction to Produce Alcohols from Carboxylic Acids
The group recently found a new and efficient soluble catalyst, based on earth-abundant cobalt, for efficient hydrogenation of esters and carboxylic acids. These are highly desirable chemical reactions relevant for fine chemical transformations and biomass conversion. The results were disclosed in the top-journal *Science*. Industrially, the catalytic hydrogenation of esters and carboxylic acids is currently performed using solid catalysts that operate at very high temperatures and pressures. Milder reaction conditions are possible with soluble (homogeneous) catalysts. However, all reported examples of such catalysts operating in solution under mild reaction conditions are based on expensive and scarce metals such as ruthenium and iridium. In addition, these previous examples perform poorly in the reduction of carboxylic acids to alcohols.



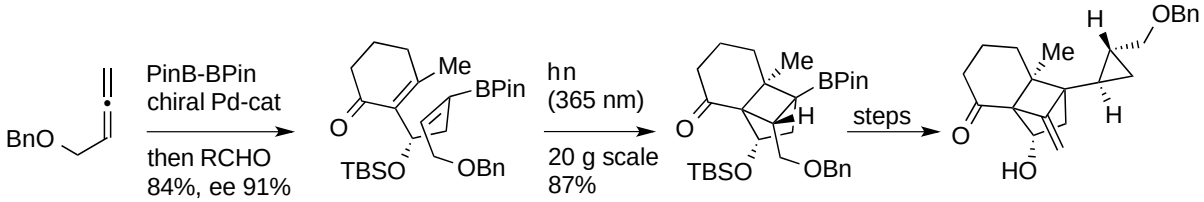
Hence, cheaper and more effective soluble catalyst, based on earth-abundant metals such as cobalt, are highly desirable. Within a project financed by CatchBio and DSM, a team of UvA-HIMS researchers decided to tackle this problem. The team (including the HIMS Molecular Inorganic Chemistry group) succeeded in the development of a novel soluble catalyst, based on earth-abundant cobalt, for efficient hydrogenation of esters and carboxylic acids. This system, pairing $Co(BF_4)_2 \cdot 6H_2O$ with a TriPhos tridentate phosphine ligand, can reduce a wide range of esters and carboxylic acids under mild reaction conditions (100 °C, 80 bar H_2) and reaches turnover numbers of up to 8000. The system outperforms known precious metal-based catalysts and thereby increases the sustainability of this transformation.

Hydrogenation of Carboxylic Acids with a Homogeneous Cobalt Catalyst
Korstanje, T.J.; van der Vlugt, J.I.; Elsevier, C.J.*; de Bruin, B.*, *Science,* **2015**, *350 (6258), 298-302. DOI: 10.1126/science.aaa8938.* [link]

Heterogeneous Catalysis and Sustainable Chemistry
As part of the SmartMix CatchBio project, we have developed a new method for solubilising lignin using liquid ammonia. Lignin is nature's richest source of aromatics, yet it is usually burned as a leftover product in biorefining. Using liquid ammonia at 80 °C, we managed to solubilise different wood and grass lignins within minutes, enabling their fractionation to useful aromatic derivatives. This project, a collaboration between the Suschem RPA and Wageningen University, opens opportunities for lignin valorisation in future biorefineries using the unique properties of liquid ammonia, a highly coordinating yet non-protic solvent. The results were published in *Green Chemistry,* the leading scientific journal in the area of sustainable chemistry.

Lignin solubilisation and gentle fractionation in liquid ammonia. Z. Strassberger, F. van der Klis, D. S. van Es, S. Tanase, P. Prinsen and G. Rothenberg, *Green Chem.*, **2015**, 17, 325-334.
DOI: 10.1039/C4GC01143K (Open Access)

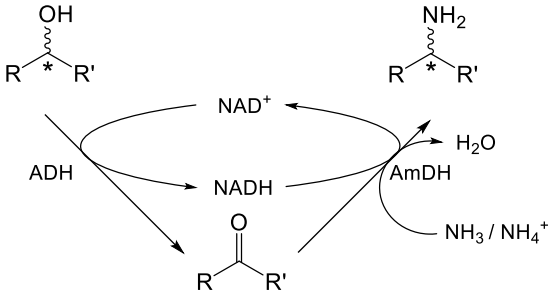
Synthetic Organic Chemistry
Formal Total Synthesis of Solanoeclepin A: In our synthetic approach to solanoeclepin A (hatching agent of potato cyst nematodes) an enantioselective synthesis of an intermediate in the Tanino total synthesis of solanoeclepin A has been developed. The key step was an intramolecular [2+2] photocycloaddition, which led to the tricyclo[5.2.1.$0^{1,6}$]decane core in six steps. The photosubstrate was prepared through a catalytic asymmetric allene diborylation in high enantiomeric excess. The [2+2] photocycloaddition proceeded in high yield on irradiation at 365 nm on 20 g scale in a flow system. Other important steps were the replacement of a boronate group at the quaternary carbon by a vinyl group and diastereoselective cyclopropanation of an allylic alcohol (see Scheme below).

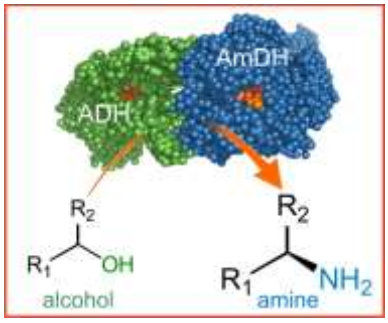


Biocatalysis

*The major highlight from the Biocatalysis group has been a publication in Science (*impact factor 33.61, DOI: 10.1126/science.aac9283). In this article, we have described the redox self-sufficient, catalytic enzymatic conversion of alcohols to amines. Amines are among the most frequently used chemical intermediates for the production of pharmaceuticals, fine chemicals, agrochemicals, polymers, dyestuffs, pigments, emulsifiers and plasticizing agents. During the past decades many academic and industrial researchers have worked on the development of efficient methods for the synthesis of these amines starting from alcohols.

In this contest, our new enzymatic method reported in *Science* outperforms all the other (non-biocatalytic) synthetic methods in terms of versatility, efficiency, selectivity and reduction of waste.

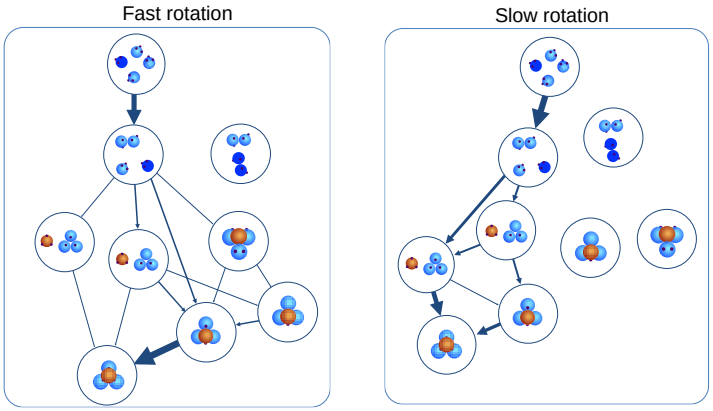




The novel method relies on two enzyme classes: alcohol dehydrogenases and amine dehydrogenases that work in tandem in a hydrogen-borrowing cascade. This is a process wherein the electrons liberated in the first oxidative step are internally recycled in the second reductive step, making the overall cycle redox self-sufficient. The biocatalytic method possesses the highest possible atom efficiency, sourcing nitrogen from ammonia and generating water as the sole by-product. One particularly important feature is that it gives direct access to highly valuable enantiopure amines which constitute the active core of a large number of pharmaceuticals and fine chemical.

Computational Chemistry

Arthur Newton et al. [Proc. Nat. Acad. Sci. **112**, 15308] describe how the rotation of nanoparticles such as proteins and colloids affects the self-assembly into complexes and clusters. In nature, molecular self-assembly plays an important role: proteins stick to each other to form viruses, or protein complexes transmit signals in cellular networks. These self-assembly results depends on the dynamics and kinetics. Usually translation and rotation of particles are linked via the so-called Stokes-Einstein relation. However, in recent years, experiments revealed that this coupling does not hold in tightly packed, crowded environments like the cytoplasm of the living cell. We investigated the effect of releasing the Stokes-Einstein coupling. While even for two particles already a strong effect on the association emerge, this gets more relevant for systems with multiple particles, where metastable intermediate states are possible. In a simulation of cluster formation of four particles, varying the rotational diffusion significantly shifts the preference for the self-assembly routes (see figure). This was generalized to clusters of any size.

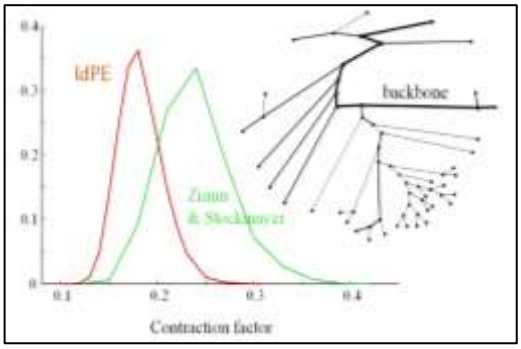


The figure shows change of assembly mechanism when reducing rotational diffusion. A circle depicts a metastable state. The black dots indicate where the particles can 'stick' to each other. One particle is colored orange in order to clarify the contrast. The thickness of the arrows reflects the probability of the assembly route. For slow rotation one route is clearly preferable compared to the other. Here 'frustrated' states (at the right) are avoided, resulting in significantly less kinetic hindrance and better yield.

The researchers argue that their results provide new opportunities for a better control of the bottom-up synthesis of functional materials. For example, it should be possible to design particles of which the rotation can be controlled with magnetic or electric fields.

Computational Polymer Chemistry & Science for Arts

The group considers a variety of branched polymers, from linseed oil (collaboration with Netherlands Institute for Conservation, Art and Sciences – NICAS) and acrylate networks (collaboration with Océ) to an industrially important branched polymer, low-density Polyethylene (ldPE). Dr. Nazila Yaghini has obtained her PhD degree on a dissertation under the title *"Towards The Architectures of Macromolecules, Modeling of Multi---dimensional Polymer Chain Distributions."* She focused on the unique hyperbranched structure of ldPE. Although this plastic is being produced for more than 60 years, still a lack of understanding of the materials properties exists. This prevents a more sustainable application of ldPE in thin film coatings for milk cartons, or the development of alternative polymers with equivalent processing and end use properties. One issue is the relation between reaction conditions and branching topology. Models have been developed by Dr. Yaghini that explain the bimodal MWD of ldPE from branching and non-random scission. Deeper knowledge of the microstructure through models turned out also to be important for polymer characterization with viscosimetry and light scattering. We provide alternatives to the famous Zimm and Stockmayer's (1949) analytical expression of contraction factor for molecules with terminal branching. The contraction factor prediction account for the kinetics of a radical polymerization with transfer to polymer and recombination termination, typical for ldPE. Thus, we observe significantly stronger contraction than predicted by the old model of Zimm and Stockmayer.



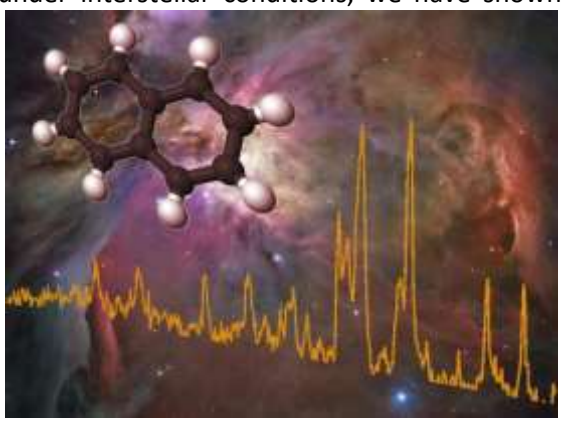
Radius of gyration contraction factor distribution for populations of terminally branched and ldPE topologies (example topology: backbone with side branches)

Yaghini, N., Iedema, P.D. (2015). Branching determination from radius of gyration contraction factor in radical polymerization. Polymer 59, 166-179.

Molecular Photonics

Fingerprints of Polycyclic Aromatic Hydrocarbons in space

PAHs are notorious for being carcinogenic byproducts of, for example, combustion and grilled meat. However, PAHs are also found throughout the universe and are important because they provide clues on how matter is formed in interstellar space and how it eventually evolves to form stars and planets. The characteristic infrared radiation emitted by interstellar PAHs is a powerful means to identify these molecules. Using advanced laser spectroscopic methods under interstellar conditions, we have shown together with colleagues from the Leiden Observatory, the Radboud University, the SETI Institute and NASA Ames Research Center that PAH infrared spectra (the fingerprints) are far more complex than expected. This also means that models used up till now to simulate them deviate strongly from the interstellar reality. To rationalize these observations, a novel quantum-chemical approach to calculate and predict PAH spectra has been developed. A scenario now coming within reach is one in which astronomical observations can be translated directly into specific PAH compositions. The breakthrough achieved now is timely, since the James Webb Space Telescope will be launched in 2018. This instrument will be able to perform astronomical observations at unprecedented spectral and spatial resolution.



1.4.3 Prizes and honours


HIMS professors Joost Reek (Homogeneous, Supramolecular and Bio-inspired Catalysis group) and Huib Bakker (Molecular Photonics group, right photograph) were installed as members of the Royal Netherlands Academy of Arts and Sciences on 28 September 2015.

Prof. Peter Schoenmakers of the Analytical Chemistry Group was awarded the Csaba Horváth Memorial award, an honorable distinction in the field of separation science recognizing his leading position in the field of Analytical Chemistry. Schoenmakers also received the 20th annual CASSS award for outstanding achievements in separation science. It honours his life-long contributions to this field, with particular consideration for his development of new methods and techniques. Finally Schoenmakers maintained his 7th position on the 'Analytical Sciences Power List' compiled by the magazine 'The Analytical Scientist'. In a European perspective he holds the third position, as in the previous edition of 2013.

In December 2015 Prof. Bas de Bruin (Bio-inspired Catalysis) was elected Faculty Lecturer of the Year 2015 by the students of the Faculty of Science. As one of the seven faculty winners he competed for the title of UvA Lecturer of the Year, which was awarded to him on 8 January 2016 during the 384th Dies Natalis after scrutiny by the Student Council and the ASVA Student Union.

At the HPLC2015 international symposium on high performance liquid-phase separations, held in Geneva in June, postdoc researcher Andrea F.G. Gargano (left at picture) of the Analytical Chemistry group won the Csaba Horváth Young Scientist Award. His colleague PhD student Henrik Cornelisson van de Ven won an Agilent Best Poster Award at the same symposium.

Jurn Heinen, PhD student in the Computational Chemistry research group, won 2000 euro with his MSc thesis on the computational modeling of a catalytic alumina surface. On 6 June 2015 he finished as runner-up in the competition for the UvA Thesis Prize 2015.

Dr. Tatu S. Kumpulainen of the Molecular Photonics group was awarded the Dick Stufkens Prijs for the best PhD thesis of the Holland Research School of Molecular Chemistry (HRSMC). It was presented to him at the annual HRSMC symposium on 5 November 2015.

At the HPLC2015 conference held in September in Beijing, PhD student Bob Pirok of the Analytical Chemistry group was awarded a Shimadzu Young Scientist Award. He was the only non-Chinese recipient among five award winners.

At the NanoCity2015 conference held 5-6 October 2015 in Amersfoort, PhD student Marta Mourão of the Analytical Chemistry group received an award for her poster 'Can we use Biomarkers in Sputum for Early Diagnosis of Tuberculosis?'. She received a certificate and 500 euro.

1.4.4 Grants

Title	**Solardam; Energy from the sun – a concerted approach**
Applicants	Prof.dr. Joost Reek et al
Partners	IoP, VU, AMOLF, ECN
Grant from	UvA-VU AAA fonds
Amount	k€ 1.000 (k€ 250; 3 year postdoc for HIMS)

Title	**Alternative plastics made from plants**
Applicants	Prof.dr. Gadi Rothenberg
Partners	Plantics BV
Grant from	STW take off
Amount	k€ 40

Title	**MANIAC – Making Analytically Incompatible Approaches Compatible**
Applicants	Prof.dr. Peter Schoenmakers, prof.dr. Ron Peters, et al
Partners	DSM, Shell, Heineken, Micronit Microfluidics, VU, RU, RuG
Grant from	NWO/TI COAST
Amount	k€ 1.038 (1 PhD student and 3 year postdoc for HIMS)

Title	**Development of a Vibrational Optical Activity analysis toolbox from chiroptical spectra to molecular stereochemistry and conformation**
Applicants	Prof.dr. Wybren Jan Buma et al
Partners	Scientific Computing & Modelling, Biotools Inc, VU
Grant from	NWO NCI TA
Amount	k€ 1.147 (1 PhD student and 3 year postdoc plus equipment for HIMS)

Title	**NANOmaterials for the RESToration works of ART**
Applicants	Dr. Katrien Keune et al
Partners	Rijksmuseum,
Grant from	H2020-Art
Amount	1 PhD

Title	**Image-Guided Surgery and Personalised Postoperative Immunotherapy To Improving Cancer Outcome (ISPIC)**
Applicants	Prof.dr. Hong Zhang et al
Partners	7 academic institutes, 2 medical centres, 4 industrial partners from 5 European countries
Grant from	ERC ITN Curie
Amount	k€ 3.500 (1 PhD student for HIMS)

Title	**Camera ready? Action!**
Applicants	Dr. Moniek Tromp
Grant from	NWO Vidi
Amount	k€ 800

Title	**Shapes and formats of extraterrestrial organic molecules**
Applicants	Dr. Annemieke Petrignani
Grant from	NWO Vidi
Amount	k€ 800

Title	**Photocuring created network Topologie**
Applicants	Prof.dr. Piet Iedema
Partners	Océ
Grant from	STW, Topsector HTSM
Amount	1 PhD student

Title	**Catalysis in Confined Spaces**
Applicants	Prof.dr. Gadi Rothenberg, prof.dr. Joost Reek et al
Partners	RuG
Grant from	NWO TOP-Punt
Amount	k€ 2.000 (6 PhD students for HIMS)

Title	**Preclinical Intraoperative Image-Guided Surgery and Postoperative Radiotherapy of Tumours**
Applicants	Dr. Hong Zhang et al
Partners	LUMC, Percuros (Dutch company), TECO Bioscience (German company)
Grant from	NWO NCI TA
Amount	k€ 1.038 (1 PhD student for HIMS)

Title	**Intact Protein Analysis**
Applicants	Dr. Andrea Gargano
Grant from	NWO Veni
Amount	k€ 250

Title	**Deterministic modelling in multiple dimensions**
Applicants	Dr. Yvan Kryven
Grant from:	NWO Veni
Amount	k€ 250

Title	**DIMPHos based transition metal catalysis for selective synthesis**
Applicant	Prof.dr. Joost Reek
Partner	InCatT
Grant from	NWO NCI LIFT
Amount	1 PhD student

Title	**Transition-metal catalyzed epimerization-free peptide C-terminal activation and fragment coupling**
Applicant	Prof.dr. Jan van Maarseveen
Partner	Enzypep
Grant from	NWO NCI LIFT
Amount	1 year postdoc

Title:	**In-situ Ageing and Conservation Studies on Metal-containing Works of Art**
Applicants	Dr. Moniek Tromp, dr. Katrien Keune, dr. Annelies van Loon et al.
Partners	Rijksmuseum Amsterdam, UvA Conservation & Restoration, Cultural Heritage Agency
Grant from	NWO - NICAS
Amount	k€ 25

Title	**PREDicting AGIng of Oil networks (PREDAGIO)**
Applicants	Prof.dr. Piet Iedema, dr. Katrien Keune, dr. Annelies van Loon et al.
Partners	Rijksmuseum Amsterdam, UvA Conservation & Restoration, Cultural Heritage Agency, TU/e
Grant from	NWO - NICAS
Amount	k€ 456

Title	**Preparation of Complex Oxide Systems/Understanding and Designing Catalysts**
Applicant	Dr. Moniek Tromp
Partner	Clariant
Grant from	NWO NCI LIFT
Amount	1 PhD student

Title	**Sustainable synthesis of biaryl compounds via aerobic cross-dehydrogenative coupling**
Applicant	Dr. Tati Fernandez
Partner	DSM
Grant from	NWO NCI LIFT
Amount	1 year postdoc

Title	**Developing novel catalytic materials for converting CO2, methane and ethane to high-value chemicals in a hybrid plasma-catalytic reactor**
Applicants	Dr. N.R. Shiju, prof.dr. A.W. Kleijn
Partner	CIDS, Chengdu, China
Grant from	NSFC-NWO Advanced Materials
Amount	k€ (1 PhD student for HIMS)

Title	**An e-infrastructure for software, training and consultancy in simulation and modelling (E-CAM)**
Applicants	Prof.dr. Peter Bolhuis
Partners	16 European universities
Grant from	EU H2020-EINFRA
Amount	k€ 4.836 (k€ 176 for equipment within HIMS)

Title	**Forensic Explosives Intelligence (FEXIN)**
Applicants	Prof.dr. Arian van Asten
Partners	TNO, NFI
Grant from	NCTV
Amount	1 PhD student

Title	**Renewable fuels by tuning nature**
Applicants	Prof.dr. Lucas Visscher, prof.dr. Wybren Jan Buma
Partners	VU
Grant from	FOM, CSER
Amount	1 PhD student at VU (no funding to HIMS)

Title	**Non-classical crystallization of gas hydrate and calcium carbonate under reservoir and transport conditions**
Applicants	Prof.dr. Peter Bolhuis
Grant from	FOM, CSER
Amount	1 PhD student

Title	**Unravelling the mechanism of biomimetic hydrogen fuel production**
Applicants	Dr. Bernd Ensing
Grant from	FOM, CSER
Amount	1 PhD student

Title	**Operando XAS measurements of a novel Iron electrode for low-cost energy storage**
Applicant	Dr. Moniek Tromp
Partners	E-Stone batteries, TU Delft
Grant from	NWO NCI KIEM
Amount	k€ 18

Title	**Solar fuel device based on molecular components**
Applicant	Dr. Remko Detz, prof.dr. Joost Reek
Grant from	Bio Solar Cells PoP Grant
Amount	k€ 36

Title	**Debottlenecking of chromatographic separations (DEBOCS)**
Applicants	Prof.dr. Peter Schoenmakers
Partners	VU Brussels and private partners DSM Coating Resins, Dow Benelux, Janssen Pharma, Research Institute for Chromatography, Abundnz
Grant from	STW/ITW (Belgium)
Amount	k€ 416 (1 PhD student and 1 year postdoc for HIMS)

Title	**Hypovalency in Catalysis; Towards Sustainable C-H Bond Functionalization & Carbene Polymerisation**
Applicant	Prof.dr. Bas de Bruin
Grant from	NWO CW TOP
Amount	k€ 780

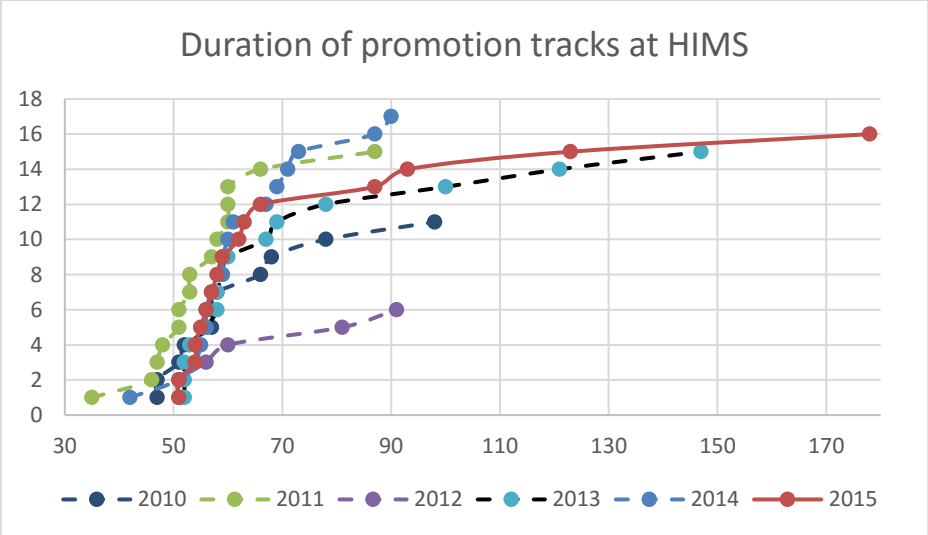
Subsidies brought by new staff members:

Title	**New strategies to sustainable procedures based on metal-catalyzed C-H functionalization**
Applicant	Dr. Tati Fernandez
Grant from	NWO Vidi 2014
Amount	k€ 800

Title	**The design and development of efficient biocatalytic cascades and biosynthetic pathways for the sustainable production of amines**
Applicants	Dr. Francesco Mutti
Grant from	ERC Starting Grant 2014
Amount	k€ 1.500

1.4.5 Dissertations

first name		Name	Promotor(es)	Co-promotor(es)	Promotion date	Duration in months
Jochem		Rutters	prof.dr. H. Hiemstra	dr. J.H. van Maarseveen	2015-01-13	87
Bart	van den	Bosch	prof.dr. J.N.H. Reek	prof.dr. S. Woutersen	2015-01-27	57
Yoshiko		Shimazu	prof.dr. J.J. Boon	dr. K. van den Berg	2015-02-05	n.a. [1]
Sander		Oldenhof	prof.dr. J.N.H. Reek	dr.ir. J.I. van der Vlugt	2015-03-10	54
Nazila		Yaghini	prof.dr. P.D. Iedema		2015-03-24	58
Stanimir		Popovic	prof.dr. H. Hiemstra	dr. J.H. van Maarseveen	2015-05-13	63
Tatu		Kumpulainen	prof.dr. A.M. Brouwer	prof.dr. S. Woutersen	2015-05-21	55
Aleksandra		Chojnacka	prof.dr.ir. P.J. Schoenmakers	prof.dr.ir. J.G.M. Janssen	2015-05-26	93
Dirk		Visser	prof.dr. P.D. Iedema	dr. C.P. Lowe	2015-06-03	178
Rudy		Vonk	prof.dr.ir. P.J. Schoenmakers		2015-06-30	51
Heleen		Meuzelaar	prof.dr. S. Woutersen	dr. J. Vreede	2015-06-30	56
Tibert	van der	Loop	prof.dr. S. Woutersen	prof.dr. H.J. Bakker	2015-09-15	66
Soraya		Sluijter	prof.dr. C.J. Elsevier	dr.ir. J.I. van der Vlugt	2015-09-18	51
Liyuan		Liu	prof.dr. H.J. Bakker		2015-10-28	n.a. [1]
Jurriaan		Luiken	prof.dr. P.G. Bolhuis		2015-11-11	62
Stephan		Lotze	prof.dr. H.J. Bakker		2015-11-19	n.a. [1]
Ivo		Jacobs	prof.dr. J.N.H. Reek		2015-11-27	123
Katja		Davydova	prof.dr.ir. P.J. Schoenmakers		2015-12-03	54
Zhou		Tang	prof.dr. B. de Bruin	dr.ir. J.I. van der Vlugt	2015-12-04	59



The graph above shows the duration of promotion tracks at HIMS (from start to *hora est*) in months for the past years. Each dot represents a single PhD. The median value decreased from 2014 to 2015 with half a month. It is the institute's ultimate aim to have a median value of 51 months (48 months to prepare a manuscript plus three months for the formalities External prepared promotions are not taken into account in these figures.

