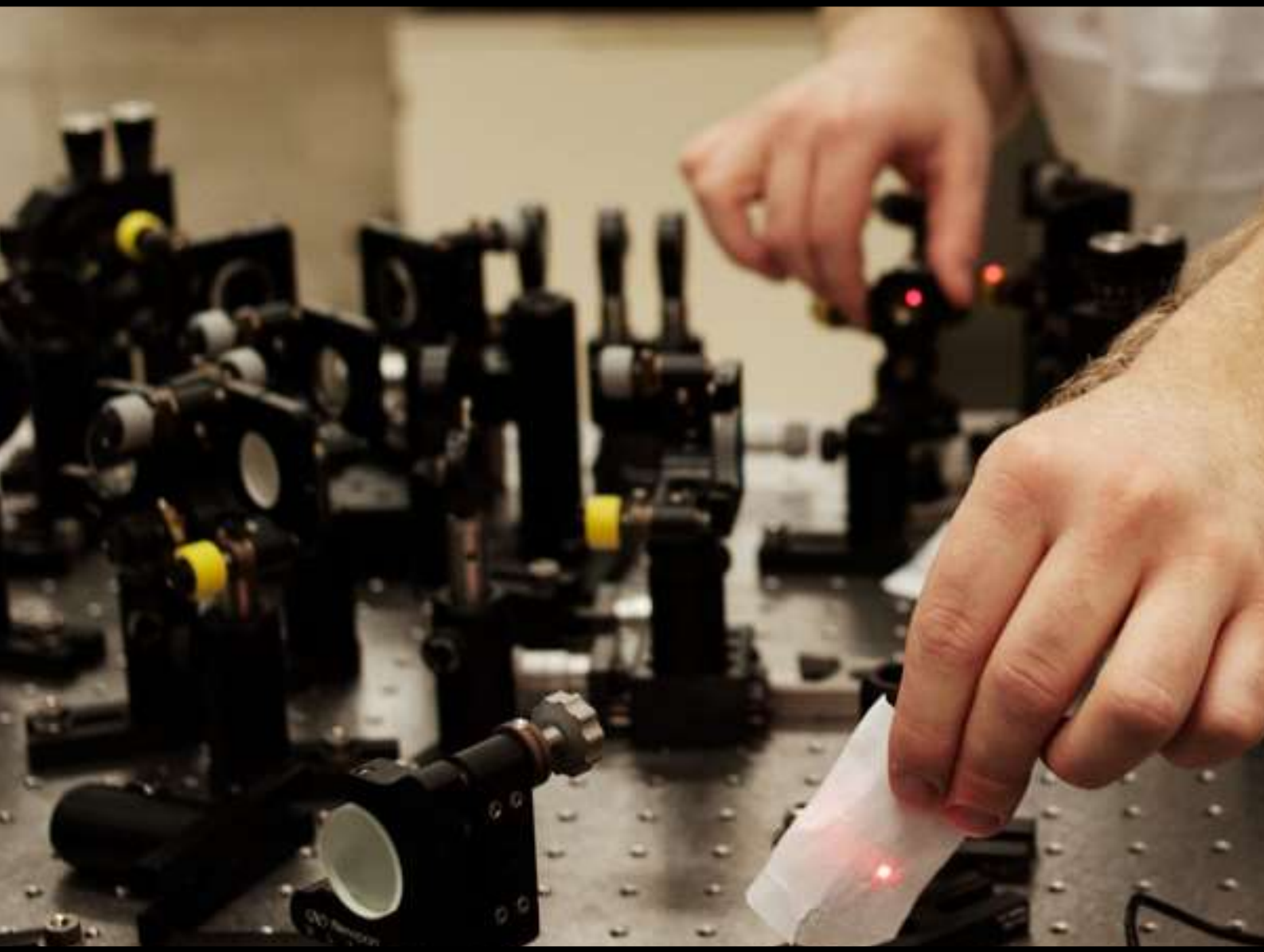
# Van ’t Hoff Institute for Molecular Sciences



# Annual report 2016

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Cover:
HIMS PhD student Benjamin Strudwick at the laserlab. Photograph by Teska Overbeeke.

June 2017

# Preface

I am proud to report that 2016 was again a great year for HIMS, in which the number of young scientific staff (PhD students and postdocs) increased with almost 20 due to expansion of external research funding. New projects were acquired and we underpinned our international position with even more appealing publications in renowned scientific journals.

As a whole HIMS has been very successful in establishing new research fields. HIMS welcomed two Vidi-fellows and one professor by special appointment. 15 new projects were acquired with a total funding of 6 million euros granted by EU, NWO and Topsector Chemistry. Amongst these was a prestigious ERC Advanced Grant. 13 projects were inspired by future applications and 9 of these projects already have participating and co-financing companies. In 2016 four new patent applications were filed based on HIMS research. A total of 12 promising valorisation opportunities were exploited.

The scientific level of HIMS research is very high, which is reflected in 216 peer-reviewed scientific publications, many of which in high impact journals, including two *Science* papers. 14 PhD students successfully defended their theses, two of them receiving their PhD *cum laude*. The quality of HIMS scientists is also reflected in the prizes and honours awarded, Prof. Bas de Bruin was named UvA Lecturer of the Year by the UvA Student Council, PhD student Jurn Heinen was one of the winners of the first Amsterdam heat of *FameLab*, The Royal Netherlands Chemical Society KNCV awarded Prof. Jan van Maarseveen its '*Van Marumpenning*', researcher Dr. Bert Wouters was awarded the '*Solvay Award*' for his groundbreaking PhD research and Prof. em. Ron Wever received the 7th *Vanadis* Award for his research on vanadium haloperoxidases.

After years of preparations we were very happy to welcome the group of Dr. Chris Slootweg from VU University Amsterdam to HIMS in November 2016. The group will be embedded within the synthetic-organic-chemistry group led by Prof. Jan van Maarseveen and its focus fits perfectly within the sustainable chemistry aims of HIMS.

The RPA Sustainable Chemistry is very active at many different levels. Together with ACE venture Labs a bootcamp week on Sustainable Chemistry entrepreneurship was organised in November 2016. Junior researchers Simon Mathew, Marissa de Boer and Monalisa Goswami were awarded financial support and mentoring during the start-up of their chemistry-based spin-off company.

At the end of 2016 I was appointed as the new director of HIMS, succeeding Prof. Joost Reek, who stepped down after three years. I thank Prof. Reek for his commitment to HIMS and the great institution that he entrusted to his successor and I am very happy that he will continue to serve as successful group leader within HIMS and as the figurehead of the UvA research priority area Sustainable Chemistry in his new role as distinguished research professor at the UvA Faculty of Science.

To conclude, 2016 was successful scientifically, and also in terms of valorisation and 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.ir. Peter Schoenmakers
Director

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# 1. General considerations and highlights

## 1.1 Key figures of HIMS in 2016

The high level of scientific output of HIMS was maintained in 2016. HIMS published 8 papers in absolute top journals (impact factor > 15) and 20 papers in top journals (impact factor 10-15). The total number of refereed and other professional publications, patents and book (chapter)s increased to 254, of which 19 where joint publications. The amount of published PhD dissertations was 13, which was slightly under the average of 2010-2015 (15.5 average).

With a total of 6.2 M€ in external funding (excluding the own matching budge) the year 2016 was even more successful than former years. These funds were acquired from funding agencies as NWO/FOM, EU/ERC, as well as from industry and other partners.

## 1.2 Personnel

In 2016 the total staff amounted to 143.2 fte. This is about 15 fte more than the former years. The increase is due to the start of the expansion in staff in the past years. Several tenure track researchers acquired projects and appointed PhD students and postdocs. In 2016 Dr. Annemieke Petrignani and Dr. Tiddo Mooibroek started as a vidi-fellows. Prof. Gert-Jan Gruter was appointed professor by special appointment of Industrial Sustainable Chemistry on behalf of the Foundation *Stichting Bèta Plus*. His research will focus primarily on making industrial chemical processes more sustainable. After elaborate preparations the group of Dr Chris Slootweg moved from VU University Amsterdam to HIMS in November 2016. Two PhD students: Dr Ariana Torres Knoop and Dr Danny Broere received their PhD Cum Laude.

## 1.3 Finances

HIMS finished the year 2016 with a slight negative financial result of - 16 k€. This result should be corrected with the costs (120k€) that find their resources in the reservations for appointments in the framework of the *Sectorplan Natuur- en Scheikunde* and the RPA Sustainable Chemistry and some other appointments. The remaining result for 2016 is 312 k€ positive.

## 1.4 Highlights

### 1.4.1 Institutional highlights

**Sino-Dutch partnership**

In a collaborative project with the Center of Interface Dynamics for Sustainability (CIDS) at the Chengdu Development Center for Science and Technology in China, HIMS researchers are exploring a new method for recycling carbon dioxide. The Sino-Dutch partnership received funding from both the Netherlands Organisation for Scientific Research (NWO) and the National Natural Science Foundation of China (NSFC).

**Japanese visit**

As part of the 'Program for Advancing Strategic International Networks to Accelerate the Circulation of Talented Researchers' Japanese scientists from Kanazawa University visited HIMS. Their visit was funded by the Japan Society for the Promotion of Science.

**Continued collaboration in forensic science**

The Netherlands Forensic Institute (NFI), the Academic Medical Center (AMC) and the UvA Science faculty continued their cooperation in the Co van Ledden Hulsebosch Center in the field of forensic

science. HIMS researchers participate in CLHC, for example in the new project FEXIN aimed at improving chemical methods for the investigation of explosives. Later in the year TU Delft also joined CLHC.

**Sustainability Workshop**
On 23 September 2016 HIMS and HRSMC (Holland Research School of Molecular Chemistry) jointly organised a successful workshop on Sustainability featuring professor Jacqueline Cramer (UvA alumnus and former Dutch minister of Housing, Spatial Planning and the Environment) as keynote speaker. Fascinating plenary lectures and engaging workshop sessions gave rise to fruitful discussions among the many participants.

**Amsterdam Chemistry Innovation Day**
HIMS hosted the Amsterdam Chemistry Innovation Day on 28 October 2016, organised in association with the Innovation Lab Chemistry Amsterdam (ILCA) and the Amsterdam Green Campus. The day offered participants from academia and industry the lowdown on progress and innovation in chemistry while providing ample opportunity for networking and scouting for PhD talent.

**Most highly cited researcher**
Prof. em. Rajamani Krishna is one of the few Dutch chemists in the list of Highly Cited Researchers 2016. The authoritative listing was compiled by Clarivate Analytics, formerly the Intellectual Property & Science business of Thomson Reuters. Throughout his career, prof. Krishna has focused on improving technologies related to reaction and separation by means of investigating physico-chemical phenomena at the molecular and microscopic levels.

**Slootweg research group moves to HIMS**
The organic chemistry research group led by Dr Chris Slootweg moved from Vrije Universiteit Amsterdam to the HIMS Synthetic Organic Chemistry group led by Prof. Jan van Maarseveen. The transfer forms a meaningful addition to the UvA research priority area Sustainable Chemistry.

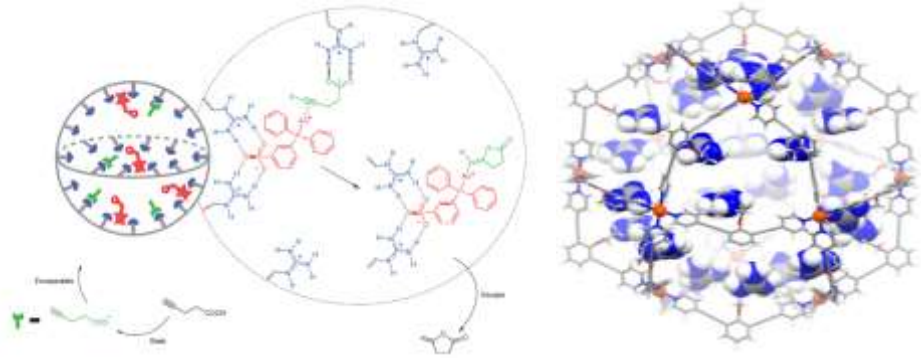
**New director**
Peter Schoenmakers was appointed as new scientific director of HIMS starting 1 January 2017, succeeding Prof. Joost Reek who will continue to be the coordinator of the UvA's research priority area Sustainable Chemistry.

**Grants awarded**
Professor Peter Schoenmakers received an ERC Advanced Grant. The Innovational Research Incentives Scheme of NWO yielded Tiddo Mooibroek a VIDI grant and Ties Korstanje a VENI grant. Other memorable awards were an ECHO grant for Jarl Ivar van der Vlugt, KIEM grants for Moniek Tromp and professor Jan van Maarseveen, TKI grants for Raveendran Shiju and professor Maarten van Bommel and CSER grants for Bernd Ensing and professor Peter Bolhuis. All in all a total of 15 research proposals of HIMS researchers where granted in 2016 (see section 1.4.4). 13 of these projects were inspired by future applications and 9 projects have already companies participating and co-financing them.

## 1.4.2 Scientific highlights

**Homogeneous and Supramolecular Catalysis**

The nanoconcentrator, a new catalytic nanosphere concept has been developed in the context of the ERC Advanced Grant research program 'Nature Inspired Transition Metal Catalysis'. The new nanocontainers are formed by self-assembly: mixing 12 palladium metals and 24 so-called ditopic nitrogen ligands leads to formation of nano-sized spheres. The ditopic nitrogen ligands are modified with guanidinium binding motifs such that the resulting nanocontainers are able to bind sulfonates and carboxylates in their interior. Sulfonate guests are bound much more strongly than carboxylates because of so-called cooperative binding (employing multiple binding sites). This has been used to firmly fix sulfonated gold-based catalyst, while the remaining binding sites are available for the pre-organisation of the carboxylate moieties that are to be converted (the substrates). The working principles of this 'nanoconcentrator' system was established using a gold-catalysed cyclization reaction. The local high concentration of the metal catalyst combined with the pre-organization of the substrate resulted in dramatically enhanced reaction rates in comparison to common systems where the catalyst and the reactants are not pre-organised but just both dissolved in a solvent. Reactions usually increase with catalyst and substrate concentration; but this is generally limited solubility issues or unfavorable catalyst/reactant ratios. This has now been solved by taking advantage of local concentrations in the self-assembled nanoconcentrator. *Nature Chemistry,* **2016**



**Heterogeneous Catalysis and Sustainable Chemistry**

**From MOFs to structured "carbon onions" – advanced material design**

A collaboration between several group members together with researchers from University of Bucharest, EPFL, and Lawrence Berkeley Laboratories in California has led to the successful development of tunable multi-shell carbon materials with a host of applications in catalysis and sustainable energy. By simple tuning of the reaction pH, a series of new materials were made based on the self-assembly of two joined metal-organic frameworks. These can be easily carbonised, giving "carbon onions" with excellent accessibility. Their structure resembles a modern highway system, with interconnected wide and narrow roads. These new materials are now being applied as supercapacitors, oxidation catalysts and fuel cell electrodes.

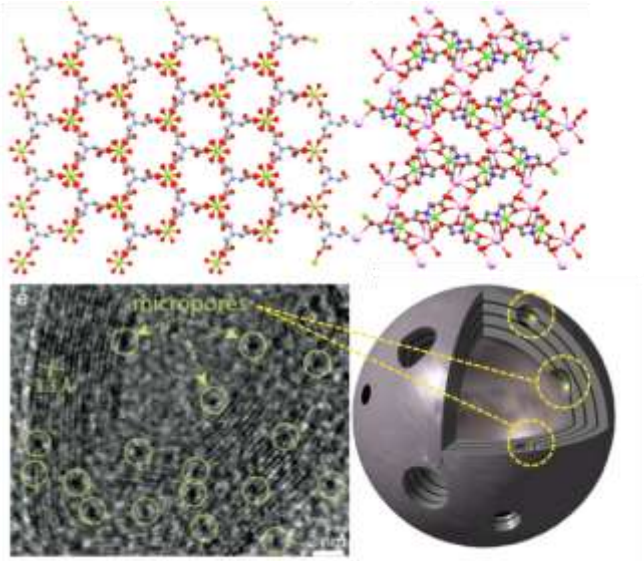
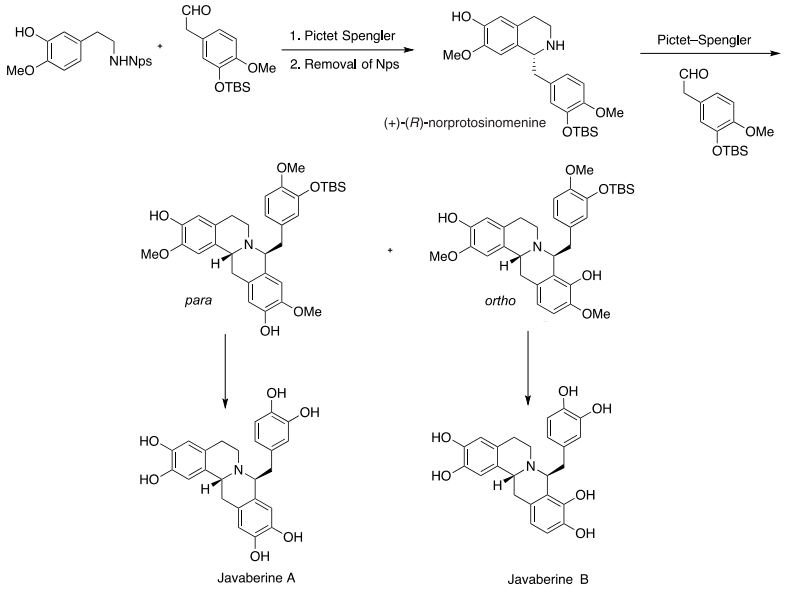



**Figure 1**. The self-assembly of two MOFs (above) and pyrolysis gives nested graphitic shells with interconnecting micropores (below).

- A rational synthesis of hierarchically porous, N-doped carbon from Mg-based MOFs: Understanding the link between nitrogen content and oxygen reduction electrocatalysis. D. Eisenberg, W. Stroek, N.J. Geels, S. Tanase, M. Ferbinteanu, S.J. Teat, P. Mettraux, N. Yan, G. Rothenberg *Phys. Chem. Chem. Phys.,* **2016**, 18, 20778-20783.

**Synthetic Organic Chemistry**

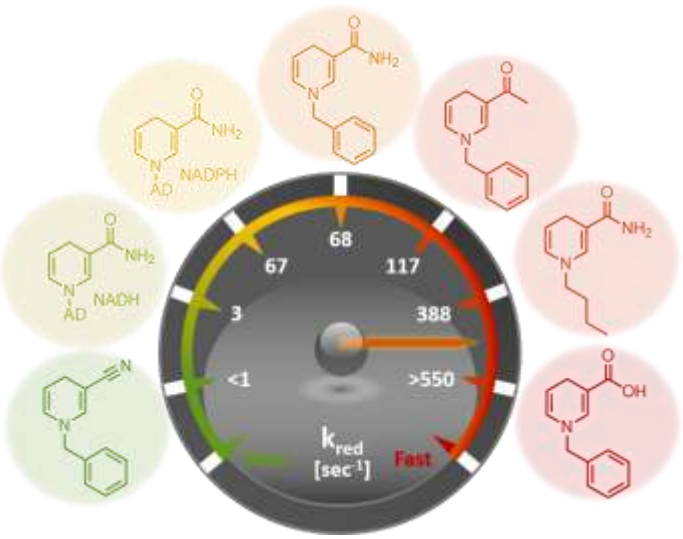
An enantioselective organocatalytic synthesis of the natural 8-benzylprotoberberines (+)-javaberine A and (+)-javaberine B was developed based on two consecutive Pictet–Spengler (PS) condensations with protected 3,4-dihydroxyphenylacetaldehydes. The first PS reaction between a dopamine derivative carrying a *N-o*-nitrophenylsulfenyl (Nps) group and an approprioately protected 3,4-dihydroacetaldehyde was catalyzed with 5 mol% of (*R*)-TRIP to afford (+)-(*R*)-norprotosinomenine in 90 % *ee.* The second PS reaction proceeded without any catalyst to form two regio isomers in a ratio that was highly dependent on the solvent. In trifluoroethanol the ratio between the *para* and *ortho* regioisomers was 99:1 while in the apolair solvent toluene we observed perefential formation of the *ortho* isomer. Subsequently, the para isomer was deprotected to afford (+)-javaberine A in 48% overall yield and the ortho isomer converted to (+)-javaberine B in 35% yield.




This synthetic work on javaberines was published in : Kayhan, J., Wanner, M. J., Ingemann, S., van Maarseveen, J. H., & Hiemstra, H. (2016). *Consecutive Pictet-Spengler Condensations toward Bioactive 8-Benzylprotoberberines: Highly Selective Total Syntheses of (+)-Javaberine A, (+)-Javaberine B, and (-)-Latifolian A*. *European Journal of Organic Chemistry*, *2016*(22), 3705-3708. This paper was highlighted in SYNFACTS, *Highlights in Current Synthetic Organic Chemistry, 2016, 12(10)* 1011.