[1] Promotion prepared outside the HIMS laboratories.

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 another two new tenure track candidates were hired in 2015. This paragraph contains the reports of the following groups:

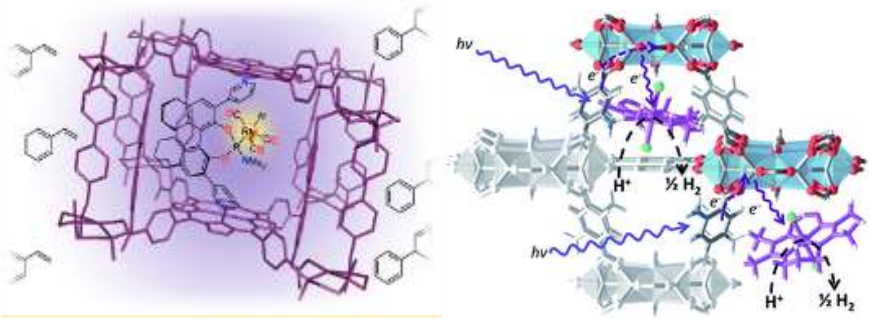
- Homogeneous and Supramolecular Catalysis
- Heterogeneous Catalysis and Sustainable Chemistry
- Synthetic Organic Chemistry
- Molecular Inorganic Chemistry
- Biocatalysis and Bio-organic Chemistry

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. M. Tromp Dr.ir. J.I. van der Vlugt		
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	1-9-2013	31-12-2015
	Dr. W.I. Dzik	1-11-2013	31-10-2016
	Dr. S. Mathew	1-9-2015	31-8-2016
	Dr. S. Gonell Gomez	1-5-2015	30-4-2016
	Dr. M.N. Devillard	1-3-2015	31-12-2016
	dr. T.J. Korstanje	1-12-2015	31-01-2017
	dr. D.J. Martin	1-10-2015	30-09-2016
	Dr. A.E. Pascui	1-1-2014	30-6-2015
	Dr. S. Raoufmoghaddam	31-1-2016	31-1-2016
	Dr. Q. Wang	31-12-2015	1-12-2015
	Dr. X. Wang	01-05-2014	30-4-2016
	Dr. B. Bagh	15-1-2015	31-12-2016
	Dr. B.G. Das	1-7-2015	30-6-2016
PhD students	Ing. R. Becker	1-3-2012	29-2-2016
	Drs. S. Bai	1-9-2015	31-8-2019
	Drs. S.Y. Boer	15-8-2011	14-8-2015
	Drs.ing. D.L.J. Broere	15-5-2012	14-5-2016
	Drs. A. Chirila	1-9-2012	31-8-2016

	Drs. J.J.M. Daubignard	1-1-2011	31-12-2015
	Drs. M. Goswami	1-8-2013	31-7-2017
	Drs. C. te Grotenhuis	1-8-2013	31-7-2017
	Drs. A.P.T. Hartendorp	1-9-2015	31-8-2019
	Drs. J. Hessels	1-10-2015	30-9-2019
	Drs. A.C.H. Jans	15-3-2014	14-3-2018
	Drs. L.S. Jongbloed	15-2-2012	14-2-2016
	Drs. L.J. Jongkind	1-9-2014	31-8-2018
	Drs. J.M. Koelewijn	1-2-2011	31-1-2016
	Drs. P.F. Kuijpers	1-10-2012	30-9-2016
	Drs. S.H.A.M. Leenders	1-10-2011	30-9-2015
	Drs. S.S. Nurttila	1-6-2014	31-5-2018
	Drs. S. Oldenhof	1-10-2010	28-2-2015
	J.P.H. Oudsen MSc	01-09-2015	30-08-2019
	Drs. R. Plessius	1-10-2015	30-9-2019
	Drs. C. Rebreyend	1-8-2013	31-7-2017
	Drs. E.C.F. Schippers	1-11-2013	31-10-2017
	Drs. V. Sinha	1-9-2014	31-8-2018
	Drs. V. Subbiah	1-1-2015	31-12-2015
	Drs. B. Sun	1-10-2015	30-9-2019
	B. Venderbosch MSc	1-11-2015	31-10-2019
	Drs. K.M. van Vliet	1-11-2015	31-10-2019
	Drs. V. Vreeken	1-5-2012	30-4-2016
	Drs. F.F. van de Watering	1-11-2012	31-10-2016
	Drs. R.Zaffaroni	1-12-2012	30-11-2016

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.

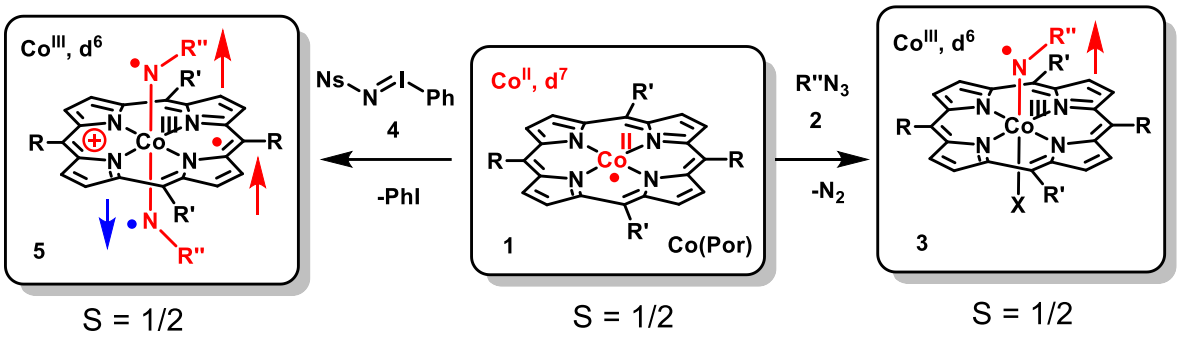
Research highlights per staff member
Prof.dr. Joost Reek
We continued our efforts to develop bio-inspired supramolecular catalysts for various transformations. In one example, we have generated a system in which a chiral rhodium complex is encapsulated in a self-assembled metallocage (figure left below). Once placed in confined space the catalyst converted styrene into chiral aldehyde with high selectivity. Also in the area of catalysis for green energy applications we have been exploring various bio-inspired supramolecular approaches. We have used METAMORphos as a proto-reactive ligand in formic acid dehydrogenation, which is important in the context of hydrogen storage. In collaboration with a Gascon from Delft, we have generated cobalt catalyst in the confined spaces of a MOF. This systems has been demonstrated to be active in the light-driven hydrogen formation reaction (right figure below), which is important in the context of our solar to fuel program.



- Enantioselective hydroformylation by a Rh-catalyst entrapped in a supramolecular metallocage García-Simón, C.; Gramage-Doria, R.; Raoufmoghaddam, S.; Parella, T.; Costas*, M.; Ribas*, X.; and Reek*, J. N.H. *J.Am. Chem. Soc.* **2015**, *137*, 2680-2687.
- Co@ NH 2-MIL-125 (Ti): cobaloxime-derived metal--organic framework-based composite for light-driven H 2 production. Nasalevich, M. A.; Becker, R.; Ramos-Fernandez, E. V.; Castellanos, S.; Veber, S. L.; Fedin, M. V.; Kapteijn, F.; Reek*, J. N. H.; van der Vlugt,* J. I.; and Gascon*, J. *Energy Environ. Sci.* **2015**, *8*, 364-375.
- Dehydrogenation of formic acid by Ir--bisMETAMORPhos complexes: experimental and computational insight into the role of a cooperative ligand. Oldenhof, S.; Lutz, M.; de Bruin, B.; van der Vlugt, J. I.; and Reek*, J. N. H. *Chem. Sci.* **2015**, *6*, 1027-1034.

Prof.dr. Bas de Bruin

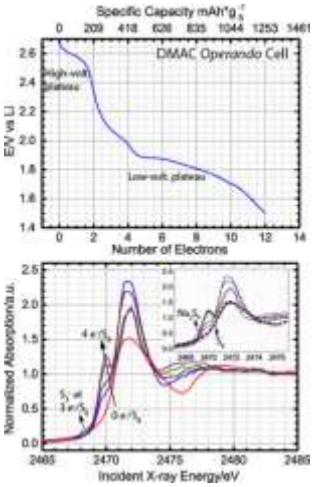
Besides the work on acid hydrogenation (as described above in the group highlight), the sub-group of de Bruin further contributed the field of metallo-radical catalysis. One of the highlights in this field is a study reported in JACS describing detailed spectroscopic characterization of the nitrene-radical intermediates of key relevance in (por)Co-catalyzed nitrene-transfer reactions. These key-intermediates were characterized with several techniques (EPR, XAS, UV-Vis, ESI-MS, IR, VCD). Several unexpected insights evolved from this study, such as the fact that mono- and bis-nitrene intermediates can be formed of which the latter are quite unstable, and the fact that mono-nitrene species are 6-coordinate. This insight is of importance for further development of efficient nitrene-transfer catalysis, in particular for selective C-H bond amination.



- *Hydrogenation of Carboxylic Acids with a Homogeneous Cobalt Catalyst, Korstanje, T.J.; van der Vlugt, J.I.; Elsevier, C.J.*; de Bruin, B.*, Science, **2015**, 350 (6258), 298-302. DOI: 10.1126/science.aaa8938. [link]*
- *Dynamic Ligand Reactivity in a Rhodium Pincer Complex, Tang, Z.; Otten, E.; Reek, J.N.H.; van der Vlugt, J.I.*; de Bruin, B.*, Chem. Eur. J., **2015**, 21, 12683–12693. [link] **'Hot Paper'. Front Cover. Cover Profile.***
- *Characterization of Porphyrin-Co(III)-'Nitrene radical' species relevant in catalytic nitrene transfer reactions. Goswami, M.; Lyaskovskyy, V.; Domingos, S.R.; Buma, W.J.; Woutersen, S.; Troeppner, O.; Ivanović-Burmazović, I.; Lu, H.; Cui, X.; Zhang, X.P.*; Reijerse, E.J.; DeBeer, S.; van Schooneveld, M.M.; Pfaff, F. F.; Ray, K.; de Bruin, B.*, J. Am. Chem. Soc., **2015**, 137, 5468–5479. [link]*

Dr. Moniek Tromp

The development, application and interpretation of X-ray absorption and X-ray emission spectroscopy has been continued and expanded (JPhysChemC2015), showing great potential in obtaining detailed electronic properties from the data directly (without complicated simulation/analysis procedures).



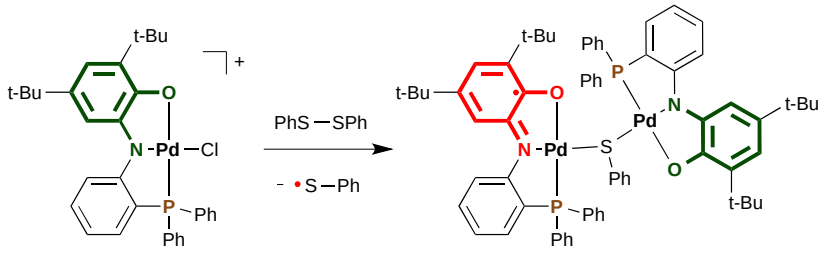
At the same time our efforts in the electrochemical field were awarded by the successful development of a spectro-electrochemical cell for the operando X-ray absorption spectroscopy study of batteries (JES2015). The cell allows spatial- and time-resolved characterization of species in the individual electrodes as well as the electrolyte, during charging and discharging, thereby providing novel insights in mechanisms and deactivation processes, important for the development of novel high capacity and stable battery systems for, for example, the automotive industry.

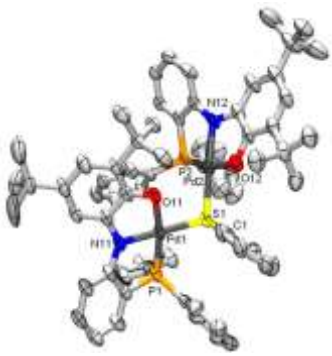
An important application of our advanced spectroscopy methods led, in the heterogeneous catalysis field, towards a breakthrough in understanding the structure and electronics of the catalytically active Cu site for the important methane to methanol (gas-to-liquid) reaction (NatureComm215).

- R. J. Thomas, J. Kas, P. Glatzel, M. Al Samarai, F. M. F. de Groot, R. A. Mori, M. Kavcic, M. Zitnik, K. Bucar, J. J. Rehr, M. Tromp, 'Resonant Inelastic X-ray Scattering of molybdenum oxides and sulfides', J. Phys. Chem. C 2015, 119(5), 2419–2426.
- Y. Gorlin, A. Siebel, M. Piana, T. Huthwelker, H. Jha, G. Monsch, F. Kraus, H. A. Gasteiger, M. Tromp, 'Operando Characterization of Intermediates Produced in a Lithium-Sulfur Battery', J. Electrochem. Soc. 2015, 162(7), A1146-A1155.
- S. Grundner, M. Markovits, G. Li, M. Tromp, E. A. Pidko, E.J.M. Hensen, A. Jentys, M. Sanchez-Sanchez, J.A. Lercher, 'Single site trinuclear copper oxygen clusters in mordenite for the selective methane to methanol conversion', Nature Commun. 2015, 6, 7546.

Dr.ir. Jarl Ivar van der Vlugt

The sub-group of van der Vlugt continued research in the field of reactive ligand-induced substrate activation. One of the highlights is a study reported in ACIE detailing the homolytic activation of homodiatomic bonds (e.g. disulfides) on closed-shell Pd(II) platforms, via redox-active ligand-to-substrate single electron transfer. This work enables the formation of unique ligand-based mixed-valent dinuclear architectures, which have interesting switchable photochemical and magnetochemical properties. Furthermore, the conceptual design of a new flexidentate ligand led to the first example of reversible facile cyclometalation on Rh(I), with isolation of a rare Rh-(C-H) agostic complex. Finally, the use of a reactive pincer ligand has allowed the activation of a well-defined nickel-azido species, with intermediacy of a transient nickel-nitrido complex. These developments and mechanistic insights are of relevance for a number of catalytic applications, which are currently under investigation.





Redox-Active Phosphine Ligand
Ligand-to-Substrate Single-Electron Transfer
Ligand-based Mixed Valent Dinuclear Pd-complex

- Efficient C-H activation of arenes by a photoactivated Ni^{II}(azide) – Formation of a transient nickel nitrido complex, V. Vreeken, M. Lutz, B. de Bruin, J. N. H. Reek, M.A. Siegler, J.I. van der Vlugt* Angew. Chem. Int. Ed. 2015, 54, 7055-7059.
- *Facile synthesis and versatile reactivity of an unusual cyclometalated Rh^{I} pincer complex, L.S. Jongbloed, B. de Bruin, J.N.H. Reek, M. Lutz, J.I. van der Vlugt* Chem. Eur. J.* 2015, *21*, 7297-7305.
- Redox-active ligand-induced homolytic bond activation, D.L.J. Broere, L.L. Metz, B. de Bruin, J.N.H. Reek, M.A. Siegler, J.I. van der Vlugt* *Angew. Chem. Int. Ed.* 2015, *54*, 1516-1520.

Other activities
Hier kunnen andere activiteiten/samenwerkingen met andere groepen (binnen en buiten HIMS) beschreven worden, die buiten de bovengenoemde activiteiten vallen.

Prof.dr. Joost Reek
Collaboration with many several groups from the BIOSOLARCEL and SOLARDAM network. Collaboration with Prof Gascon TU Delft, Prof Ivanovic-Burmazovic Univeristy Erlangen, Prof Ribas, IFP, Lyon, EASTAN USA.
- 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.*
- 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 form
- Steering committee Co van Ledden Hulsebosch Center
- Member of the World economic forum

Dr. Moniek 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)
- Visiting Professor Technical University Munich (Germany)
- Member of NWO TOP-ECHO review panel.
- Secretary of the organizing committee of the EuCheMS International Conference on Organometallic Chemistry 2017 in Amsterdam.
- Secretary of the organizing committee of the International Symposium on Homogeneous Catalysis 2018 in Amsterdam.
- Member of the Spectroscopy Village Beamlines Review Committee, Diamond Light Source.
- Chair of the Peer Review Panel (incl. all sub-committees) of the Swiss Light Source. Chair of the hard X-ray panel.
- Member of the Scientific Advisory Panel of the Swiss Light Source.
- Board member of the Dutch Catalysis Society.
- Member of the core-committee for the Dutch Belgium (DUBBLE) beamline at the ESRF in France.
- Member of BMW Diesel IAS-TUM focus group on ‘Electrochemical Interfaces in Batteries’
- Member of the Scientific Advisory Committee of the SOLEIL synchrotron.

- Member ‘Agentschap voor Innovatie door Wetenschap en Technologie’ (IWT) evaluation panel PhD proposals.
- Member of the European Synchrotron User Organisation Committee.
- Member of the international user committee of the ANKA research facility (Karlsruhe, Germany).
- Member of the MAX Laboratory (Lund, Sweden) Program Advisory Committee.
- Member of the Swiss Light Source Peer Review Panel (2009-current). Chair of the Hard X-ray Committee of the Pair Review Panel since 2011.

Dr.ir. Jarl Ivar van der Vlugt

Collaboration with Prof Gascon TU Delft, prof. Meyer/dr. Demeshko (Goettingen), dr. Siegler (John Hopkins), dr. Carbo (Tarragona)

- Member, Board of Examinations, Chemistry UvA/VU
- Member, Advisory Board Technology Center FNWI, UvA
- Member, Sounding Board to the Dean, FNWI, UvA
- Member, Management Team, COST Action CHAOS

Dissertations

Bart van den Bosch, (co-)promotors: prof.dr. J.N.H. Reek, prof.dr. S. Woutersen
Sander Oldenhof, (co-)promotors: prof.dr. J.N.H. Reek, dr.ir. J.I. van der Vlugt
Soraya Sluijter, (co-)promotors: prof.dr. C.J. Elsevier, dr.ir. J.I. van der Vlugt
Ivo Jacobs, (co) promotors: prof.dr. J.N.H. Reek, prof.dr. B. de Bruin
Zhou Tang, (co-)promotors: prof.dr. B. de Bruin, dr.ir. J.I. van der Vlugt

Grants

Title	Solardam; Energy from the sun – a concerted approach
Applicants	Prof.dr. Joost Reek et al
Partners	IoP, VU, AMOLF, ECN
Grant from	UvA-VU AAA fonds
Amount	k€ 1.000 (k€ 250; 3 year postdoc for HIMS)

Title	Camera ready? Action!
Applicants	Dr. Moniek Tromp
Grant from	NWO Vidi
Amount	k€ 800

Title	Catalysis in Confined Spaces
Applicants	Prof.dr. Gadi Rothenberg, prof.dr. Joost Reek et al
Partners	RuG
Grant from	NWO TOP-Punt
Amount	k€ 2.000 (6 PhD students for HIMS)

Title	DIMPHos based transition metal catalysis for selective synthesis
Applicant	Prof.dr. Joost Reek
Partner	InCatT
Grant from	NWO NCI LIFT
Amount	1 PhD student

Title:	In-situ Ageing and Conservation Studies on Metal-containing Works of Art
Applicants	Dr. Moniek Tromp, dr. Katrien Keune, dr. Annelies van Loon et al.
Partners	Rijksmuseum Amsterdam, UvA Conservation & Restoration, Cultural Heritage Agency
Grant from	NWO - NICAS
Amount	k€ 25

Title	Preparation of Complex Oxide Systems/Understanding and Designing Catalysts
Applicant	Dr. Moniek Tromp
Partner	Clariant
Grant from	NWO NCI LIFT
Amount	1 PhD student

Title	Solar fuel device based on molecular components
Applicant	Dr. Remko Detz, prof.dr. Joost Reek
Grant from	Bio Solar Cells PoP Grant
Amount	k€ 36

Title	Hypovalency in Catalysis; Towards Sustainable C-H Bond Functionalization & Carbene Polymerisation
Applicant	Prof.dr. Bas de Bruin
Grant from	NWO CW TOP
Amount	k€ 780

Title	Operando XAS measurements of a novel Iron electrode for low-cost energy storage
Applicant	Dr. Moniek Tromp
Partners	E-Stone batteries, TU Delft
Grant from	NWO NCI KIEM
Amount	k€ 18

Prizes

Prof.dr. Joost Reek was elected member of the KNAW.
Prof.dr. Bas de Bruin was elected as 'UvA teacher of the year 2015', in a university-broad competition organized by the students of the University of Amsterdam.

Invited lectures

Joost Reek

1. Plenary lecture farewell symposium Prof van Leeuwen," Supramolecular strategies in transition metal catalysis, with a focus on hydroformylation" Barcelona, february 2015.
2. Plenary lecture at the GEQO meeting on organometallics and catalysis," Supramolecular strategies in transition metal catalysis" Madrid, May 2015.
3. Invited lecture at the Gordon conference organometallics," Supramolecular strategies in transition metal catalysis" New port US, July 2015.
4. Invited lecture at Eastman, "Supramolecular strategies in transition metal catalysis" Kingsport,September 2015.
5. Plenary lecture Ernst Hage symposium," Supramolecular asymmetric transition metal catalysis" Mulheim, Germany, december 2015.
6. Invited lecture at CHAINS, "Towards solar to fuel devices based on molecular components: Veldhoven December 2015
7. Invited lecture Amsterdam-china symposium on sustainability "catalysis in confined spaces" Amsterdam December, 2015
8. Lecture at the pacifichem 2015," Towards solar to fuel devices based on molecular components" Honolulu US, december 2015.
9. Plenary lecture at the pacifichem 2015," Supramolecular asymmetric transition metal catalysis" Honolulu US, december 2015.

Bas de Bruin

1. Pacifichem 2015, Honolulu, Hawai, USA. Special symposium "Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications." December 15-20, 2015. Title: Radical-type catalytic reactions involving substrate radicals. **Invited speaker**
2. Reedijk Symposium 2015, Leiden, The Netherlands, October 30, 2015. Title: Catalytic Radical-Type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Radicals'. **Key Lecture**
3. 10th International School of Organometallic Chemistry (ISOC), Camerino, Italy, September 2-9, 2015. Title: New catalytic developments involving carbene reactivity.
4. Euchem Inorganic Chemistry Conference (EICC), Wroclaw, Poland, June 28-July 1, 2015. Title: Reactivity of Substrate Radicals. **Keynote Lecture**
5. Seminar at the ETH Zürich (LAC lecture series), Switzerland, May 19, 2015. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of 'Carbene and Nitrene Radicals'. Host: Hansjörg Grützmacher.
6. Seminar at the University of Toronto, Canada, April 7, 2015. Title: Catalytic Reactivity of Carbene & Nitrene Radicals. Host: Bob Morris.
7. Gordon Research Conference on Reaction Mechanisms, Texas, USA, Hotel Galvez, March 1-6, 2015. Title: New Catalytic Reactions with Carbene & Nitrene Radicals. Organizer: Paul Chirik.
8. 13th IBN SINA International Conference on Pure and Applied Heterocyclic Chemistry (13th IBN SINA), Hurghada, Egypt, February 14-17, 2015. Title: New Catalytic Reactions with Carbene Radicals. **Plenary Lecture**
9. Seminar at the Freie Universität Berlin (Inorganic Chemistry department). Febr.10, 2015. Host
10. Prof. Biprajit Sarkar. Title: New Catalytic Reactions with Carbene Radicals.
11. KAUST Research Conference on Catalytic Carbon and Hydrogen Management (KRC-CCHM), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia, February 1-4, 2015, Title: New Catalytic Reactions with Carbene Radicals. Keynote Lecture.