**Biocatalysis**

The Biocatalysis group has published a study on a range of synthetic biomimetic compounds that can replace the relatively expensive natural nicotinamide coenzymes (NADH and NADPH) in asymmetric enzymatic redox processes of industrial relevance. In the *Journal of the American Chemical Society*, the Biocatalysis group showed the great potential of the biomimetics in an extensive study with a range of oxidoreductase enzymes. In particular, they investigated the performance of the biomimetic compounds with enzymes belonging to the family of the "ene"-reductases, which catalyse the asymmetric reduction of activated alkenes. The group elucidated the performance of the biomimetics through steady-state and rapid-reaction kinetics as well as the analysis of the X-ray



crystal structures of the biomimetics in complex with the ene-reductase XenA. Notably, the analysis of the kinetic parameters showed that, in selected cases, these biomimetics surpasses the catalytic efficiency of the natural coenzymes. The biomimetic coenzymes are inexpensive to manufacture and more stable than their biological counterparts, that are required as hydride source in enzymatic redox reactions. The implementation of these synthetic biomimetics – as well as the design of more sophisticated analogues capable of operating with a variety of other oxidoreductases – will facilitate the use of redox biocatalysts in chemicals production. It is expected that the "Better-than-Nature" biomimetics can find widespread application in fine and specialty chemicals production by harnessing the power of high stereo-, regio-, and chemoselective redox biocatalysts and enabling reactions under mild conditions and at low cost.

**Computational Chemistry**

**The role of colloidal bond hybridization and anisotropy in self-assembly of microcapsules**

Particles with directional interactions are important building blocks for novel functional materials and may serve as models for biological structures. For example, mutually attractive deformable nanoparticles may spontaneously order themselves in a variety of structures, such as strings, sheets and large vesicles. Moreover, anisotropic colloids with attractive patches can self-assemble into open lattices, "colloidal" molecules, and micelles. However, to date model systems that combine mutual attraction, anisotropy and deformability have not been reported. This paper reported on synthesis and simulations of colloidal particles that combine these three characteristics and obtain self-assembled microcapsules. Mutual attraction and deformability induce directional interactions via colloidal bond hybridization. The particles contain both mutually attractive and repulsive surface groups that are flexible. In analogy to the simplest chemical bond—in which two isotropic orbitals hybridize into the molecular orbital of $H_2$—these flexible groups rearrange on binding. Through colloidal bond hybridization several structures can be formed: isotropic spheres self-assemble into planar monolayers, whereas anisotropic snowman-shaped particles self-assemble into hollow monolayer microcapsules. A modest change in the building blocks yield a much greater complexity of the self-assembled structures. Hence, these relatively simple building blocks self-assemble into markedly more complex structures than do similar particles that are isotropic or non-deformable.
C.H. J. Evers, J.A. Luiken, P.G. Bolhuis, W.K. Kegel, Nature **534**, 364–368 (2016)

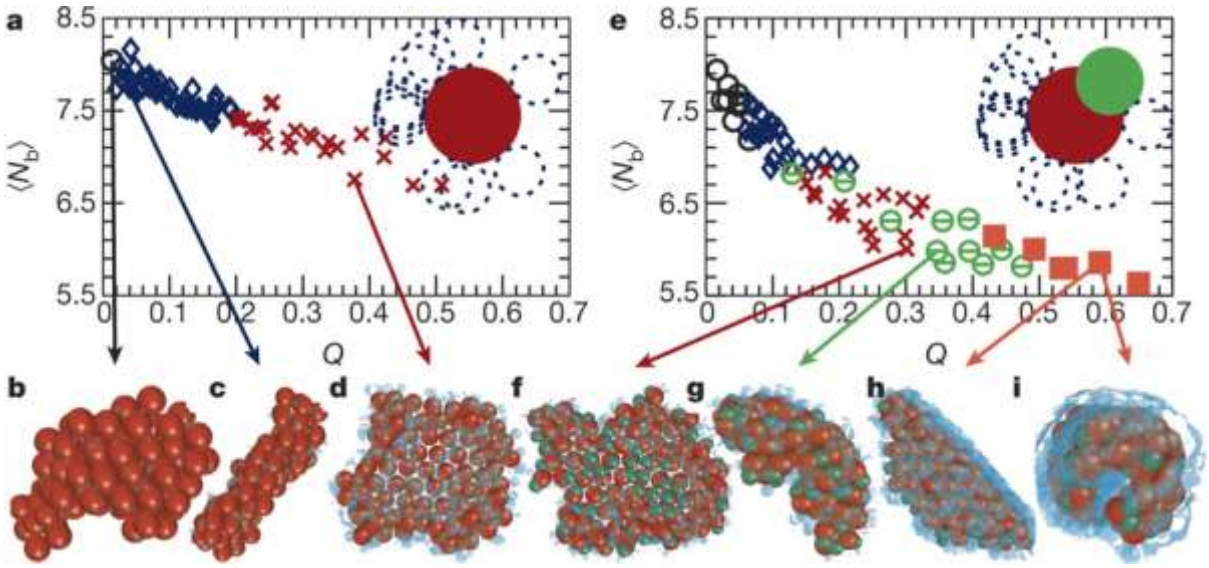


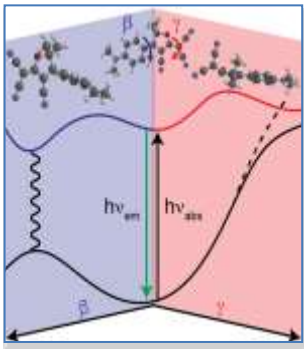

Figure: Monte Carlo simulation of anisotropic deformable mutually attractive colloidal particles. Modifying anisotropy and deformability yields a large variety of self-assembled structures.

**Computational Polymer Chemistry & Science for Arts**

One theory for percolating polymer networks: Polymer networks feature strong dependence of the material properties on the underlying network topology. These properties are qualitatively distinguished in the non-percolating phase (a 'liquid' sol) and percolating phase (a 'solid' gel), although both phases are comprised of the same molecular units in terms of chemical composition. The phase transition from liquid to solid can thus be observed not only with a change of standard thermodynamic quantities, as temperature or pressure, but also with a change of chemical state of the network precursors (monomers).

The phase diagram shown (gel fractions in color) spans a triangle between extremes of the monomer's connectivity's. Available kinetic theories could only solve a few special cases up to now: $A_n$, $A_nB_2$ and $AB_3$ polycondensation. Rather than tackling such individual cases, recent research in the Computational Polymer Chemistry group solved the whole puzzle with one shot. This was possible by a clever combination of various analytical results from random graphs and polymerization kinetics. The resulting theory regards an arbitrary mixture of monomers with arbitrary functionalities; it explains precisely how and when a sparse network that occupies only a tiny fraction of the total material weight percolates the whole volume and therefore trigger the phase transition.

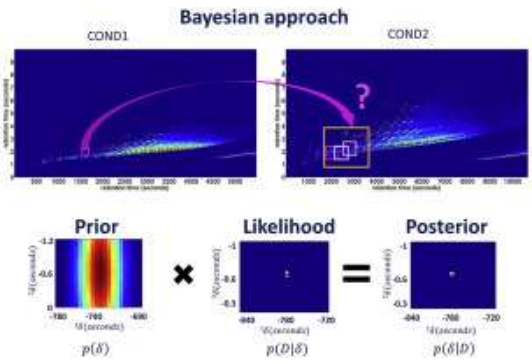
**Molecular Photonics**



The fluorescence intensity of molecular rotors increases strongly with solvent viscosity. Single-bond and double-bond rotations have been proposed as pathways of nonradiative decay for molecular rotors. Using a combination of photophysical experiments and quantum-chemical calculations we show here that both are involved in the case of DCDHF rotors, which we use in our research on contact mechanics with Daniel Bonn (Institute of Physics): fluorescence is quenched by rotation around the dicyanomethylene double bond in nonpolar solvents, but in a sufficiently polar environment rotation about a formally single bond leads to a dark internal charge-transfer state (*J. Phys. Chem. Lett.* **2016**, *7*, 4285–4290). (LiveSlides presentation: http://pubs.acs.org/doi/suppl/10.1021/acs.jpclett.6b02277)).

**Analytical Chemistry**

Great progress was made at the interfaces between chemistry and mathematics ("chemometrics") and between chemometrics and forensics ("forensimetrics"). Often in collaboration with the Korteweg-de-Vries Institute for Mathematics (Prof. M. Sjerps). A novel peak-tracking method based on Bayesian statistics has been proposed. The method consists of assigning (*i.e.* tracking) peaks from two GC×GC-FID data sets of the same sample recorded under different conditions. Opposed to traditional (*i.e.* deterministic) peak-tracking algorithms, in which the assignment problem is solved with a unique solution, the proposed algorithm is probabilistic. In other words, the uncertainty of matching two peaks is quantified without excluding other possible candidates, ranking the possible peak assignments regarding their posterior probability. This represents a significant advantage over existing deterministic methods. Two algorithms are presented, the blind-peak-tracking algorithm (BPTA) and the peak-table-matching algorithm (PTMA). The PTMA method was able to assign correctly 78% of a selection of peaks in a GC×GC-FID chromatogram of a diesel sample and proved to be extremely fast. (A. Barcaru, E. Derks and G. Vivó-Truyols, Anal. Chim. Acta **940** (2016) 46-55)



## 1.4.3 Prizes and honours

During the 384th Dies Natalis Professor on 8 January 2016 Bas de Bruin was named UvA Lecturer of the Year by the UvA Student Council and the ASVA Student Union. The jury lauded De Bruin for his lecturing qualities.

A jury of scientists and science communication professionals chose Jurn Heinen (PhD candidate at UvA-HIMS) as one of the winners of the first Amsterdam heat of FameLab, the international competition in science communication for young scientists. Heinen gave a lively and creative three-minute pitch of his research to a general audience.

Ariana Torres-Knoop and Danny Broere received their PhD degrees with the distinction 'Cum Laude'. Knoop successfully defended her thesis entitled Entropy -driven separations in nanoporous materials. Broere, whose thesis was titled New ave nues for redox-active ligands, also received a NWO Rubicon grant enabling him to conduct research for a period of two years at Yale University (US).

The Royal Netherlands Chemical Society KNCV awarded professor Jan van Maarseveen its 'Van Marumpenning' in recognition of his contributions to the societal relevance and the public image of chemistry. It was presented to him during the national 'Evening of Chemistry' event in Leiden.

Postdoc researcher Bert Wouters was awarded the 'Solvay Award' for his groundbreaking PhD research on the development of a microfluidic chip for spatial three-dimensional liquid chromatography. The prize was presented to him on 23 October 2016 in Brussels during the Solvay Public Event on ‘Chemistry for the World of Tomorrow'.

During the 10th International Vanadium Symposium held from 6-9 November 2016 in Taipei (Taiwan) emeritus professor Ron Weve r received the 7th Vanadis Award for his research on vanadium haloperoxidases. The award honors contributions to innovative research and the development of new applications of vanadium.

PhD Student Fleur van Beek was awarded the COAST prize for best analytical chemistry poster during the annual Dutch chemistry conference CHAINS 2016 held 6-8 December 2016. She designed an "interactive" poster explaining the MAnIAC project of the HIMS Analytical Chemistry group.

Following his stepping down as HIMS director professor Joost Reek was appointed as distinguished research professor at the UvA Faculty of Science. Reek is the eighth professor awarded this position since 2005, enabling him to make a contribution to academic development within the Faculty of Science. He will continue to serve as the figurehead of the UvA research priority area Sustainable Chemistry.

Researchers Simon Mathew, Marissa de Boer and Monalisa Goswami (f.l.t.r.) were the three winners of the ACE Venture Lab bootcamp Sustainable Chemistry that was organised in November 2016. They were awarded financial support and mentoring during the start-up of their chemistry-based businesses.

## 1.4.4 Grants

| | |
|---|---|
| Title | **Chemistry of Light-Induced Degradation (COLD)** |
| Applicants | prof.dr. Peter Schoenmakers, prof.dr. Maarten van Bommel |
| Partner | Unilever |
| Grant from | TKI Chemie, TKI Toeslag |
| Amount | k€ 40 |

| | |
|---|---|
| Title | **Design of heterogeneous catalysts for chemo-selective synthesis of cyclohexylamines** |
| Applicant | dr. N.R. Shiju |
| Partner | DSM |
| Grant from | TKI Chemie, TKI Toeslag |
| Amount | k€ 103 |

| | |
|---|---|
| Title | **Separation Technology for A Million Peaks (STAMP)** |
| Applicant | prof.dr. Peter Schoenmakers |
| Grant from | ERC Advanced Grant |
| Amount | k€ 2,500 |

| | |
|---|---|
| Title | **Conversion of levulinic acid from biomass in to valuable base chemicals** |
| Applicant | Dr. N.R. Shiju |
| Partner | Green Future Biochemicals |
| Grant from | EFRO Kansen voor West |
| Amount | k€ 199 (1 PD for HIMS) |

| | |
|---|---|
| Title | **Identification of potential salt sensors in plants** |
| Applicants | dr. J. Vreede, K. de Groot, S. Spoelstra |
| Grant from | NWO Topsector chemistry student competition |
| Amount | k€ 18 |

| | |
|---|---|
| **Title** | **Making amines out of thin air** |
| Applicant | dr. D.L.J. Broere |
| Grant from | NWO Rubicon |
| Amount | 24 month postdoc at Yale University |

| | |
|---|---|
| Title | **Chemical industry made natural!** |
| Applicant | dr. T.J. Korstanje |
| Grant from | NWO Veni |
| Amount | k€ 250 |

| | |
|---|---|
| Title | **Higher Order Structure Analysis (HOSAna)** |
| Applicant | Prof.dr. Peter Schoenmakers, prof.dr. Govert Somsen (VU) |
| Partners | VU, DSM, Postnova, Bruker |
| Grant from | NWO / PTA-COAST |
| Amount | k€ 557 (1 PhD student for HIMS) |

| | |
|---|---|
| **Title** | **Gamification of participatory science for training and education purposes -GAPARS** |
| Applicant | Prof.dr. Garry Corthals |
| Partners | Consortium of eight European research institutes and companies |
| Grant from | EU - H2020 |
| Amount | k€ 240 |

| | |
|---|---|
| **Title** | ***Synthese van volledig L-geconfigureerde gespannen kleine cyclische peptiden gebaseerd op asymmetrische hydrogenering van dehydro aminozuren*** |
| Applicant | Prof.dr. Jan van Maarseveen |
| Partner | InCatT |
| Grant from | NWO NCI-Kiem |
| Amount | k€ 35 |

| | |
|---|---|
| **Title** | **Operando XAS measurements of a novel Iron electrode for low-cost energy storage** |
| Applicant | Dr. M. Tromp |
| Partner | E-Stone Batteries B.V. |
| Grant from | NWO NCI-KIEM, 2016 |
| Amount | k€ 18,75 |

| | |
|---|---|
| **Title** | **Redox Mediators in Dye-sensitized Photoelectrochemical Cells for $CO_2$-reduction** |
| Applicants | Prof.dr. Joost Reek, dr. Remko Detz, prof.dr. Fred Brouwer, prof.dr. Wim Sinke (IoP, |
| ECN), | dr. Erik Garnett (AMOLF) |
| Partners | AMOLF, ECN, Merck |
| Grant from | NWO Solar to Products (CW/FOM) |
| Amount | k€ 557 (2 PhD students for HIMS) |

| | |
|---|---|
| **Title** | **Against the Odds: Regioselective Hydroaddition via Single-Electron Catalysis with** |
| **Noble** | **Metals** |
| Applicant | Dr. J.I. van der Vlugt |
| Grant from | NWO CW ECHO |
| Amount | k€ 260 (1 PhD student for HIMS) |

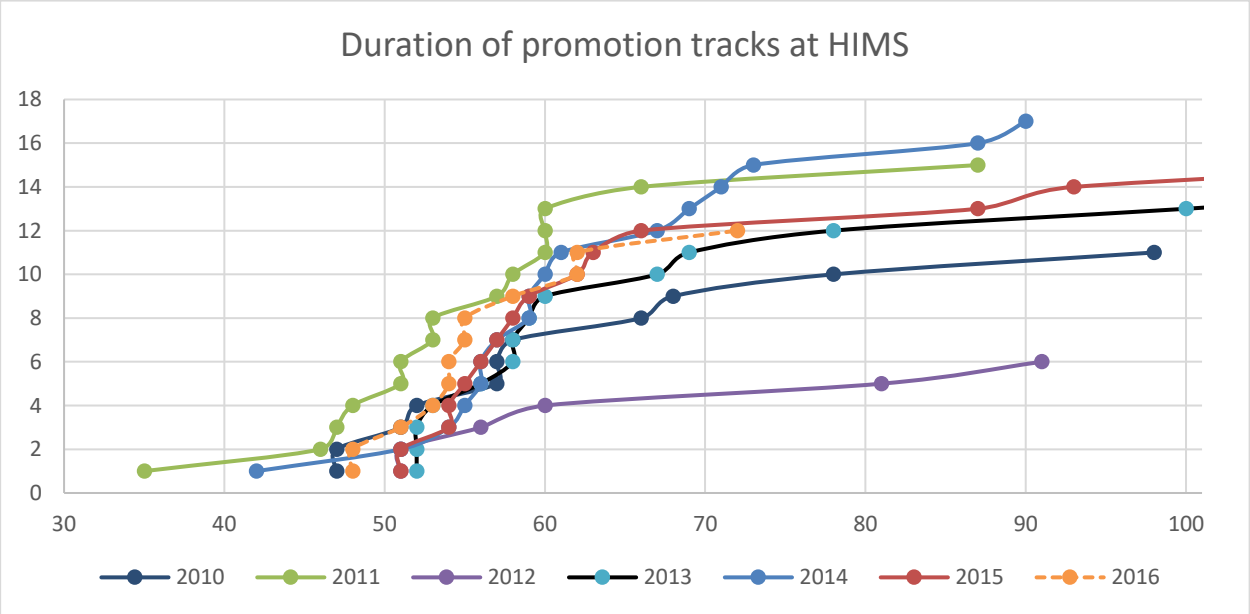
| | |
|---|---|
| **Title** | **ELENA Low energy electron driven chemistry for the advantage of emerging nano-fabrication methods** |
| Applicants | Prof.dr. Fred Brouwer and ELENA Consortium |
| Grant from | European Commission, HORIZON 2020 program, |
| Amount | k€ 1.067 (1 PhD student at ARCNL) |

*Subsidy brought by new staff members:*

| | |
|---|---|
| **Title** | **Supramolecular catalysts for the one-pot selective synthesis of carbohydrate** |
| **derivatives** | |
| Applicant | dr. T.J. Mooibroek |
| Grant from | NWO Vidi |
| Amount | k€ 800 |

## 1.4.5 Dissertations

| First name | Name | Promotor(es) | Co-promotor(es) | Promotion date | Duration in months |
|---|---|---|---|---|---|
| Hung-Cheng | Chen | prof.dr. A.M. Brouwer, prof.dr. J.N.H. Reek | dr. R.M. Williams | 2016-01-14 | 53 |
| Julien | Daubignard | prof.dr. J.N.H. Reek | prof.dr. B. de Bruin | 2016-02-19 | 62 |
| Stefan | Leenders | prof.dr. J.N.H. Reek | prof.dr. B. de Bruin | 2016-03-11 | 54 |
| Martin | Koelewijn | prof.dr. J.N.H. Reek | dr. R. Detz | 2016-03-29 | 62 |
| Ariana | Torres Knoop | prof.dr. E.J. Meijer | dr. D. Dubbeldam | 2016-04-28 (cum laude) | 48 |
| Kush | Singhal | prof.dr. P.G. Bolhuis | dr. J. Vreede | 2016-04-28 | 72 |
| Danny | Broere | prof.dr. J.N.H. Reek | dr.ir. J.I. van der Vlugt | 2016-06-07 (cum laude) | 48 |
| Sandra | de Boer | prof.dr. J.N.H. Reek | dr.ir. J.I. van der Vlugt | 2016-06-28 | 58 |
| Martin | Lopatka | prof.dr. M.J. Sjerps | dr. G. Vivo Truyols | 2016-06-30 | 51[1] |
| René | Becker | prof.dr. J.N.H. Reek | dr.ir. J.I. van der Vlugt | 2016-09-14 | 54 |
| Linda | Jongbloed | prof.dr. J.N.H. Reek | dr.ir. J.I. van der Vlugt | 2016-09-28 | 55 |
| Wilbert | Smit | Prof.dr. H. Bakker | prof.dr. M. Bonn | 2016-11-24 | [2] |
| Vincent | Vreeken | prof.dr. J.N.H. Reek | dr.ir. J.I. van der Vlugt | 2016-12-01 | 55 |
| Simona | Strazdaite | Prof.dr. H. Bakker | | 2016-12-21 | [2] |




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. After four years with a median value of almost 59, the median decreased to 54.5 in 2016. 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. Externally prepared promotions are not taken into account in these figures.

[1] Promotion prepared administrated at Korteweg de Vries Institute.
[2] 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:

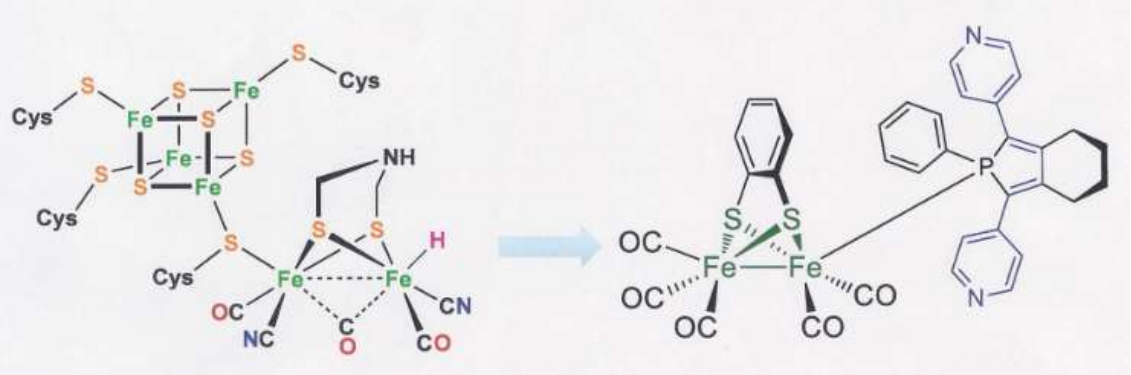
- Homogeneous and Supramolecular Catalysis
- Heterogeneous Catalysis and Sustainable Chemistry
- Synthetic Organic Chemistry
- Biocatalysis and Bio-organic Chemistry
- Sustainable Materials Characterisation

| Group | Homogeneous and Supramolecular Catalysis | | |
|---|---|---|---|
| Academic staff | Prof.dr. J.N.H. Reek<br>Prof.dr. B. de Bruin<br>Dr. J.I. van der Vlugt<br>Dr. T.J. Mooibroek (Vidi fellow, 01-08-2016 -31-07-2021) | | |
| Associated academic staff | Prof.dr. C.J. Elsevier (0,4 FTE, only education)<br>Prof.dr. B. van der Zwaan (BHL, 0.2 FTE) | | |
| Support staff | F. Ait El Maate<br>E. Duin-Berteling<br>C. Mahabiersing<br>J.M. Ernsting | | |
| Temporary staff | | Start date | (foreseen) end date |
| Postdocs | Dr. C.B. Bheeter | 01-09-2016 | 31-08-2017 |
| | Dr. W.I. Dzik | 01-11-2013 | 31-10-2016 |
| | Dr. S. Mathew | 01-09-2015 | 31-08-2017 |
| | Dr. S. Gonell Gomez | 01-05-2015 | 30-04-2017 |
| | Dr. M.N. Devillard | 01-03-2015 | 31-12-2016 |
| | Dr. S. Raoufmoghaddam | 01-02-2014 | 31-01-2016 |
| | Dr. X. Wang | 01-05-2014 | 30-04-2016 |
| | Dr. B. Bagh | 15-01-2015 | 14-01-2017 |
| | Dr. B.G. Das | 01-07-2015 | 30-06-2017 |
| PhD students | R. Becker, MSc. | 01-03-2012 | 29-02-2016 |
| | S. Bai, MSc. | 01-09-2015 | 31-08-2019 |
| | Drs. T. Bouwens | 01-11-2016 | 31-10-2020 |
| | D.L.J. Broere, MSc. | 15-05-2012 | 14-05-2016 |
| | Drs. A. Chirila | 01-09-2012 | 31-08-2016 |
| | Drs. P.R. Linnebank | 15-02-2016 | 14-02-2020 |
| | M. Goswami, MSc | 01-08-2013 | 31-07-2017 |
| | C. te Grotenhuis, MSc. | 01-08-2013 | 31-07-2017 |
| | A.P.T. Hartendorp, MSc. | 01-09-2015 | 31-08-2019 |

| | | | |
|---|---|---|---|
| | Drs. J. Hessels | 01-10-2015 | 30-09-2019 |
| | Drs. A.C.H. Jans | 15-03-2014 | 14-03-2018 |
| | Drs. L.S. Jongbloed | 15-02-2012 | 14-02-2016 |
| | L.J. Jongkind, MSc. | 01-09-2014 | 31-08-2018 |
| | P.F. Kuijpers, MSc | 01-10-2012 | 30-09-2016 |
| | S.S. Nurttila, MSc. | 01-06-2014 | 31-05-2018 |
| | R. Plessius, MSc. | 01-10-2015 | 30-09-2019 |
| | Drs. C. Rebreyend | 01-08-2013 | 31-07-2017 |
| | Drs. E.C.F. Schippers | 01-11-2013 | 31-10-2017 |
| | Drs. V. Sinha | 01-09-2014 | 31-08-2018 |
| | B. Sun, MSc. | 01-10-2015 | 30-09-2019 |
| | K.M. van Vliet, MSc. | 01-11-2015 | 31-10-2019 |
| | Drs. V. Vreeken | 01-05-2012 | 30-04-2016 |
| | F.F. van de Watering, MSc. | 01-11-2012 | 31-10-2016 |
| | Drs. R. Zaffaroni | 01-12-2012 | 30-11-2016 |
| | N.P. van Leest, MSc. | 01-09-2016 | 31-08-2020 |
| | V. Mouarrawis, MSc. | 01-01-2016 | 31-12-2019 |
| | D. A. Poole, MSc. | 01-10-2016 | 30-09-2020 |

**Mission of the group:**
The mission of the research group is the development of supramolecular and bio-inspired tools and concepts to advance the field of transition metal catalysis. Eventually these new tools should lead to the discovery of new catalyst systems and novel strategies that enable 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 the bio-based economy.

**Research highlights per staff member**
**Joost Reek**
The transition from a fossil-based to sustainable energy economy would be greatly accelerated if systems for direct solar to fuel generation becomes available. In this context we have an interest in water oxygenation, and proton and $CO_2$ reduction catalysis, as well the implementation of such molecular catalyst in devices by immobilization on electrodes. We have reported detailed kinetic studies on water oxidation catalysis (*ACS Catalysis; ChemPhysPhysChem*), as well immobilization strategies for such systems (*ChemPlusChem*). Also, we reported on a dye sensitized photoelectrode for proton reduction catalysis (*ChemCatChem*). The biggest breakthrough in this area is the development of a novel hydrogenase model (*Science Adv*.). Nature shows that iron-based catalysts in the form of iron-iron hydrogenase (H2ase) enzymes can catalyzes hydrogen evolution with rates similar to platinum with low overpotential. However, existing synthetic H2ase mimics generally suffer from low efficiency and oxygen sensitivity, and generally operate in organic solvents. We reported on a synthetic H2ase mimic that contains a redox-active phosphole ligand as an electron reservoir, a feature also crucial for the operation of the natural enzyme. Using a combination of (spectro)electrochemistry and time-resolved infrared spectroscopy we elucidate the unique redox behavior of the catalyst. We find that the electron reservoir actively partakes in the reduction of protons and that its electron-rich redox states are stabilized through ligand protonation. In dilute sulfuric acid, the catalyst has a turnover frequency of 7.0·104 s–1 at an overpotential of 0.66 V. This catalyst is tolerant to the presence of oxygen, thereby paving the way for a new generation of synthetic H2ase mimics that combine the benefits of the enzyme with synthetic versatility and improved stability. In the next phase we will encapsulate such catalyst in molecular container, another field were we made important contributions this year (*Nature Chem, Chem. Eur. J, Acs Catalysis*)




**Key publications**

- Q. Wang, S. Gonell Gomez, S.H.A.M. Leenders, M. Dürr, I. Ivanović-Burmazović & J.N.H. Reek, "Self-assembled nanospheres with multiple endohedral binding sites pre-organize catalysts and substrates for highly efficient reactions." *Nature Chemistry*, **2016** *8*, 225-230
- *R. Becker, S. Amirjalayer, P. Li, S. Woutersen, J.N.H. Reek* "An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media" Science Adv.* ***2016****, 2, e1501014 DOI: 10.1126/sciadv.1501014*
- Koelewijn, J. M.; Lutz, M.; Dzik, W. I.; Detz, R. J.; and Reek, J. N. H. Reaction Progress Kinetic Analysis as a Tool To Reveal Ligand Effects in Ce(IV)-Driven IrCp*-Catalyzed Water Oxidation. *ACS CATALYSIS* **2016**, *6*, 3418-3427.
- Leenders, S. H. A. M.; Duerr, M.; Ivanovic-Burmazovic, I.; and Reek, J. N. H. Gold Functionalized Platinum M12L24-Nanospheres and Their Application in Cyclization Reactions. *ADVANCED SYNTHESIS & CATALYSIS* **2016**, *358*, 1509-1518.

**International collaborations (2016)**

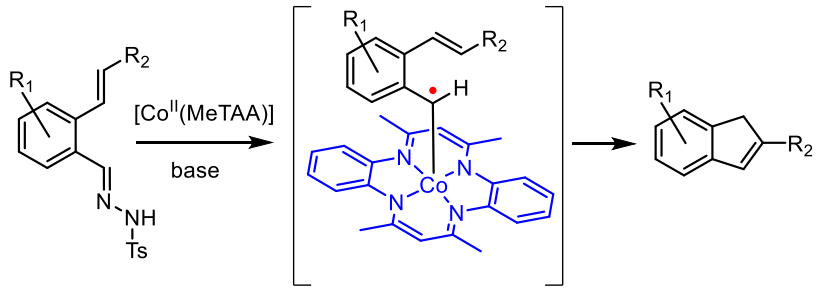
- Prof C. Moberg, Stockhom university, Sweden
- Prof Ivanovic-Burmazovic Erlangen, Germany
- Prof He/Prof Duan Key state laboratory Dalian, CHina
- Prof Sun Stockholm University, Sweden
- Prof Spiccia, Monash Univ, Melbourne, Australia.
- Prof Brudvig Yale USA
- Prof Sakai, Kyushu Univ, Fukuok, Japan.
- Prof Nolan University of Gent (formal st Andrews) Belgium

**Other activities**

- Director HIMS institute (122 FTE)
- Scientific director InCatT
- Director of research priority area Sustainable Chemistry UvA
- Board member Eur. J. Inorg Chem.
- NWO work group Coordination and Catalysis
- Management team BioSolarCell (Dutch artificial leaf program)
- Chair UOC UvA (till june)
- Steering committee Co van Ledden Hulsebosch Center
- KNAW Raad NTW
- Member Sector raad chemistry

**Bas de Bruin**

Research in the context of the VICI project of Bas de Bruin, in close collaboration with researchers active in the research priority area Sustainable Chemistry (SusChem) developed a new catalysts for easy synthesis of substituted 1*H*-indenes. The catalysts is a cheap and easy to prepare complex, based on the cheap and abundant element cobalt. Indenes are valuable building blocks of a variety of natural products, pharmaceuticals and other bioactive compounds, and find application as ligands of other metal complexes for use in e.g. olefin polymerization. As such, there is a demand for the development of short, efficient and broadly applicable methods for indene synthesis from readily available starting materials. The strategy reported by the team contributes to the development of a sustainable catalytic route to 1*H*-indene synthesis.




The team made use of so called metalloradical catalysis to synthesize indenes; a method of making use of the intrinsic radical-type reactivity of first row transition metals instead of trying to prevent it. This is a new (bio-inspired) way of thinking about catalysis, crucial to move away from using expensive noble metal catalysts using cheap metals instead.

**Key publications**

- *$Co^{III}$-Carbene Radical Approach to Substituted 1H-Indenes Das, B.G.; Chirila, A.; Tromp, M.; Reek, J.N.H; de Bruin, B., J. Am. Chem. Soc.,* ***2016****, 138, 8968–8975.* [link]
- *A Self-Assembled Molecular Cage for Size-Selective Epoxidation Reactions in Aqueous Media Kuijpers, P.F.; Otte, M.; Dürr, M.; Ivanović-Burmazović, I.; Reek, J.N.H.; de Bruin, B. ACS Catalysis,* ***2016****, 6, 3106–3112.* [link]
- *Deprotonation Induced Ligand Oxidation in a $Ni^{II}$ Complex of a Redox Non-innocent N1-(2-aminophenyl)benzene-1,2-diamine and its Use in Catalytic Alcohol Oxidation Sikari, R.; Sinha, S.; Jash, U.; Das, S.; Brandão, P.; de Bruin, B.; Paul, N.D. Inorg. Chem.,* ***2016****, 55, 6114–6123.* [link]
- *Reactivity of Me-pma Rh(I)- and Ir(I)-complexes upon deprotonation and their application in catalytic carbene carbonylation reactions Tang, Z.; Tejel, C.; Martinez de Sarasa Buchaca, M.; Lutz, M.; van der Vlugt, J.I.; de Bruin, B., Eur. J. Inorg. Chem,* ***2016****, 7, 963-974.* [link]

**Other activities**

**Bas de Bruin**

**Committee/organisational activities (2016)**

- Co-organizer NWO CHAINS 2016 conference
- Chair of the Editorial Board *European Journal of Inorganic Chemistry*
- Editorial Advisory Board *Organometallics*
- Editorial Advisory Board *ACS Catalysis*
- Scientific committee EuCOMC-2017
- Co-organiser ISHC-2018 conference

**International collaborations (2016)**

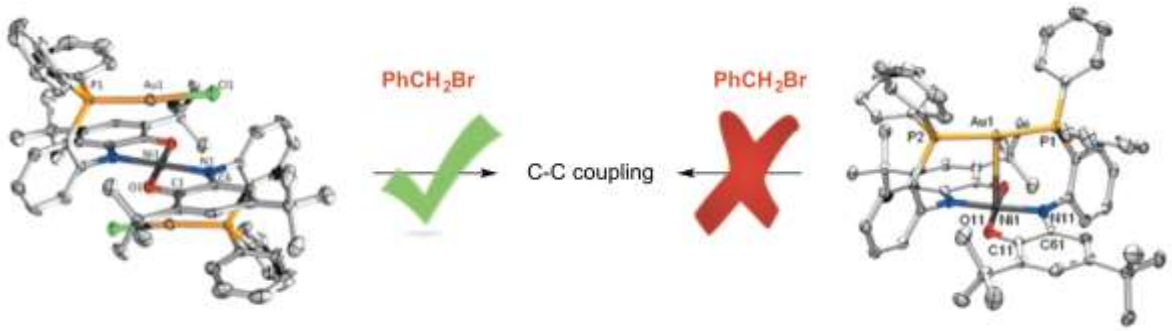
- Prof. Hansjörg Grützmacher, ETH Zürich (Switzerland).
- Prof. Peter Budzelaar, University of Manitoba (Canada).
- Dr. Ed Reijerse, MPI Chemical energy Conversion, Mülheim a/d Ruhr (Germany).
- Prof. Miguel Ciriano & Dr. Cristina Tejel, University of Zaragoza (Spain).
- Prof. Sven Schneider, University of Göttingen (Germany).
- Dr. Robert Wolf, University of Regensburg (Germany).
- Prof X. Peter Zhang, University of South California (USA).
- Prof Kallol Ray (Humboldt University of Berlin (Germany).
- Prof Serena DeBeer, MPI Chemical energy Conversion, Mülheim a/d Ruhr (Germany).
- Dr. Eckhard Bill, MPI Chemical energy Conversion, Mülheim a/d Ruhr (Germany).

**Invited book Chapters (2016)**

- *Redox Non-innocent Ligands: Reactivity and Catalysis, de Bruin, B.; Gualco, P.; Paul, N.D., in Ligand Design In Metal Chemistry: Reactivity and Catalysis, Wiley, (edited by Stradiotto, M. & Lundgren, R.),* ***2016****, ISBN: 978-1-118-83983-6, p.46-65.*
- *Multiple Spin State Scenarios in Organometallic Reactivity, Dzik, W.I.; Böhmer, W.; de Bruin, B.* in Spin States in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity, Wiley, (edited by Swart, M. & Costas, M.),* ***2016****, ISBN: 978-1-118-89831-4, p.103 – 130.*

**Jarl Ivar van der Vlugt**

Research in the context of the ERC project of Jarl Ivar van der Vlugt has continued to focus on novel concepts for small molecule activation and catalysis, with an emphasis on reactive ligand design strategies. The team exploits the modular power of organic ligands that are accessible in three different oxidation states and that are capable of redox-active ligand centered one-electron transfer. This affords selective radical-type chemistry with metal-bound substrates. Furthermore, the ligands are ditopic, allowing the construction of multinuclear metal complexes and catalysts. unique ligand-mediated tunable metal-metal interactions have become accessible.




Trinuclear Au-Ni-Au assemblies have been shown to enable selective electrocatalytic C-C coupling. The conversion of mononuclear azido-complexes into unprecedented trinuclear bis(nitride) architectures and the construction of dinuclear complexes supported by a multidentate ligand offering two electronically insulated binding pockets are two other examples from this research. The latter research has opened avenues for the construction of innovative intra-ligand mixed-valent architectures. The group has also designed improved dinuclear gold catalysts for cyclization reactions, which have proven superior over existing designs, by taking advantage of redox-active ditopic ligands to preorganize the metal centers.

**Key publications**

1. *Localized mixed-valence and redox-activity within a triazole-bridged dinucleating ligand upon coordination to palladium D.L.J. Broere, R. Plessius, J. Tory, S. Demeshko, B. de Bruin, M.A. Siegler, F. Hartl, J.I. van der Vlugt* Chem. Eur. J.* ***2016****, 22, 13965-13975.*
2. *Well-defined dinuclear gold complexes for preorganization-induced selective dual-gold catalysis V. Vreeken, D.L.J. Broere, A.C.H. Jans, M. Lankelma, J.N.H. Reek, M.A. Siegler, J.I. van der Vlugt* Angew. Chem. Int. Ed.* ***2016****, 55, 10042-10046.*
3. *Redox-active ligand mediated formation of an acyclic trinuclear ruthenium complex with bridging nitrido ligands B. Bagh, D.L.J. Broere, M.A. Siegler, J.I. van der Vlugt* Angew. Chem. Int. Ed.* ***2016****, 55, 8381-8385.*
4. *Metal-metal interactions in heterobimetallic complexes with dinucleating redox active ligands D.L.J. Broere, D.K. Modder, E. Blokker, M.A. Siegler, J.I. van der Vlugt* Angew. Chem. Int. Ed.* ***2016****, 55, 2406-2410.*

**Other activities**

Committee/organisational activities (2016)

- Management Team, COST Network CHAOS (2016-2020)
- Organizer, International Mini-Symposium 'RADICALS: Redox-Active Designs in Chemistry and Life Sciences', Amsterdam, June 6, 2016
- Guest-editor, ACS Catalysis Virtual Special Issue 'Catalysis in the Netherlands'
- Scientific committee EuCOMC-2017
- Co-organiser ISHC-2018 conference

International collaborations (2016)

- Prof. Frantisek Hartl, University of Reading (UK).
- Prof. Axel Klein, University of Cologne (Germany).
- Dr. Jordi Carbo, University of Tarragona (Spain)
- Dr. Maxime Siegler, John Hopkins University (USA).
- Prof Laurent Maron, University of Toulouse (France).
- Prof Franc Meyer, Dr. Serhiy Demeshko, University of Goettingen (Germany).
- Prof. Phillip Dauban, Gif-sur-Yivette (France)

**Bob van der Zwaan**

- van der Zwaan, B.C.C. and R. Gerlagh, "Offshore CCS and Ocean Acidification: A Global Long-Term Probabilistic Cost-Benefit Analysis of Climate Change Mitigation", *Climatic Change*, 137, 2016, 157-170.
- van der Zwaan, B.C.C., K. Calvin, L. Clarke (Guest Editors), "Climate Mitigation in Latin America: implications for energy and land use", Preface to the Special Issue on the findings of the CLIMACAP-LAMP project, *Energy Economics*, 56, 2016, 495-498.
- Clarke, L., J. McFarland, C. Octaviano, B. van Ruijven, R. Beach, K. Daenzer, S. Hernandez, A.F.P. Lucena, A. Kitous, M. Labriet, A. Maria Loboguerrero Rodriguez, A. Mundra, B.C.C. van der Zwaan, "Long-Term Abatement Potential and Current Policy Trajectories in Latin American Countries", *Energy Economics*, 56, 2016, 513-525.
- Kober, T., J. Falzon, B. van der Zwaan, K. Calvin, A. Kanudia, A. Kitous, M. Labriet, "A Multi-Model Study of Energy Supply Investments in Latin America under Climate Control Policy Energy Economics", *Energy Economics*, 56, 2016, 543-551.
- van der Zwaan, B.C.C., T. Kober, S. Calderon, L. Clarke, K. Daenzer, A. Kitous, M. Labriet, A.F.P. Lucena, C. Octaviano, N. Di Sbroiavacca, "Energy Technology Roll-Out for Climate Change Mitigation: A Multi-Model Study for Latin America", *Energy Economics*, 56, 2016, 526-542.
- Veysey, J., C. Octaviano, K. Calvin, S. Herreras Martinez, A. Kitous, J. McFarland, B. van der Zwaan, "Pathways to Mexico's Climate Change Mitigation Targets: A Multi-Model Analysis",

*Energy Economics*, 56, 2016, 587-599.

- Jewell, J., V. Vinichenko, D. McCollum, N. Bauer, K. Riahi, T. Aboumahboub, O. Fricko, M. Harmsen, T. Kober, V. Krey, G. Marangoni, M. Tavoni, D.P. van Vuuren, B. van der Zwaan, A. Cherp, "Energy Independence and Climate Change Mitigation", *Nature Energy*, 16073, 1, 6 June 2016, 1-9.