Moniek Tromp

1. M. Tromp, 'Probing dynamic species in homogeneous catalysis', Invited Lecture, Winterschool Hubert Gasteiger (TUM Electrochemistry), Austria, March 2015.
2. M. Tromp, 'Multitechnique Approach to Understand Selective Oligomerisation Mechanisms', Invited Lecture, Operando V Conference, France, May 2015.
3. M. Tromp, 'Towards understanding selective Oligomerisation Catalysts', ISHHC 2015, Utrecht, June 2015.
4. M. Tromp, 'Operando XAS Characterisation of LiS Batteries', Invited Lecture, International XAFS 16 Conference, Germany, August 2015.
5. M. Tromp, "Towards Understanding Selective Cr-based Oligomerisation Catalysis", Invited Lecture, Leuven University, Heverlee, Belgium, September 2015.

Jarl Ivar van der Vlugt

1. 3rd COST CARISMA Annual Symposium, Tarragona, Spain (Mar 2015) *Redox-Active and Reactive Ligands – Attractive & Versatile Concepts for Small Molecule Activation and Much More*
2. 11th International Conference on Heteroatom Chemistry *(ICHAC), Caen, France – keynote* (June 2015) *Redox-Active Ligand Induced Single Electron Reactivity on Closed-Shell Noble Metals*
3. 3rd EuCheMS Inorganic Chemistry Conference (EICC), Wroclaw, Poland (July 2015) *Odd Electron Reactivity at Late Transition Metals Mediated by Redox-Active Ligand-to-Subtrate Single Electron Transfer*
4. 6th EuCheMS Conference on Nitrogen Ligands, Beaune, France (Sep 2015) *Odd Electron Reactivity at Late Transition Metals Mediated by Redox-Active Ligand-to-Subtrate Single Electron Transfer*
5. International Chemical Congress, Pacific Basin Societies (PACIFICHEM), Honolulu HI, USA (Dec 2015)
   - *Facile Synthesis and Versatile Reactivity of Cyclometalated Rh^{I} and Ni^{II} Pincer Complexes*
   - *Efficient C-H Activation of Arenes by a Photoactivated Ni^{II}(azide)*
   - *Redox-Active Ligand Induced Single-Electron Reactivity on Closed-Shell Noble Metals*

Patents and utilization

Topic	Photosensitiser based on Cu and Ni
Staff members	Prof.dr. Fred Brouwer, Prof.dr. Joost Reek, Hung-Cheng Chen M.Sc.
Activities	Patent filed. SBI student identified and contacted 22 companies that may be interested. Discussions with 8 of them started, two companies are serious interested in collaboration with HIMS.

Topic	Olefin oligomerisation catalysts
Staff members	Prof.dr. Joost Reek, Pierre Boulens M.Sc.
Activities	Shared IP agreement with IFP Energies Nouvelles was drafted.

Topic	Cobalt based catalyst converts carboxylic acids to alcohols
Staff members	Prof.dr. Bas de Bruin, prof.dr. Kees Elsevier, dr. Jarl Ivar van der Vlugt, dr. Ties Korstanje
Activities	Patent was drafted, but company retracted in final stage. Other valorisation options are being explored.

Topic	In-situ and operando X-ray services
Staff members	Dr. Moniek Tromp
Activities	Investigation of possibilities for Spin-off company.

Outreach

Joost Reek

Proefstuderen december 2015

Bas de Bruin

UvA 2 April 2015, Gastcollege voor 4 VWO scholieren uit Zaandam. Titel: “Drinken Vampieren ook Blauw Bloed?”

Moniek Tromp

- M. Tromp, ‘The active site in the spotlight’, NWO VIDI pitch at KNCV event ‘Chemie tussen de Sterren’, Invited lecture, Sterrenwacht Leiden, November 2015.
- M. Tromp and E. Manders, ‘Het onzichtbare belicht’, UvA-FNWI Colloquium for general audience, SPUI25, Amsterdam, November 2015.
- M. Tromp and S. Kluwer, ‘Hoe maak je vuurwerk?’, Wakker worden Kinderlezingen, Nemo, Amsterdam, December 2015.

Jarl Ivar van der Vlugt

Press release 2015 *Faculty of Science* (website) (related to *Angew. Chem. Int. Ed.* **2015**, *54*, 7055)
C2W coverage on our group (related to first prize of M.Sc. student Raoul Plessius at PAC symposium 2015 for his poster on ‘Dinucleating redox-active ligands for dinuclear Pd complexes’)

Group	Heterogeneous Catalysis and Sustainable Chemistry		
Groupleader	Prof.dr. G. Rothenberg		
Academic staff	Dr. N.R. Shiju Dr. S. Grecea Dr. N. Yan		
Support staff	Ing. P.F. Collignon Ing. N.J. Geels		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. D.Eisenberg Dr. Z.Guo Dr. A. Narani Dr. J. Pandey Dr. P.L.K. Prinsen Dr. E.G.K. Solomon Raja	1-2-2015 1-6-2015 1-6-2015 1-7-2015 1-2-2014 1-7-2014	31-1-2016 31-5-2016 31-5-2016 30-6-2016 31-1-2016 30-6-2016
PhD students	Y. Tang MSc W. Zhang MSc Drs. Y. Gao Drs. V. Santacroce	1-10-2015 1-10-2015 1-9-2014 15-9-2014	30-9-2019 30-9-2019 31-8-2018 15-3-2015

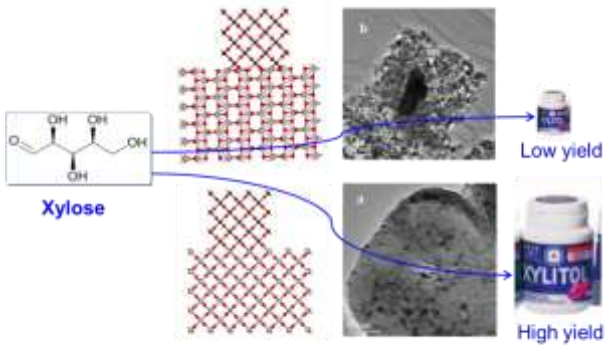
Mission of the group:

Our mission is to discover new catalysts and materials for sustainable chemistry applications by understanding what makes catalysis tick. We work chiefly on fundamental processes that relate to bulk chemicals and sustainable energy solutions. The applications include chemicals from biomass, fuel cells, multifunctional materials and finding new catalytic routes to a variety of industrial chemicals. Our strengths are in catalyst design, catalyst synthesis and testing, and characterization under real-life conditions. HCSC is interdisciplinary (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. N. Raveendran Shiju

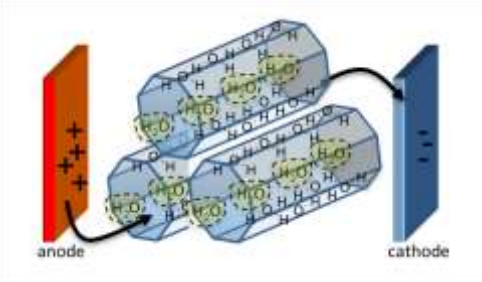
As part of our programme for converting lignocellulosic biomass into various industrially important chemicals, we studied the hydrogenation of xylose (a sugar obtained by the hydrolysis of beech wood hemicellulose) to xylitol, an extensively used compound in the food, cosmetics, and pharmaceutical sectors. With an estimated market of $340m, xylitol is one of the most popular sweeteners. Currently, xylitol is made via catalytic hydrogenation over RANEY® nickel. Although this catalyst is cheap, it deactivates quickly due to leaching and/or poisoning. Any leached Ni must be removed, leading to additional costs. In this work, we found that Ru supported on TiO_2 is a highly efficient catalyst. However, we also found that the same TiO_2 support with different crystal structures (anatase or rutile) gives very different catalytic efficiency. Characterization of catalysts showed that (mis)matching between the active species and the support is the secret. Similar crystal structures of RuO_2 and rutile titania ensure a better interaction during the heating steps of catalyst synthesis. This helps maintain the initial good dispersion of the active species on the support, leading to better activity and selectivity.



Better matching between rutile RuO_2 and rutile titania support leads to smaller Ru particles and higher catalytic activity.

- Ru/TiO_2-catalysed hydrogenation of xylose: the role of crystal structure of the support. C. Hernandez-Mejia, E.S. Gnanakumar, A. Olivos-Suarez, J. Gascon, H. Greer, W. Zhou, G. Rothenberg and N.R. Shiju, *Catal. Sci. Technol.*, 2016, 6, 577-582.
- Catalytic acetoxylation of lactic acid to 2-acetoxypropionic acid, en route to acrylic acid. R. Beerthuis, M. Granollers, D.R. Brown, H.J. Salavagione, G. Rothenberg and N.R. Shiju, *RSC Adv.*, 2015, 5, 4103-4108.
- Catalytic routes towards acrylic acid, adipic acid and ε-caprolactam starting from biorenewables. R. Beerthuis, G. Rothenberg and N.R. Shiju, *Green Chem.*, 2015, 17, 1341-1361.

Dr. Stefania Grecea

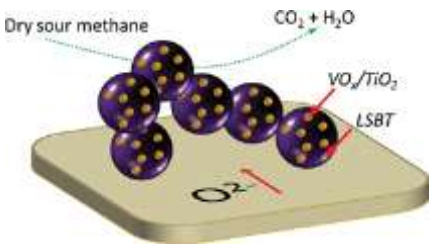


We have shown that metal organic frameworks (MOFs) with cyanide-bridges and highly hydrophilic open channels are excellent proton conductive materials. They enable high proton conductivity, as much as 10^{-3} Scm^{-1}. The MOF's channels contain two types of water molecules: coordinated ('in-the-framework') water and lattice (absorbed) water. Our studies show that it is the lattice water which is critical for the proton conductivity. The lattice water molecules form a hydrogen-bonding network, through which protons hop along *via* the Grotthuss mechanism. The fact that (unlike most MOFs) this material is also stable both in water and at relatively high temperatures (up to 150 °C) makes it a promising candidate for real-life applications. As we showed earlier, this class of materials has also special luminescence and magnetic properties. Combining these with ionic conductivity opens opportunities for designing proton-conducting switches controlled by temperature, light and/or external magnetic fields.

- A novel one-dimensional chain built of vanadyl ions and pyrazine-2,5-dicarboxylate. M. Lankelma, J. de Boer, M. Ferbinteanu, A. L. Dantas Ramos, R. Tanasa, G. Rothenberg, S. Tanase, Dalton Trans., 2015, 44, 11380-11387.
- High proton conductivity in cyanide-bridged metal-organic frameworks: understanding the role of water. Y. Gao, R. Broersen, W. Hageman, N. Yan, M.C. Mittelmeijer-Hazeleger, G. Rothenberg, S. Tanase J. Mater. Chem. A, 2015, 3, 22347-22352.
- Metal-organic frameworks with d-f cyanide bridges: structural diversity, bonding regime and magnetism. M. Ferbinteanu, F. Cimpoesu, S. Tanase, *Struct. Bond.*, 2015, *163*, 185-230.

Dr. Ning Yan

The fuel cells research was launched at HIMS in the year of 2015 during which we completed the constructions of two electrochemical setups. Regarding the research, we started with developing the sulfur/coke-resisting anode catalyst of solid oxide fuel cells. In particular, we discovered that the doped $SrTiO_3$ catalyst exhibited excellent stability and moderate activity towards methane electro-oxidation in the presence of sulfur poisons. Through an *in-situ* measurement, we understood that the sulfur adsorbates on the electrocatalyst actually promoted the activation of methane. To further enhance the activity of the titanate anode, we then developed a "vanadia grafting" technique. In addition, we succeeded in understanding the degradation mechanism of protonic ceramic electrolyte at ambient conditions, performing the first "metal-free" electrocatalyst trial for the cathode of proton-exchange membrane fuel cells, and developing a novel electrochemical route for "CO_2 to fuels" while generating electricity.



- Electrochemical oxidation of sour natural gas over $La_{0.4}Ce_{0.6}O_{1.8}$-$La_{0.4}Sr_{0.6}TiO_{3\pm\delta}$ anode in SOFC: A mechanism study of H_2S effects. M. Roushanafshar, N. Yan, K.T. Chuang & J.L. Luo, *Appl. Catal., B*, 2015. 176-177, 627-636.

- Highly cost-effective and sulfur/coking resistant VO_x-grafted TiO_2 nanoparticles as an efficient anode catalyst for direct conversion of dry sour methane in solid oxide fuel cells. A. Garcia, N. Yan, A. Vincent, A. Singh, J.M. Hill, K. T. Chuang & J.L. Luo. *J. Mater. Chem. A*, 2015, 3, 23973-23980.
- Discovery and understanding of the ambient-condition degradation of doped barium cerate proton-conducting perovskite oxide in solid oxide fuel cells. N. Yan, Y.M. Zeng, B Shalchi, W. Wang, T Gao, G. Rothenberg & J.L. Luo, *J. Electrochem. Soc.*, 2015. 162, F1408-F1414.

Other activities

HCSC has strong ongoing collaborations with Fudan University (Shanghai, China) and with the Center of Interface Dynamics for Sustainability (Chengdu, China) with joint research projects funded by NWO and by the NSFC and the local Shanghai government. The group also has a long-term ongoing collaboration funded by Solvay on catalysis for sustainable processes.

Grants

Title	Alternative plastics made from plants
Applicants	Prof.dr. Gadi Rothenberg
Partners	Plantics BV
Grant from	STW take off
Amount	k€ 40

Title	Catalysis in Confined Spaces
Applicants	Prof.dr. Gadi Rothenberg, prof.dr. Joost Reek
Partners	RuG
Grant from	NWO TOP-Punt
Amount	k€ 2.000 (6 PhD students for HIMS)

Title	Developing novel catalytic materials for converting CO_2, methane and ethane to high-value chemicals in a hybrid plasma-catalytic reactor
Applicants	Dr. N.R. Shiju, prof. dr. G. Rothenberg, prof.dr. A.W. Kleijn
Partner	CIDS, Chengdu, China
Grant from	NSFC-NWO Advanced Materials
Amount	k€ 300 (1 PhD student for HIMS)

Invited lectures (international)

Prof.dr. Gadi Rothenberg

1. Practical catalyst design: From nanometers to megatons. CNRS lab for eco-efficient products and processes, Shanghai, November 2015.
2. A practical approach to metal-free oxygen reduction catalysts. 1st International Symposium on Energy Chemistry & Materials, Fudan University, Shanghai, October 2015.
3. A new type of bioplastic made from plants. European Bioenergy Research Institute, Aston University, Birmingham, February 2015.
4. A new type of bioplastic made from plants. Reading University, Reading, February 2015.

Dr. N. R. Shiju

1. Catalysis in action: a few short stories. Max-Planck-Institut fuer Eisenforschung GmbH, Dusseldorf, March 2015.

Dr. Stefania Grecea

1. Proton conductive lanthanide-based metal-organic frameworks.1st International Caparica Christmas Congress on Translational Chemistry. Lisbon, December 2015.
2. Octacyanometallates - versatile building-blocks for constructing multifunctional molecular materials. 6th North America-Greece-Cyprus Workshop on Paramagnetic Materials, Athens, June 2015.

Dr. David Eisenberg

1. The black art of energy storage: Rational design of porous carbons for electrochemical applications. Department of Chemistry, Ben Gurion University, Beer Sheva, December 2015.
2. The black art of energy storage: Rational design of porous carbons for electrochemical applications. Department of Chemistry, Tel Aviv University, Tel Aviv, December 2015.
3. The black art of energy storage: Rational design of porous carbons for electrochemical applications. Department of Chemistry, Schulich Faculty of Chemistry, Technion, Haifa, December 2015.
4. A simple synthesis of an N-doped carbon ORR catalyst: Hierarchical pores lined with graphitic walls. Electrochemical Society Meeting. Glasgow, July 2015.

Dr. Pepijn Prinsen

1. Lignin depolymerisation in liquid ammonia: challenges and benefits. 1st International Workshop on Biorefinery of Lignocellulosic Materials, University of Cordoba, Cordoba, June 2015.

Patents and utilization

Topic	Catalyst to reduce CN levels in wastewater treatment
Staff members	Dr. Raveendran Shiju (co-inventor) Prof.dr. Gadi Rothenberg (co-inventor),
Activities	Follow-up research and pilot projects with the steel- and precious metals industry (patent filed in 2014; ongoing projects with several industrial partners, including Heimerle+Meule GmbH).

Topic	Plantics B.V.
Staff members	Prof.dr. Gadi Rothenberg
Activities	HIMS spin-off company received UvA Proof-of-Concept loan and has signed a licence agreement for transfer of IP. The company has started production on ton scale at its new facility in the Amsterdam harbor area. See http://www.plantics.com

Topic	Amsterdam Green Campus (AGC)
Staff members	Prof.dr. Michel Haring (SILS), dr. Shiju et al
Activities	HIMS participates in new platform for collaborating on education and valorisation.

Outreach

The group is involved in several high-profile projects that strongly connect the themes “Science & Society” and “Science & Industry”. For example, together with Utrecht University, WaterNet and the waste-to-energy company in Amsterdam (*afvalenergiebedrijf*) E. van der Roest (joint MSc student with Utrecht University) Prof. Gadi Rothenberg and Prof. Bob van der Zwaan (HIMS/ECN) have carried out a techno-eocnomic analysis on the conversion of waste toilet paper to electricity using a two step process of gasification followed by high-temperature fuel cells. The work is currently being considered for piloting by the *aeb* and has raised the interest in practical solutions of converting true waste streams to useful products.

Prof. Rothenberg was invited to the “Kamera Kultura” program of *Het Nutshuis* in The Hague, where he spoke about the bioplastic invention and the waste toilet paper project.

Group	Synthetic Organic Chemistry		
Group leader	Prof. dr. H. Hiemstra		
Academic staff	Prof. dr. J.H. van Maarseveen Prof. dr. P. Timmerman (bijzonder hoogleraar vanwege GdNGH) Dr. S. Ingemann Jørgensen Dr. M.A. Fernández Ibáñez		
Support staff	R. Klein Nijenhuis M.J. Wanner E. Zuidinga		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. C. Valderas Cortina	1-5-2015	31-7-2016
PhD students	K. Naksomboon MSc. S. Popović MSc. G.J.J. Richelle MSc. L. Steemers MSc. D.E. Streefkerk MSc. L. Wijsman MSc. S. Žari MSc. (Tallinn, Estonia)	1-9-2015 1-2-2010 1-11-2013 1-9-2012 1-6-2014 1-3-2015 1-11-2014	31-8-2019 31-5-2015 31-10-2017 31-8-2016 31-5-2018 28-2-2019 31-3-2015
MSc students	K. Vos M.L. Corrado M. Acquesta T.K. Slot J. Kayhan S.O. Ori M. de Bruijn T. van den Enk	1-9-2014 1-9-2014 1-9-2014 1-3-2015 1-3-2015 1-7-2015 1-9-2015 1-8-2015	30-6-2015 30-6-2015 30-6-2015 31-10-2015 31-12-2015 31-1-2016 30-6-2016 31-5-2016
Stagiair	V. Mudde (Hogeschool Utrecht)	1-9-2015	29-2-2016

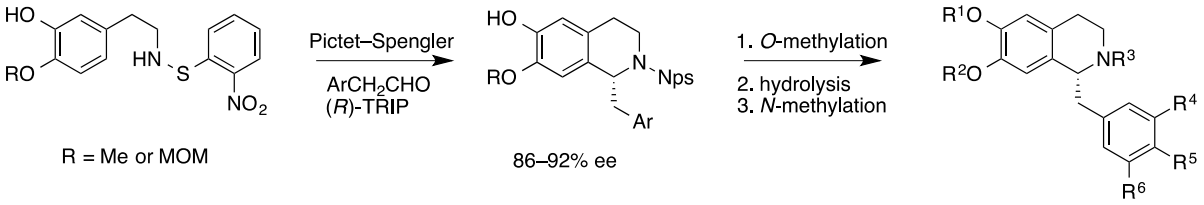
Mission of the group:

The research in the Synthetic Organic Chemistry group is directed at the development of efficient and selective, diversity-oriented synthetic methodology, in particular catalytic procedures, and target-oriented preparation of molecules of relevance in chemistry, biology and medicine. The main target molecules are novel enantiopure organocatalysts, indole and tetrahydroisoquinoline 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. A new research line is directed at the discovery and development of robust methods for the synthesis of high value chemicals and materials using the C-H functionalization strategy.

Research highlights per staff member

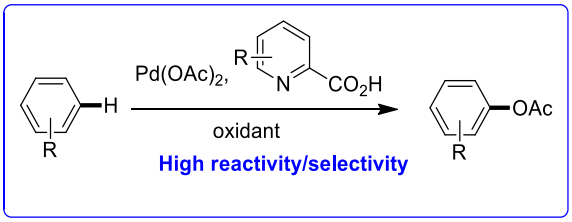
Dr. S. Ingemann Jørgensen

A general procedure for the synthesis of 1-benzyl-1,2,3,4-tetrahydroisoquinolines was developed, based on organocatalytic, regio- and enantioselective Pictet-Spengler reactions (86–92% ee) of *N*-(*o*-nitrophenylsulfenyl)-2-arylethylamines with arylacetaldehydes. The presence of the *o*-nitrophenylsulfenyl group, together with the MOM-protection in the catechol part of the tetrahydroisoquinoline ring system appeared to be a productive combination. To demonstrate the versatility of this approach, ten biologically and pharmaceutically relevant alkaloids were prepared using (*R*)-TRIP as the chiral catalyst: (*R*)-norcoclaurine, (*R*)-coclaurine, (*R*)-norreticuline, (*R*)-reticuline, (*R*)-trimemetoquinol, (*R*)-armepavine, (*R*)-norprotosinomenine, (*R*)-protosinomenine, (*R*)-laudanosine and (*R*)-5-methoxylaudanosine.



Dr. M. Ángeles (Tati) Fernández Ibáñez

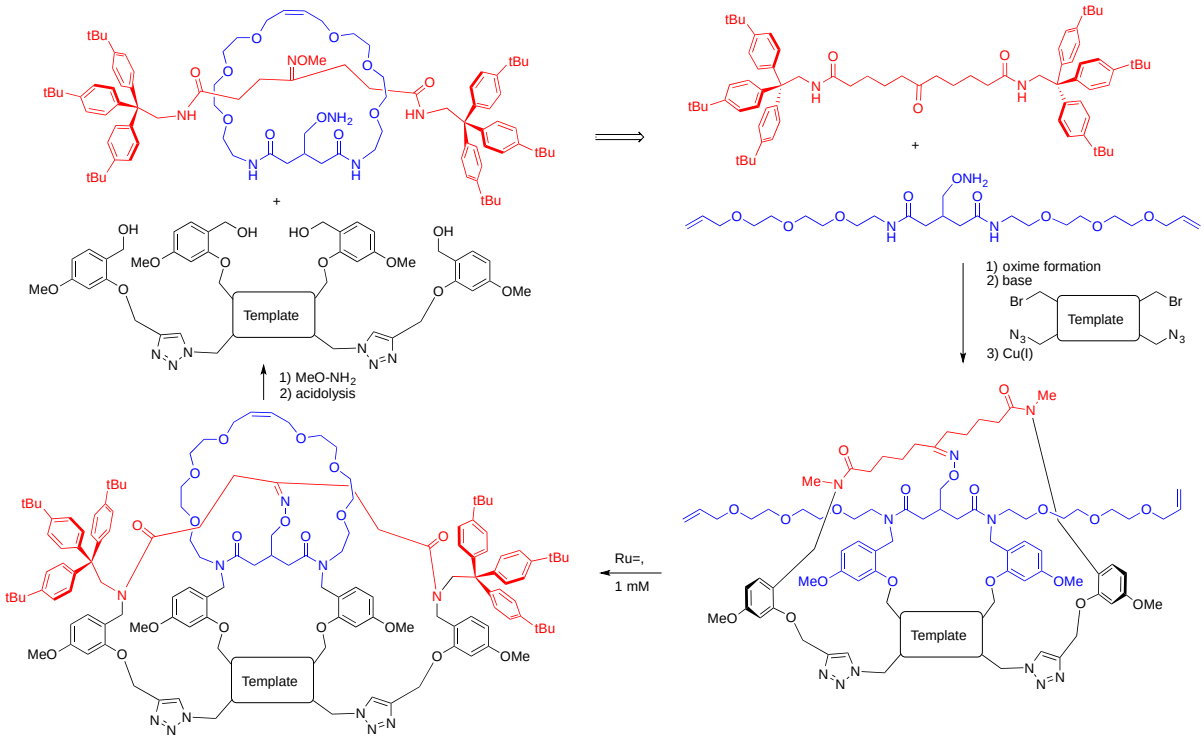
A new catalytic system for the direct C-H acetoxylation of simple arenes based on $Pd(OAc)_2$ and picolinic acid ligand was developed, that shows high reactivity and site selectivity. This system proved to be active at low catalyst loading leading to the highest TON reported to date for palladium-catalyzed C-H acetoxylation of benzene.