**Dissertations**

14-01-2016 Hung-Cheng Chen (prof.dr. A.M. Brouwer, prof.dr. J.N.H. Reek, dr. R.M. Williams)
19-02-2016 Julien Daubignard (prof.dr. J.N.H. Reek, prof.dr. B. de Bruin)
11-03-2016 Stefan Leenders (prof.dr. J.N.H. Reek, prof.dr. B. de Bruin)
29-03-2016 Martin Koelewijn (prof.dr. J.N.H. Reek, dr. R. Detz)
07-06-2016 Danny Broere (prof.dr. J.N.H. Reek, dr.ir. J.I. van der Vlugt) – Cum laude
28-06-2016 Sandra de Boer (prof.dr. J.N.H. Reek, dr.ir. J.I. van der Vlugt)
14-09-2016 René Becker (prof.dr. J.N.H. Reek, dr.ir. J.I. van der Vlugt)
28-09-2016 Linda Jongbloed (prof.dr. J.N.H. Reek, dr.ir. J.I. van der Vlugt)
01-12-2016 Vincent Vreeken (prof.dr. J.N.H. Reek, dr.ir. J.I. van der Vlugt)

**Grants**

| | |
|---|---|
| **Title** | **Supramolecular catalysts for the one-pot selective synthesis of carbohydrate derivatives** |
| Applicant | dr. T.J. Mooibroek |
| Grant from | NWO Vidi |
| Amount | k€ 800 |

| | |
|---|---|
| **Title** | **Making amines out of thin air** |
| Applicant | dr. D.L.J. Broere |
| Grant from | NWO Rubicon |
| Amount | 24 month postdoc at Yale University |

| | |
|---|---|
| **Title** | **Redox Mediators in Dye-sensitized Photoelectrochemical Cells for $CO_2$-reduction** |
| Applicants | Prof. dr. Joost Reek, dr. Remko Detz, prof.dr. Fred Brouwer, prof.dr. Wim Sinke (IoP, ECN), dr. Erik Garnett (AMOLF) |
| Partners | AMOLF, ECN, Merck |
| Grant from | NWO Solar to Products (CW/FOM) |
| Amount | k€ 557 (2 PhD students for HIMS) |

| | |
|---|---|
| **Title** | **Against the Odds: Regioselective Hydroaddition via Single-Electron Catalysis with Noble Metals** |
| Applicant | Dr. J.I. van der Vlugt |
| Grant from | NWO CW ECHO |
| Amount | k€ 260 (1 PhD student for HIMS) |

**Prizes**

- Prof. dr. Joost Reek was elected Member of the Advanced Research Centre Chemical Building Blocks Consortium (ARC CBBC).
- Prof. dr. Bas de Bruin was elected Member of the Advanced Research Centre Chemical Building Blocks Consortium (ARC CBBC).

**Invited lectures**

**Bas de Bruin**

1. Ernst Haage Symposium, Mülheim a/d Ruhr, Germany. November 22-24, 2016. Title: Radical-type Catalysis with CoII Metallo-Radicals. Plenary Lecture
2. ICC 2016, Beijing, China. 16th International Conference on Catalysis. July 3-8, 2016. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of CoII & 'Carbene and Nitrene Radicals'. Invited speaker
3. 2016 International Symposium for Metal Porphyrins and Phthalocyanines; Beijing, China; July 1-2, 2016. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of CoII & 'Carbene and Nitrene Radicals'. Plenary Lecture
4. Summerschool XLI International Summer School on Organic Synthesis "A. Corbella", Gargnano, Italy, June 12-16, 2016. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of CoII & 'Carbene and Nitrene Radicals'. Invited speaker
5. FUSION 2016, Cancun, Mexico. 2nd small molecules activation conference. May 20-23, 2016. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of CoII & 'Carbene and Nitrene Radicals'. Invited speaker
6. Girona Seminar 2016: Predictive Catalysis, Girona, Spain. April 17-20, 2016. Title: Catalytic (Radical-type) Transformations at Cobalt(II); Catalytic Reactivity of 'Carbene and Nitrene Radicals'. Plenary speaker
7. Seminar at the Universität zu Köln, Cologne, Germany, January 27, 2016. Title: Catalytic Radical-type Transformations; Catalytic Reactivity of CoII, 'Carbene and Nitrene Radicals'. Host: Axel Klein.

**Joost Reek**

1. Invited lecture CDL, "From Supramolecular to Nature inspired approaches in Transition metal catalysis" Leiden, march 2016
2. Colloquium lecture AMOLF, "Towards solar to fuel devices based on molecular components", Amsterdam, April 2016.
3. IMM Colloquium RU Nijmegen, "From Supramolecular to Nature inspired approaches in Transition metal catalysis" Nijmegen, April 2016
4. SYNCOM colloquium, "Supramolecular apporaches in transition metal catalysis" Groningen, May, 2016
5. Invited lecture, "Supramolecular Control of Selectivity in Transition Metal Catalysis" Osaka, Japan, July 2016.
6. Oral contribution, ISHC XX, "Catalysis at extreme high local concentrations in self-assembled nano-spheres, Kyoto Japan, 2016, July 2016
7. Invited lecture at the 9th Asian-European Symposium on Metal-Mediated Efficient Organic Synthesis, "Supramolecular approaches to control selectivity in transition metal catalysis" September, 2016, Stockholm, Sweden.
8. Keynote lecture 5th International Symposium on Solar Fuels and Solar Cells; "Towards solar to fuel devices based on molecular components" October 2016, Dalian, China
9. Invited lecture at CHAINS, "Supramolecular Transition Metal Catalysis: control of activity and selectivity by second coordination sphere" Veldhoven December 2016

**Jarl Ivar van der Vlugt**

1. 3rd International Symposium on C-H Activation, Montreal, Canada (Jun **2016**), *C-H Amination involving Redox-Active Ligand Mediated One-Electron Transfer*
2. International Coordination Chemistry Conference, Brest, France – keynote speaker (Jul **2016**) *Dinuclear Chemistry and Catalysis with Redox-Active Ligands*
3. 11th Conference on Catalysis and Fine Chemical Catalysis, Lyon, France – keynote speaker (Sep **2016**) *C-H Amination Catalysis using Redox-Active Ligands*

4. 34th GEQO Congress of the Organometallic Chemistry Group, Girona, Spain (Sep **2016**) *Well-defined Organometallic Dinuclear Gold Complexes - Application in Dual-Gold Catalysis*
5. Seminar at the Universität Köln Germany *Host* Prof. Klein (Nov **2016**) *Reactive And Redox-Active Ligands - New Avenues for Organometallic Chemistry, Selective Bond Activation and Homogeneous Catalysis*

**Patents and utilization**

| | |
|---|---|
| Topic | Catalysts and Processes for Producing Aldehydes |
| Staff members | Prof.dr. Joost Reek, together with dr. Xiaowu Wang and dr. Jody Rodgers (Eastman). |
| Activities | Patent filed on June 24, 2016 by Eastman |

**Outreach**

**Bas de Bruin**

- IVN Woerden, Gastcollege voor IVN leden. Woerden, 26 november 2016. Titel: 'Hoe werkt een spinnendraad en andere vormen van chemische oorlogsvoering in de wereld van ínsecten'.
- INTREE week, Gastcollege voor aankomende masterstudenten. NEMO Science Museum, Amsterdam. 30 Augustus 2016. Titel: 'Vampires, Blue Blood, and chemical ware fare in biology'.
- BETA Break college, Universiteitsdag UvA, Gastcollege voor Alumni, OMHP, Amsterdam. 4 juni 2016. Titel: 'Bloed, heem en katalyse; Inspiratie uit de Natuur'.
- UvA 17 maart 2016, Gastcollege voor docenten en leerlingen middelbare scholen op congres 'chemie in Amsterdam'. Titel: Bio-geïnspireerde katalyse: gecontroleerde radicaalreacties met cobalt

**Joost Reek**

KNCV lecture at the "Avond van de chemie"

**Joint Publications**

Within SusChem Research priority

1. Becker, R.; Amirjalayer, S.; Li, P.; Woutersen, S.; and Reek, J. N. H. An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media. SCIENCE ADVANCES 2016, 2.
2. Chen, H. -C.; Reek, J. N. H.; Williams, R. M.; and Brouwer, A. M. Halogenated earth abundant metalloporphyrins as photostable sensitizers for visible-light-driven water oxidation in a neutral phosphate buffer solution. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 2016, 18, 15191-15198.
3. Das, B. G.; Chirila, A.; Tromp, M.; Reek, J. N. H.; and de Bruin, B. Co-III-Carbene Radical Approach to Substituted 1H-Indenes. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 2016, 138, 8968-8975.
4. Chen, H. -C.; Williams, R. M.; Reek, J. N. H.; and Brouwer, A. M. Robust Benzo[g,h,i]perylenetriimide Dye-Sensitized Electrodes in Air-Saturated Aqueous Buffer Solution. CHEMISTRY-A EUROPEAN JOURNAL 2016, 22, 5489-5493.

Within Solardam

1. Khoram, P.; Brittman, S.; Dzik, W. I.; Reek, J. N. H.; and Garnett, E. C. Growth and Characterization of PDMS-Stamped Halide Perovskite Single Microcrystals. *JOURNAL OF PHYSICAL CHEMISTRY C* **2016**, *120*, 6475-6481.

With other collaborators.

1. Hetterscheid, D. G. H.; van der Ham, C. J. M.; Diaz-Morales, O.; Verhoeven, M. W. G. M.; Longo,

A.; Banerjee, D.; Niemantsverdriet, J. W.; Reek, J. N. H.; and Feiters, M. C. Early stages of catalyst aging in the iridium mediated water oxidation reaction. *PHYSICAL CHEMISTRY CHEMICAL PHYSICS* **2016**, *18*, 10931-10940.

2. Theveau, L.; Bellini, R.; Dydio, P.; Szabo, Z.; van der Werf, A.; Sander, R. A.; Reek, J. N. H.; and Moberg, C. Cofactor-Controlled Chirality of Tropoisomeric Ligand. *ORGANOMETALLICS* **2016**, *35*, 1956-1963.
3. Wang, Q. -Q.; Gonell, S.; Leenders, S. H. A. M.; Duerr, M.; Ivanovic-Burmazovic, I.; and Reek, J. N. H. Self-assembled nanospheres with multiple endohedral binding sites pre-organize catalysts and substrates for highly efficient reactions. *NATURE CHEMISTRY* **2016**, *8*, 225-230
4. Yu, H.; He, C.; Xu, J.; Duan, C.; and Reek, J. N. H. Metal-organic redox vehicles to encapsulate organic dyes for photocatalytic protons and carbon dioxide reduction. *INORGANIC CHEMISTRY FRONTIERS* **2016**, *3*, 1256-1263.
5. Detz, R. J.; Sakai, K.; Spiccia, L.; Brudvig, G. W.; Sun, L.; and Reek, J. N. H. Towards a Bioinspired-Systems Approach for Solar Fuel Devices. *CHEMPLUSCHEM* **2016**, *81*, 1024-1027
6. Brudvig, G. W.; Reek, J. N. H.; Sakai, K.; Spiccia, L.; and Sun, L. Catalytic Systems for Water Splitting. *CHEMPLUSCHEM* **2016**, *81*, 1017-1019.
7. Leenders, S. H. A. M.; Becker, R.; Kumpulainen, T.; de Bruin, B.; Sawada, T.; Kato, T.; Fujita, M.; and Reek, J. N. H. Selective Co-Encapsulation Inside an M6L4 Cage. *CHEMISTRY-A EUROPEAN JOURNAL* **2016**, *22*, 15468-15474.
8. Jans, A. C. H.; Gomez-Suarez, A.; Nolan, S. P.; and Reek, J. N. H. A Switchable Gold Catalyst by Encapsulation in a Self-Assembled Cage. *CHEMISTRY-A EUROPEAN JOURNAL* **2016**, *22*, 14836-14839.
9. Mannathan, S.; Raoufmoghaddam, S.; Reek, J. N. H.; de Vries, J. G.; and Minnaard, A. J. Palladium(II) Acetate Catalyzed Reductive Heck Reaction of Enones; A Practical Approach (vol 7, pg 3923, 2015). *CHEMCATCHEM* **2016**, *8*, 2572.
10. van den Bosch, B.; Rombouts, J. A.; Orru, R. V. A.; Reek, J. N. H.; and Detz, R. J. Nickel-Based Dye-Sensitized Photocathode: Towards Proton Reduction Using a Molecular Nickel Catalyst and an Organic Dye. *CHEMCATCHEM* **2016**, *8*, 1392-1398.
11. Leenders, S. H. A. M.; Duerr, M.; Ivanovic-Burmazovic, I.; and Reek, J. N. H. Gold Functionalized Platinum M12L24-Nanospheres and Their Application in Cyclization Reactions. *ADVANCED SYNTHESIS & CATALYSIS* **2016**, *358*, 1509-1518.
12. Kuijpers, P. F.; Otte, M.; Duerr, M.; Ivanovic-Burmazovic, I.; Reek, J. N. H.; and de Bruin, B. A Self-Assembled Molecular Cage for Substrate-Selective Epoxidation Reactions in Aqueous Media. *ACS CATALYSIS* **2016**, *6*, 3106-3112.

| Group | Heterogeneous Catalysis and Sustainable Chemistry | | |
|---|---|---|---|
| Groupleader | Prof.dr. G. Rothenberg | | |
| Academic staff | Dr. S. Grecea<br>Dr. N.R. Shiju<br>Dr. N. Yan | | |
| Associated academic staff | Prof.dr. G.J.M. Gruter (BHL, 0.2 FTE, > 01-12-2016) | | |
| Support staff | ing. P.F. Collignon<br>ing. N.J. Geels | | |
| Temporary staff | | Start date | (foreseen) end date |
| Postdocs | Dr. D. Eisenberg<br>Dr. Z. Guo<br>Dr. A. Narani<br>Dr. J. Pandey<br>Dr. M.C. Mittelmeijer-Hazeleger<br>Dr. P.L.K. Prinsen<br>Dr. E.G.K. Solomon Raja | 01-02-2015<br>01-06-2015<br>01-06-2015<br>01-07-2015<br>01-05-2013<br>01-02-2014<br>01-07-2014 | 31-01-2017<br>31-05-2016<br>31-05-2016<br>30-06-2016<br>30-04-2017<br>31-01-2016<br>30-06-2017 |
| PhD students | Y. Tang MSc<br>W. Zhang MSc<br>A. Gheorghe, MSc.<br>M. Ronda Lloret, MSc.<br>T.K. Slot, MSc.<br>Drs. Y. Gao | 01-10-2015<br>01-10-2015<br>01-01-2016<br>01-09-2016<br>15-10-2016<br>01-09-2014 | 30-09-2019<br>30-09-2019<br>31-12-2019<br>31-08-2020<br>14-10-2020<br>31-08-2018 |

**Mission of the group:**
Our mission is to discover new catalysts and materials for sustainable chemistry and sustainable energy applications. We start from fundamental concepts and develop practical applications. This includes the synthesis of fuels and chemicals from biomass, clean energy, and advanced materials. Our strengths are in catalyst design, materials design, catalyst synthesis and testing, and characterisation under real-life conditions. HCSC is a highly interdisciplinary group (organic chemists, physicists, chemical engineers, electronics experts, materials scientists, chemometricians and computational chemists) and all our projects benefit from this.

**Research highlights per staff member**

**Prof. Gadi Rothenberg** / catalyst design
The catalyst design team has focused on oxygen activation using first-row transition metals, and has made important steps in 2016. We have developed a new type of hierarchical porous material made from carbon and nitrogen that can catalyse an electron transfer to oxygen molecules. By placing metal oxide nanoparticles on this active support, we effected the selective oxidation of alcohols to aldehydes using air. The cooperative catalytic effect is the result of an 'active doughnut' surrounding the metal oxide particle (see Figure 2). Selective oxidation with oxygen is an important challenge in catalysis, and this subject will be one focal point of our research in the coming years.

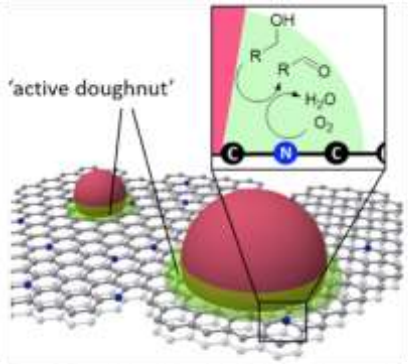


Figure 2. The catalytic oxidation of alcohols by molecular oxygen is a dual-site process, where the oxygen molecule is first reduced at the nitrogen-doped carbon surface, and subsequently reacts with the alcohol inside a doughnut-shaped active region that surrounds the metal catalyst particle.

- A Simple Synthesis of an N-Doped Carbon ORR Catalyst: Hierarchical Micro/Meso/Macro Porosity and Graphitic Shells. D. Eisenberg, W. Stroek, N. J. Geels, C. S. Sandu, A. Heller, N. Yan and G. Rothenberg, *Chem. Eur. J.*, **2016**, 22, 501-505.
- The evolution of hierarchical porosity in self-templated nitrogen-doped carbons and its effect on oxygen reduction electrocatalysis. D. Eisenberg, P. Prinsen, N.J. Geels, W. Stroek, N. Yan, B. Hua, J.-L. Luo and G. Rothenberg, *RSC Adv.*, **2016**, 6, 80398-80407.
- Cooperative catalysis for selective alcohol oxidation with molecular oxygen. T.K. Slot, D. Eisenberg, D. van Noordenne, P. Jungbacker and G. Rothenberg, *Chem. Eur. J.*, **2016**, 22, 12307–12311.

**Dr. Raveendran Shiju** / catalysis engineering

The catalysis engineering team made important progresses in various research lines. Within the biomass conversion programme, we have provided new insights into the development of stable catalysts that are selective under demanding hydrothermal conditions. Within our programme to tackle the $CO_2$ pollution, one of the major societal problems, a new NWO-NSFC project for developing a plasma-catalytic hybrid reactor was started with the appointment of a PhD student in September 2016. The importance of a collective effort to solve this difficult problem was highlighted in the summer school organised at Chengdu jointly by the Dutch and Chinese partners with the participation of international experts. The team also entered into the exploration of synergy between electrocatalysis and heterogeneous catalysis by receiving a HRSMC short-term grant in collaboration with the University of Leiden. The research efforts of the team were recognised by the invitation to give a Keynote Lecture at the Green and Sustainable Chemistry international conference in Berlin.

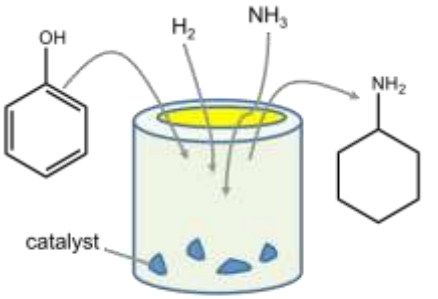


**Figure 3.** In the 'Catamine' project, we will develop efficient solid catalysts for the hydroamination of phenols to anilines in collaboartion with DSM.

- 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.F. Greer, W. Zhou, G. Rothenberg and N.R. Shiju, *Catal. Sci. Technol.,* **2016**, 6, 577-582.
- Silica-supported sulfonic acids as recyclable catalyst for esterification of levulinic acid with stoichiometric amounts of alcohols. R. Maggi, N.R. Shiju, V. Santacroce, G. Maestri, F. Bigi, G. Rothenberg, Beilstein *J. Org. Chem.,* **2016**, 12, 2173-2180.
- N. R. Shiju, Tuning selectivity in heterogeneous catalysis by understanding structural features, Green and Sustainable Chemistry Conference, Berlin, April 2016.

**Dr. Stefania Grecea** / inorganic materials

The inorganic materials team continued to develop synthetic strategies for the synthesis of metal-organic frameworks (MOFs) with tailored properties. Specifically, we highlighted the rational design of porous molecular structures built from lanthanide ions and organic linkers with appropriate geometries and functionalities. These materials are attractive candidates for molecular and bio-sensing, optical and proton-conduction applications. We foresee that the isoreticular and building-block approaches are the most efficient ones because they give the possibility to finely tune the pore sizes and the network topologies of the MOFs.

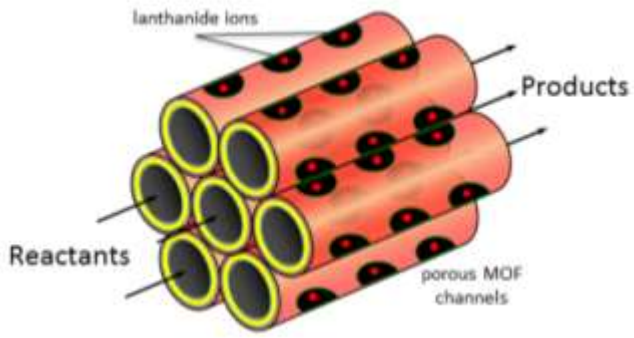
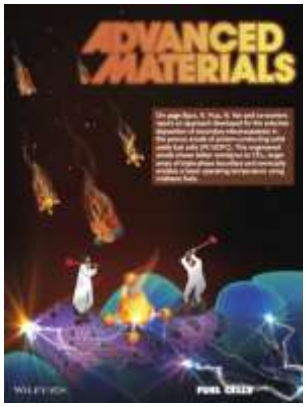



**Figure 4.** Combining the Lewis acidity of the lanthanide ions with appropriate organic ligands having specific acidic or basic functionalities allows to promote faster and more efficient substrate activation.

- Lanthanide-based metal organic frameworks: synthetic strategies and catalytic applications. C. Pagis, M. Ferbinteanu, G. Rothenberg, S. Tanase, *ACS Catal.,* **2016**, 6, 6063-6072.
- A rational synthesis of hierarchically porous, N-doped carbon from Mg-based MOFs: Understanding the link between nitrogen content and oxygen reduction electrocatalysis. D. Eisenberg, W. Stroek, N. J. Geels, S. Tanase, M. Ferbinteanu, S. J. Teat, P. Mettraux, N. Yan, G. Rothenberg *Phys. Chem. Chem. Phys.,* **2016**, 18, 20778-20783.

**Dr. Ning Yan** / fuel cells




The fuel cells team continued to focus on three research projects in 2016: The first project centred on a new nitrogen-doped carbon catalyst for oxygen reduction reaction (ORR). The systematic studies were published in three peer-reviewed papers. In the second research line, we tailored the crystallographic structure of perovskite and developed a series of robust perovskite oxides for oxygen catalysis and methane oxidation reactions. These results were published in top journals including *Advanced Materials* (impact factor 18.96) and *Advanced Functional Materials* (impact factor 11.80). The third project focused on the $CO_2$ valorization. We pioneered the electrochemical dry reforming process in fuel cells with electrical power cogeneration.. These results were published *Energy Environ. Sci.* (impact factor 25.42).

- B. Hua, N. Yan, M. Li, Y.-Q. Zhang, Y. F. Sun, J. Li, T. Etsell, P. Sarkar, K. T. Chuang, J. L. Luo, Energy Environ. Sci., 2016, 9, 207-215.
- N. Yan, J. Pandey, Y.M. Zeng, B. S. Amirkhiz, B. Hua, N. J. Geels, J. L. Luo, G. Rothenberg, ACS Catal., 2016, 6, 4630-4634.
- B. Hua, N. Yan, M. Li, Y.-F. Sun, Y.-Q. Zhang, J. Li, T. Etsell, P. Sarkar, J. L. Luo, Adv. Mater., 2016, 28, 8922-8926. Featured on the issue cover.

**Other activities**

Collboration with the Catalan Institute of Nanoscience and Nanotechnology (Barcelona, Spain) for the synthesis of nanostructered MOFs for applications in molecular sensing and catalysis.

**Grants**

| | |
|---|---|
| Title | **Design of heterogeneous catalysts for chemo-selective synthesis of cyclohexylamines** |
| Applicant | Dr. N.R. Shiju |
| Partner | DSM |
| Grant from | TKI Chemie, TKI Toeslag |
| Amount | k€ 104 |

| | |
|---|---|
| Title | **Conversion of levulinic acid from biomass in to valuable base chemicals** |
| Applicant | Dr. N.R. Shiju |
| Partner | Green Future Biochemicals |
| Grant from | EFRO Kansen voor West |
| Amount | k€ 119 (1 PD for HIMS) |

**Invited lectures**

- N. Yan: Perovskite oxide and electrocatalysts in fuel cells. EMN Meeting on Perovskite and Devices, Xiamen, China. December 2016.
- G. Rothenberg: Shades of red: Selective oxidation with molecular oxygen. University of Alicante, November 2016.
- G. Rothenberg: Plantics: Plastics made from plants. Bioplastics 2016, Alicante, November 2016 (keynote lecture).
- N.R. Shiju: Catalysis in action: a few short stories. M.G. University, Kottayam, October 2016.
- N.R. Shiju: Catalysis engineering for sustainable chemical processes. National Conference on Current Trends in Catalysis for Energy (CTCE-2016), CSIR-NCL, Pune, October 2016.
- N.R. Shiju: Metal oxide catalysed selective oxidations-probing the structure-activity relationships. SABIC, Bangalore, October 2016.
- S. Grecea: Building metal-organic frameworks from lanthanide ions and octacyanometallate building-blocks. CMD26 MOFs Colloquium, Groningen, September 2016.
- G. Rothenberg: Designing efficient catalysts for syn-gas conversion. Sinopec Shanghai, September 2016.
- G. Rothenberg: A simple method for finding good catalysts. East China Normal University, Shanghai, September 2016.
- G. Rothenberg: Selective oxidation with molecular oxygen: A 20¬-year quest. Fudan University, Shanghai, September 2016.
- N.R. Shiju: Tuning selectivity in heterogeneous catalysis by understanding structural features. 1st Green and Sustainable Chemistry Conference, Berlin, April 2016 (keynote lecture).
- G. Rothenberg: Break the bark: New catalytic routes from biomass to chemicals. 26th ORCS Conference, Miami, March 2016 (Keynote lecture).
- D. Eisenberg: A practical approach to metal-free oxygen reduction electrocatalysts. Israel Materials Engineering Conference (IMEC17), February 2016.
- G. Rothenberg: Practical tools for predicting catalyst performance. University of Glasgow, Glasgow, February 2016.
- N.R. Shiju: Catalysis in action: from nylon to paracetamol. Neste, Espoo, February 2016.
- N.R. Shiju: Designing heterogeneous catalysts for sustainable chemical processes. DSM, Geleen, January 2016.

**Patents and utilization**

Topic: F*uel cells and supercapacitors.*
Staff members: Rothenberg, Eisenberg (PD)
Activities: Invention of new supercapacitor and fuel cell electrode material. Supercapacitor and porous material. D. Eisenberg and G. Rothenberg, Eur. Pat. Appl. EP16171357, 05/2016.

Topic: *New carbon-based materials for advanced chromatography.*
Staff members: Rothenberg, Eisenberg (PD), Camenzuli (Analytical Chemistry group)
Activities: Invention of new column material, joint patent application in progress.

Topic: *Cyanide removal from industrial wastewater streams*
Staff members: Shiju, Rothenberg.
Activities: partners Industrial pilot plant under construction with partners, discussions with industrial on commercialisation route.

**Outreach**
HCSC staff participated in a variety of outreach activities, including teaching evening courses to high-school chemistry teachers (Rothenberg) and giving general and inorganic chemistry lectures for the students representing the Netherlands at the 48th International Chemistry Olympiad (Grecea).

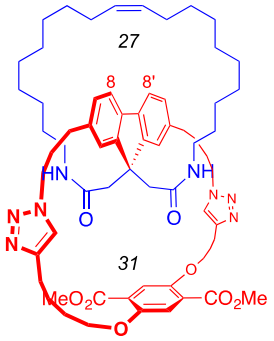
| Group | Synthetic Organic Chemistry | | |
|---|---|---|---|
| Groupleader | Prof.dr. J.H. van Maarseveen | | |
| Academic staff | Prof.dr. H. Hiemstra<br>Prof.dr. P. Timmerman (BHL)<br>Dr. S. Ingemann Jørgensen<br>Dr. M.A. Fernández Ibáñez | | |
| Support staff | R.A. Klein Nijenhuis<br>M.J. Wanner<br>E. Zuidinga | | |
| Temporary staff | | Start date | (foreseen) end date |
| Postdocs | Drs. L. Steemers (PD position)<br>Dr. C. Valderas Cortina<br>Dr. Y. Alvarez<br>Dr. P. Gajewski | 1-9-2016<br>1-5-2015<br>1-10-2016<br>1-5-2016 | 31-8-2018<br>31-10-2016<br>30-9-2017<br>31-3-2017 |
| PhD students | K. Naksomboon MSc.<br>Drs. G.J.J. Richelle<br>Drs. L. Steemers<br>Drs. D.E. Streefkerk<br>Drs. L. Wijsman<br>W.-L. Jia MSc.<br>M. Gomez MSc. (guest PhD)<br>Drs A.P.T. Hartendorp (with HomKat | 1-9-2015<br>1-11-2013<br>1-9-2012<br>1-6-2014<br>1-3-2015<br>1-10-2016<br>1-9-2016<br>1-9-2015 | 31-8-2019<br>31-10-2017<br>31-8-2016<br>31-8-2018<br>31-8-2016<br>30-09-2020<br>30-11-2016<br>31-8-2019 |
| MSc students | S.O. Ori<br>M. de Bruijn<br>T. van den Enk<br>J. Kayhan<br>D. Hagedoorn | 1-7-2015<br>1-9-2015<br>1-8-2015<br>1-3-2015<br>1-7-2016 | 31-1-2016<br>30-6-2016<br>31-5-2016<br>31-1-2016<br>28-2-2017 |
| HBO Stagiaires | V. Mudde<br>J. Visser<br>B. van Leeuwen<br>R. Klijn<br>D. Verdoorn | 1-9-2015<br>1-1-2016<br>1-1-2016<br>1-9-2016<br>1-10-2016 | 29-2-2016<br>31-7-2016<br>31-7-2016<br>31-1-2017<br>31-7-2017 |

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

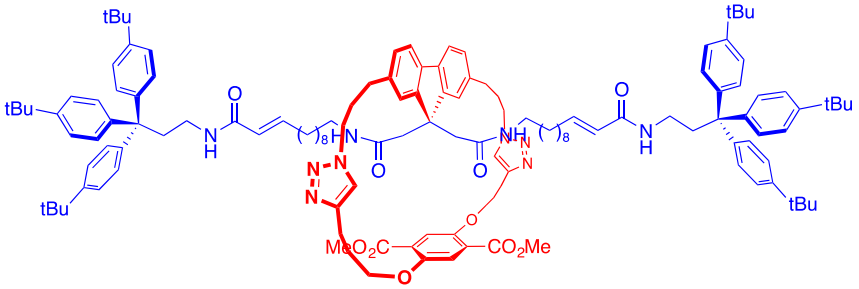
**Research highlights per staff member**

**Prof.dr. Jan H. van Maarseveen**
During our methodology development studies towards the total synthesis of the naturally occurring lasso peptides a new molecule class was revealed. Along the road we realized that our backfolding strategy to make interlocked molecules may also provide access to the unprecendented inverted spiro geometry. We have successfully disclosed this new class of molecules that we coined quasi [1]catenanes. Although the regular spiro and quasi [1]catenane geometries only differ by inversion

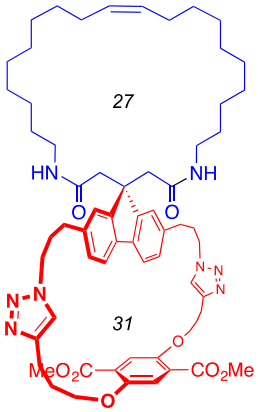
of the configuration of the center-of-symmetry tetrahedral carbon they relate as diastereomers with inherent different physical properties. By starting from the same tetrahedral C-centered acyclic precursor and the same backfolding concept the structurally related mechanically locked quasi [1]rotaxane and its unwinded conformer were obtained.



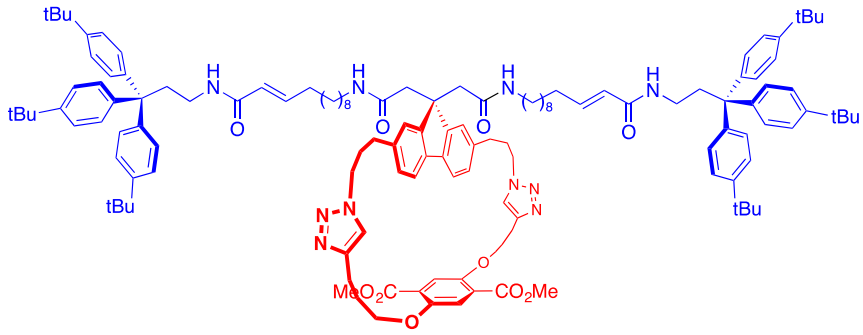

quasi [1]catenane




quasi [1]rotaxane




spiro bicycle




**Grants**

| | |
|---|---|
| **Title** | *Synthese van volledig L-geconfigureerde gespannen kleine cyclische peptiden gebaseerd op asymmetrische hydrogenering van dehydro aminozuren* |
| Applicant | Prof.dr. Jan van Maarseveen |
| Partner | InCatT |
| Grant from | NWO NCI-Kiem |
| Amount | k€ 35 |

**Prizes**

Prof.dr. Jan van Maarseveen received the KNCV Van Marumpenning in recognition of his contributions to the societal relevance and the public image of chemistry.

**Invited lecture**

Methodology development towards the lasso peptide series, L. Steemers, J.H. van Maarseveen, FLOHET 2016, Gainesville, March 2nd 2016.

**Publication**

Popovic, S., Wijsman, L., Landman, I. R., Sangster, M. F., Pastoors, D., Veldhorst, B. B., Hiemstra, H., van Maarseveen, J. H. (2016). *Fine-tuning the balance between peptide thioester cyclization and racemization*. *European Journal of Organic Chemistry*, *2016*(3), 443-446.

**Patents and utilization**
*Multicyclic CLIPS Peptides: Next Generation Therapeutic Peptide Drugs*. D.E.S. Streefkerk, G.J.J. Richelle, Jan H. van Maarseveen, Peter Timmerman. EP16202466.

**Outreach**
1. *Over koolstof en de moleculen van het leven*, Helen Parkhurst College, Almere, 20 januari.
2. *Over koolstof en de moleculen van het leven*, 4e-Gymnasium, Amsterdam, 26 januari.
3. *Development of new tools for peptide synthesis.* Studievereniging De chemische Binding, Groningen, 8 februari.
4. *Hoe zijn de eerste bouwstenen van het leven ontstaan?* Museum Natura Docet, Denekamp, 16 februari.
5. *Recente highlights uit de organische chemie en nieuws vanuit het front.* Bossche Chemische Kring, 17 februari.
6. *Waarom stinken scheten?* NEMO, 13 maart.
7. *Koolstof heeft de toekomst!* Scheikunde Docenten Symposium, Nijmegen, 5 april.
8. *Recente highlights uit de organische chemie en nieuws vanuit het front.* Zwolse Chemische Kring, 24 mei.
9. *Water lost alles op*. Museum Cruquius, Hoofddorp, 2 oktober
10. *Zonder kooldioxide geen leven*. IMC Weekendschool, Science Park, 30 oktober.
11. *Over het maken van geuren en smaken*. Nacht van de Wetenschap, NEMO, 5 november.
12. *Synthetic Organic Chemistry at the UvA*. ChemTogether, Havengebouw Amsterdam, 30 november.
13. *Stereochemie, van plat naar tetraëder*. Zaanlands Lyceum, Zaandam, 13 december.

**Prof.dr. Henk Hiemstra**
Research highlight, see paragraph 1.4.1.

**Other activities**
- Elected Member of the Royal Holland Society of Sciences (KHMW, Haarlem)
- Member of the International Advisory Board of the Organic division of the Czech Chemical Society
- Member of the Editorial Board of Molecules (Open Access Organic Chemistry Journal)
- Chairman of the Research Committee of the HRSMC
- Member of the Program Committee of the 27th European Colloquium on Heterocyclic Chemistry, Amsterdam, July 2016
- Member of the Organizing Committee, 5th HRSMC Summer School on Organic Synthesis, Maastricht, July 2017
- Member of the vici jury, NWO The Hague, 2016
- Member of the jury of the AkzoNobel Afstudeerprijs voor Chemie en Procestechnologie, KHMW Haarlem, 2016.

**Publications**
Kleinnijenhuis, R. A., Timmer, B. J. J., Lutteke, G., Smits, J. M. M., de Gelder, R., van Maarseveen, J. H., & Hiemstra, H. (2016). *Formal synthesis of solanoeclepin A: enantioselective allene diboration and intramolecular [2+2] photocycloaddition for the construction of the tricyclic core*. *Chemistry - A European Journal*, *22*(4), 1266-1269.

Lutteke, G., Kleinnijenhuis, R. A., Beuving, R. J., de Gelder, R., Smits, J. M. M., van Maarseveen, J. H., & Hiemstra, H. (2016). *Enantioselective Approach to the Right-Hand Substructure of Solanoeclepin A. European Journal of Organic Chemistry*, *2016*(35), 5845-5854.

Pauli, G. F., Niemitz, M., Bisson, J., Lodewyk, M. W., Soldi, C., Shaw, J. T., Tantillo, D. J., Saya, J. M., Vos, K., Kleinnijenhuis, R. A., Hiemstra, H., Chen, S.-N., McAlpine, J. B., Lankin, D. C., Friesen, J. B. (2016). *Toward Structural Correctness: Aquatolide and the Importance of 1D Proton NMR FID Archiving*. *Journal of Organic Chemistry*, *81*(3), 878-889.

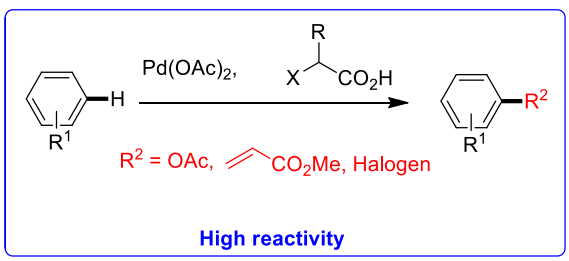
**Dr. Steen Ingemann Jørgensen**
Research highlight, see paragraph 1.4.1**.**

**Other activities**
Member of the European Chemistry Thematic Network (on behalf of the Faculty of Science)
Member of the FNWI Working Group on Governance Innovation
Program director Master Chemistry (single degree, UvA – VU)
Coordinator of the Master Chemistry Track: Molecular Sciences
Head of the Structure Analysis group at HIMS comprising the instrumental methods: MS, NMR, X-Ray and EPR

**Invited Lecture**
Asymmetric Synthesis of Natural Tetrahydroisoquinolines and Tetrahydroprotoberberines, Lecture at the 27th European Colloquium on Heterocyclic Chemistry, Amsterdam, July 3 – 6, 2016, Beurs van Berlage, Amsterdam

**Publication**
Breman, A. C., van der Heijden, G., van Maarseveen, J. H., Ingemann Jorgensen, S., & Hiemstra, H. (2016). *Synthetic and Organocatalytic Studies of Quinidine Analogues with Ring-Size Modifications in the Quinuclidine Moiety*. *CHEMISTRY-A EUROPEAN JOURNAL*, *22*(40), 14247-14256.

**Dr. M. Ángeles (Tati) Fernández Ibáñez**
A general and efficient synthesis of alpha-substituted phosphinoacetic acids using simple esters and diphenylchlorophosphine-borane as readily available starting materials has been reported. These compounds will be used in a variety of metal-catalyzed transformations.
A new catalytic system for the direct C-H acetoxylation of simple arenes based on $Pd(OAc)_2$ and picolinic acid ligand has been reported. The presence of the picolinic acid ligand enhance the reactivity, providing the highest TON (7800) reported for the $Pd(OAc)_2$-catalyzed C-H acetoxylation of benzene, and increase the site selectivity of the reaction with substituted arenes.
A new bidentate ligand capable of promoting a variety of Pd-catalyzed C-H functionalization reactions of aromatic compounds has been developed. To demonstrate the applicability of this new system, large-scale reactions as well as the late C-H functionalization of naproxene and estrone derivatives have been performed successfully.




- C. Valderas, K. Naksomboon, M. Á. Fernández-Ibáñez "Ligand-Promoted Palladium-Catalyzed C-H Acetoxylation of Simple Arenes" *Chem. Cat. Chem*. **2016**, *8*, 3213.
- M. Veguillas, R. Solà, M. Á. Fernández-Ibañez, B. Maciá "Catalytic enantioselective addition of methyltriisopropoxititanium to aldehydes" *Tetrahedron: Asymm.* **2016**, *27*, 643.

**Other activities**

- Collaborations with Dr. Beatriz Macia (Manchester, UK), Dr. Franceso Mutti (HIMS, UvA), Dr. Stefania Grecea (HIMS, UvA).
- MC Member, EU COST-network -C-H Activation in Organic Synthesis (CHAOS)
- Session Chair: HRSMC Symposium 2016 and CHAINS 2016.
- Member of the Editorial Board of Scientific Reports (Nature Publishing Group)
- Member of the Organizing Committee, 5th HRSMC Summer School on Organic Synthesis, Summer 2017
- Member of the core team 'Task force Sustainability' UvA
- Member of the board Women in FNWI (WiF), University of Amsterdam

**Grants**

| | |
|---|---|
| Title | Artificial Metalloenzyme for the Selective C-H Alkenylation of Arenes |
| Applicant | Dr. M. A. (Tati) Fernandez |
| Partner | Dr. Francesco Mutti |
| Grant from | HRSMC |
| Amount | 6 month postdoc |

**Invited lectures**

- *Design of New Ligands for Palladium-Catalyzed C-H Fuctionalization reactions* University of Antwerp, Antwerp (Belgium)/ Oct. 2016
- Ligand-promoted Pd-catalyzed C-H Functionalization COST action meeting, Vienna (Austria)/ Sep.2016
- Ligand-promoted Pd-catalyzed C-H Functionalization CAFC-11 International Congress on Catalysis and Fine Chemicals, Lyon (France)/ Sep. 2016
- Ligand-promoted Pd-catalyzed C-H Acetoxylation ECHC 2016XXVII European Colloquium on Heterocyclic Chemistry, Amsterdam (The Netherlands)/ July 2016
- Ligand-promoted palladium-catalyzed C-H acetoxylation of simple arenes RSEQ Organic Chemistry Symposium, Punta Umbria (Spain)/ June. 2016

**Prof.dr. Peter Timmerman** (professor by special appointment)

**Lectures**

- "CLIPS-constrained Peptides: Excellent Mimics of Complex Protein Surfaces", Invited lecture at the 3rd Belgian Peptide Symposium, Brussels, Belgium, 17 February 2016.
- "Discovery & Optimization of CLIPS-constrained Macrocycles using Pepscan Peptide Arrays", Invited lecture at the 24th EFMC International Symposium Medicinal Chemistry (ISMC), Manchester, UK, 28 August – 1st September 2016.
- "CLIPS-constrained Peptides: Excellent Mimics of Complex Protein Surfaces", Invited lecture at the 34th European Peptide Symposium, Leipzig, Germany, 6th September 2016.
- "CLIPS-constrained Peptides: Excellent Mimics of Complex Protein Surfaces", Invited lecture op 20th National Fall Meeting of the Norwegian Chemical Society, Division Organic Chemistry, Oslo, Norway, 28th October 2016.
- "Multicyclic Peptides: Excellent Mimics of Complex Protein Surfaces", Invited lecture at the 6th Austrian Peptide Symposium, Vienna, Austria, 1st December 2016.