Prof. dr. J. H. van Maarseveen

Conditions have been found to ring-close small peptides in an epimerization-free fashion leading to strained 7-membered bislactams. Key were the use of peptides activated as 4-OMe-phenyl thioesters and high dilution (1 mM) conditions at pH = 6,8.

In the project towards the development of the templated synthesis of peptide rotaxanes considerable progress has been made. The concept relies on the covalent constraining of the ring and thread fragment onto a template to force the final clipping reaction around the thread. The ring and thread fragments are connected by oxime formation followed by template attachment via subsequent Williamson ether formation and Cu-catalyzed azide-alkyne cycloaddition (CuAAC). All these reactions have been optimized, are robust and run well on a preparative scale. Unfortunately, after Ru-catalyzed ring-closing metathesis and template detachment no rotaxane formation was detected. Presumably due to too much felixibility in the system both CuAAC reactions had occurred at the same side of the ring fragment. The current end-game focusses on more rigid templates and/or ketal instead of oxime linkage between the thread and ring fragments.



Key publications:

- Reconstructing the Discontinuous and Conformational β1/β3-Loop Binding Site on hFSH/hCG by Using Highly Constrained Multicyclic Peptides, L.E.J. Smeenk, D. Timmers-Parohi, J.J. Benschop, W.C. Puijck, H. Hiemstra, J.H. van Maarseveen, P. Timmerman, ChemBioChem, 16, 91–99 (2015).
- Enantioselective synthesis of tunable chiral clickphine P,N-ligands and their application in Ir-catalyzed asymmetric hydrogenation, J. Wassenaar, R.J. Detz, S.Y. de Boer, M. Lutz, J.H. van Maarseveen, H. Hiemstra, J.N.H Reek, J. Org. Chem. 80, 3634–3642 (2015).
- Organocatalytic enantioselective Pictet–Spengler approach to biologically relevant 1-benzyl-1,2,3,4-tetrahydroisoquinoline alkaloids, A. Ruiz-Olalla, M.A. Würdemann, M.J. Wanner, S. Ingemann, J.H. van Maarseveen, H. Hiemstra, J. Org. Chem. 80, 5125–5132 (2015).
- Total synthesis of aquatolide, J.M. Saya, K. Vos, R.A. Kleinnijenhuis, J.H. van Maarseveen, S. Ingemann, H. Hiemstra, Org. Lett. 17, 3892–3894 (2015).
- Cinchona alkaloid catalyzed sulfa-Michael addition reactions leading to enantiopure β-functionalized cysteines, A.C. Breman, S.E.M. Telderman, R.P.M. van Santen, J.I. Scott, J.H. van Maarseveen, S. Ingemann, H. Hiemstra, J. Org. Chem. 80, 10561–10574 (2015).
- Targeting the Parasite's DNA with Methyltriazenyl Purine Analogs Is a Safe, Selective, and Efficacious Antitrypanosomal Strategy, B. Rodenko, M.J. Wanner, A.A.M. Alkhaldi, G.U. Ebiloma, R.L. Barnes, M. Kaiser, R. Brun, R. McCulloch, G.J. Koomen, H.P. de Koning, Antimicr. Agents Chemother. 59, 6708–6716 (2015).

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 Program 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 (until September 1st 2015)
- Chairman of the Research Committee of the HRSMC
- Member of the Organizing Committee, 5th HRSMC Summer School on Organic Synthesis, Summer 2017

Prof. dr. P. Timmerman

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

Prof. 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
- Member of the Organizing Committee, 5th HRSMC Summer School on Organic Synthesis, Summer 2017

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

Dr. M. Ángeles (Tati) Fernández Ibáñez

- Member of the Organizing Committee, 5th HRSMC Summer School on Organic Synthesis, Summer 2017
- Management Committee Member, EU COST-network C-H Activation in Organic Synthesis (CHAOS)
- Member of the Editorial Board of Advances in Chemistry (Organometallic Chemistry section)
- Member of the core team 'Task force Sustainability' UvA
- Member of the board Women in FNWI (WiF), University of Amsterdam

Dissertations

Jochem P. A. Rutters (13-01-2015), Auxiliary mediated synthesis of ring-strained lactams, (co-) promotors: prof. dr. H. Hiemstra, prof. dr. J.H. van Maarseveen

Stanimir Popovic (13-05-2015), Epimerization-free C-terminal peptide activation, elongation and cyclization, (co-)promotors: prof. dr. H. Hiemstra, prof. dr. J.H. van Maarseveen

Grants

Title	Transition-metal catalyzed epimerization-free peptide C-terminal activation and fragment coupling
Applicant	Prof. dr. Jan H. van Maarseveen
Partner	Enzypep
Grant from	NWO NCI LIFT
Amount	1 year postdoc

Title	Sustainable synthesis of biaryl compounds via aerobic cross-dehydrogenative coupling
Applicant	Dr. Tati Fernandez
Partner	DSM
Grant from	NWO NCI LIFT
Amount	1 year postdoc

Title	New strategies to sustainable procedures based on metal-catalyzed C-H functionalization
Applicant	Dr. Tati Fernandez
Grant from	NWO Vidi 2014
Amount	k€ 800

Invited lectures

Prof. dr. H. Hiemstra

- *"Formal total synthesis of solanoeclepin A"*, Plenary lecture at the Beilstein Organic Chemistry Symposium 2015, Natural Products, Prien (Chiemsee), Germany, September 29th, 2015.

Prof. dr. J.H. van Maarseveen

- *"Epimerization-free Cu-catalyzed peptide activation and cyclization"*, Lecture at the The 25th ISHC Congress, Santa Barbara, USA, August 27th, 2015.
- *"Development of new tools for peptide synthesis"*, Syncom, Groningen, June 18th, 2015.
- *"Development of new tools for peptide synthesis"*, Mercachem, Nijmegen, September 14th, 2015.
- *"Van de Oerknal naar het leven"*, Plenary lecture Woudschoten conferentie, Zeist, November 7th, 2015.

Prof. dr. P. Timmerman

- *"2-CLIPS peptides: Shaping peptides to perfection",* Lecture at Bachem AG, Bubendorf, Switzerland, 12 March 2015.

- *"2-CLIPS peptides: a novel class of biopharmaceuticals",* Lecture at the 12th German Peptide Symposium, Darmstadt, Germany, 21 March 2015.
- *"2-CLIPS peptides: a novel class of biopharmaceuticals",* Lecture at the Voorjaarsbijeenkomst van de KNCV-sectie farmacochemie, Utrecht, 27 March 2015.
- *"3D-structured peptides as functional mimics of protein surfaces",* Lecture at the 'Biomedical Primate Research Center', Rijswijk, 14 April 2015.
- *"Functional mimics of protein surfaces using constrained peptides",* Lecture at the '3rd European Workshop on Peptide Signalling and Activity in Plants', Ghent, Belgium, 4 September 2015.
- *"Protein surface mimics using constrained peptides",* Lecture at the Symposium on the Occasion of the 225th anniversary of the Genootschap voor Natuur-, Heel-, en Geneeskunde, Amsterdam, 21 November 2015.

Dr. M. Ángeles (Tati) Fernández Ibáñez

- "*Ligand-Promoted C-H Functionalization*" Sustainable Chemistry, Amsterdam meets China, The Netherlands,
- "*Synthetic and Mechanistic Studies on the Pd-Catalyzed C(sp^3)–H γ-Arylation of Amino Acid Derivatives with Arl*" NextGenChem@NL, Leiden, The Netherlands,
- *"New strategies to sustainable procedures based on C-H functionalization"* PAC Symposium, Amsterdam, The Netherlands, March 5th, 2015.

Outreach

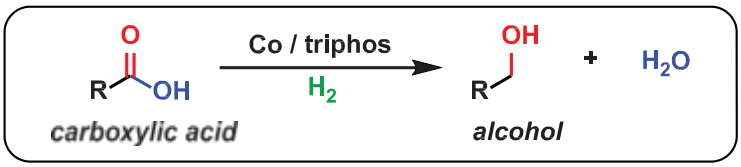
Prof. dr. J. H. van Maarseveen

- Sketches for television program "Proefkonijnen".
- Several lectures at highschools.
- Assistance at the Science Park open day in October.

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	30-9-2015
PhD students	Drs. S.N. Sluijter	1-6-2011	31-5-2015

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.

Research highlights per staff member
Prof.dr. Kees Elsevier
Homogeneous catalysts for the hydrogenation of esters and acids under mild reaction conditions are internationally pursued with vigor, especially varieties involving first-row transition metals. Such reactions are still hardly known, especially involving metals such as cobalt or iron. We have now reached a major break-through by employing $Co(BF_4)_2{\cdot}6H_2O$ together with a tridentate
phosphine, obviating the use of ruthenium-based catalysts. A special feature of this catalyst is that it even hydrogenates a host of carboxylic acids, which are even harder to reduce than esters. Our studies have resulted in a paper in Science.



- T.J. Korstanje, J.I. van der Vlugt, C.J. Elsevier, B. de Bruin; Hydrogenation of carboxylic acids with a homogeneous cobalt catalyst. *Science*, **2015**, 350, 298-302.
- R.M. Drost, V. Rosar, S.D. Marta, M. Lutz, N. Dimitri, B. Milani, B. de Bruin, C.J. Elsevier; Pd-catalyzed *Z*-selective semihydrogenation of alkynes: determining the type of active species. *Chem.Cat.Chem*., **2015**, *7*, 2095-2107.
- S.N. Sluijter, Jongkind, C.J. Elsevier; Synthesis of BINAM-based chiral di-1,2,3-triazolylidene complexes and application of the di-NHC Rh(I) catalyst in enantioselective hydrosilylation. *Eur.J.Inorg.Chem*., **2015**, *18*, 2948-2955.

Other activities
- Cooperation with: HomKat staff (de Bruin, v.d. Vlugt, Reek) on general aspects of organometallic chemistry and catalysis, sharing of equipment and work discussions; discussions and collaboration with prof. P. Braunstein (Strasbourg) 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
Soraya Sluijter, 18 september 2015; (co-)promotors: prof.dr. C.J. Elsevier, dr.ir. J.I. van der Vlugt
Multidentate di-*N*-heterocyclic carbene ligands for transition metal catalyzed hydrogenation reactions.

Invited lectures
1. Invited lecture “Low valent metal species and applications in catalysis” at the Technion Haifa, Israel, February 19, 2015.
2. Keynote lecture “TM[tzNHC] and Cobalt[Triphos] for hydrogenation of acids and esters” at the XXI International Conference on Organometallic Chemistry, EuCHEMS/EuCOMC, Bratislava, July 5-9, 2015.

3. Invited lecture “Cobalt[Triphos] for hydrogenation of acids and esters” ate the Universidad de Valladolid, Spain, December 10, 2015

Patents and utilization

Topic	Cobalt based catalyst converts carboxylic acids to alcohols
Staff members	Prof.dr. Bas de Bruin, prof.dr. Kees Elsevier, dr. Jarl Ivar van der Vlugt, dr. Ties Korstanje
Activities	Patent was drafted, but company retracted in final stage. Other valorisation options are being explored.

Outreach

An interview with pupils of a vwo school as part of an assignment of theirs.
One consultation with local media about chemistry subjects.

Group:	Biocatalysis		
Group leader:	dr. F. Mutti (1-7-2015)		
Academic staff:	Prof. dr. R. Wever (Emeritus)		
Support staff:	A.F. Hartog (< 26-07-2015) dr. L.C. Pham (>1-9-2015)		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	dr. T. Knaus	01-07-2015	30-06-2020
PhD students:	drs. W. Böhmer V. Tseliou M.Sc. J. Vilím M.Sc.	01-09-2015 01-10-2015 01-10-2015	31-08-2019 30-09-2019 30-09-2019

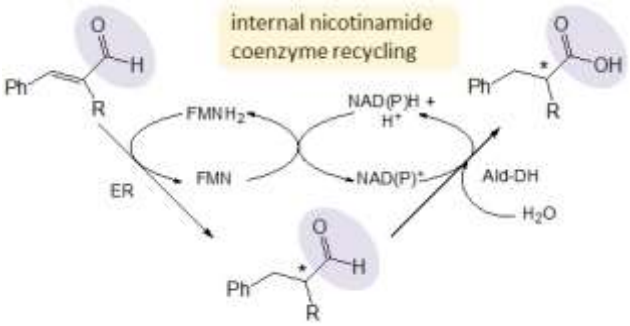
Mission of the group:

The Biocatalysis group carries out cutting-edge research at the interphase between the chemical and the biological sciences. The research focuses on the development of novel biocatalytic systems for the sustainable manufacture of chemical products, identification and characterisation of novel enzymes, engineering of enzymes to improve existing activities or introduce new activities, kinetic and thermodynamic measurements of enzymatic reactions, elucidation of enzymatic reaction mechanisms and creation of artificial enzymes.

Research highlights per sub project

Dr. Francesco Mutti and Dr. Tanja Knaus

Since July 2015, Dr. Francesco Mutti has taken a position as tenure-track chair of the Biocatalysis at HIMS. Together with Dr. Tanja Knaus, he has authored the previously mentioned publication on the biocatalytic hydrogen-borrowing amination of alcohols (*Science* **2015**). Furthermore, they have demonstrated that the “hydrogen-borrowing” concept is applicable to different biocatalytic systems as in the case of the two-step cascade for the conversion of α-β unsaturated aldehydes to chiral α-substituted carboxylic acids employing ene-reductases and aldehyde dehydrogenases (*Org. Biomol. Chem.* **2015**).



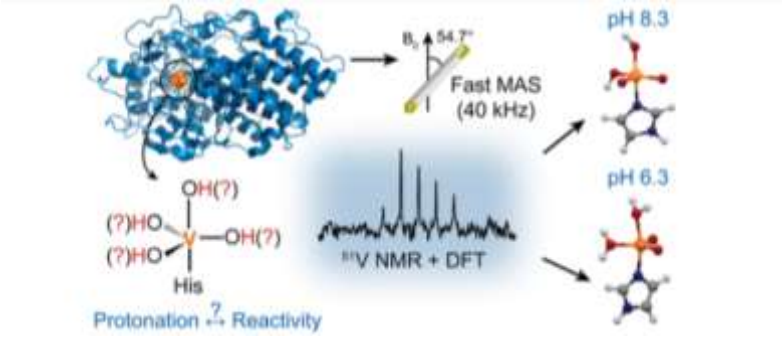
Finally, in a collaboration with the University of Graz, the group has presented a new approach for the asymmetric reductive amination of ketones employing ω-transaminases. The method relies on a sophisticated network constituted by three enzymes: a ω-transaminase, an alanine dehydrogenase and a

Fe/S dioxygen tolerant hydrogenase. The system requires 5 equivalents of alanine and a catalytic amount of NAD (nicotine adenine dinucleotide) as cofactor, the latter recycled at the expense of molecular hydrogen (*Org. Lett.* **2015**).

- Mutti, F. G. *; Knaus, T.; Scrutton, N. S.; Breuer, M.; Turner, N. J; *Science*, **2015**, *359*, 1525-1529.
- Holzer, A. K.; Hiebler, K.; Mutti, F. G.; Simon, R. C.; Lauterbach, L.: Lenz, O.; Kroutil, W; *Org. Lett.*; **2015**, *17*, 2431-2433.
- Knaus, T.; Mutti, F. G.; Humphreys, L.; Turner, N. J.; Scrutton, N. S.; *Org. Biomol. Chem.*, **2015**, *13*, 223-233

Em Prof.dr. Ron Wever and Louis Hartog

Ron and Louis have coauthored two publications in peer-reviewed international journals: *Advanced in Synthesis and Catalysis* **2015** and *European Journal of Organic Chemistry* **2015**. In these studies, the bacterial arylsulfate sulfotransferase (AST) from *Desulfitobacterium hafniense* was used as a catalytic tool to derivatize poorly soluble aromatic compounds (polyphenols). As examples, they sulfated the natural occurring compounds p-coumaric acid, 6-hydroxyflavone, resveratrol, phloretin, and quercetin, using p-nitrophenylsulfate as the sulfate donor. The water-soluble sulfate esters were purified and characterized. The use of substrate engineering also allowed the enzymatic sulfation of a number of carbohydrate derivatives. This simple enzymatic one-step sulfation method is easy to use and it allows a convenient and simple production of sulfated compounds with improved solubility.



In another work in collaboration with the University of the Delaware, Ron and collaborators have employed an NMR crystallography approach based on 51V magic angle spinning NMR spectroscopy and Density Functional Theory, to gain insights into the structure and coordination environment of the cofactor in the resting state of vanadium-dependent chloroperoxidases (*JACS* **2015**).

- Hartog, A.F., Wever, R.; *Adv. Synth. Catal.* **2015**, *357*, 2629-2632.
- Van Der Horst, M.A., Hartog, A.F., El Morabet, R., Marais, A., Kircz, M., Wever, R.; *Eur. J. Org. Chem.* **2015**, 534-541.
- Gupta, R., Hou, G., Renirie, R., Wever, R., Polenova, T.; *J. Am. Chem. Soc.* **2015**, *137*, 5618-5628.

Other activities

- The Biocatalysis group has started collaborations within other groups at UvA (HIMS and SILS). Among the others, the Biocatalysis group has interaction with the Organic Chemistry group (Prof. Henk Hiemstra, Prof. Jan van Maarseveenm, Dr. Steen Ingemann, Dr. Tati Fernandez). The chemistry-oriented PhD students of the Biocatalysis group and the group leader co-organise joined regular weekly research seminars and literature seminars with the Organic Chemistry group. Participation is active in a way that the members of the Biocatalysis group present their research achievements and discuss their literature review. Research collaborations on specific projects between the groups have been initiated.
- The Biocatalysis group shares scientific equipment with the Swammerdam Institute of Life Sciences (SILS) and discussion for research collaborations with SILS's groups have been started. Furthermore, the Biocatalysis group is involved in the initiative Amsterdam Green Campus (theme Green Chemistry) in which HIMS and SILS are both involved.
- The Biocatalysis group has started collaborations with academic groups from other Dutch Universities. In particular, a close collaboration has been initiated with the Protein Crystallography group at the University of Groningen (emeritus Prof. Bauke Dijkstra, Dr. Andy-Mark Thunnissen). This collaboration is aimed at solving the crystal structure of new amine dehydrogenases and related enzymes. The

outcome will allow for understanding the reaction mechanism of these enzymes and planning further studies on enzyme engineering.
- Other international academic collaborations have been continued, in particular with groups at The University of Manchester – UK (Prof. N. Scrutton, Prof. Nick Turner, Prof. S. Flitsch), at the TU Graz – Austria (Prof. P. Macheroux) and at the University of Magna Graecia (Prof. A. Procopio).
- Industrial collaborations are with BASF (Ludwigshaven, Germany) and GSK (Stevenage, UK). Initial contacts with DSM (Gelen, Netherlands) have been taken.
- Finally, the group has joined the Holland Research School of Molecular Chemistry (HRSMC).

Grants

Title	The design and development of efficient biocatalytic cascades and biosynthetic pathways for the sustainable production of amines
Applicants	Dr. Francesco Mutti
Grant from	ERC Starting Grant 2014 (moved to UvA in July 2015)
Amount	k€ 1.500

Title	Sustainable routes to enantiopure amino-alcohols through biocatalytic cascades
Applicants	Dr. Francesco Mutti
Grant from	NWO Echo-Stip (reallocated in 2015)
Amount	k€ 260

Prizes and Honours

Honorary Research Fellow from The University of Manchester (Dr. Francesco Mutti)

Patents and utilization

Topic	Redox self-sufficient bioamination of alcohols
Activities	Patent pending PCT/EP**2015**/65101
Staff members	Dr. Francesco Mutti & Dr. Tanja Knaus
Industrial partner	BASF (Ludwigshafen, Germany)
Full Applicants List	BASF SE, Baldenius, Kai-Uwe; Breuer, Michael; Ditrich, Klaus; Navickas, Vaidotas; Mutti, Francesco; Knaus, Tanja; Turner, Nicholas.

Topic	Expression system Shigella flex
Staff members	Em. prof.dr. Ron Wever
Activities	Sample sold to commercial catalogue house.

Outreach

The Biocatalysis group has been engaged in outreaching activity in relation to assuming an educational role within the Dutch society (as a part of HIMS) and raising the awareness on issue related to sustainable chemistry. For instance, during the period July-December 2015, the Biocatalysis group has regularly communicated with the Dutch press.
Among the others:
http://www.kennislink.nl/publicaties/efficiente-enzymen-voor-schonere-kunststoffen
http://www.duurzaambedrijfsleven.nl/chemie/9127/uva-ontwikkelt-duurzame-chemie-voor-amines-uit-biomassa

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.

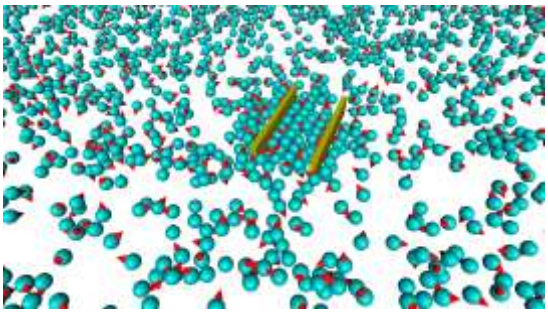
Group	Computational Chemistry		
Groupleaders	Prof.dr. P.G. Bolhuis Prof.dr. E.J. Meijer		
Academic staff	Prof.dr. R. Krishna (em.) Dr. D. Dubbeldam Dr. B. Ensing Dr. C.P. Lowe Dr. J. Vreede		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. A.J. Cruz Cabeza (VIDI)	1-11-2011	22-2-2015
	Dr. E.C. Mastbergen	16-6-2014	31-8-2015
	Dr. R. Ni (VENI)	1-9-2014	31-8-2017
	Dr. D. Sun	21-10-2013	30-9-2015
	Dr. D.W.H. Swenson	1-1-2012	30-6-2015
	Dr. T. Wassenaar	1-3-2014	31-7-2015
	Dr. N. Yachini	1-1-2015	29-2-2016
	Dr. A. Rudavskyi	1-10-2015	30-9-2016
PhD students	Drs. Z.F. Brotzakis	1-9-2012	31-8-2016
	Drs. N.C. Burtch	1-6-2015	1-9-2015
	Drs. J. Heinen	1-9-2014	31-8-2018
	Drs. W. Homsi Brandeburgo	15-1-2011	31-12-2015
	Drs. A. Kumar	1-9-2010	31-1-2016
	Drs. A. Newton	15-4-2012	15-4-2016
	Drs. M. Nowosielski	15-4-2011	14-7-2015
	Drs. A. Tiwari	1-7-2015	30-6-2019
	Drs. A. Torres Knoop	1-3-2012	29-2-2016
	Drs. A. Vijaykumar	1-6-2013	31-5-2017

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.

Soft (Bio)Matter (Peter Bolhuis, Ran Ni, Christopher Lowe)

VENI laureate Ran Ni et al. [Phys. Rev. Lett. **114**, 018302] predicted the existence of a new effective force in active nanomaterials. In computer simulations they discovered the ability of randomly moving self-propelling nanoparticles to collectively move larger microscopic objects. Such active nanoparticles might be used to realize high-tech materials with complex structures, in a 'natural' fashion. Inspired by nature, scientists have developed active materials consisting of small dispersed nanoparticles, propelling themselves for instance by means of a chemical reaction at their surface. Such active systems can show unexpected behaviour not observed in comparable dispersions of passive particles.



Active nanoparticles (in blue), propelling themselves in a random direction (red arrows). Because the particles have a tendency to maintain their direction they accumulate around and in between two larger rectangular objects. This leads to a repulsive force between these objects, driving them apart.