**Publications**

1. The sclerostin-neutralizing antibody AbD09097 recognizes an epitope adjacent to sclerostin's binding site for the Wnt co-receptor LRP6. Bosschert V, Frisch C, Back JW, van Pee K, Weidauer SE, Muth EM, Schmieder P, Beerbaum M, Knappik A, Timmerman P, Mueller TD. Open Biol. 2016, 6(8), 160120.

2. Targeted vaccination against the bevacizumab binding site on VEGF using 3Dstructured peptides elicits efficient antitumor activity. Wentink MQ, Hackeng TM, Tabruyn, SP, Puijk WC, Schwamborn K, Altschuh D, Meloen RH, Schuurman T, Griffioen AW, Timmerman P. PNAS 2016, 113(44), pp. 12532-12537.

**Patent**
See above, together with Van Maarseveen

**Outreach**
Guest lecturer at the "Synthesis" workshop of the ITN-training network "BIOGEL"; Amphitheater Vergina, CERTH, Thessaloniki, Greece, 15-16 September 2016.

**Contribution to RPA Sustainable Chemistry**
Development of new catalysis systems for the direct C-H acetoxylation and C-H alkenylation of aromatic compounds

| | | | |
|---|---|---|---|
| Theme: | Sustainable Chemistry | | |
| Group: | Biocatalysis | | |
| Group leader: | Dr. F. Mutti | | |
| Associated academic staff | Prof.dr. R. Wever (Emeritus) | | |
| Support staff: | dr. L.C. Pham (<1-9-2016)<br>J.A. Houwman MSc (>01-10-2016) | | |
| Temporary staff | | Start date | (Foreseen) end date |
| Postdocs: | dr. T. Knaus | 01-07-2015 | 30-06-2020 |
| PhD students: | drs. W. Böhmer<br>V. Tseliou M.Sc.<br>J. Vilím M.Sc.<br>M.L. Corrado, MSc. | 01-09-2015<br>01-10-2015<br>01-10-2015<br>01-02-2016 | 31-08-2019<br>30-09-2019<br>30-09-2019<br>31-01-2020 |

**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 staff member**
**Dr. Francesco Mutti**
As reported in section 1.4.2, it was demonstrated that man-designed nicotinamide biomimetics are able to outperform the natural coenzymes in biocatalytic redox reactions, hence facilitating the implementation of oxidoreductases in chemical manufacturing.
In another work published in *Angewandte Chemie Int. Ed.*, the group presented a one-pot multi-enzyme cascade using a single bacterial whole cell system to carry out the formal regio- and stereoselective amination of benzylic C-H bonds. That was achieved via the combination of a P450 monooxygenase, an alcohol dehydrogense and an omega-transaminase in the same host organism.

**Publications**
- Knaus, T.; Paul, C. E.; Levy, C.W.; de Vries, S.; Mutti, F. G.; Hollmann, F.; Scrutton, N.S.; "Better than nature: Nicotinamide biomimetics that outperform natural coenzymes" *J. Am. Chem. Soc.*, **2016**, 138, 1033-1039.
- Both, P.; Busch, H.; Kelly, P. P.; Mutti, F. G.; Turner, N. J.; Flitsch, S. L.; "Whole-cell biocatalysts for stereoselective C-H amination reactions" *Angew. Chem. Int. Ed.*, **2016**, *55*, 1511-1513.

**Other activities**
Dr. Francesco Mutti from the Biocatalysis group and Dr. M. Ángeles (Tati) Fernández-Ibáñez from the Synthetic Organic Chemistry group received funding for a joined proposal from the Holland Research School of Molecular Chemistry (HRSMC). The research fellow, Dr. Alejandro Orden (assistant professor at the University of San Louis – Argentina), will carry out six months research at HIMS. The project aims at developing new artificial metalloenzymes capable of promoting the selective functionalization of C-H bonds.
The Biocatalysis group is involved in a number of international academic collaborations, in particular with groups at TU Delft (Prof. F. Hollmann), at The University of Manchester – UK (Prof. N. S. Scrutton,

Prof. N. J. Turner), at the TU Graz – Austria (Prof. P. Macheroux) and at the University of Magna Graecia (Prof. A. Procopio). Industrial collaborations are with EnginZyme (Stockholm, Sweden), EnzyPep and DSM (Geleen), BASF (Ludwigshafen, Germany) and GSK (Stevenage, UK).

**Prizes**

Prof.dr. Ron Wever received Vanadis award for his seminal research on vanadium haloperoxidases.

**Invited lectures**

Dr. Francesco Mutti has been invited speaker at the following international conferences:

- "Biocatalytic hydrogen-borrowing cascades for the efficient synthesis of high value chiral compounds", OxiZymes 2016, forthcoming: 3 July – 6 July, 2016, Wageningen (Netherlands)
- "Biocatalytic asymmetric hydrogen-borrowing cascades", Biotransformations 2016, 30 June – 2 July, 2016, Warsaw (Poland)

**Patents and utilization**

| | |
|---|---|
| Topic | Redox self-sufficient biocatalytic amination of alcohols |
| Staff members | Dr. F. Mutti and dr. T. Knaus |
| Activities | Patent application filed by BASF: PCT Int. Appl. (2016), WO 2016001362 A1 |
| 20160107; | Eur. Pat. Appl. (2016), EP 2963121 A1 20160106. |

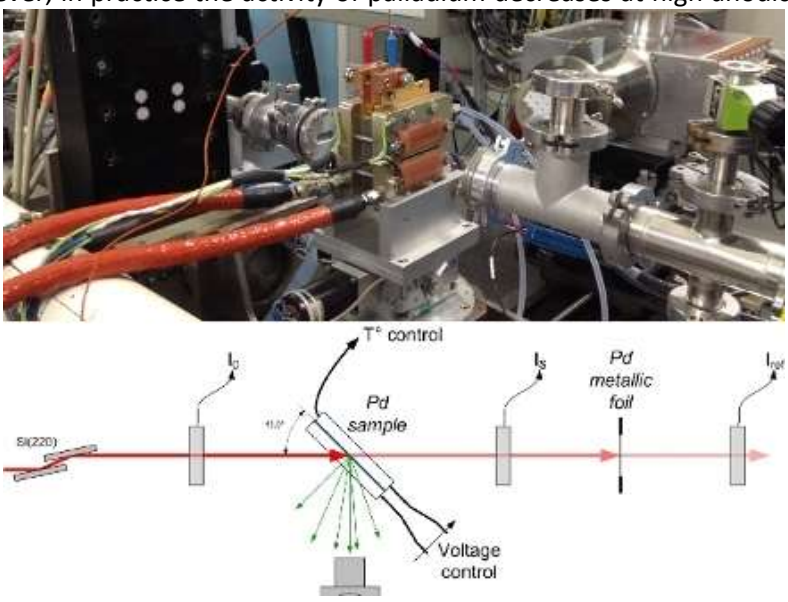
**Outreach**

In 2016, Dr. Francesco Mutti was nominated Associate Editor of the magazine "Amsterdam Science". Amsterdam Science gives Master's students, PhD students and researchers a platform for communicating their latest and most interesting findings to the Dutch society. It represents the opportunity to show each other and the rest of the world the enormous creativity, quality, diversity and enthusiasm that characterises the scientific community in Amsterdam. Amsterdam Science covers all the active research areas in Amsterdam universities and research institutes: mathematics, chemistry, astronomy, physics, biological and biomedical sciences, health sciences, ecology, earth and environmental sciences, forensic science, computer science, logic and cognitive sciences.
The Biocatalysis group has also been engaged in outreaching activity in collaboration with the Dutch press (e.g. http://www.alphagalileo.org/ViewItem.aspx?ItemId=160556&CultureCode=en).

| | | | |
|---|---|---|---|
| Theme | Sustainable Chemistry | | |
| Group | Sustainable Materials Characterisation | | |
| Groupleader | Dr. M. Tromp | | |
| Support staff | D.S. Tromp | | |
| Temporary staff | | Start date | (foreseen) end date |
| Postdocs | Dr. T.J. Korstanje<br>Dr. D.J. Martin | 01-12-2015<br>01-10-2015 | 31-01-2017<br>30-09-2018 |
| PhD students | M. Hammerton, MSc.<br>J.P.H. Oudsen, MSc.<br>B.Venderbosch, MSc. | 01-05-2016<br>01-09-2015<br>01-11-2015 | 30-04-2020<br>31-08-2019<br>31-10-2019 |

**Mission of the group:**
To understand the fundamentals of the chemical processes, i.e. derive structure-performance relationships and as such allow rational design, to enable the conversion of sustainable raw materials into useful products and energy the group focuses on development of different (operando) spectroscopic technologies and methodologies.

**Research highlight Moniek Tromp**
In addition to our work on operando spectroscopy in catalysis, we have put much effort towards electrochemistry, i.e. batteries and fuel cells, recently. Operando spectroscopy during battery cycling, using a specially designed spectro-electrochemical cell, provided valuable information on the charge and discharge mechanisms as well as deactivation pathways (e.g. J. Electrochem. Soc. 2016, 163(6), A930-A939, J. Mater. Chem. A 2016, 4, 18300-18305).
In proton exchange membrane fuel cells (PEMFC) electrons are generated by means of the electrochemical oxidation of hydrogen, thus producing the electrical power to drive an electric car or provide electricity for industry or households. The best currently known electro-catalysts for reaction are the so-called platinum-group metals, with platinum itself as the most active catalyst. Palladium provides an interesting alternative for platinum since it is only slightly less active but more widely available and less expensive. However, in practice the activity of palladium decreases at high anodic potentials. This has until now been explained by a change in its catalytic properties, mainly hydride decomposition in the bulk of the material and oxide formation at the surface.
These explanations are however based on laboratory experiments in liquid electrolytes at room temperature. Typical operating conditions of a low temperature PEMFC involve temperatures up to 80 °C. We have therefore developed an improved operando spectroscopy cell, based on a full fuel cell, rather than the half-cells typically used.




The operando X-ray Absorption Spectroscopy (XAS) characterization during hydrogen oxidation unequivocally demonstrates that the hydride phase is maintained under practical operating conditions of a fuel cell anode, even at high anodic potentials. The transition from a hydride to a metallic state, previously observed in electrochemical cells based on a liquid electrolyte, does not occur. The

differences in results can be explained by the fact that the reaction environment of operating PEMFC's is so much unlike that in room-temperature liquid electrolytes cells that the chemical state of the Pd catalyst is completely different. One important feature explaining this is the orders of magnitude higher mass-transport rates in PEMFC's.
This study demonstrates the necessity of characterizing the properties of electro-catalysts under realistic operating conditions. Moreover, for all electro-catalytic reactions in which the reactant is supplied in a gaseous form - not just for the hydrogen oxidation in a fuel cell – it is crucial that appropriate mass transfer regimes are maintained when establishing structure-activity relationships.

**Key publications**


- S. A. Bartlett, J. O. Moulin, M. Tromp, G. Reid, A. J. Dent, G. Cibin, D. S. McGuinness, J. Evans, 'Activation of [CrCl3{(PPh2)2NiPr} for the selective oligomerisation of ethene: a Cr K-edge XAFS study', Cat. Sci. Tech. 2016, 6, 6237-6246, DOI: 10.1039/c6cy00902f.
- Siebel, Y. Gorlin, J. Durst, O. Proux, F. Hasché, M. Tromp, H. A. Gasteiger, 'Determination of HOR catalyst structure using operando EXAFS', ACS Catal. 2016, 6, 7326-7334.
- J. Wandt, A. Freiber , R. Thomas, Y. Gorlin, A. Siebel, R. Jung, H. A. Gasteiger, M. Tromp, "Transition metal dissolution and deposition in Li-ion batteries investigated by operando x-ray absorption spectroscopy', J. Mater. Chem. A 2016, 4, 18300-18305.


**Grants**

| | |
|---|---|
| **Title** | **Chemical industry made natural!** |
| Applicant | dr. T.J. Korstanje |
| Grant from | NWO Veni |
| Amount | k€ 250 |

| | |
|---|---|
| **Title** | **Operando XAS measurements of a novel Iron electrode for low-cost energy storage** |
| Applicant | Dr. M. Tromp |
| Partner | E-Stone Batteries B.V. |
| Grant from | NWO NCI-KIEM, 2016 |
| Amount | k€ 18,75 |

**Invited lectures**

- M. Tromp, 'Probing Materials in Action – Operando Spectroscopy Providing Insights in Structure/Electronic-Performance Relationships and Mechanisms', **Invited Lecture**, Göch Colloquium, Innsbrueck University, Austria, January 2016.
- M. Tromp, Beta-Break on 'De Toekomst van vervoer', Panel discussion at University of Amsterdam – Faculty of Science, January 2016.
- M. Tromp, 'Probing Materials in Action – Operando Spectroscopy Providing Insights in Structure/Electronic-Performance Relationships and Mechanisms', **Invited Lecture**, Institutskolloquium, University Giessen, Germany, February 2016,
- M. Tromp, 'Understanding aging and conservation processes in art', **Invited Lecture**, Winterschool H. Gasteiger, Austria, March 2016.
- M. Tromp, 'The active site in the spotlight', **Invited Lecture,** UvA FNWI Faculty Colloquium, Amsterdam, April 2016.
- M. Tromp, 'Dynamic Processes in Batteries – Using operando spectroscopy to obtain detailed mechanistic insights', **Invited Lecture (plenary)**, Munich Battery Discussions 2016, BMW/TUM, March 2016.
- M. Tromp, 'The active site in the spotlight!', **Invited lecture (plenary)**, International Symposium on Homogeneous Catalysis, Japan, July 2016.
- M. Tromp, 'Advanced spectroscopic characterization of important homogeneous Cu catalysts – time and energy resolved', **Invited Lecture**, (DFG) FOR1405 Symposium, RWTH Aachen,

September 2016.
- M. Tromp, 'The active site in the spotlight! – Improving battery performance', **Invited Lecture**, Chains 2016: Chemistry Matters for the Future – the Dutch Chemistry Conference, Veldhoven, December 2016.
- M. Tromp, 'Probing sustainable materials using advanced spectroscopies', **Invited Lecture**, Materials Colloquium, ETH Zurich, December 2016.

**Outreach**

M. Tromp, 'Hoe maak je vuurwerk?', Kinderlezing, Basisschool De Boomgaard, Utrecht, December 2016.

## 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<br>Prof.dr. E.J. Meijer | | |
| Academic staff | Prof.dr. R. Krishna (em.)<br>Dr. D. Dubbeldam<br>Dr. B. Ensing<br>Dr. C.P. Lowe<br>Dr. J. Vreede | | |
| Temporary staff | | Start date | (foreseen) end date |
| Postdocs | Dr. R. Ni (VENI)<br>Dr. D. Sun<br>Dr. D.W.H. Swenson<br>Dr. N.Yachini<br>Dr. A. Rudavskyi | 01-09-2014<br>21-10-2013<br>01-03-2016<br>01-01-2015<br>01-10-2015 | 17-03-2016<br>21-10-2016<br>28-02-2017<br>29-02-2016<br>30-09-2016 |
| PhD students | Drs. Z.F. Brotzakis<br>A.Arjun, MSc.<br>Drs. J. Heinen<br>R.C. Puthenkalathil, MSc.<br>C. Dong, MSc.<br>Drs. A. Newton<br>Drs. A. Tiwari<br>Drs. A. Torres Knoop<br>Drs. A. Vijaykumar | 01-09-2012<br>01-07-2016<br>01-09-2014<br>01-04-2016<br>01-09-2016<br>15-04-2012<br>01-07-2015<br>01-03-2012<br>01-06-2013 | 31-08-2016<br>30-06-2020<br>31-08-2018<br>31-03-2020<br>31-08-2017<br>14-04-2016<br>30-06-2019<br>29-02-2016<br>31-05-2017 |

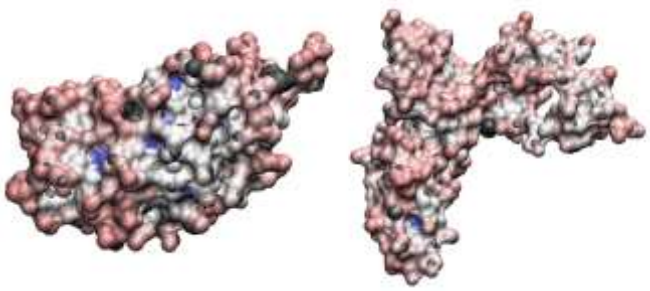
**Mission of the group:**

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.

**Research highlights per staff member**

**Peter Bolhuis**

The research of Peter Bolhuis concerns the modelling of self-assembly and conformational transitions, structure and dynamics of complex system including soft matter and proteins. In 2016 his research group published 5 regular research articles. In collaboration with Chris Evers and Willem Kegel from Utrecht University, Jurriaan Luiken and Peter Bolhuis published a Nature article in which it was shown that the combination of mutual attraction, deformability and asymmetry of biomolecular building blocks is crucial for the formation of complex biological nanostructures such as virus particles (See Group Highlight in



Water reorientation dynamics around folded and misfolded proteins. Blue is slowest, red is fastest.

paragraph 1.4.2). Faidon Brotzakis and Peter Bolhuis developed a novel transition path-sampling shooting algorithm for the efficient sampling of complex (biomolecular) activated processes with asymmetric free energy barrier (J. Chem Phys. **145**, 164112).
As water is an essential ingredient in protein structure, dynamics, and functioning, knowledge of its behavior near proteins is crucial. Faidon Brotzakis investigated water dynamics around bovine α-lactalbumin by combining molecular dynamics simulations with polarization-resolved femtosecond infrared (fs-IR) spectroscopy of the group of Huib Bakker (J. Phys. Chem. B, **120**, 4756-4766). Intrinsic rate constants play a dominant role in the theory of diffusion-influenced reactions, but usually as abstract quantities that are implicitly assumed to be known. However, recently it has become clear that modeling complex processes requires explicit knowledge of these intrinsic rates. In a paper in the Faraday Discussions, Adithya Vijaykumar and Peter Bolhuis, together with Pieter Rein ten Wolde from AMOLF, provide microscopic expressions for the intrinsic rate constants for association and dissociation processes of isotropically interacting particles and illustrate how these rates can be computed efficiently using rare event simulations techniques.

Key publications:

1. C. H. J. Evers, J.A. Luiken, P.G. Bolhuis, W.K. Kegel, *Self-assembly of microcapsules via colloidal bond hybridization and anisotropy*, Nature **534**, 364 (2016).
2. Z. F. Brotzakis, P.G. Bolhuis, *A one-way shooting algorithm for transition path sampling of asymmetric barriers*, J. Chem. Phys. **145**, 164112 (2016).
3. Z.F. Brotzakis, C.C.M. Groot, W.H. Brandeburgo , H.J. Bakker and P.G. Bolhuis, *Dynamics of Hydration Water around Native and Misfolded alpha-Lactalbumin*, J. Phys. Chem. B **120**, 4756-4766 (2016).
4. A. Vijaykumar, P.G. Bolhuis, P.R. ten Wolde, *The intrinsic rate constants in diffusion-influenced reactions*, Faraday Discuss. **195**, 421-441 (2016).