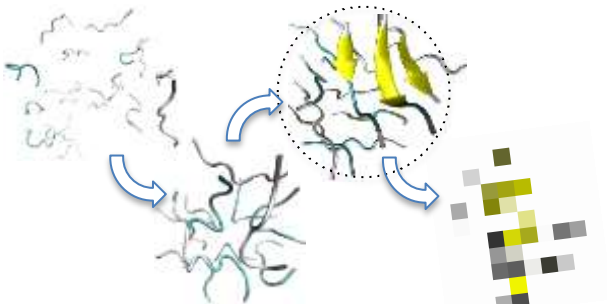
Surprisingly, the scope of these forces significantly exceeds expectations based on the size of the active particles. Furthermore, it is possible to invert forces from attractive to repulsive, simply by modifying the concentration of the active particles. The researchers explain their finding by a 'memory effect' regarding the active nanoparticles. Because of rotational inertia they need some time to 'forget' their direction of movement. In interaction with the larger passive particles this leads to collective effects resulting in the rather strong forces. (Ni et al, PRL 2015).

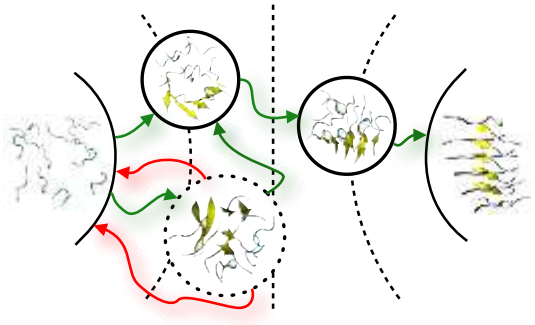
Key publications:

1. R. Ni, M.A. Cohen Stuart, and P.G. Bolhuis, *Tunable Long Range Forces Mediated by Self-Propelled Colloidal Hard Spheres*, Phys. Rev. Lett., **114**, 018302 (2015).
2. A.C. Newton, J. Groenewold, W.K. Kegel & P.G. Bolhuis, *Rotational diffusion affects the dynamical self-assembly pathways of patchy particles*. Proc. Natl. Acad. Sci. USA, **112**, 15308 (2015).
3. R. Ni, J.M. Kleijn, S. Abeln, M.A. Cohen Stuart & P.G. Bolhuis, *Competition between surface adsorption and folding of fibril-forming polypeptides*, Phys. Review E **91**, 022711 (2015).

Biomolecular Systems (Peter Bolhuis and Jocelyne Vreede)

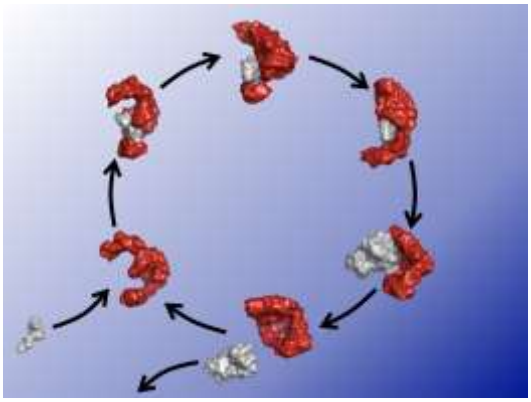
Jurriaan Luiken and Peter Bolhuis published two papers on amyloid nucleation and fibril formation. Amyloid fibril formation is believed to be a nucleation-controlled process. Depending on the nature of peptide sequence fibril nucleation can occur in one step, straight from a dilute solution, or in multiple steps via oligomers or disordered aggregates. In the first paper (Phys. Chem. Chem. Phys.) investigated the phase behavior of three short peptide sequences with increasing side-chain hydrophobicity. They found evidence of a novel additional transition to a liquid phase consisting of clusters of aligned peptides (see figure), implying a three-step nucleation process. The peptide clusters in the associated liquid tend to be slow and long-lived, which may give the oligomer droplet more time to act as a toxic oligomer, before turning into a fibril.





Employing forward flux sampling Luiken and Bolhuis (J. Phys. Chem. B, 119, 12568-12579) analyzed the reactive pathways from the solvated state to the fibril, increasing the overall side-chain hydrophobicity switches the fibrillization mechanism from one- to two-step nucleation. Overall, in this mechanism, peptides first form dimers and trimers, which then grow into a beta-sheet. This sheet serves as a template for nucleation of additional β-sheets until the fibril nucleus is fully formed. Our simulations indicate that the presence of the recently predicted polymerized phase in the nucleation pathway of intermediately hydrophobic peptides slows down the dynamics of fibril formation considerably, which may influence the timescale on which toxic early oligomers exist.

Trigger Factor (TF) is an ATP-independent chaperone protein that assists in folding and prevents misfolding. Up to now, it is a general unsolved question how chaperones assist in the folding of protein chains. Experimental methods that can probe at the length and timescales of inter-residue interactions are scarce, while the systems are too large—and the folding process too long—to be studied by computer simulations. To overcome these obstacles, we performed molecular dynamics simulations at key moments along the folding pathway, and address the changes in the folding and unfolding dynamics of protein chains while in contact with TF. Our results provide the first detailed view on a chaperone-protein complex in different stages of folding and offers an explanation for the ability of TF to guide chains to their native state. Moreover, the results demonstrate the role of TF's flexibility in interacting with a wide range of client states. Overall, it explains how TF can interact with many types of substrates in various stages of folding, without the need for an ATP cycle to switch between encapsulation and liberation of client proteins.



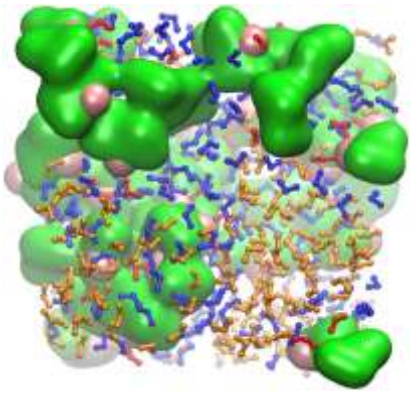
The figure illustrates the mechanism of TF assisted protein folding, with TF in red and the client protein in white. The cycle starts with TF interacting with an unfolded protein, which binds first to TF's outer appendages, followed by encapsulation. This way, TF stabilizes secondary structure elements, such as beta-sheets. TF releases the client protein upon folding, thus becoming available for binding another unfolded protein.

Key publications:

1. K. Singhal, J. Vreede, A. Mashaghi, S.J. Tans & P. Bolhuis, *The Trigger Factor chaperone encapsulates and stabilizes partial folds of substrate proteins*, PLoS Comput. Biol. **11**, e1004444,
2. J.A. Luiken and P.G. Bolhuis (2015), *Primary Nucleation Kinetics of Short Fibril-Forming Amyloidogenic Peptides*, J. Phys. Chem. B **119**, 12568 (2015).
3. J. Zhu, J. Vreede, M. Hospes, J. Arents, J.T. Kennis, I.H. van Stokkum, K.J. Hellingwerf , M.L. Groot,
4. *Short hydrogen bonds and negative charge in photoactive yellow protein promote fast isomerization but not high quantum yield.* J. Phys. Chem. B., **119**, 2372 (2015).
5. W. Du and P.G. Bolhuis*, Equilibrium Kinetic Network of the Villin Headpiece in Implicit Solvent.* Biophys. J., **108**, 368 (2015).

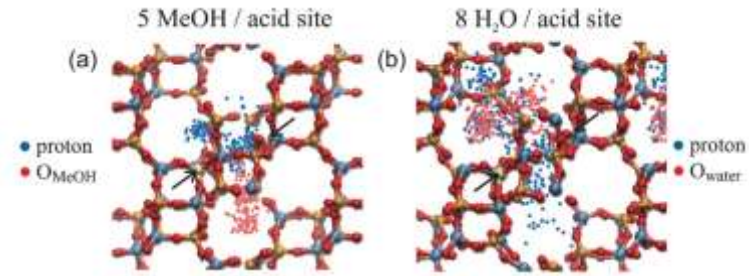
Chemical Processes in Complex Environment (Evert Jan Meijer and Bernd Ensing)

Aqueous solvation of small amphiphilic molecules exhibits a unique and complex dynamics that is only partially understood. A recent series of studies on the hydration of small organic com- pounds, such as tetramethylurea (TMU), trimethylamine N-oxide (TMAO) and urea, has provided strong evidence of a slowdown of the dynamics of the hydrating water molecules. However, the mechanism of this slowdown was still a matter of debate. We analyzed the slowdown mechanism by *ab initio* and classical force field simulations [Brandeburgo et *al*, PCCP **17**, 24968]. Aqueous solutions of TMU and of urea were studied, in which we decomposed the contribution of different solvating groups to the orientational dynamics. Our results reveal that two competing processes govern the H-bond breaking mechanism: H-bond switching through an associative partner exchange and a dissociative breaking characterized by an unbound state. H-bond switches are shown to occur less often near hydrophobic groups, thus creating a subset of OH groups that do not switch and therefore do not significantly reorient within the lifetime of one H-bond, but will require at least a second H-bond to be formed and broken before it may switch. Our results shed new light on the role of hydrophobic solvation in the water



orientational dynamics and help to conciliate the controversy regarding the timescale separation, providing a mechanistic explanation for the observed slow component.

Chemical conversions in zeolites play an essential role in today's industrial catalysis. Within the field of heterogeneous catalysis, the conversion of methanol to hydrocarbons (MTH) or olefins (MTO) over acidic zeolites has received a lot of attention over the last decades because of its relevance in the search for alternative processes to produce hydrocarbon products. It can be considered a showcase example of complex zeolite-catalyzed chemistry as many factors affect the reactivity. These include framework flexibility, adsorption of various guest molecules, and competitive reaction pathways. We have demonstrated [De Wispelaere et *a*l, Chem. Eur. J, **21**, 9385] that by using first principle molecular dynamics techniques to capture this complexity can be elucidated, shown by means of two case studies. Firstly, the adsorption behavior of methanol and water in H-SAPO-34 at 350 ^{0}C is investigated. Hereby an important degree of framework flexibility and proton mobility was observed. Secondly, the methylation of benzene by methanol through a competitive direct and stepwise path- way in the AFI topology was studied. Both case studies clearly show that a first-principle molecular dynamics approach enables unprecedented insights into zeolite-catalyzed reactions at the nanometer scale to be obtained.



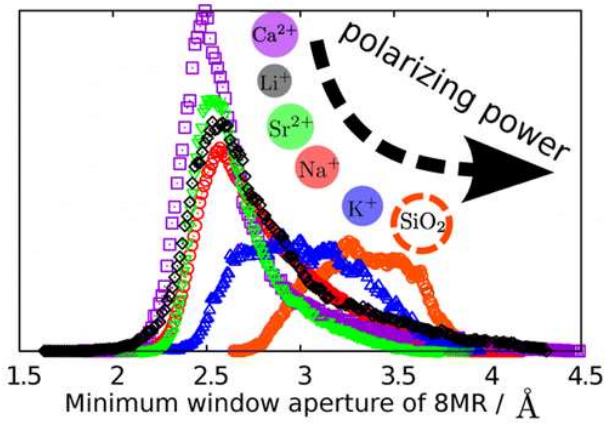
The Figure shows representations of the displacement of a proton (blue) and a methanol or water oxygen atom (red) as observed in a 50 ps MD simulation of H-SAPO-34 zeolite filled with five methanol molecules (left) or eight water molecules (right) per acid site.

Publications:

1. K. De Wispelaere, B. Ensing, A. Ghysels, E.J. Meijer, and V. Van Speybroeck, *Complex reaction environments and competing reaction mechanisms in zeolite catalysis: insights from advanced molecular dynamics*, Chem. Eur. J. **21,** 9385 (2015).
2. W. H. Brandeburgo, S. T. van der Post, E.J Meijer, and B. Ensing, *On the slowdown mechanism of water dynamics around small amphiphiles*, Phys. Chem. Chem. Phys. **17,** 24968 (2015).
3. J.A. van den Ende, M.M.H. Smets, D.T. de Jong, S.J.T. Brugman, B. Ensing, P.T. Tinnemans, H. Meekes, and H.M. Cuppen, *Do solid-to-solid polymorphic transitions in DL-norleucine proceed through nucleation?*, Faraday Discuss. **179,** 421 (2015).
4. T.T. Trinh, K.Q. Tran, X.Q. Zhang, R.A. van Santen, and E.J. Meijer, *The role of a structure directing agent tetramethylamonium template in the initial steps of silicate oligomerization in aqueous solution*, Phys. Chem. Chem. Phys. **17**, 21810–21818 (2015).

Nanoporous Materials (David Dubbeldam and R. Krishna)

Molecular valves are becoming popular for potential biomedical applications. However, little is known concerning their performance in energy and environmental areas. Zeolite RHO shows unique pore deformations upon changes in hydration, cation siting, cation type, or temperature–pressure conditions. By varying the level of distortion of double eight-rings, it is possible to control the adsorption properties, which confer a molecular valve behavior to this material [Balestra et al, Chem. Mater **27**, 5657].



We reviewed [Torres-Knoop and Dubbeldam, ChemPhysChem **16**, 2046] the molecular mechanisms behind adsorption and the separations of mixtures in metal–organic frameworks and zeolites. Separation mechanisms can be based on differences in the affinity of the adsorbate with the framework and on entropic

effects. To develop next-generation adsorbents, the separation efficiency of the materials needs to be improved. The performance under industrially relevant conditions largely depends on two factors: 1) the separation selectivity and 2) the pore volume capacity of the material. Enthalpic mechanisms can lead to increased selectivities, but these are mostly restricted to the low loading regime, and hence these mechanisms are unable to make use of all of the large-pore volume that a metal–organic framework can provide. Industrial processes routinely operate in the pore saturation regime. In this Review, we focused on entropic molecular separation mechanisms that are effective under these conditions and, in particular, on a recent methodology to obtain high selectivities at high pore loading.
Separating acetylene from ethylene/acetylene mixtures containing is a technologically very important, but highly challenging task. We [R. Krishna] have contributed to a study of a microporous metal–organic framework that in which the suitable pore/cage spaces preferentially take up much more acetylene than ethylene while the functional amine groups on the pore/cage surfaces further enforce their interactions with acetylene molecules, leading to its superior performance for this separation. The combination of simulations and and experimental characterizations collaboratively support this claim, underlying the potential of this material for the industrial usage of the removal of acetylene from ethylene/acetylene mixtures.

Publications:

1. RHO, S. Balestra, S. Hamad, A. Rabdel Ruiz-Salvador, V. Domínguez-García, P. Merkling, D. Dubbeldam and S. Calero, *Understanding nanopore window distortions in the reversible molecular valve zeolite*, *Chem. Mater.* **27**, 5657 (2015).
2. Torres-Knoop and D. Dubbeldam, *Exploiting Large-Pore Metal-Organic Frameworks for Separations using Entropic Molecular Mechanisms*, *Chem. Phys. Chem.*, **16**, 2046 (2015).
3. D. Dubbeldam and K.S. Walton, *On the Application of Classical Molecular Simulations of Adsorption in Metal-Organic Frameworks*, Book chapter in *Metal-Organic Frameworks: Materials Modeling towards Engineering Applications* edited by Jiang Jianwen, Pan Stanford Publishing Pte Ltd, (2015).
4. T.-L. Hu, H. Wang, B. Li, R. Krishna, H. Wu, W. Zhou, Y. Zhao, Y. Han, X. Wang, W. Zhu, Z. Yao, S. Xiang, and B. Chen, *Microporous metal–organic framework with dual functionalities for highly efficient removal of acetylene from ethylene/acetylene mixtures*, Nature Comm. **6**, 7328 (2015).
5. J.J. Gutierrez-Sevillano, S. Calero; R. Krishna, *Selective Adsorption of Water from Mixtures with 1-Alcohols by Exploitation of Molecular Packing Effects in CuBTC*, J. Phys. Chem. C 119, 3658.

Other activities

- Jocelyne Vreede co-organized the ACMM symposium June 25, 2015.
- Bernd Ensing organized the Graduate Winterschool on Theoretical Chemistry and Spectroscopy, December 8-12, 2015 (Han-sur-Lesse, Belgium)
- Bernd Ensing co-organized the ACMM symposium in honour of Evert-Jan Baerends 70th birthday.
- Peter Bolhuis is director of the Dutch CECAM node.
- Peter Bolhuis is chair of the CW study group Soft Matter
- Peter Bolhuis co-organized the ESI/CECAM Workshop “From trajectories to reaction coordinates: making sense of molecular simulation data”, September 16-18, 2015, Erwin-Schrödinger-Institute in Vienna, Austria
- Evert Jan Meijer, Bernd Ensing, David Dubbeldam organized the Graduate winterschool on Understanding Molecular Simulation, January 5-16, 2015; Amsterdam.

Dissertations

Dirk Visser, (co-)promotors: prof.dr. P.D. Iedema, dr. C.P. Lowe
Jurriaan Luiken, promotor: prof.dr. P.G. Bolhuis

Grants

Title	An e-infrastructure for software, training and consultancy in simulation and modelling (E-CAM)
Applicants	Prof.dr. Peter Bolhuis
Partners	16 European universities
Grant from	EU H2020-EINFRA
Amount	k€ 4.836 (k€ 176 for equipment within HIMS)

Title	Non-classical crystallization of gas hydrate and calcium carbonate under reservoir and transport conditions
Applicants	Prof.dr. Peter Bolhuis
Grant from	FOM, CSER
Amount	1 PhD researcher

Title	Unravelling the mechanism of biomimetic hydrogen fuel production
Applicants	Dr. Bernd Ensing
Grant from	FOM, CSER
Amount	1 PhD researcher

Prizes

Jurn Heinen (now PhD student) wins 2nd prize at UvA competition for best Master thesis.

Invited lectures

Peter Bolhuis

- CMTC - Free Energy Workshop – Muenster, Germany 9-11 March 2015
- *Free energy, kinetics and mechanisms of protein self-assembly*
- Seminar at U of Cambridge, UK, March 17, 2015
- *Condensation, polymerization and fibrillization of amyloidogenic peptides*
- New Frontiers in the Characterization of Molecular Systems workshop, 9th-10th April 2015
- *Efficient sampling of dynamical pathways in kinetic rare event networks*
- Seminars at SISSA, Trieste, Italy, 4-8 May 2015
- *Sampling rare event pathways: from single barriers to kinetic networks*
- Seminar at Leiden Chemistry & Data Science Meeting, May 28th 2015
- *Bridging length and time scales in biomolecular systems*
- CECAM workhop on “The Physics of Protein Self-Assembly ” , Lausanne Switserland from June 22-24. 2015
- *Kinetics versus thermodynamics in amyloid and protein self-assembly*
- ACS Symposium on” Hydrophobicity, Ion Solvation, and Interfaces: Theory, Simulations, and Experiments” the 250th National ACS Meeting in Boston, August 16-20, 2015,
- *Water dynamics at surfaces: vapor, small amphiphiles and proteins*
- Lorentz workshop on The future of multi-scale soft matter modeling, 31 Aug- 4 sept 2015
- *Bridging scales in biomolecular and soft matter simulations*
- Molecular and Chemical Kinetics Workshop, 7-9 september 2015
- *The Influence of Rotational Diffusion on the Self-Assembly Pathways of (Protein) Complexes*
- CECAM workshop "Free energy landscapes for protein folding. Consensus or dissensus?", ETH Zurich, October 12-14 2015
- *Sampling the equilibrium kinetic network of small model proteins: Trp-cage and Villin*
- Computational Science Seminar, University of Amsterdam, 27 November 2015
- *Bridging length and time scales in biomolecular systems*

Jocelyne Vreede

- Seminar at NIH, Rockwel, USA; February 12, 2015.
- Seminar at NTNU, Trondheim, Norway; April 17, 2015.

Evert Jan Meijer

- Seminar at Nanjing University, Nanjing, China; June 17, 2015. *Ab Initio Simulation of Aqueous Ions*
- AMNM2015 - Advances in Modeling of Nano Materials, Hefei, China; June 14-17, 2015 *Understanding the Role of the Solvent in Catalytic Reactions*
- Seminar at Beijing Computational Science Research Center, Beijing, China; June 11, 2015. Carbon Phase Diagram. *Modeling Transformations at Extreme Conditions*
- Challenges in Computational Homogeneous Catalysis, Stockholm, Sweden; September 2-4, 2015*. Solvent Effects in Chemical Reactions.*
- Seminar at IIT Delhi; India; December 14, 2015. *Ab Initio Molecular Dynamics of Chemical Reactions.*

Bernd Ensing

- September 2015, ESI/CECAM Workshop, “From trajectories to reaction coordinates: making sense of molecular simulation data” at the Erwin- Schrödinger-Institute in Vienna, Austria.
- September 2015, FISMAT 2015 conference in Palermo, Sicily, Italy.
- July 2015, Cecam workshop “Modeling activity vs. selectivity in metalloproteins“ in Paris, France.
- April 2015, at the Dipartimento di Chimica Industriale "Toso Montanari", Bologna, Italy
- February 2015, at the University of Pretoria, Pretoria, South Africa.

David Dubbeldam

- Seminar, 28 July 2015; Delft. “Developing Entropy-driven Separations”.
- Seminar, March 27, 2015; Shell Amsterdam. “Separating Xylene Isomers using Nanoporous Materials”.
- Seminar, October 6, 2015; Shell Amsterdam. "Exploiting Large-Pore Metal-Organic Frameworks for Separations using Entropic Molecular Mechanisms”.

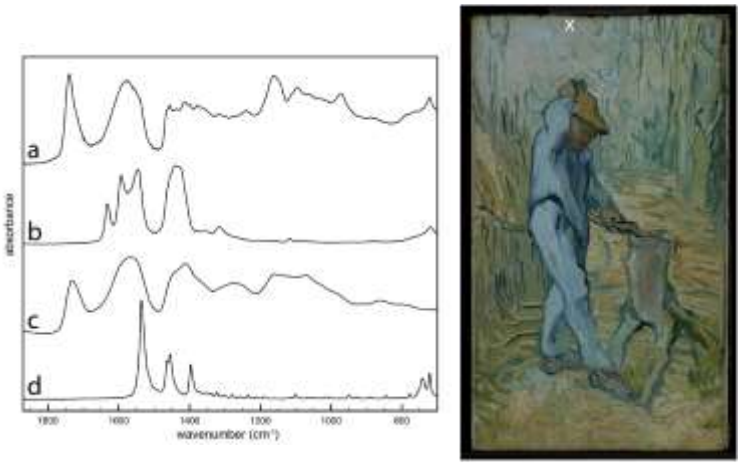
Contribution to RPA Sustainable Chemistry

- Ensing) Hiring of PhD student Ambuj Tiwari on the CSER/FOM/Shell grant entitled “Probing the electrochemical reaction dynamics in solar water splitting cells“
- (Ensing) Hiring of postdoctoral fellow Andrii Rudavskyi, funded by the SusChem RPA, and start of research project on “Water splitting and hydrogen production reactions with silane catalyzed by silver-oxide nano-particles” (in collaboration with Dr. R.N. Shiju, Heterogeneous Catalysis).
- (Ensing) Start of research project on “Quantumchemical study of proton reduction and molecular hydrogen formation by biomimetic di-iron complexes”, with Dr. Mihaljo Etinski, visiting researcher from the University of Belgrade (collaboration with PhD student R. Beckers and Prof. dr. J. Reek, Homogeneous Catalysis).
- (Meijer) Initiating collaboration with DIFFER on water splitting on hematite surfaces.
- (Meijer) Initiating collaboration with SHELL-India on High-Throughput Computational Design of Materials for Energy.
- Ensing) Winning a second CSER/FOM/Shell grant entitled “Unraveling the mechanism of biomimetic hydrogen fuel production”
- (Ensing) Winning HRSMC Fellowship, with Dr. S. Grecea (Heterogeneous Catalysis) and Prof. dr. S. Woutersen (Molecular Photonics) entitled “Unraveling the mechanism of proton transport in proton-conducting MOFs” and start of research project with visiting postdoctoral fellow Saeed Amirjalayer.

Group	Computational Polymer Chemistry		
Groupleader	Prof.dr. P.D. Iedema		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. K. Keune Dr. A. van Loon Dr. I. Kryven (veni-fellow)	1-8-2012 1-8-2012 1-4-2015	31-7-2016 31-7-2016 1-1-2019
PhD students	Drs. J.J. Hermans	1-12-2012	31-12-2016

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 highlights per staff member
Prof. Dr. P.D. Iedema
The formation of metal soaps is a prominent issue for oil painting conservators and the topic of the PhD research of drs. Joen J. Hermans. Metal soap defects appear in many different forms: as large aggregates that deform paint layers, as deposits on the paint surface, or homogeneously spread throughout paint layers. We have shown that variations in metal soap appearance and location within paints can be explained by understanding the pathways of metal soap formation and subsequent crystallization from the paint matrix. Our research concentrates on structural aspects of metal soaps, phase behavior of metal soap-linseed oil systems and transport of metal through polymerized oil films. We have studied structure and composition of zinc alkanoates formed in oil paint using a combination of FTIR (Fourier Transform Infrared spectroscopy, see Figure) and PXRD (Powder X-ray Diffraction).[6] We explained the broad va COO- band commonly observed in FTIR spectra of zinc white paint layers. We reproduced the broadening in two paint reconstructions: ZnO-containing linseed oil polymer (ZnO-LO) synthesized in presence of water, causing hydrolysis of ester bonds, and Zn-ionomer made by polymerizing a mixture of zinc sorbate and linseed oil.