**David Dubbeldam**

The subgroup of David Dubbeldam has >10 papers published in 2016 on topics such as “controlling thermal expansion” (Chem. Mater.), DFT based material research (energy-decomposition applied on open-metal sites in MOFs), and many papers on method and theory-development (Continuous Fractional Component Monte Carlo). As a highlight I have chosen the publication: “RASPA: Molecular Simulation Software for Adsorption and Diffusion in Flexible Nanoporous Materials”.
RASPA is a software package, developed in our subgroup, for simulating adsorption and diffusion of molecules in flexible nanoporous materials is presented. The code implements the latest state-of-the-art algorithms for Molecular Dynamics and Monte Carlo in various ensembles including symplectic/measure-preserving integrators, Ewald summation, Configurational-Bias Monte Carlo, Continuous Fractional Component Monte Carlo, Reactive Monte Carlo, and Baker's minimization. Applications of RASPA include computing coexistence properties, adsorption isotherms for single and multiple components, self- and collective diffusivities, reaction systems, and visualization. After 10 years of development, the software is now released as open source under the GNU General Public License in 2016 and includes the methodologies developed in my VIDI project (700.10.428). The package is now in use by over 30 research groups and institutions, including groups at the University of Amsterdam, Technical University of Delft, Georgia Tech (Atlanta, USA), Northwestern University (Evanston, USA), Shell (Amsterdam), and CSIRO (Melbourne, Australia). The package is described in "RASPA: Molecular Simulation Software for Adsorption and Diffusion in Flexible Nanoporous Materials" by D. Dubbeldam, S. Calero, D.E. Ellis, and R.Q. Snurr, *Mol. Simulat.*, **42(2)**, 81-101, (2016). (By December 2016, cited 75 times - google scholar)

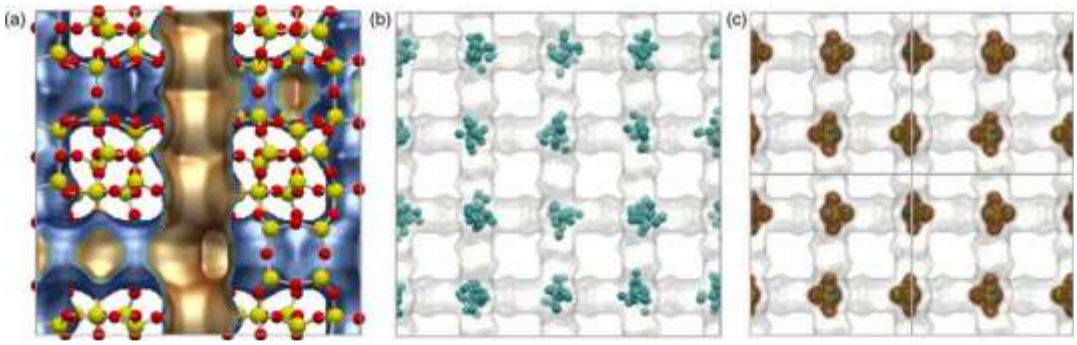



Figure: RASPA: computational package for computation and visualization of adsorption and diffusion in nanoporous materials, (a) the MFI-type zeolites consisting of oxygen (red) and silicon (yellow), (b) snapshots of adsorbing di-branched alkanes at 433K and high loading, (c) density plot.

Key publications:

1. S. Balestra; R. Bueno-Pérez, S. Hamad, D. Dubbeldam, A.R. Ruiz-Salvador, and S. Calero, *Controlling Thermal Expansion: a Metal Organic Frameworks Route*, *Chem. Mater.* **28**, 8296-8304 (2016).
2. J. Heinen, N. Burtch, C.F. Guerra, K.S. Walton, and D. Dubbeldam, *Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials using Force Field Calculations based on Energy Decomposed Density Functional Theory*, *Chem. Eur. J.* **22**, 18045-18050 (2016).
3. J. Heinen and D. Dubbeldam, *Understanding and Solving Disorder in Substitution Pattern of Amino Functionalized MIL-47(V)*, *Dalton Transactions* **45**, 4309-4315, (2016).

**Bernd Ensing**

The subgroup of Bernd Ensing published 5 papers in 2016 on the research theme of multiscale modeling of molecular transitions. Enhanced sampling techniques were developed and applied in combination with quantum chemical (DFT-based) molecular dynamics (MD) and with force-field based (MM) molecular dynamics simulations, to study e.g. electron and proton transfer reactions, methanol-olefin conversion in zeolites, molecular hydrogen activation by frustrated Lewis pairs, and solid-solid phase transitions in crystalline norleucine (see Figure). A new methodological advance by the group made it possible to simulate for the first time electron transfer between a donor and an acceptor species in water solution.

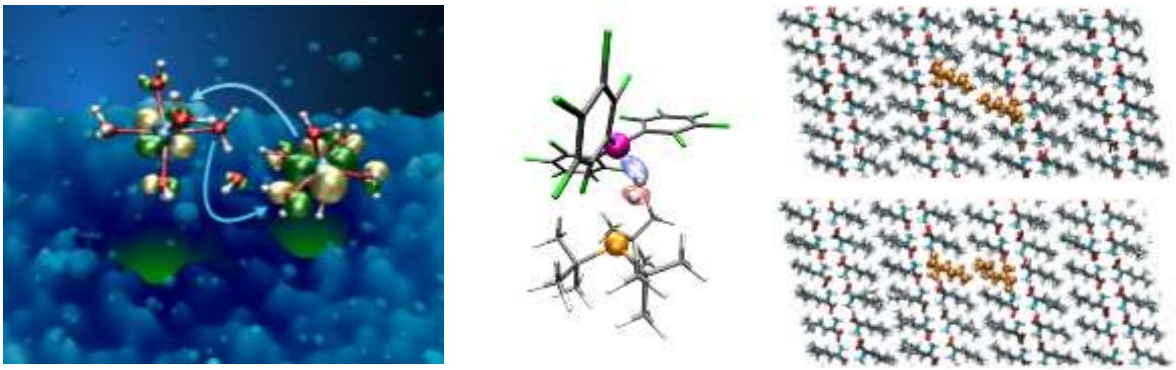


Figure. Development and applications of enhanced sampling simulations. Left: artistic impression of electron transfer between two $Ru^{2+/3+}$ ions for the cover of Faraday Discussions [3]. Center: charge transfer during $H_2$ dissociation inside a frustrated Lewis pair [1]. Right: Polymorph phase transition in crystalline norleucine revealed by metadynamics simulation [2].

Until now, it was only possible to study a (redox) half-reaction at the DFT-MD level of theory, because the random motions in the water solution that drive the spontaneous transfer of an electron between two non-covalently bonded solutes is too rare to observe in a straight-forward simulation. The new

technique, a modified version of Transition Path Sampling, generates a large number of independent reactive trajectories, which are analyzed to reveal the rare solvent and ligand fluctuations. For the prototypical self-exchange reaction between two $Ru^{2+/3+}$ ions in water, we discovered that the electron transfer is concerted with a proton transfer reaction from one of the water ligands of the $Ru^{2+}$ complex to a deprotonated ligand of the $Ru^{3+}$ complex. Hereafter, this technique can be used to unravel the mechanistic details of electron transfer in various types of redox chemistry, including electrochemical reactions at electrode surfaces and electron transfer in enzymes and between biomolecules.

Key Publications


1. L. Liu, B. Lukose, and B. Ensing, *Hydrogen Activation by Frustrated Lewis Pairs Revisited by Metadynamics Simulations*, *J. Phys. Chem. C* (2016) accepted.
2. 2), J.A. van den Ende, B. Ensing, and H.M. Cuppen, *Energy barriers and mechanisms in solid-solid polymorphic transitions exhibiting cooperative motion*, CrystEngComm, 18 (2016), 4420 – 4430.
3. A. Tiwari and B. Ensing, *Reactive trajectories of the $Ru^{2+/3+}$ self-exchange reaction and the connection to Marcus' theory*, *Faraday Discuss.*, (2016) accepted**.**


**R. Krishna**

The trade-off between physical adsorption capacity and selectivity of porous materials is a major barrier for efficient gas separation and purification through physisorption. We report control over pore chemistry and size in metal coordination networks with hexafluorosilicate and organic linkers for the purpose of preferential binding and orderly assembly of acetylene molecules through cooperative host-guest and/or guest-guest interactions. The specific binding sites for acetylene are validated by modeling and neutron powder diffraction studies. Their efficiency for the separation of acetylene/ethylene mixtures is demonstrated by experimental and simulated breakthrough curves.
Transient breakthrough curves were determined to demonstrate the C2H2/C2H4 separation performances of the SIFSIX materials in column adsorption processes. Two C2H2/C2H4 mixtures (1/99 and 50/50) were used as feeds to mimic the industrial process conditions. Clean separations were realized with all five SIFSIX MOFs; C2H4 first eluted through the bed to yield a polymer-grade gas, then C2H2 broke through from the bed at a certain time tbreak (see Figure)

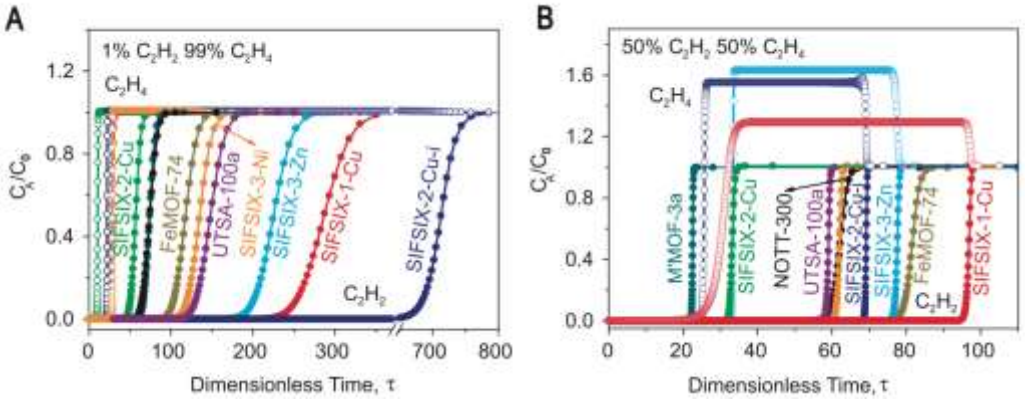
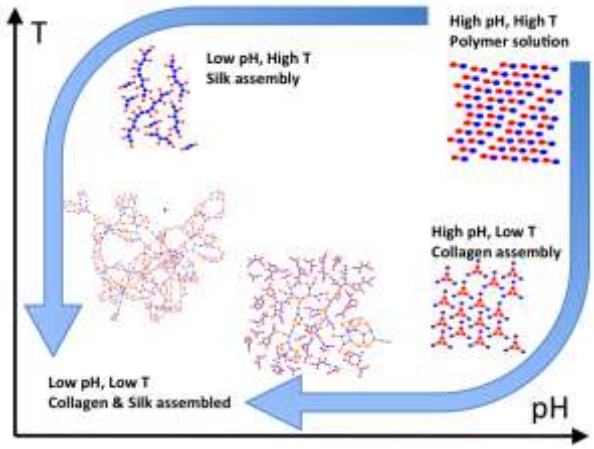



Figure: C2H2/C2H4 separation by SIFSIX materials in column adsorption processes. Simulated breakthrough curves comparing SIFSIX against previously reported best-performing materials.

**Key Publications**

1. X. Cui, K. Chen, H. Xing, Q. Yang, R. Krishna, Z. Bao, W. Zhou, X. Dong, Yu Han, Bin Li, Q. Ren, M.J. Zaworotko, B. Chen, *Pore chemistry and size control in hybrid porous materials for acetylene capture from ethylene*. Science, **353**, 141-144.
2. R. Krishna, *Describing mixture permeation across polymeric membranes by a combination of Maxwell-Stefan and Flory-Huggins models*. Polymer **103**, 124-131 (2016).
3. R. Krishna, *Tracing the origins of transient overshoots for binary mixture diffusion in microporous crystalline materials*, Phys. Chem. Chem. Phys., 18(23), 15482-15495 (2016) . DOI: 10.1039/c6cp00132g

**Christopher Lowe**




Although during 2016 Christopher Lowe has been very limited active in research and teaching, due to illness, he published together with Aatish Kumar, Peter Bolhuis, and Martien Cohen Stuart from Wageningen University, a research paper in Soft Matter on a numerical study of polymer network formation of asymmetric biomimetic telechelic polymers. This type of polymer has two reactive ends, in this case based on a self-assembling collagen, elastin or silk-like polypeptide sequence. The two reactive ends of the polymer can be activated independently using physicochemical triggers such as temperature and pH. Using a simple coarse-grained model, the work showed that the order in which this triggering occurs influences the final morphology. For both of collagen-silk and elastin-silk topologies it was found that for relatively short connector chains the morphology of the assembly is greatly influenced by the order of the trigger, whereas for longer chains the equilibrium situation is more easily achieved. Moreover, self-assembly is greatly enhanced at moderate collagen interaction strength, due to facilitated binding and unbinding of the peptides. This finding indicates that both the trigger sequence and strength can be used to steer self-assembly in these biomimetic polymer systems.

**Key publication**

Kumar, A., Lowe, C. P., Cohen Stuart, M. A., & Bolhuis, P. G. (2016). Trigger sequence can influence final morphology in the self-assembly of asymmetric telechelic polymers. Soft Matter, 12(7), 2095-2107.

**Evert Jan Meijer**

An important research line in the group focusses on understanding chemical transformations in a complex environment. Metal catalyzed asymmetric transfer hydrogenation in aqueous solution is a prime example, where the complexity involves both the nature of the catalyst as well as the aqueous environment. In this context, ruthenium compounds can efficiently catalyze asymmetric transfer hydrogenation via a metal–ligand bifunctional mechanism with either 2-propanol or formate as hydrogen donors. In a computational study we provide novel insight for two key steps in the catalytic cycle of transfer hydrogenation cycle, using a model of Ru(p-cymene)[TsDPEN] with an explicit aqueous solvent. Employing ab initio molecular dynamics simulations, the hydride transfer between formate and the protonated and deprotonated catalyst *and* the dissociation of the ruthenium-formato complex is elucidated. It is shown that solvent water molecules play an important role, provides a significant contribution to the reaction barriers. The induce an increasing the hydride transfer barrier, while decreasing the dissociation barrier for ruthenium-formato complex, when compared with gas-

phase models. These effects can be attributed to hydrogen-bond structure around the formate, which favors the formate to be in solution. Furthermore, the hydride transfer barrier was significantly higher for the deprotonated catalyst, suggesting that the catalyst protonation state is an important factor. In a more general context the study demonstrate that a first-principles molecular dynamics approach, incorporating a molecular description of the solvent, is able to capture the full complexity of catalytic reactions in an aqueous solvent. This approach can provide an important contribution to understanding the reactions as well as provide directions for novel developments in catalysis.

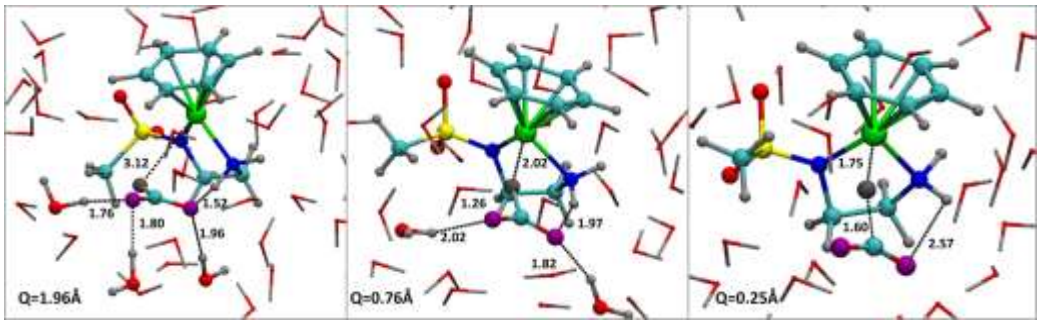



Figure: Ab initio molecular dynamics of ruthenium-formate hydrogen transfer in aqueous solution. Representative snapshots of key steps along the reaction pathway.

**Key Publications**

A.Pavlova, E.Rosler,and E.J.Meijer, *Mechanistic Aspects of Using Formate as a Hydrogen Donor in Aqueous Transfer Hydrogenation*, ACS Catal. **6**, 5350–5358 (2016).

K. DeWispelaere, C.S. Wondergem, B. Ensing, K. Hemelsoet, E.J. Meijer, B.M. Weckhuysen, V. Van Speybroeck, and J. Ruiz-Martinez, *Insight in the effect of water on the methanol-to-olefins conversion in H-SAPO-34 from molecular simulations and in-situ micro-spectroscopy*, ACS Catal. **6**, 1991-2002 (2016).

C. Zhang, X. Liu, X. Lu, E.J. Meijer, K. Wang, M. He, and R. Wang, *Cadmium(II) Complexes Adsorbed on Clay Edge Surfaces: Insight from First-Principles Molecular Dynamics Simulation*. Clays and Clay Minerals **64**, 337-347 (2016).

**Jocelyne Vreede**

The research highlight of the subgroup of Jocelyne Vreede was a study on the effect of salt bridges on the stability and folding kinetics of model alpha-helices, in collaboration with Sander Woutersen. The following link directs to a movie of an alpha-helix unfolding and refolding:
https://www.dropbox.com/s/f3zi2d3mhnz4ziy/ERi4.mp4?dl=0

She supervised an NWO-funded student project on the identification of potential salt sensors in plants, in collaboration with prof. dr. Christa Testerink of the Plant Cell Biology group in the Swammerdam Institute for Life Sciences. Jocelyne obtained an HRSMC visiting research fellow grant to host Dr. Enrico Riccardi from NTNU, Trondheim, Norway to perform rate calculations on the DNA binding by the bacterial DNA organizing protein H-NS.

**Key Publication**

H. Meuzelaar, J. Vreede and S. Woutersen. *Influence of Glu/Arg, Asp/Arg, and Glu/Lys Salt Bridges on α-Helical Stability and Folding Kinetics*, Biophys. J. (2016) 110:2328 .

**Other activities**

Peter Bolhuis is

- director of the Dutch CECAM node.
- chair of the CW study group Soft Matter
- member of the FOM WGC Physics of Life
- member of the steering committee NWA Route 5
- member of the international programme committee of the Faraday discussion on "Reaction Rate theory"
- member of the CSER programme committee
- editorial advisory board member of JPCB

Evert Jan Meijer is

- member of the scienctific council of CECAM
- member of the board of the ATOSIM Erasmus Mundus Consortium
- member of Scientific Committee for the Computational Sciences for Future Energy (FE) conference

Peter Bolhuis organised the Lorentz Centre Workshop "Reaction coordinates from molecular trajectories" in Leiden, Aug 2016.

Bernd Ensing organized the Graduate Winterschool on Theoretical Chemistry and Spectroscopy, December 6-10, 2016 (Han-sur-Lesse, Belgium)

Evert Jan Meijer, Bernd Ensing, and David Dubbeldam organized the Graduate winter school on Understanding Molecular Simulation, January 4-15, 2016; Amsterdam.

**Dissertations**

28-04-2016 Ariana Torres Knoop (dr. D. Dubbeldam, Prof.dr. E.J. Meijer) – Cum laude
28-04-2016 Kush Singhal (prof.dr. P.G. Bolhuis, dr. J. Vreede)

**Grants**

| | |
|---|---|
| Title | Identification of potential salt sensors in plants |
| Applicants | dr. J. Vreede, K. de Groot, S. Spoelstra |
| Grant from | NWO Topsector chemistry student competition |
| Amount | k€ 18 |

| | |
|---|---|
| Title | Upconversion mechanism of lanthanide-based nanomaterials |
| Applicants | Prof. E.J. Meijer, Prof. H. Zhang, Dr. Tu Langping |
| Grant from | HRSMC |
| Amount | k€ 18 |

| | |
|---|---|
| Title | Research on Mechanism of Thermal Dissociation of Tertiary Amine Hydrochlorides Using Molecular Simulation Techniques |
| Applicants | C. Dong (MSc), Prof. E.J. Meijer, Prof. Jianguo Yu, Prof Xingfu Song |
| Grant from | China Research Council |
| Amount | 12 month PhD Scholarship |

**Invited lectures**

**P.G. Bolhuis**

- Lecture at Mini-Statistical Mechanics meeting, UC Berkeley, 8-10 Jan 2016,
- Seminar ENS Paris 28 Jan 2016
- Lecture at CECAM workshop "Models for protein dynamics" 15 Feb 2016 to 18 Feb 2016
- Lecture at RESIM Rare Event workshop, Eindhoven, 29 Mar 2016 to 01 Apr 2016
- Lecture at Statistical Mechanics meeting, Rutgers Univ, New Jersey, 9-11 May 2016
- Lecture at Gordon Conference on Computational Chemistry, Girona, 25-28 July 2016
- Lecture at CMD conference, Groningen, 5-9 September 2016
- Lecture at Erice International School on Physics, Sicily, Italy, 7-12 October 2016

**D. Dubbeldam**

- Mini-symposium, HIMS “Innovative Material Science Based on Supramolecules”, (January 19, 2016)
- Workshop TU-Delft, “Molecular Simulation of Nanoporous Materials and Ionic Liquids” (December 19, 2016)

**B. Ensing**

- Seminar series of the Institute for Theoretical Chemistry, Universitat de Barcelona, (Barcelona, Spain; February 2, 2016)
- Physical Chemistry seminar, Department of Chemistry, Norwegian University of Science and - Technology (Trondheim, Norway; March 3, 2016)
- TACC 2016 conference 28/8–2/9, (Seattle, USA; August 30, 2016)

**E.J. Meijer**

- Seminar at DIFFER/FOM Institute (Eindhoven; June 2016).
- Seminar at East China Normal University, School of Chemistry and Molecular Engineering (Shanghai, China; June 2016)
- Seminar at East China University of Science and Technology, School of Chemical Engineering (Shanghai, China; June 2016)
- Lecture at mini-symposium "Molecular-scale Properties of Mineral-Water interfaces: Recent Progress and Future Challanges for Computer Simulations; State Key Laboratory for Mineral Deposits Research, Nanjing University (Nanjing, China; June 2016)
- Lecture at symposium "Mechanisms in heterogeneous catalysis" (Heeze, September 7-9, 2016).
- Lecture at "EMN Meeting on Computation and Theory" (Las Vegas, USA; October 10-13, 2016).
- Lecture at "International Symposium of Computational Organometallic Catalysis" (Beijing, October 20-24; 2016)
- Lecture at "HRSMC Annual Symposium (Leiden, November 2016)