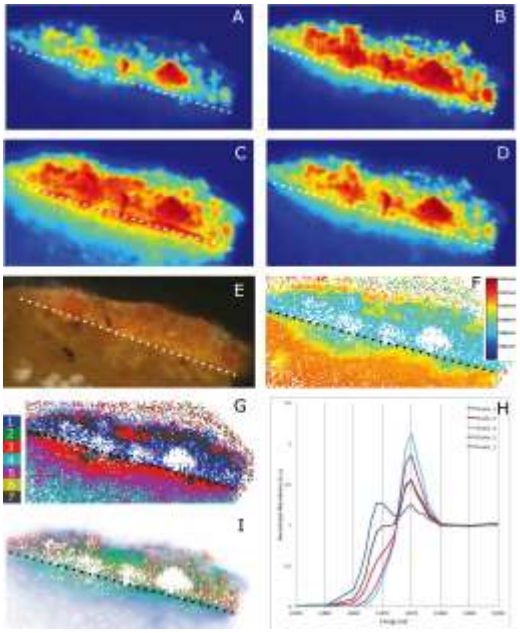


(left) ATR-FTIR spectra[6] of (a) zinc soaps formed in a cured film of ZnO in linseed oil (ZnO-LO), (b) molten zinc palmitate at 160°C, (c) area 1 in sample from *The Woodcutter,* (d) zinc palmitate at room temperature. (right) *'The Woodcutter (after Millet)'* by Vincent van Gogh, 1889, van Gogh Museum (Vincent van Gogh Foundation). X marks sample spot.

- Yaghini, N., Iedema, P.D. (2015). *New Models of Radical Polymerization with Branching and Scission Predicting Molecular Weight Distribution in Tubular and Series of Continuous Stirred Tank Reactors Allowing for Multiradicals and Gelation.* Chemical Engineering Science 130, 301–309.
- Yaghini, N., Iedema, P.D. (2015). *Predicting Molecular Weight Distribution by Deterministic Modeling and Monte Carlo Simulations of Radical Polymerization with Branching and Scission Allowing for Multiradicals and Gelation in Various Reactor Configurations***.** Chemical Engineering Science 130, 310–318.
- Hermans, J.J., Keune, K., Van Loon, A., Iedema, P.D. (2015) *An infrared spectroscopic study of the nature of zinc carboxylates in oil paintings.* J. Anal. At. Spectrom., 30, 1600–1608.

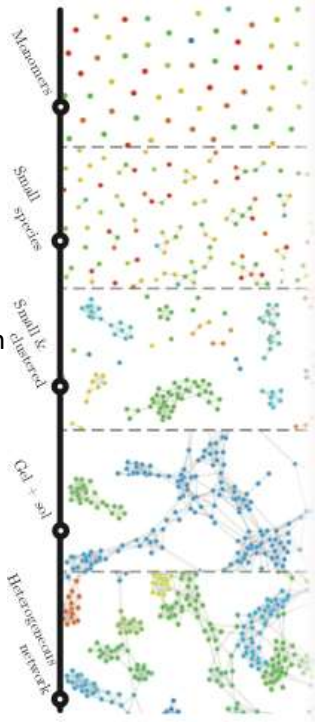
Dr. Katrien Keune

Realgar and orpiment, arsenic sulfide pigments used in historic paints, degrade under the influence of light, resulting in transparent, whitish, friable and/or crumbling paints. So far, para-realgar and arsenic trioxide have been identified as the main oxidation products of arsenic sulfide pigments. This work shows that after photo-degradation, various oxidation and migration processes are taking place. Synchrotron radiation (SR) micro X-ray fluorescence (µ-XRF, see Figure) reveals arsenic to be distributed throughout the whole multi-layered paint system. Arsenic (As) K-edge micro X-ray absorption near edge structure (µ-XANES) analyses indicate the presence of intact AsxSy pigment, arsenite compounds (As^{3+}; As_2O_3), and arsenate compounds (As^{5+}); the latter are certainly present as calcium, lead, aluminium and iron arsenates. Sulfur (S) K-edge µ-XANES point to the conversion of the sulfide (S^{2-}) group to a sulfate (SO42-) group, probably via an elemental sulfur (S) or sulfoxide (OS) compound. Principal Component Analysis (PCA) and subsequent k-means clustering of multi-energy SR µ-XRF maps and µ-XANES was performed to identify the various arsenic species and visualize their distribution. The arsenates (As^{5+}) are spread throughout the entire paint system and dominate the photo-degraded paint and ground layers, while the arsenite compounds (As^{3+}) are located close to the intact arsenic sulfide pigment. The oxidation of arsenic trioxide into arsenates is likely taking place in aqueous solution. The presence of (As^{5+}) compounds in the paint systems indicates that the arsenic trioxide is dissolved by ambient water present in the paint. Arsenite and arsenate compounds are water soluble and are transported by water throughout the paint system. This knowledge is crucial for the conservation field, as this is the first time that (indirect) evidence of water transport within paintings has been given.



- Keune, K., Mass, J., Meirer, F., Pottasch, C., Loon, A. van, Hull, A., Church, J., Pouyet, E., Cotte, M. & Mehta, A. (2015). Tracking the transformation and transport of arsenic sulfide pigments in paints: synchrotron-based X-ray micro-analyses. Journal of analytical atomic spectrometry, 30 (3), 813-827. doi: 10.1039/c4ja00424h

Dr. Ivan Kryven

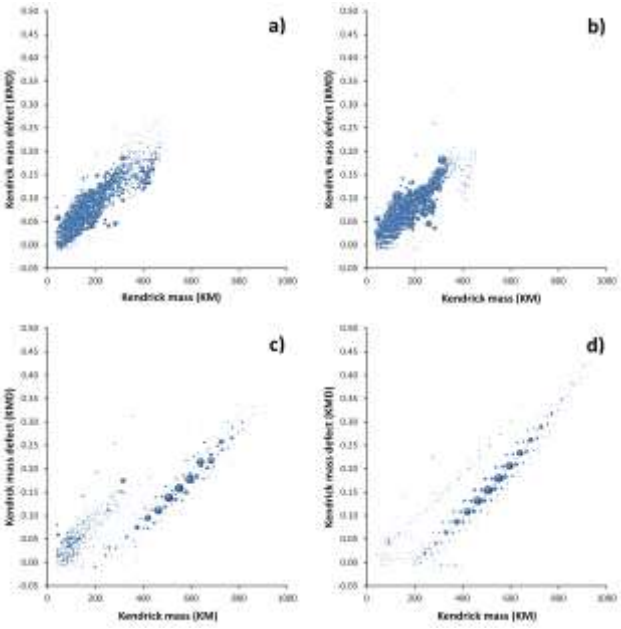


Polymerised oil paint is a strongly cross-linked network and direct observation of the molecular topology is impossible. Insight in the structure/topology is crucial to explain the degradation process. This study develops absolutely new approach to molecular network modelling. The approach takes the graph theory as its core and permits to study the kinetics of polymerisation on the broadest range of timescales: from microseconds to centuries. The random graph model favours reactivity for monomers that are positioned close in the network topology, and disfavours reactivity for those that are obscured by the surrounding. The phenomena of conversion-dependant reaction rates, gelation, and micro-gelation are thus naturally predicted by the model and do not have to be imposed. Resulting non-homogeneous network topologies are analysed to extract such descriptors as: size distribution, crosslink distances, and gel-point conversion. Furthermore, new to the molecular simulation community descriptors are invented. These descriptors are especially useful for understanding evolution of pure gel, amongst them: cluster coefficient, network modularity, cluster size distribution. The output of the model is compatible with graph theory oriented mechanical models, that might be used to study elastic, transport, or rheological properties of the binding medium. Even though the main outcome of this work is an algorithm generating molecular topologies, we have also introduced a new vocabulary allowing a new way of discussing and comparing random molecular topologies, regardless the methodology adopted to construct the.

- Kryven, I., Iedema, P.D. (2015) *Transition into the gel regime for crosslinking radical polymerization in a continuously stirred tank reactor*. Chemical Engineering Science, 126, 296–308.
- Kryven, I., Iedema, P.D. (2015) *Deterministic modelling of copolymer microstructure: composition drift and sequence patterns.* Macromolecular Reaction Engineering, 9, 285–306.

Dr. Annelies van Loon

Direct temperature-resolved mass spectrometry (DTMS) is an analytical technique in which small (µg) amounts of sample are applied to a filament and introduced into the ion source of a mass spectrometer. It is a fast fingerprinting method particularly suitable for the characterization of oils, resins, waxes and other classes of organic compounds in tiny and complex samples of paintings. DTMS results reported thus far have been obtained almost exclusively by instruments with nominal mass resolution. Through collaboration with Shell Technology Centre Amsterdam, however, we could make use of a modern time-of-flight mass spectrometer, which provides high resolution and high sensitivity simultaneously. The availability of accurate mass information adds another dimension to DTMS. The difference between the nominal and accurate mass, the mass defect, may be graphically presented in so-called 'Kendrick plots'. These can be used as fingerprints, enabling a quick overview of the main features in high-resolution mass spectra of complex mixtures. The work combines DTMS with Kendrick mass defect analysis applied to a series of reference compounds commonly found in paintings, and to samples taken from the painting of Saul and David by Rembrandt van Rijn (c.1650-55, Mauritshuis, The Hague) that has been recently subjected to intensive conservation treatment. Its appearance was severely compromised by the presence of old restoration layers. DTMS



proved to be a useful technique for the identification and interpretation of these thin, non-original surface layers. This information was crucial for guiding conservation strategies.

- Van Loon, A., Genuit, W., Pottasch, C., Smelt, S., Noble, P. (2016, online 2015*) Analysis of Old Master Paintings by Direct Temperature-Resolved Time-of-Flight Mass Spectrometry: Some Recent Developments.* Microchem. J., 26, 406-414. doi:10.1016/j.microc.2015.12.025

Dissertations

- Shimazu, Y. (2015, Februari 05). Chemical and optical aspects of appearance changes in oil paintings from the 19th and early 20th century. Universiteit van Amsterdam (xi, 194 pag.). Prom./coprom.: prof.dr. J.J. Boon & K.J. van den Berg.
- Visser, D.C. (2015, Juni 03). Multiphase flow in a confined geometry with Dissipative Particle Dynamics. Universiteit van Amsterdam (132 pag.). Prom./coprom.: prof.dr. P.D. Iedema & dr. C.P. Lowe.
- Yaghini, N. (2015, Maart 24) Towards the architectures of macromolecules: Modeling of multi-dimensional polymer chain distributions. Universiteit van Amsterdam (175 pag.). Prom./coprom.: prof.dr. P.D. Iedema & Prof. dr. P.G. Bolhuis.

Grants

Title	Photocuring created network Topologies - PhoTo
Applicants	Prof.dr. Piet Iedema
Partners	Océ
Grant from	STW, Topsector HTSM
Amount	1 PhD student

Title	Deterministic modelling in multiple dimensions
Applicants	Dr. Ivan Kryven
Grant from:	NWO Veni
Amount	k€ 250

Title	PREDicting AGIng of Oil networks (PREDAGIO)
Applicants	Prof.dr. Piet Iedema, dr. Katrien Keune, dr. Annelies van Loon et al.
Partners	Rijksmuseum Amsterdam, UvA Conservation & Restoration, Cultural Heritage Agency, TU/e
Grant from	NWO - NICAS
Amount	k€ 456

Title	NANOmaterials for the RESToration works of ART
Applicants	Dr. Katrien Keune et al
Partners	Rijksmuseum,
Grant from	H2020-Art
Amount	1 PhD

Title	IRES: US-Dutch Research Collaboration in Cultural Heritage Science
Applicants	Dr. Katrien Keune et al
Partners	Northwestern University
Grant form	IRES NSF
Amount	k€ 220

Title	In-situ Ageing and Conservation Studies on Metal-containing Works of Art
Applicants	Dr. Moniek Tromp, dr. Katrien Keune
Partners	Rijksmuseum Amsterdam, UvA Conservation & Restoration, Cultural Heritage Agency,
Grant from	NWO - NICAS
Amount	k€ 10

Title	Multi isotopic analysis of early modern art: linking origin, trade and production of raw materials with provenance research
Applicants	Prof. G. Davies (VU). dr. Katrien Keune, dr. Annelies van Loon et al
Partners	Rijksmuseum Amsterdam, UvA Conservation & Restoration, Cultural Heritage Agency.
Grant from	NWO - NICAS
Amount	k€ 249

Invited lectures

1. K. Keune, 'High-Resolution 3-Dimensional Backscattered-Electron Imaging of Paint Cross Sections Analytical challenge', Analytical Challenge 2015, KNCV section forensics, 7 October 2015
2. K. Keune, 'Verf en Licht', Jaar van het Licht, Spui 25, 29 September 2015
3. K. Keune, 'Surface chemical reactions in paintings', Dag van de oppervlaktetechnologie, ION, 12 November 2015

2.3 Molecular Photonics

Groups:	Molecular Spectroscopy; Spectroscopy and Photonic materials; Time Resolved Vibrational Spectroscopy		
Group leaders:	Prof. dr. A.M. Brouwer[2] Prof. dr. W.J. Buma		
Academic staff:	Prof. dr. M.C.G. Aalders (BHGL) Prof. dr. H.J. Bakker (BHGL) Prof. dr. J. Oomens (BHGL) Dr. R.M. Williams Prof. dr. S. Woutersen (BHGL) Dr. H. Zhang[3]		
Support staff:	Drs. ing. M.F. Hilbers Ing. P.P. Reinders Drs. H.J. Sanders		
Temporary staff		Start date	(Foreseen) end date
Postdocs:	Dr. R. Bloem Dr. V.P. Nicu Dr. S. Shen	03-07-2015 01-06-2015 01-05-2015	31-12-2015 31-12-2018 30-04-2016
PhD students:	H.C. Chen, MSc. R.O. Gutierrez Gota, MSc. Drs. M.A.J. Koenis E. Maltseva, MSc. D. Petrova, M.Sc. Drs. S.J. Roeters M. Raeisolsadati Ouskoui, M.Sc. B.H. Strudwick, M.Sc. D. Zheng, MSc.	01-09-2011 01-06-2015 01-09-2015 01-08-2012 01-04-2015 15-10-2011 01-11-2012 01-08-2014 01-09-2014	31-08-2015 31-05-2019 31-08-2019 31-07-2016 31-03-2019 14-07-2016 30-09-2015 31-07-2019 31-08-2018
MSc + BSc students:	C. O'Bryen (Erasmus student) A. Elci J.P. Oudsen O. Lugier C.M.P. Talavera Ormeno (guest) Martijn Tros F. Veenstra (HBO) Sander Westerveld	16-08-2015 01-09-2015 20-03-2015 18-08-2014 01-09-2014 18-08-2014 01-10-2014 30-03-2105	29-06-2016 01-10-2015 20-07-2015 24-02-2015 31-01-2015 01-07-2015 01-07-2015 09-07-2015

Mission of the group

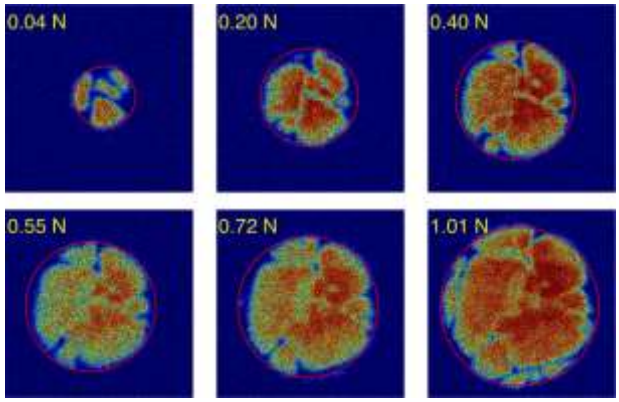
The Molecular Photonics group aims to advance the fundamental knowledge of the dynamics of excited states in molecules and nano-sized objects, and to contribute with its expertise to applications of the photosciences. Light-induced chemical conversions play a key role in many technological and biological 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 highlights Molecular Photonics

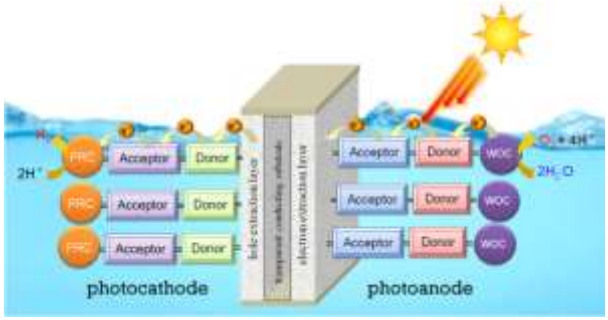
[2] Per July 2014 professor Brouwer is also part time group leader Nanophotochemistry at the Advanced Research Center for Nanolithography (ARCNL).

[3] Zhang is also chair professor at Northeast Normal University (China) and professor at Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences

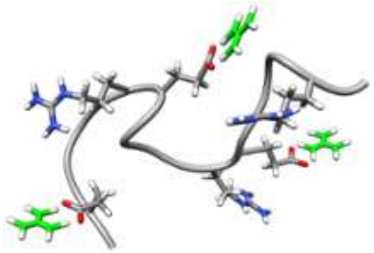
We describe the first **direct visualization of mechanical contacts at the microscale by means of fluorescence microscopy**, using specifically developed probe molecules that fluoresce when confined in a contact. The figure shows how a roughly circular contact area is formed (with a radius increasing up to ~70 micrometers) when a plastic bead is pressed onto a glass slide to which the fluorescent molecules are covalently attached. The molecules light up where the bead touches the glass. The size of the contact is in perfect agreement with Hertz' classical theory of elastic deformation. We can also see details within the overall contact, related to the surface structure of the bead. The paper was published in *Angew. Chem. Int. Edit.* **2015**, *54*, 3688–3691. It opens up possibilities to directly observe mechanical contacts with high spatial and temporal resolution for the study of important physical phenomena such as friction.



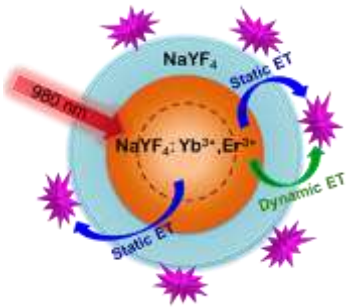
Holding on to the electrons in artificial photosynthesis
We designed new clever molecules that can play a key role in the conversion of Solar-to-Fuel. The molecules hold on to an extra electron in such a way that these are not quickly trapped by oxygen and water, but can still be transported easily inside the material. Natural photosynthesis provides a blueprint for the construction of efficient artificial solar-to-fuel conversion systems: an "artificial leaf". The essence of molecule-based artificial photosynthetic devices is photo-induced electron transfer between donor and acceptor molecules in the photoelectrodes (see Figure). This generates charged intermediate species that can activate the catalyst for the water oxidation (WOC) and catalyst for proton reduction (PRC) for oxygen and hydrogen production. PhD student Hung-Cheng Chen developed a series of novel molecules (called benzo[ghi]perylenetriimides (BPTI's)) that strongly absorb light in the blue-green area of the sunlight spectrum. BPTI's are excellent electron acceptors for use as the photoanode. Studies show the potential of BPTI compounds as electron acceptors in devices for artificial photosynthesis aiming for water splitting and also are interesting electron-transport materials for organic solar cells. (see also references 1 and 2).
http://atlasofscience.org/holding-on-to-the-electrons-in-artificial-photosynthesis/



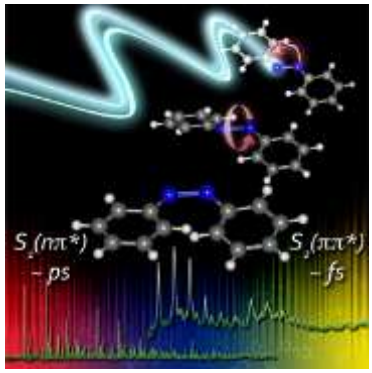
How guanidinium unfolds proteins Guanidinium is a commonly used denaturant, but the mechanism by which it unfolds proteins is still largely unknown. By studying specifically tailored peptides we have been able to solve this mystery. We find that guanidinium disrupts the folded protein conformation by breaking salt bridges. Two-dimensional infrared spectroscopy shows that guanidinium binds in a competitive manner to the carboxylate side groups involved in these salt bridges. The low guaninidium:carboxylate association constant explains the high guandininum concentrations that are typically required to denature proteins. We could even design peptides that fold (rather than unfold) upon adding guanidinium, simply by inserting salt bridges in the sequence that stabilize the unfolded state. This result was published in *Angewandte Chemie,* and contributes to our understanding of protein unfolding, which is believed to be involved in the pathogenesis of many diseases.



Biophotonic nanomaterials Understanding the excitation energy migration and interaction mechanisms in photonic nanomaterials as well as developing novel functional nanomaterials are an important research topic for application of these materials. In 2015 we have focused on (1) exploration of new luminescence upconversion mechanisms in space-confined systems, typically in $NaFY_4$ based upconversion nanocomplexes. Experimental discoveries have led to new nano-constructions with potentially high upconversion efficiencies (*Chem. Soc. Rev.* **2015**, *44*, 1331); (2) understanding at a subcellular level the translocation of the upconversion nanoparticles and their interaction with a biological environment. Relevant dynamical processes have been monitored. The subcellular picture of cytotoxicity provides a firm and sound basis for the biomedical application of this sort of nanomaterials; (3) how to improve the excitation energy utilization in FRET-related biomedical applications of upconversion nanoplatforms. For typical core-shell nanostructures dynamic- and static energy transfer were separated for the first time and excitation energy utilization efficiency was improved by more than an order of magnitude (*J. Phem. Chem. Letters* **2015**, *6*, 2518).



Azobenzene: fast dynamics probed by slow spectroscopies Azobenzene is the *prima donna* amongst photoswitches finding extensive applications in areas ranging from molecular probes to molecular nanotechnology and photopharmacology. Despite its huge popularity, the operational mechanism behind the structural changes was not at all clear. Using jet-cooled molecular beam and multiphoton ionization techniques we have been able to obtain the first high-resolution excitation spectra of the electronically excited states that control and steer photoisomerisation (*Nat. Commun.* **2015**, *6*, 5860). These spectra reveal directly the forces the molecule is subjected to upon photon absorption and allow to study dynamics occurring on a femtosecond timescale with nanosecond lasers. From the results it becomes clear that (i) dynamics occur on a completely different time scale than assumed up till now, (ii) changes in spatial structure are considerably different from what has been previously proposed, and (iii) out of the many proposed photoisomerisation pathways an inversion-assisted torsional pathway with a barrier of ~2 kcal/mol is the correct one. The studies on azobenzene are also important because there is a vast amount of photoresponsive systems for which high-resolution spectroscopy was thought to be out of reach because of prohibitively short lifetimes. The present studies show the potential of our methodologies for the study of their photodynamics.



Key publications

1. Chen, H.-C.; Hsu, C.-P.; Reek, J. N. H.; Williams, R. M.; Brouwer, A. M. Highly Soluble Benzo[Ghi]Perylenetriimide Derivatives: Stable and Air-Insensitive Electron Acceptors for Artificial Photosynthesis. *ChemSusChem* **2015**, *8* (21), 3639–3650.
2. Chen, H.-C.; Hetterscheid, D. G. H.; Williams, R. M.; van der Vlugt, J. I.; Reek, J. N. H.; Brouwer, A. M. Platinum(II)-Porphyrin as a Sensitizer for Visible-Light Driven Water Oxidation in Neutral Phosphate Buffer. *Energy Environ. Sci.* **2015**, *8*, 975–982.
3. Ding, Y.; Wu, F.; Zhang, Y.; Liu, X.; de Jong, E.M.L.D.; Gregorkiewicz, T.; Hong, X.; Liu, Y.; Aalders, M.C.G.; Buma, W.J.; Zhang, H. Interplay between static- and dynamic energy transfer in biofunctional upconversion nanoplatforms. *J. Phys. Chem. Lett.* **2015**, *6*, 2518-25232.
4. Domingos, S.R.; Hartl, F.; Buma, W.J.; Woutersen, S. Elucidating the structure of chiral molecules by using amplified vibrational circular dichroism: from theory to experimental realization. *ChemPhysChem* **2015**, *16*, 3363 (invited Concept article).
5. Hennig, R.; Heidrich, J.; Saur, M.; Schmüser, L.; Roeters, S.J.; Hellmann, N.; Woutersen S.; Bonn, M.; Weidner, T.; Markl, J.; Schneider, D. IM30 triggers membrane fusion in cyanobacteria and chloroplasts. *Nature Commun.* **2015**, *6*, 7018.

6. Kiawi, D.M.; Bakker, J.M.; Oomens, J.; Buma, W.J.; Jamshidi, Z.; Visscher L., Waters, L.B.F.M. Water adsorption on free cobalt cluster cations probed by IR multiple-photon dissociation spectroscopy and density functional theory calculations. *J. Phys. Chem A* **2015**, *119*, 10828-10837.
7. Liu, X.; Chen, H.-C.; Kong, X.; Zhang, Y.; Tu, L.; Chang, Y.; Wu, F.; Wang, T.; Reek, J. N. H.; Brouwer, A. M.; Zhang, H. Near Infrared Light-Driven Water Oxidation in a Molecule-Based Artificial Photosynthetic Device Using an Upconversion Nano-Photosensitizer. *Chem. Commun.* **2015**, *51*, 13008–13011.
8. 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.* **2015**, *27*, 1389-1394.
9. Maltseva, E.; Petrignani, A.; Candian, A.; Mackie, C.J.; Huang, X.; Lee, T.J.; Tielens, A.G.G.M.; Oomens, J.; Buma, W.J. High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons: the realm of anharmonicity. *Astrophys. J.* **2015**, *814*, 23.
10. Meuzelaar, H.; Panman, M.R.; Woutersen, S. Guanidinium-Induced Denaturation by Breaking of Salt Bridges. *Angew. Chem. Int. Ed.* **2015**, 54, 15255-15259.
11. Panman, M.R.; van Dijk, C.N.; Meuzelaar, H.; Woutersen, S. Nanosecond folding dynamics of an alpha helix: Time-dependent 2D-IR cross peaks observed using polarization-sensitive dispersed pump-probe spectroscopy. *J. Chem. Phys.* **2015**, *142*, 041103.
12. Suhina, T.; Weber, B.; Carpentier, C. E.; Lorincz, K.; Schall, P.; Bonn, D.; Brouwer, A. M. Fluorescence Microscopy Visualization of Contacts Between Objects. *Angew. Chem. Int. Edit.* **2015**, *54*, 3688-3691.
13. Tan, E.M.M.; Amirjalayer, S.; Smolarek, S.; Vdovin, A.; Zerbetto, F.; Buma, W.J. Fast photodynamics of azobenzene probed by scanning excited state potential energy surfaces using slow spectroscopy. *Nat. Commun.* **2015**, *6*, 5860.
14. Tu, L.; Liu, X.; Wu, F.; Zhang, H. Excitation energy migration dynamics in upconversion nanomaterials. *Chem. Soc. Rev.* **2015**, *44*, 1331-1345
15. Yamaguchi, T.; Hilbers, M.; Reinders, P.; Kobayashi, Y.; Brouwer, A. M.; Abe, J. Nanosecond Photochromic Molecular Switching of a Biphenyl-Bridged Imidazole Dimer Revealed by Wide Range Transient Absorption Spectroscopy. *Chem. Commun.* **2015**, 1375–1378.

Other activities

A.M. Brouwer

- Collaborations with J. Qian (Shanghai, China), T. Ogoshi (Kanazawa, Japan), J. Abe (Kanagawa, Japan), D. Bléger and S. Hecht (Berlin), 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
- Member Editorial Board European Journal of Organic Chemistry
- Organizer of EPA/HRSMC Summer Schools on Photochemistry 1998, 2003, 2008, 2012, 2016
- Organizer of LEELIS workshops (Low-Energy Electrons: Lithography, Imaging and Soft matter), Amsterdam, 2014, 2016
- 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

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), H. Overkleeft (RUL), S. Amirjalayer (University of Münster), M. Pryce (University of Dublin), F. Zerbetto (University of Bologna), L. Nafie and R. Dukor (BioTools)
- Organizer HRSMC and ESF Graduate School "Modern Developments in Spectroscopy" 2001, 2003, 2006, 2009, 2012, 2015

- Member International Advisory Committee “International Symposium on Molecular Beams”, 2017
- Member Editorial Advisory Board of ChemPhysChem
- 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.

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 Scientific World Journal”.

S. Woutersen
- Collaborations with Prof. M. Bonn (Max Planck Instituut, Mainz), dr. Gertien Smits (SILS, UvA), prof. D. Bonn (IoP, UvA) on structure and dynamics of water in living systems; Dr. T. la Cour Janssen (RuG) on 2D-IR spectroscopy of solute-solvent interactions; Dr. P.W.J.M. Frederix (RuG) on 2D-IR spectroscopy to characterize bio-compatible nanomaterials based on self-assembling peptides; Prof. M. Claessens (TU Twente) on amyloid formation by alpha-synucleine; Dr. M. T. Pryce (Dublin City University) on photo-catalytic CO_2 reduction; Profs. G. Knoer (Universiteit van Linz), J.N.H. Reek and B. de Bruin (UvA) on foto-catalytic H_2 generation; Prof. D. Schneider (Johannes Gutenberg-Universiteit, Mainz) on spectroscopy of proteins in membranes; Dr. S. Amirjalayer (Universiteit van Muenster) on 2DIR spectroscopy on metal-organic frameworks; Dr. W. Sager (Universiteit van Juelich) and prof H.J. Bakker (AMOLF) on structure and dynamics of water in nanostructures; Dr. A. Cruz-Cabeza and prof. R. Davey (Manchester University) on molecular mechanism of crystal polymorphism; Prof. dr. C. Austen Angell (University of Arizona) on liquid-liquid transitions in water.
- Member of the scientific advisory committee of the Max-Planck-Institut in Mainz
- Member of the international organizing committee of the European Conference on Spectroscopy of Biological Molecules (ECSMB)
- Member of the organizing committee of the Conference on Multi-Dimensional Spectroscopy 2016 (CMDS2106)
- Member of the Program Advisory Committee (PAC) of the free-electron laser FELIX

Hong Zhang
- Collaboration with A. Vahrmeijer, F. Ossendorp, L. Crus (LUMC), C. Löwik (Erasmus University Medical Center), P. di Martino, R. Censi (Univ. Camerino), E. McCormack (Bergen), E. Cubikovskaya (EPFL), B. Lelieveldt and M. Reinders (TU Delft), C. Lewism (Univ. Sheffield), R. Heeren (Univ. Maastricht), P. Prosposito and M. Casalboni (Univ. Rome), X.G. Kong (CIOMP/CAS), H.J. Zhang (CIAC/CAS), Y.C. Liu (NENU), A. Szemik-Hojniak (Univ. Wroclaw), T. Gregorkiewicz (IoP, UvA), Joost Reek, S. Grecea, G. Rothenberg (HIMS)
- Member of editorial board J. Rare Earths
- Member of Rare Earth Society of China / Luminescence Branch
- 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
- Member of Advisory committee of 3rd International Workshop on Persistent and Photostimulable Phosphors (Arlington, USA)

- Chairing research theme “Luminescence Dynamics of spatially confined systems” at CIOMP/CAS
- 4 PhD students under supervision received PhD degree at CIOMP/CAS in 2015

Dissertations

Bart van den Bosch, (co-)promotors: prof.dr. J.N.H. Reek, prof.dr. S. Woutersen
Tatu Kumpulainen, (co-) promotors: prof.dr. A.M. Brouwer, prof.dr. S. Woutersen
Heleen Meuzelaar, (co-) promotors: prof.dr. S. Woutersen, dr. J. Vreede
Tibert van der Loop, (co-) promotors: prof.dr. S. Woutersen, prof.dr. H.J. Bakker
Liyuan Liu, promotor: prof.dr. H.J. Bakker
Stephan Lotze, promotor: prof.dr. H.J. Bakker

Grants

Title	Development of a Vibrational Optical Activity analysis toolbox from chiroptical spectra to molecular stereochemistry and conformation
Applicants	Prof. dr. Wybren Jan Buma et al
Partners	Scientific Computing & Modelling, Biotools Inc, VU
Grant from	NWO NCI TA
Amount	k€ 1.147 (1 PhD student and 3 year postdoc plus equipment for HIMS)

Title	Image-Guided Surgery and Personalised Postoperative Immunotherapy To Improving Cancer Outcome (ISPIC)
Applicants	Prof. dr. Hong Zhang et al
Partners	7 academic institutes, 2 medical centres, 4 industrial partners from 5 European countries
Grant from	ERC ITN Curie
Amount	k€ 3.500 (1 PhD student for HIMS)

Title	Shapes and formats of extraterrestrial organic molecules
Applicants	Dr. Annemieke Petrignani
Grant from	NWO Vidi
Amount	k€ 800

Title	Preclinical Intraoperative Image-Guided Surgery and Postoperative Radiotherapy of Tumours
Applicants	Dr. Hong Zhang et al
Partners	LUMC, Percuros (Dutch company), TECO Bioscience (German company)
Grant from	NWO NCI TA
Amount	k€ 1.038 (1 PhD student for HIMS)

Title	Renewable fuels by tuning nature
Applicants	Prof. dr. Lucas Visscher, prof. dr. Wybren Jan Buma
Partners	VU
Grant from	FOM, CSER
Amount	1 PhD student at VU (no funding to HIMS)

Prizes

Tatu Kumpulainen was awarded the 2015 Dick Stufkens Prize for the best PhD thesis of the Holland Research School of Molecular Chemistry (HRSMC).

Invited lectures

A.M. Brouwer

- “In touch with fluorescent probe molecules: visualizing contact and friction", International Conference on Functional Polymers and Materials, Marrakech, Morocco, March 30 - April 2, 2015.

- "Fluorescence in confinement: observation of mechanical contact", Minisymposium 'Photophysics of Solar Fuel Materials', Vrije Universiteit, Amsterdam, November 2, 2015.
- "Fluorescence in confinement: observation of mechanical contact", 3rd International Workshop on Nano and Bio-photonics, Cabourg, France, December 6-11, 2015.

W.J. Buma
- "Fast photodynamics probed by slow spectroscopy", XXVI International Symposium on Molecular Beams, Segovia, Spain, June 28-July 3, 2015.
- "High-resolution spectroscopy of the complex, fast and furious", DESY, Hamburg, Germany, September 3, 2015.
- "High-resolution fingerprints of photo(re)activity", Opening and user meeting FELIX Laboratory, October 28-30, 2015, Radboud University.

S. Woutersen
- "New light on liquids, protein folding, and chirality", Max-Planck-Institut für Polymerforschung, Mainz, March 3, 2015.
- "New light on liquid structure, solvation, and protein denaturation", Ruhr Universität Bochum, October 23, 2015.
- "Water at its weirdest", HRSMC symposium, November 5, 2015.

H. Zhang
- "*Application of rare earth based upconversion nanomaterials: restrictions and possibilities*", 8th International Conference on Nanophotonics, May 24-28, 2015, Changchun, China.
- "*Photostable organic photosynthesis employing near infrared nanotransducer*", 3rd International Workshop on Persistent and Photostimulable Phosphors, November 9-11, 2015, UT Arlington, USA.
- "*Light Upconversion in Nanomaterials: Applications & Fundamental Challenges*, XIV National Conference on Chemical Dynamics, August 21-24, 2015, Xian, China.

Patents and utilization

Topic	Photosensitiser
Staff members	Prof. dr. Fred Brouwer, Prof. dr. Joost Reek, Hung-Cheng Chen M.Sc.
Activities	Patent filed. SBI student identified and contacted 22 companies that may be interested. Discussions with 8 of them started, two companies are serious interested in collaboration with HIMS.

Topic	Improving sunscreens
Staff members	Prof. dr. Wybren Jan Buma
Activities	Cold acquisition to potentially interested personal care companies.

Outreach

A.M. Brouwer

Fred Brouwer gave a *Spui 21* lecture on November 25, 2016 on *Licht en Moleculen*, and hosted a visit of the Stedelijk Gymnasium Hilversum on November 19.

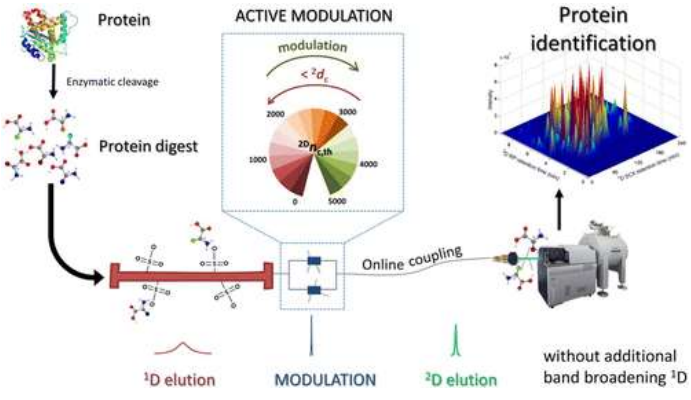
R.M. Williams
- Proefstuderen, December 11, 2015 (practicum).
- Profielwerkstuk *Kunstmatige fotosynthese*. Grätzel cel practicum, November 25, 2015, Lucy Tao en Jin Smeding, 6VWO, Dominicus College (Nijmegen).

2.4 Analytical Chemistry

Group	Analytical Chemistry		
Groupleader	Prof.dr.ir. P.J. Schoenmakers		
Academic staff	Prof.dr. G.L. Corthals Prof.dr. M.R. van Bommel (0,2 FTE) Prof.dr.ir. J.G.M. Janssen (BHL) Prof.dr. A.C. van Asten (BHL) Prof.dr. R.A.H. Peters (BHL, > 5-11-2015) Prof.dr. S. van der Wal (em. BHL) Dr. W.Th. Kok Dr. G.I. Vivo Truyols Dr. M. Camenzuli		
Support staff	T. Aalbers P. Aarnoutse P.G. Verschuren P.J. Jansen (>19-1-2015)		
Temporary staff		Start date	(foreseen) end date
Postdocs	Dr. A. Astefanei Dr. I. Dapic Dr. A.F.G. Gargano Dr. B. Wouters	15-9-2015 1-11-2015 1-9-2013 1-11-2015	15-9-2017 30-9-2017 31-1-2016 31-10-2016
PhD students	Ir. K.D.B. Bezemer Drs. J. Králová Drs. M. Marioli Drs. B.W.J. Pirok Drs. H. Cornelisson van de Ven Drs. M.G.Gerritsen Drs. E. Davydova Drs. A.A.S. Sampat Drs. M. Woldegebriel Drs. M.Pacheco Bothelho Mourao Drs. A.A. Baglai Drs. Barcaru	1-10-2015 1-8-2011 1-8-2011 1-4-2015 1-10-2012 1-5-2014 1-6-2011 1-2-2012 1-4-2013 1-9-2013 1-10-2012 1-4-2013	31-3-2017 31-7-2015 31-7-2015 30-9-2016 30-9-2016 30-4-2016 30-9-2015 31-1-2016 31-3-2017 30-6-2016 30-9-2016 31-3-2017

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

Group highlight: Stationary-Phase-Assisted Modulation in 2D LCMS
The increasing complexity of mixtures encountered in biomedical and environmental samples often exceeds the limits of peak capacity, required for analyses of such complex samples. The Analytical Chemistry group combined a slow and a fast one dimensional liquid chromatography method into a 2D LCMS which leads to high speed and sensitive analysis.



Dissertations

Yoshiko Shimazu, (co-)promotors: prof.dr. J.J. Boon, dr. K. van den Berg
Aleksandra Chojnacka, (co-)promotors: prof.dr.ir. P.J. Schoenmakers, prof.dr.ir. J.G.M. Janssen
Rudy Vonk, promotor: prof.dr.ir. P.J. Schoenmakers (joint doctorate with VU Brussel)
Katja Davydova, promotor prof.dr.ir. P.J. Schoenmakers (joint doctorate with VU Brussel)

Grants

Title	MANIAC – Making Analytically Incompatible Approaches Compatible
Applicants	Prof.dr. Peter Schoenmakers, prof.dr. Ron Peters, et al
Partners	DSM, Shell, Heineken, Micronit Microfluidics, VU, RU, RuG
Grant from	NWO/TI COAST
Amount	k€ 1.038 (1 PhD student and 3 year postdoc for HIMS)

Title	Intact Protein Analysis
Applicants	Dr. Andrea Gargano
Grant from	NWO Veni
Amount	k€ 250

Title	Forensic Explosives Intelligence (FEXIN)
Applicants	Prof.dr. Arian van Asten
Partners	TNO, NFI
Grant from	NCTV
Amount	1 PhD student

Title	Debottlenecking of chromatographic separations (DEBOCS)
Applicants	Prof.dr. Peter Schoenmakers
Partners	VU Brussels and private partners DSM Coating Resins, Dow Benelux, Janssen Pharma, Research Institute for Chromatography, Abundnz
Grant from	STW/ITW (Belgium)
Amount	k€ 416 (1 PhD student and 1 year postdoc for HIMS)

Prizes

Prof.dr. Peter Schoenmakers was ranked number 7 in Analytical scientist world ranking
Prof.dr. Peter Schoenmakers received Csaba Horváth Memorial Award
Prof.dr. Peter Schoenmakers received CASSS award
Bob Pirok received Young-Scientist Award at HPLC 2015 Beijing
Andrea Gargano received Csaba Horváth Young Scientist Award
Henrik Cornelisson van de Ven received HPLC2015 poster award
Marta Mourao received NanoCity 2015 poster award

Patents and utilization

Topic	Modulation Approach in Two-Dimensional Liquid Chromatography
Staff members	Prof.dr. Peter Schoenmakers, Henrik Cornelisson van de Ven M.Sc.
Activities	Patent filed, acquisition of industrial companies prepared.

Topic	IP workshop
Staff members	Prof.dr. Peter Schoenmakers et al
Activities	Workshop on valorisation and IP by IXA for CASA members.

3. Evaluation

After the mid-term evaluation in 2013, there were only light assessments by the Scientific Advisory Board (WAR) of HIMS in 2014 and 2015. In fact the year 2015 was evaluated in January 2016. This meeting was the last meeting of prof. Reinhoudt as WAR member and the first of prof. Arends who succeeds him.
Based upon a presentations on the follow-up of the 2014 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 has several of positive developments in the past year. The appointment of a significant number of new young staff members demonstrates the viability of HIMS. After years of budget limitations, it is good to see growth and an influx of young talents. Coaching of the new tenure track staff members will be important for the future of HIMS. The research continues to be of a high scientific level with a large number of high quality publications. In the present climate where publications in the highest impact journals serve as an important criteria to measure the success of research groups, it is important to continue to strive for even more publications in this category journals. The success in obtaining funding from a variety of external sources has been impressive in the past year, both for fundamental research as well as funding in programs requiring industrial participation.
In the past evaluation several recommendations of the WAR have stimulated action:

- *<u>Stronger cooperation between groups</u> – There is an increase in joint publications. Regular staff lunches and the joint housing are expected to further stimulate interaction between groups within HIMS and to also lead to more joint research proposals. The WAR is positive about the actions taken.*
- *<u>Stimulate entrepreneurship</u> – A number of measures has been taken, such as courses for PhD students and post-docs, participation in Innovation Labs, the HIMS Industry Day, support for staff members, also through a dedicated budget, for spin-off activities. Results are not clearly visible yet, which may be because of the short period since implementation. It is important to closely monitor the success of the measures taken and also to set clear (yearly) targets for expected results.*
- *<u>The time to obtain a PhD degree</u> has been significantly longer than four years. To reduce the delays, a stricter policy for extension of contracts has been implemented and a bonus of €2000 is offered if a manuscript is submitted within four years. So far, this has not resulted in a measurable improvement. It is recommended to monitor the developments closely and also to set ambitious (but realistic) targets for the coming years and, if the targets are not realized, implement additional measures.*
- *<u>The appointment of new staff members</u> within the 'Sectorplan Natuur- en Scheikunde' has been problematic and a sense of urgency was expressed by the WAR. It is encouraging to see that now all position have been filled with the appointment of Dr. Mutti in July 2015.*

A special point of action for the future is the appointment of a female professor/female professors within HIMS. It is important to increase the number of female staff members and some of the newly appointed young staff members are women which is encouraging. However, within the present HIMS staff of 24 professors, there is no female professor. This needs to change in the near future and immediate action is required.

<u>Composition of the WAR</u>
Prof. dr. Andries Meijerink (chair), Utrecht University
Dr. Tom van Aken, Avantium
Prof. dr. Isabel Arends, Delft University of Technology
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. HIMS received funding for 28 research proposals (see section 1.4.4). 20 of these projects were inspired by future applications and 14 of these projects have already companies participating and co-financing them. One of the granted projects is a collaboration with HIMS spin-off InCatT. On top of that two new contract research projects were started for companies.

In 2015 two new patent applications were filed, in collaboration with research consortia or companies. 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 IXA 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.

On 30 October 2015, HIMS organised its annual Industry Day. About 30 companies (from Amsterdam SMEs to multinationals) were introduced into the research themes of the UvA chemistry research institute. The Industry Day contained a talent lunch with PhD students and postdocs, active workshops and an informal poster session. The RPA Sustainable Chemistry discussed valorisation and possibilities for cooperation with its Industrial Advisory Board on 30 October 2015.

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. In 2015 HIMS made its analytical infrastructure available to ILCA members. Via ILCA HIMS became member of the Amsterdam Chemie Café where chemists from the Metropolitan area.

On top of the valorisation activities that focus on direct public-private collaboration or application of HIMS knowledge as mentioned above, there are more activities within HIMS that give besides scientific output value to society. Like other years HIMS trained in 2015 (together with TI-COAST and HRSMC) many talented people at bachelor, master and PhD and postdoc level. These young scientist left the Science Park for jobs in industry or academia nearby or else in the world.

That chemical knowledge of HIMS is of value for other disciplines can be shown by the many multi-disciplinary collaborations. Numerous are with the sister-institutes of our faculty. Outside our university HIMS collaborates in consortia like Solardam, BioSolar Cells, Co van Ledden Hulsebosch Center, Netherlands Institute for Conservation, Art and Science, Quantivision, LaserLaB Amsterdam, Advanced Research Center for Nanolithography.

Valorisation of research results

Topic	Photosensitiser based on Cu and Ni
Staff members	Prof.dr. Fred Brouwer, Prof.dr. Joost Reek, Hung-Cheng Chen M.Sc.
Activities	Patent filed. SBI student identified and contacted 22 companies that may be interested. Discussions with 8 of them started, two companies are serious interested in collaboration with HIMS.

Topic	Olefin oligomerisation catalysts
Staff members	Prof.dr. Joost Reek, Pierre Boulens M.Sc.
Activities	Shared IP agreement with IFP Energies Nouvelles was drafted.

Topic	Modulation Approach in Two-Dimensional Liquid Chromatography
Staff members	Prof.dr. Peter Schoenmakers, Henrik Cornelisson van de Ven M.Sc.
Activities	Patent filed, acquisition of industrial companies prepared.

Topic	In-situ and operando X-ray services
Staff members	Dr. Moniek Tromp
Activities	Investigation of possibilities for Spin-off company.

Topic	Catalyst to reduce CN levels in waste water treatment
Staff members	Prof.dr. Gadi Rothenberg, Dr. Shiju
Activities	Follow-up research projects with steel- and with precious metals industry (patent filed in 2014).

Topic	Improving sunscreens
Staff members	Prof.dr. Wybren Jan Buma
Activities	Cold acquisition to potentially interested personal care companies.

Topic	Expression system Shigella *flex*
Staff members	Em. prof.dr. Ron Wever
Activities	Sample sold to commercial catalogue house.

Topic	Plantics B.V.
Staff members	Prof.dr. Gadi Rothenberg
Activities	HIMS spin-off company received UvA Proof-of-Concept loan and a licence agreement for transfer of IP was drafted.

Topic	Cobalt based catalyst converts carboxylic acids to alcohols
Staff members	Prof.dr. Bas de Bruin, prof.dr. Kees Elsevier, dr. Jarl Ivar van der Vlugt, dr. Ties Korstanje
Activities	Patent was drafted, but company retracted in final stage. Other valorisation options are being explored.

Topic	Amsterdam Green Campus (AGC)
Staff members	Prof.dr. Michel Haring (SILS), dr. Shiju *et al*
Activities	HIMS participates in new platform for collaborating on education and valorisation.

Topic	IP workshop
Staff members	Prof.dr. Peter Schoenmakers *et al*
Activities	Workshop on valorisation and IP by IXA for CASA members.

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 leaders of the four HIMS themes and education are represented in management team. Per 31 December 2015 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 2015 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 ultimo 2015 (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 2015:

- 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 2016 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) was founded in 1994 and is legally represented by the University of Amsterdam. The research school was accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW) and is currently in its fourth accreditation period.

The HRSMC comprises research groups of the van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam (UvA); the Institute for Electrons and Molecular Structure (EMS) of the VU University (VU); and the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Leiden University (UL). 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 students, which offers a seamless connection to the Master degree programme. The primary aim is to teach PhD researchers to answer key questions in molecular science and to use their insights in a multidisciplinary approach. This is one of the aspects that makes the HRSMC unique in the Netherlands since it does not exclusively focus on a single research area as other graduate research schools do (e.g. polymers, catalysis, materials).
The extensive educational programme offered by the HRSMC means that for all practical purposes the school takes care of the educational program of its PhD students at HIMS, EMS, LO, and LION. Importantly, the educational activities of the HRSMC are also accessible for (advanced) MSc students and thereby seamlessly connect to the undergraduate programs of the participating universities.

The HRSMC has been elected in 2012 as one of the thirteen Graduate Schools to receive substantial funding from NWO. With this funding the HRSMC can offer PhD students the opportunity to develop their research ideas within the framework of the interuniversity and multidisciplinary Excellence MSc programme *"Sustainability, the Molecular Approach"*. In 2015, the HRSMC has granted two proposals for PhD research written by chemistry students Hans de Bruijn (appointed at the UL) and Kaj van Vliet (appointed at the UvA). Furthermore, in 2015 the HRSMC has established a Fellowship Programme that attracts international researchers to the Netherlands for a period up to six months. With its broad educational activities as well as its Graduate and Fellowship programmes, the HRSMC offers an excellent platform for interuniversity and multidisciplinary cooperation, and provides an incentive for world-class education and research in molecular chemistry and physics.

Major activities 2015

1. The annual HRSMC symposium (5 November, 2015), organized at the VU University. The symposium, which was attended by ca. 190 scientists, also included poster sessions with 44 posters. At the symposium, the annual Dick Stufkens prize for the best thesis within the HRSMC was awarded to Dr. Tatu Kumpulainen (former UvA PhD student, presently University of Geneva, Switserland).
2. The HRSMC educational activities of 2015 consisted of:
   - The Course '*Molecular Simulation*', organized under the auspices of CECAM (5-16 January 2015, UvA)
   - The Course '*Physical Methods in Inorganic Chemistry*' (29 January - 6 February 2015, UL/UvA)
   - The TULIP School '*Modern Developments in Spectroscopy*' (14-17 April 2015, Noordwijk)
   - The first 4-day *Proposal Writing Course* in combination with 1-day *Peer Review Course* (5-9 October 2015, UL)
   - The KNCV/HRSMC *Career Advice Activity* for PhD students and postdocs (13 October 2015, UL Gorlaeus; the KNCV is the Royal Dutch Chemistry Association).

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 advances Dutch excellence in innovation by providing pivotal analytical instruments and expertise to multiple economic sectors. COAST does this by securing and improving Dutch expertise in analytical science and technologies. Its strategic agenda combines efforts in R&D, human capital and infrastructure,

- advancing R&D and innovation in analytical technologies and encouraging cross-fertilization between analytical technologies and application areas (see also position photo with COAST focus), and
- improving education in analytical science and to increase the number of graduates, while
- providing access to (high-end) research facilities and knowledge for players within and across application areas.

The COAST research agenda connects knowledge institutes and companies in three ambitions for analytical science: “Revolutions in Resolutions”, “Analyzing Intact Systems” and “Bringing the Lab to the Sample”. In 2015 the COAST these three themes in the research portfolio comprised 15 public-private scientific research projects in which 34 companies (including 11 SMEs) collaborate with 19 academic groups. In the human-capital program approximately 80 students were enrolled in the COAST BSc and MSc talent programs for analytical chemistry, ASTP and MSc+. Moreover, more than 20 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. As a first step of this project, a 950 MHz instrument was installed in Utrecht in 2015. In addition, the web facility on analytical infrastructure presents 64 rare or unique high-end facilities available in the laboratories of COAST participants for use by other COAST participants. In 2015 COAST grew to 80 participants (47 companies, 28 academic groups at universities and 5 universities for applied sciences [hbo] with a Bachelor of Applied Science education). The groups of HIMS full professors Schoenmakers and Corthals are members of COAST.

5.1.3. Co van Ledden Hulsebosch Center

The Co van Ledden Hulsebosch Center (CLHC) is an initiative of the Faculty of Science (FNWI), the Academic Medical Center (AMC) and the Netherlands Forensic Institute (NFI). The CLHC encompasses the collaborative forensic science activities of the three institutes also including several national and international partnerships.
The center officially started in September 2013 and after an evaluation after two years all three partners unanimously decided in 2015 to continue the successful partnership. In a short period of time the CLHC has quickly developed into a nationally and internationally acknowledged forensic science center with a diverse and successful forensic science program.

In 2013-2015 a total of 8 PhD students successfully defended their PhD thesis in forensic science areas such as biophysics and physics, radiology, biology, digital forensics, medicine and chemistry.
In total over thirty PhD students published 100+ peer reviewed publications in forensic science together with their supervisors in the various FNWI institutes and AMC and NFI teams.
Currently under the umbrella of the CLHC six special chairs in forensic science have been realized in forensic

statistics, forensic data science, forensic biophysics, forensic biology, forensic radiology and forensic analytical chemistry.

The CLHC and its coordinators and professors contribute to the Forensic Science Master (FSM) of the Institute for Interdisciplinary Studies (IIS), together with the FSM the CLHC organises the successful lecture series Frontiers in Forensic Science. During the EAFS 2015 conference in Prague (European Academy of Forensic Sciences) the CLHC was presented to over 1000 participants from forensic laboratories, law enforcement agencies and academic institutes. In the scientific program a CLHC presentation focused on the novel matrix approach which has been developed in Amsterdam to create a diverse forensic science program that includes all main expertise areas.

A new international folder and annual report was produced and distributed during the conference to establish an international network.

Although the CLHC is an FNWI-AMC-NFI center there is a strong connection to HIMS. The center is physically located within HIMS and HIMS supports the development and maintenance of the CLHC website and assists in the financial administration.
Within HIMS three professors are directly involved in forensic science : prof Peter Schoenmakers (analytical chemistry and its forensic applications), prof Arian van Asten (forensic analytical chemistry) and prof Maurice Aalders (forensic biophysics). Additionally, dr Gabriel Vivo Truyols, prof dr Garry Corthals and prof dr Fred Brouwer are involved in forensic science projects as part of their research activities.

Fields of expertise and research topics include explosives profiling and intelligence, the forensic application of comprehensive chromatography, portable, rapid methods for chemical analysis at the scene of crime, the hyperspectral imaging and dating of biological forensic traces, the use of chemometric methods for the analysis of large forensic analytical datasets, Bayesian statistics in peak detection, forensic biochemical mass spectrometry and fluorescence and chemiluminescence applications in forensic science (the latter two topics in close collaboration with the AMC).

Within HIMS in 2015 in total 2 PhD students were fully (FEXIN and COMFOR project) and 2 PhD students were partly (Chromametrics project) involved in forensic research and numerous forensic and chemistry master students conducted literature thesis studies and research projects on forensic chemistry topics.
In 2015 two new forensic projects were granted : FEXIN - Forensic Explosives Intelligence (EU funding via the Internal Security Fund) and Age determination of forensic biological traces at the crime scene (STW OTP).

In 2016 the main priority of the CLHC is to maintain and develop its forensic science program by applying for national and international (H2020) funding for new forensic science projects.
Additionally, the CLHC will expand nationally by allowing new partners in Amsterdam and in the Netherlands with a strong interest in forensic science to join the CLHC network.
Within Amsterdam the University of Applied Sciences (HvA) and VU Amsterdam University are scheduled to become primary partners within the center thereby further strengthening forensic science in Amsterdam.
Furthermore, the CLHC will develop its international contacts and initiatives have already been undertaken to establish a global network of academic forensic science centers.

The CLHC is managed by directors prof dr Maurice Aalders and prof dr Arian van Asten.
The CLHC website (www.clhc.nl) is maintained by Ineke Weijer of the HIMS secretariat.
Prof dr Joost Reek is member of the CLHC steering group on behalf of FNWI and HIMS.

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 2015 of the HIMS themes, per employment type (fte)[a]

	SC	COMP	ACF	MOLP	Other	**Total**
Tenured staff	11,1	6,0	5,0	4,8	1,0	27,9
Non-tenured staff	6,3	3,0	1,7	0,0	2,0	12,9
PhD candidates	24,2	6,8	7,8	9,1	1,8	49,7
Total research staff	**41,6**	**15,8**	**14,5**	**13,9**	**4,8**	**90,6**
Technicians [b]	11,6	0,0	2,5	3,2	0,0	17,3
Visiting fellows [c]	0,0	0,0	0,2	1,3	0,0	1,5
Total research	**53,1**	**15,8**	**17,2**	**18,5**	**4,8**	**109,4**
Supporting staff					5,8	5,8
Total staff	**53,1**	**15,8**	**17,2**	**18,5**	**10,5**	**115,1**

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

Research- and supporting staff 2015 of HIMS and the HIMS groups, per employment type (fte)[a]

	HH	FM	JR	CE	GR	PB	EJM	PS	WJB	FB	Other	**Total**
Tenured staff	1,6	0,0	2,0	0,5	1,5	2,0	1,0	2,5	1,4	1,0	0,5	14,0
Non-tenured staff	0,0	0,2	3,4	0,6	1,5	2,1	0,7	1,5	00	0,0	1,8	11,6
PhD candidates	2,5	0,0	14,3	0,5	0,9	5,1	0,0	5,9	3,5	3,3	1,3	37,3
Total research staff	**4,0**	**0,2**	**19,6**	**1,6**	**3,9**	**9,1**	**1,7**	**9,9**	**4,9**	**4,4**	**3,6**	**62,9**
Technicians [b]	3,1	0,3	4,4	1,8	2,0	0,0	0,0	2,5	2,2	1,0	0,0	17,3
Visiting fellows [c]	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,1	0,7	0,0	0,0	0,8
Total research	**7,1**	**0,4**	**24,0**	**3,4**	**5,9**	**9,1**	**1,7**	**12,5**	**7,8**	**5,4**	**3,6**	**80,9**
Supporting staff											5,8	5,8
Total staff	**7,1**	**0,4**	**24,0**	**3,4**	**5,9**	**9,1**	**1,7**	**12,5**	**7,8**	**5,4**	**9,4**	**86,7**

Research groups: HH = group Hiemstra; FM = group Mutti/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.	**Total**	**%**
Direct funding [1a]	17,6	2,6	4,8	5,7	0,5	**31,1**	**38**	4,5	35,6	
Indirect funding [1b]	1,8	0,0	0,0	0,0	0,0	**1,8**	**2**	0,0		**2**
Direct [1a] + indirect [1b]	**19,4**	**2,6**	**4,8**	**5,7**	**0,5**	**33,0**	**41**	**4,5**	**37,5**	
Research grants 2	15,4	6,6	4,8	2,5	2,6	**31,9**	**39**	0,0	31,9	**37**
Contract research [3]	2,9	0,8	2,1	0,1	0,0	**5,9**	**7**	1,2	7,1	**8**
Other [4]	3,1	0,8	0,9	4,8	0,6	**10,2**	**13**	0,0	10,2	**12**
Total	**40,8**	**10,8**	**12,5**	**13,1**	**3,6**	**80,9**	**100**	**5,8**	**86,7**	**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	FM	JR	CE	GR	PB	EJM	PS	WJB	FB	**Other**	**Total research**	Supp staff	**Total**	**%**
Direct funding [1a]	4,5	0,4	7,0	2,2	3,5	1,6	1,0	4,8	3,3	2,4	0,5	**31,1**	4,5	**35,6**	***41***
Indirect funding [1b]	0,0	0,0	1,5	0,3	0,0	0,0	0,0	0,0	0,0	0,0	0,0	**1,8**	0,0	**1,8**	***2***
Direct [1a] + indirect	**4,5**	**0,4**	**8,6**	**2,5**	**3,5**	**1,6**	**1,0**	**4,8**	**3,3**	**2,4**	**0,5**	**33,0**	**4,5**	**37,5**	***43***
Research grants 2	2,3	0,0	12,7	0,0	0,5	5,9	0,7	4,8	2,0	0,5	2,6	**31,9**	0,0	**31,9**	***37***
Contract research [3]	0,1	0,0	2,1	0,7	0,1	0,8	0,0	2,1	0,1	0,0	0,0	**5,9**	1,2	**7,1**	***8***
Other [4]	0,3	0,0	0,7	0,2	1,9	0,8	0,0	0,9	2,4	2,5	0,6	**10,2**	0,0	**10,2**	***12***
Total	**7,1**	**0,4**	**24,0**	**3,4**	**5,9**	**9,1**	**1,7**	**12,5**	**7,8**	**5,4**	**3,6**	**80,9**	**5,8**	**86,7**	***100***

HH = group Hiemstra; FM = former 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/Sectorplan/Sustainable Chemistry)
[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 2015 (mln €) per funding type[1]

HIMS themes	SC	COMP	ACF	MOLP	Other	**Total[5]**
1st - NRSC-C [1]	0.00	0.00	0.00	0.00	0.00	**0.00**
1st - Other [2]	0.00	0.00	0.00	0.00	0.00	**0.00**
2nd [3]	4.59	0.16	1.46	1.20	0.88	**8.28**
3rd [4]	1.48	0.26	0.37	0.12	0.06	**2.29**
Total	**6.06**	**0.42**	**1.83**	**1.32**	**0.94**	

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	FM	JR	CE	GR	PB	EJM	PS	WJB	FB	PI	Total[5]
1st - NRSC-C [1]	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 [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**
2nd [3]	0.35	0.26	2.94	0.00	1.03	0.08	0.08	1.46	1.20	0.00	0.88	**8.28**
3rd [4]	0.00	1.46	0.12	0.00	0.02	0.26	0.00	0.37	0.12	0.00	0.06	**2.29**
Total	**0.35**	**1.72**	**2.94**	**0.00**	**1.05**	**0.34**	**0.08**	**1.83**	**1.32**	**0.00**	**0.94**	**10.57**

HH = group Hiemstra; FM = group Mutti (former groupWever); 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 5,11 mln € foreseen) excluded; own contributions HIMS (in kind and cash/from reserves) included
[2] NRSC-C (TOP Research School Catalysis);
[3] NWO-CW, FOM, STW, KNAW, ERC
[4] EU, DPI, AGENTSCHAP.NL, NanoNext, NFI, Industry
[5] Budgets were obtained for fte 23 PhD's, 19 PD and 1,1 staff.

6.2.2 Research output of the HIMS themes

Research output 2015 per type of publication source: METIS

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint [1]	Total
Refereed articles	81	57	27	57		-10	**221**
Non-refereed articles	1	1	1	0	0		**3**
Books	0	0	0	0	0		**0**
Book chapters	4	0	0	2	0		**6**
PhD-theses	8	5	3	7	3	-7	**19**
Conference papers	0	0	0	0	0		**0**
Patents	4	0	0	1	0		**5**
Professional publications	5	0	1	1	0		**7**
Publications general public	0	1	0	0	0		**1**
Other research output	4	0	1	2	0		**7**
Total		**64**	**33**	**70**		**-17**	**269**

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	5		50	4	11	1	15		29	27	49	8	9	-10	**221**
Non-ref. articles	0	0	1	0	0	0	1	0	0	1	0	0	0		**3**
Books	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Book chapters	0	2	0	0	2	0	0	0	0	0	2	0	0		**6**
PhD-theses	2	0	5	1	0	0	4	1	0	3	6	1	3	-7	**19**
Conference papers	0	0	0	0	0	0	0	0	0	0	0	0	0		**0**
Patents	0	1	3	0	0	0	0	0	0	0	0	1	0		**5**
Prof. publications	0	0	4	0	1	0	0	0	1	1	1	0	0		**7**
Publ. general public	0	0	0	0	0	0	0	0	1	0	0	0	0		**1**
Other output	1	0	2	0	0	1	3	0	0	1	2	0	0		**7**
Total			**65**	**5**	**14**	**2**	**20**		**30**	**33**	**60**	**10**	**12**		**269**

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 2015, in ranges of different impact factor Source: METIS

HIMS themes	SC	COMP	ACF	MOLP	Other	Joint [1]	**Total**
>15		2	0		0	-2	**10**
10-15		6	0		0	-1	**21**
5-10	28	16		11	0	-4	**58**
<5	42	35	22	39	9	-10	**137**
Total		**59**	**29**	**58**	**9**	**-17**	**226**

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/F	JR	CE	GR	AK	PB	EJM	RK	PS	GC	WJB	FB	PI	Joint[1]	**Total**
>15	0	1	5	1	0	0	0	0	2	0	0	2	1\	0	-2	**10**
10-15	0	2	9	0	0	0	0	0	6	0	0	4	1	0	-1	**21**
5-10	1	2	17	0	8	0	3	5	8	7		8	3	0	-4	**58**
<5	5	5	24	3	4	1	13	8	14	22		36	3	9	-10	**137**
Total	6	10	55	4	12	1	16	13	30	29	41	50	8	12	-17	**226**

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; GC= groep Corthals; WJB = group Buma; FB=group Brouwer; PI= group Iedema

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

The total of joint publications increased from 9 in 2014 to 17 in 2015. This is a result of more joint projects within the institute.

6.2.3 Efficiency of the doctoral research path

The following tables show the efficiency of the doctoral research path (period of appointment 2007-2011; planned PhD defence 2011-2015). Note that these numbers are arranged per starting date of the PhD students, while the figure in paragraph X counts the length of the PhD tracks based on PhD defences in each year.

Employed PhD-candidates of HIMS

Enrolment				Success rates of graduation in years after start							
Start	**M**	**F**	**Total**	**< 4**	**4-5**	**5-6**	**6-7**	**>7**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
2007	9	5	**14**	3	2	1	0	2	1		
2008	4	9	**13**	0	3	3	4	0	1	0	3
2009	4	8	**12**	0	7	2	0	0	0	0	3
2010	10	4	**14**	0	5	3	0	0	3	2	1
2011	8	8	**16**	2	3	1	0	0	0	9	2
Total	**35**	**34**	**69**	**5**	**20**	**10**	**4**	**2**	**5**	**11**	**12**
Cumulative 2007-2011											
SC	13	13	**26**	0	13	4	0	1	0	4	4
COMP	8	5	**13**	0	2	2	3	0	0	3	3
MBA	4	10	**14**	2	3	1	1	1	0	2	4
MOLP	9	5	**14**	3	0	3	0	0	5	2	1
Others	1	1	**2**	0	2	0	0	0	0	0	0
Total	**35**	**34**	69	**5**	**20**	**10**	**4**	**2**	**5**	**11**	**12**
%	***51***	***49***	***100***	***7***	***29***	***15***	***6***	***3***	***7***	***16***	***17***

Non-employed PhD-candidates of HIMS

Enrolment				Success rates of graduation in years after start							
Start	**M**	**F**	**Total**	**< 4**	**4-5**	**5-6**	**6-7**	**>7**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
2007	2	0	**2**	1	2	0	1	0	0	0	0
2008	3	0	**3**	0	1	1	0	0	0	0	0
2009	3	0	**3**	0	1	1	0	0	0	0	1
2010	2	2	**4**	0	1	3	0	0	0	0	0
2011	4	1	**5**	1	0	0	0	0	0	2	1
Total	**14**	**3**	**17**	**2**	**5**	**5**	**1**	**0**	**0**	**2**	**2**
Cumulative 2007-2011											
SC	3	2	**5**	1	0	3	1	0	0	0	0
COMP	0	0	**0**	0	0	0	0	0	0	0	0
MBA	3	1	**4**	1	1	0	0	0	0	0	2
MOLP	8	0	**8**	0	4	2	0	0	0	2	0
Others	0	0	**0**	0	0	0	0	0	0	0	0
Total	**14**	**3**	**17**	**2**	**5**	**5**	**1**	**0**	**0**	**2**	**2**
%	**82**	**18**	**100**	**12**	**29**	**29**	**6**	**0**	**0**	**12**	**12**

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

Enrolment (numbers)				Success rates of graduation in years after start							
Starting year	**M**	**F**	**Total**	**< 4**	**4-5**	**5-6**	**6-7**	**>7**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
Sustainable Chemistry (SC)											
2007	1	0	**1**	0	0	0	0	1	0	0	0
2008	3	4	**7**	0	4	0	1	0	0	0	2
2009	3	5	**8**	0	5	2	0	0	0	0	1
2010	5	3	**8**	0	3	4	0	0	0	0	1
2011	4	3	**7**	1	1	1	0	0	0	4	0
Total	**16**	**15**	**31**	**1**	**13**	**7**	**1**	**1**	**0**	**4**	**4**
%	**52**	**48**	**100**	**3**	**42**	**23**	**3**	**3**	**0**	**13**	**13**
Computational Chemistry (COMP)											
2007	1	1	**2**	0	1	0	1	0	0	0	0
2008	1	2	**3**	0	0	1	2	0	0	0	0
2009	0	2	**2**	0	1	0	0	0	0	0	1
2010	3	0	**3**	0	0	1	0	0	0	2	0
2011	3	0	**3**	0	0	0	0	0	0	1	2
Total	**8**	**5**	**13**	**0**	**2**	**2**	**3**	**0**	**0**	**3**	**3**
%	**62**	**38**	**100**	**0**	**16**	**15**	**23**	**0**	**0**	**23**	**23**
Analytical Chemistry (incl its application in Forensic Science)											
2007	4	4	**8**	2	1	1	0	1	0	0	3
2008	1	1	**2**	0	0	0	1	0	0	0	1
2009	1	1	**2**	0	1	0	0	0	0	0	1
2010	0	0	**0**	0	0	0	0	0	0	0	0
2011	1	5	**6**	1	2	0	0	0	0	2	1
Total	**7**	**11**	**18**	**3**	**4**	**1**	**1**	**1**	**0**	**2**	**6**
%	**39**	**61**	**100**	**17**	**22**	**6**	**6**	**6**	**0**	**11**	**32**
Molecular Photonics (MOLP)											
2007	5	0	**5**	2	2	0	0	0	1	0	0
2008	2	2	**4**	0	0	3	0	0	1	0	0
2009	3	0	**3**	0	1	1	0	0	0	0	1
2010	3	2	**5**	0	1	1	0	0	3	0	0
2011	4	1	**5**	1	0	0	0	0	0	4	0
Total	**17**	**5**	**22**	**3**	**4**	**5**	**0**	**0**	**5**	**4**	**1**
%	**77**	**23**	**100**	**14**	**18**	**23**	**0**	**0**	**23**	**18**	**4**
Others											
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	2	0	0	0	0	0	0
2011	0	0	**0**	0	0	0	0	0	0	0	0
Total	**1**	**1**	**2**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
%	**50**	**50**	**100**	**0**	**100**	**0**	**0**	**0**	**0**	**100**	**0**

Total HIMS

Enrolment				Success rates of graduation in years after start							
Start	**M**	**F**	**Total**	**< 4**	**4-5**	**5-6**	**6-7**	**>7**	**Outside UvA**	**Not yet finished**	**Discon-tinued**
2007	11	5	**16**	4	4	1	1	2	1	0	3
2008	7	9	**16**	0	4	4	4	0	1	0	3
2009	7	8	**15**	0	8	3	0	0	0	0	4
2010	12	6	**18**	0	6	6	0	0	3	2	1
2011	12	9	**21**	3	3	1	0	0	0	11	3
Total	**49**	**37**	**86**	**7**	**25**	**15**	**5**	**2**	**5**	**13**	**14**
Cumulative 2007-2011											
SC	16	15	**31**	1	13	7	1	1	0	4	4
COMP	8	5	**13**	0	2	2	3	0	0	3	3
ACF	7	11	**18**	3	4	1	1	1	0	2	6
MOLP	17	5	**22**	3	4	5	0	0	5	4	1
Others	1	1	**2**	0	2	0	0	0	0	0	0
Total	**49**	**37**	**86**	**7**	**25**	**15**	**5**	**2**	**5**	**13**	**14**
%	**57**	**43**	**100**	**8**	**29**	**17**	**6**	**2**	**6**	**15**	**16**

6.3 Finance 2015

The table below shows the HIMS financial result 2015.

HIMS result 2015 (k€)

	1st (1 structural	1st (2 Other	1st total	2nd (3	3rd (4	Total
HIMS						
Budget (fixed)	3.850		3.850			**3.850**
Budget (variable[5])	5.613		5.613	2.623	2.070	**10.306**
Other income		255	255			**255**
Matching contract research	-3.856		-3.856	2.581	1.275	**0**
Budget total	**5.607**	**255**	**5.862**	**5.204**	**3.345**	**14.411**
Percentage	**39**	**2**	**41**	***36***	**23**	***100***
Personal costs	*-3.802*	-109	*-3.911*	*-1.841*	*-1.413*	***-7.165***
Other costs (projects)	*-1.197*	-147	*-1.344*	*-821*	*-561*	***-2.726***
Overhead (central)	*791*		*791*	*-510*	*-281*	**0**
Overhead (faculty)	*-921*		*-921*	*-978*	*- 526*	***-2.425***
Overhead (institute)	*1.627*		*1.627*	*-1.050*	*- 577*	**0**
Various costs						
Other (secundary) costs	*- 2.112*		*-2.112*		*-27*	***-2.139***
Costs total	***-5.614***	**-256**	***-5.870***	***-5.200***	***-3.385***	***-14.455***
Percentage	**39**	**2**	**41**	**36**	**23**	**100**
Result 2015	***-7***	**-1**	***-8***	**4**	**-40**	**-44**
Reservations[6]	-120		-120			-120
Result inclusive reservation	**113**	**-1**	**112**	4	**-40**	**76**

1 Direct funding (1st, eerstegeldstroom; university/direct funding,
2 Various contibutions for 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 From reservations incl. SectorPlan and Sustainable Chemistry

The HIMS result for 2015 amounts to +76 k€. This result includes the spending from reservations of -120 k€. These are reservations for costs to be made in the coming years mainly from the budget for appointments in the framework of the 'Sectorplan Natuur- en Scheikunde' and the Research Priority Area Sustainable Chemistry.