**J. Vreede**

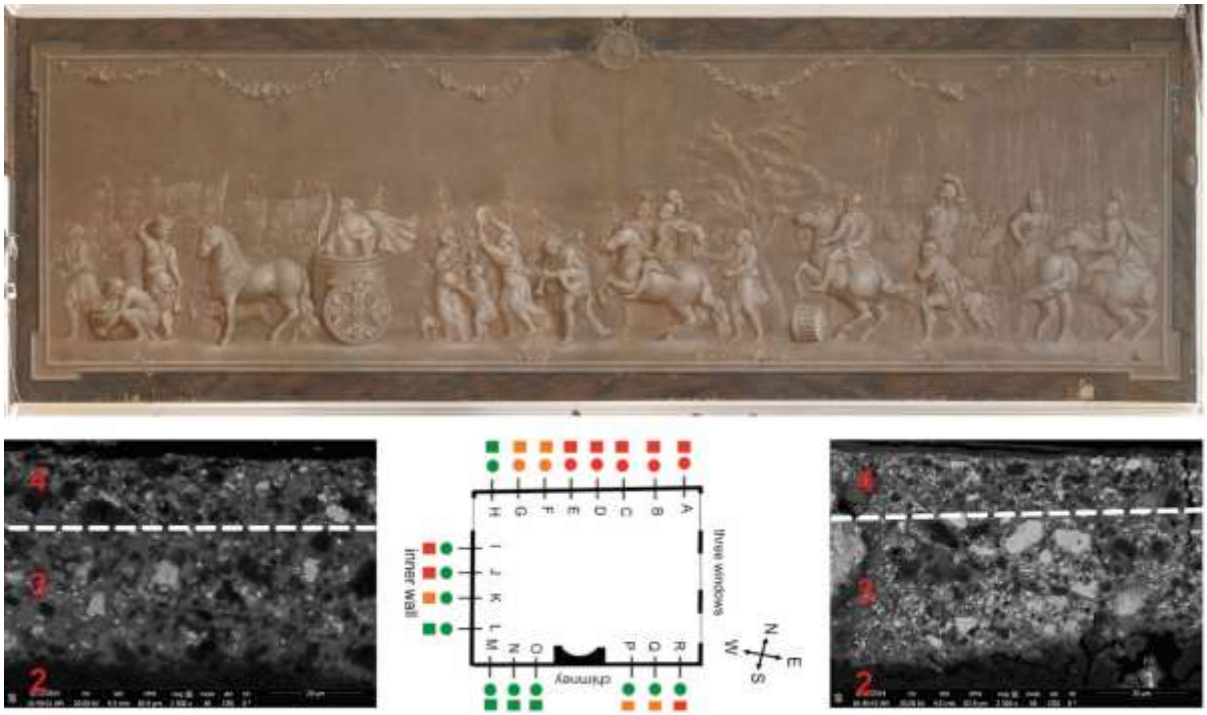
- Lecturer at the Graduate Days of the Center for Ultrafast Imaging, Hamburg, Germany (March 2016)
- Presentation at the Lorentz Workshop “Reaction Coordinates from Molecular Trajectories” (Leiden; August 2016)
- Speaker at Support4Research Masterclass (Erasmus University Rotterdam; October 2016)
- Lecture at ICREA (Barcelona, Spain; November 2016)

| Group | Computational Polymer Chemistry | | |
|---|---|---|---|
| Groupleader | Prof.dr. P.D. Iedema | | |
| Temporary staff | | Start date | end date |
| Postdocs | Dr. K. Keune (NWO/PAinT) | 1-8-2012 | 31-7-2016 |
| | Dr. A. van Loon (NWO/PAinT) | 1-8-2012 | 31-7-2016 |
| | Dr. I. Kryven (VENI) | 1-4-2015 | 1-1-2019 |
| | Dr. A. Torres Knoop (NWO/PREDAGIO) | 1-6-2016 | 1-6-2019 |
| | Dr. A. Gambardella (Rijksmuseum) | 1-1-2016 | 1-1-2019 |
| PhD students | Drs. J.J. Hermans (NWO/PAinT) | 1-12-2012 | 31-12-2016 |
| | V. Schamböck (STW/PHOTo) | 1-5-2016 | 1-5-2020 |
| | Y. Orlova, MSc (NWO/PREDAGIO) | 1-7-2016 | 1-7-2020 |
| | Drs. L. Baij (Rijksmuseum) | 1-7-2016 | 1-7-2020 |
| | Drs. S. Hageraats (Rijksmuseum) | 1-9-2016 | 1-9-2020 |

**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**
*Metal soap research* (**P. Iedema, K. Keune, A. van Loon**)
The formation of metal soaps in oil paintings is the central topic of the PhD project of Joen Hermans (defense in May 2017). Using differential scanning calorimetry (DSC) and infrared spectroscopy (FTIR) we found that metal soaps exhibit near-ideal solubility behaviour, and that polymerisation of the oil increased the supercooling needed for the start of crystallisation. In the case of zinc soaps, it even seems likely that the complexes could remain kinetically trapped in an amorphous state in oil paints.
*Direct Temperature-Resolved Time-of-Flight Mass Spectrometry of old paintings* (**A. van Loon, P. Iedema**)
Direct temperature-resolved mass spectrometry (DTMS) is a fast analytical particularly suitable for the characterization of oils, resins, waxes in tiny and complex samples of paintings. Our work combines DTMS with other techniques 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.

*Lead soaps on location* (**K. Keune, P. Iedema**)
We have studied the relationship between the lead soap formation and the local indoor environmental condition for old paintings. For several Hofkeshuis paintings (Almelo), the relative amount of intact lead white pigments and degree of lead soap areas (LW/LS ratio) is deduced from backscatter electron together with a newly developed computational image analysis methods (see Figure). The highest degree of lead white degradation in the room was found in samples from the north wall close to the windows, while the degradation diminishes further away from the window, demonstrating a strong relationship between chemical degradation of the paint and the location of the paint in the room. It is for the first time that the degradation of lead white pigment in mature oil paint has been used as an internal marker for the chemical degradation of oil paint.




**Key Publications** (**P. Iedema and I. Kryven**)

- I. Kryven, *Emergence of the giant weak component in directed random graphs with arbitrary degree distributions*, Phys. Rev. E **94**, 012315 (2016).
- J.J. Hermans, K. Keune, A. van Loon, P.D. Iedema, *Ionomer-like structure in mature oil paint binding media*, RSC Adv. **6**, 93363 (2016).
- N. Yaghini, P.D. Iedema, *Three-dimensional chain-length-branching-combination points distribution modeling of low density polyethylene in a continuous stirred tank reactor allowing for gelation,* Chem. Eng. Sci. **140**, 348–358 (2016).
- J.J. Hermans, K. Keune, A. van Loon, P.D. Iedema, *The crystallization of metal soaps and fatty acids in oil paint model systems,* Phys. Chem. Chem. Phys. **18**, 10896–10905.
- I. Kryven, J. Duivenvoorden, J.J. Hermans, P.D. Iedema *Random Graph Approach to Multifunctional Molecular Networks,* Macromol. Theory Simul. **25**, 449−465.

**Joint publications**

- Van Loon, A., Genuit, W., Pottasch, C., Smelt, S., Noble, P., 2016, 'Analysis of Old Master Paintings by Direct Temperature-Resolved Time-of-Flight Mass Spectrometry: Some Recent Developments', Microchemical Journal 26: 406-414.
- Keune, K., Mass, J., Metha, A., Church, J., Meirer, F. (2016). "Analytical imaging studies of the migration of degraded orpiment, realgar, and emerald green pigments in historic paintings and related conservation issues." Heritage Science 4.1 (2016): 1.
- Keune, K., Kramer, R.P., Huijbregts, Z., Schellen, H.L., Stappers, M.H.L. and van Eikema Hommes, M.H. (2016) 'Pigment Degradation in Oil Paint Induced by Indoor Climate: Comparison of Visual and Computational Backscattered Electron Images', Microscopy and Microanalysis, 22(2), pp. 448–457.

## 2.3 Molecular Photonics

| | | | |
|---|---|---|---|
| Groups: | Molecular Spectroscopy; Spectroscopy and Photonic materials;<br>Time Resolved Vibrational Spectroscopy | | |
| Group leaders: | Prof.dr. A.M. Brouwer[3]<br>Prof.dr. W.J. Buma | | |
| Academic staff: | Prof.dr. S. Woutersen<br>Prof.dr. M.C.G. Aalders (BHGL)<br>Prof.dr. H.J. Bakker (BHGL)<br>Prof.dr. J. Oomens (BHGL)<br>Dr.ir. A. Petrignani – Taube (Vidi-fellow, > 01-03-2016)<br>Dr. R.M. Williams<br>Dr. H. Zhang | | |
| Support staff: | Drs. ing. M.F. Hilbers<br>Ing. P.P. Reinders<br>Drs. H.J. Sanders | | |
| Temporary staff | | Start date | (Foreseen) end date |
| Postdocs: | Dr. V.P. Nicu | 01-06-2015 | 31-12-2018 |
| | Dr. W.J. Roeterdink | 01-05-2016 | 30-04-2018 |
| | Dr. S. Shen | 01-05-2015 | 30-04-2016 |
| | Dr. L. Tu | 01-09-2016 | 31-01-2017 |
| | Dr. R. Becker | 15-04-2016 | 15-04-2017 |
| PhD students: | H.C. Chen, MSc. | 01-09-2011 | 31-08-2015 |
| | Y. Feng, MSc. | 01-03-2016 | 28-02-2020 |
| | R.O. Gutierrez Cota MSc. | 01-06-2015 | 31-05-2019 |
| | Drs. M.A.J. Koenis | 01-09-2015 | 31-08-2019 |
| | E. Maltseva, MSc. | 01-08-2012 | 31-07-2016 |
| | Drs. D. Petrova | 01-04-2015 | 31-03-2019 |
| | Drs. S.J. Roeters | 15-10-2011 | 14-07-2016 |
| | M. Raeisolsadati Oskoui | 01-11-2012 | 30-09-2015 |
| | L. Song, MSc. | 01-07-2016 | 30-06-2017 |
| | Drs. B.H. Strudwick | 01-08-2014 | 31-07-2019 |
| | T. Suhina, Msc. | 01-11-2012 | 31-10-2016 |
| | Drs. S. Wiersma | 01-09-2016 | 31-08-2020 |
| | Y. Wu, MSc. | 01-09-2016 | 31-08-2020 |
| | D. Zheng, MSc. | 01-09-2014 | 31-08-2018 |
| | J. Zuo, MSc. | 01-04-2016 | 31-03-2020 |

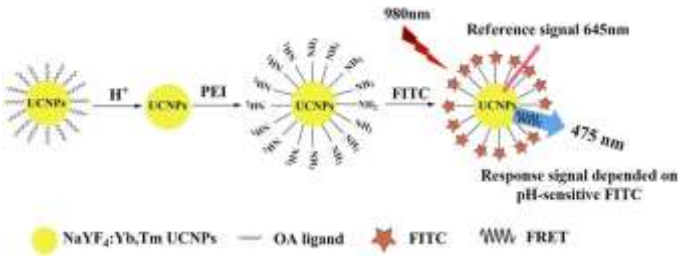
**Mission of the group:**

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**

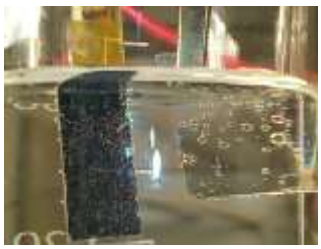
[3] Per July 2014 professor Brouwer is part time group leader Nanophotochemistry at the Advanced Research Center for Nanolithography (ARCNL).

**Molecular graphene** The interaction of delocalized π-electrons with molecular vibrations is key to charge transport processes in π-conjugated organic materials based on aromatic monomers. The application of advanced infrared multiple-photon dissociation action spectroscopic techniques and quantum-chemical calculations has allowed us to show how the molecular edge topology is ultimately responsible for determining how the electron distribution is linked to the vibrational dynamics of the carbon skeleton. These results rationalize the differences of electronic properties of armchair- versus zigzag-type families of technologically relevant organic molecules, and allow for a rational design of new materials (*Nat. Commun*. **2016**, 7, 1263).




**Nanoprobes for self-ratiometric pH sensing** The accurate quantification of the intracellular pH ($pH_i$) is of great importance in revealing the cellular activities and early warning of diseases. A series of fluorescence-based nano-bioprobes composed of different nanoparticles or/and dye pairs have already been developed for $pH_i$ sensing. Till now, biological auto-fluorescence background upon UV-Vis excitation and severe photo-bleaching of dyes are the two main factors impeding an accurate quantitative detection of $pH_i$. We have developed a self-ratiometric luminescence nanoprobe based on Förster resonant energy transfer (FRET) in which upconversion nanoparticles (UCNPs) (as energy donor) were covalently conjugated with pH-sensitive Fluorescein isothiocyanate (FITC) (as energy acceptor) for an accurate and quantitative probing of $pH_i$. Under 980 nm excitation upconversion emission bands at 475 nm and 645 nm of $NaYF_4:Yb^{3+},Tm^{3+}$ UCNPs were used as $pH_i$ response and self-ratiometric reference signal, respectively. This direct sensing approach has circumvented the traditional software-based subsequent processing of images which may lead to relatively large uncertainty of the results. Due to efficient FRET and the absence of fluorescence background, a highly sensitive and accurate sensing has been achieved, featured by 3.56 per unit change in $pH_i$ value 3.0-7.0 with deviations less than 0.43. This approach will facilitate the intracellular researches and development of the intracellular drug delivery systems (*Scientific Reports* **2016**, 6:38617).

**Vibrational Circular Dichroism.** Vibrational Circular SDichroism (VCD) is one of the most powerful tools to determine and study the stereochemistry of chiral molecular systems but its routine application suffers from the extensive theoretical efforts that need to be made to come to an unambiguous assignment of experimental spectra. In collaboration with Scientific Computing & Modelling N.V. and BioTools Inc. we have developed new theoretical methods that enable a faster and more reliable analysis. With these methodologies we have shown that the currently employed analysis methods that consider the molecule as conformationally static in general lead to an incorrect interpretation of the spectrum. Indeed, only when the conformational dynamics are explicitly taken into account full agreement between experiment and theory can be obtained (*Chem. Eur. J.* **2016**, *22*, 704; *Physical Chemistry Chemical Physics* **2016**, *18*, 21202; *ibid* 21213).



**Solar Fuels.** In 2016 the Molecular Photonics group contributed to the development of light driven water oxidation for solar fuels. We made new robust photoactive chromophores that absorb light and drive photo-catalysis. We anchored highly electron-deficient benzo[ghi]-perylene-tris-imide (BPTI) chromophores to a metal oxide electrode surface and showed that reversible formation of their radical anions can occur in air-saturated aqueous buffer solution. BPTI is a robust molecular chromophore that can function as the electron acceptor in water

splitting artificial photosynthetic devices in aqueous phase. Next to these perylene tris-imides, we also used new beta substituted porphyrins. Very photo-stable tetra-chloro-metallo-porphyrins (Cu(II) and Ni(II)) were used as sensitizers for visible-light-driven water oxidation coupled to cobalt based water-oxidation catalysts in concentrated phosphate buffer solution. We successfully demonstrated long-term (>3 h) visible-light-driven water oxidation using a molecular system (*Chemistry - A European Journal* **2016**, *22*(16), 5489-5493; *Physical Chemistry Chemical Physics* **2016**, *18*(22), 15191-15198).

**Surprising finding under the hood of molecular motors**. Time-resolved vibrational-spectroscopy experiments on the molecular motor of Nobel laureate Ben Feringa show that its operation cycle involves an electronic 'dark state', that results in a short (picosecond) stutter at the onset of its rotational movement, and strongly influences the quantum efficiency of the molecular motor. This knowledge is essential for the design of the next generation of these motors: to improve the efficiency of the photon-to-rotation conversion one should focus on the 'dark state', and not on the optically accessible excited electronic state that was the focus of attention so far (*J. Phys. Chem. A* **2016**, *120*, 8606-8612).

**Key Publications (3 per staff member)**


1. Amirjalayer, S.; Cnossen, A.; Browne, W.R.; Feringa, B.L.; Buma, W.J.; Woutersen, S. Direct observation of a dark state in the photocycle of a light-driven molecular motor. *J. Phys. Chem. A* **2016**, *120*, 8606-8612.
2. Becker, R.; Amirjalayer, A.; Li, P.; Woutersen, S.; Reek, J.N.H. An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media, *Sci. Adv.* **2016**, *2*, e1501014.
3. Bruijn, J.R.; Van der Loop, T.H.; Woutersen, S. Changing Hydrogen-Bond Structure during an Aqueous Liquid–Liquid Transition Investigated with Time-Resolved and Two-Dimensional Vibrational Spectroscopy. *J. Phys. Chem. Lett.* **2016**, *7*, 795–799.
4. Chen, H.-C.; Williams, R. M.; Reek, J. N. H.; Brouwer, A. M. Robust Benzo[Ghi]Perylenetriimide Dye-Sensitized Electrodes in Air-Saturated Aqueous Buffer Solution. *Chem. Eur. J.* **2016**, *22*, 5489-5493.
5. Chen, H-C., Reek, J. N. H., Williams, R. M., & Brouwer, A. M. Halogenated earth abundant metalloporphyrins as photostable sensitizers for visible-light-driven water oxidation in a neutral phosphate buffer solution. *Phys. Chem. Chem. Phys.* **2016**, *18*(22), 15191-15198.
6. Cong, T.; Ding, Y.; Xin, S.; Zhang; Liu Y. Solvent-Induced Luminescence Variation of Upconversion Nanoparticles. *Langmuir* **2016**, *32*, 13200-13206.
7. Galué, H.A.; Oomens, J.; Buma, W.J.; Redlich, B. Electron-flux infrared response of varying $\pi$-bond topology in charged aromatic monomers. *Nat. Commun.* **2016**, *7*, 12633.
8. Kiawi, D.M.; Chernyy, V.; Oomens, J.; Buma, W.J.; Jamshidi, Z.; Visscher, L.; Waters, L.B.F.M.; Bakker, J.M. Water dissociation upon adsorption onto free iron clusters is size dependent. *J. Phys. Chem. Lett.* **2016**, *7*, 2381.
9. Li, C.; Zuo, J.; Zhang, L.; Chang, Y.; Zhang, Y.; Tu, L.; Liu, X.; Xue, B.; Li, Q.; Zhao, H.; Zhang, H.; Kong, X. Accurately Quantitative Sensing of Intracellular pH based on Upconversion Self-ratiometric Luminescent Nanoprobe. *Scientific Reports* **2016**, *6*, 38617.
10. Limburg, B.; Hilbers, M.; Brouwer, A. M.; Bouwman, E.; Bonnet, S. The Effect of Liposomes on the Kinetics and Mechanism of the Photocatalytic Reduction of 5,5′-Dithiobis(2-Nitrobenzoic Acid) by Triethanolamine. *J. Phys. Chem. B* **2016**, *120*, 12850-12862.
11. Maltseva, E.; Petrignani, A.; Candian, A.; Mackie, C.J.; Huang, X.; Lee, T.J.; Tielens, A.G.G.M.; J. Oomens, J.; Buma, W.J. High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons in the 3-$\mu$m region: Role of periphery". *Astrophys. J.* **2016**, *831*, 58.
12. Martens, J.; Grzetic, J.; Berden, G.; Oomens, J. Structural identification of electron transfer dissociation products in mass spectrometry using infrared ion spectroscopy. *Nat. Commun.* **2016**, *7*, 11754.

13. Nicu, V.P.; Domingos, S.R.; Strudwick, B.H.; Brouwer, A.M.; Buma, W.J. Interplay of exciton coupling and large-amplitude motions in the vibrational circular dichroism spectrum of dehydroquinidine. *Chem. Eur. J.* **2016**, *22*, 704-715.
14. Suhina, T.; Amirjalayer, S.; Mennucci, B.; Woutersen, S.; Hilbers, M.; Bonn, D.; Brouwer, A. M. Excited-State Decay Pathways of Molecular Rotors: Twisted Intermediate or Conical Intersection? *J. Phys. Chem. Lett.* **2016**, *7*, 4285–4290.
15. Weerd, C. de; Gomez, L.; Zhang, H.; Buma, W.J.; Nedelcu, G.; Kovalenko, M.; Gregorkiewicz, T. Energy Transfer Between Inorganic Perovskite Nanocrystals. *J. Phys. Chem. C* **2016**, 120, 13310-13315.

**Other activities**

**A.M. Brouwer**

- Collaborations with J. Qian (Shanghai, China), T. Ogoshi (Kanazawa, Japan), S. Bonnet (Leiden), T. Gacoin (Ecole Polytechnique, Palaiseau, F), D. Bonn (IoP, UvA), B. Mennucci (Pisa), Y. Ekinci (PSI, Villigen, Switzerland), P. Audebert (Cachan), A. Spangenberg (Mulhouse).
- 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
- Chair IUPAC project Measurement of Photoluminescence Quantum Yields 2014-2018
- Member of the board of the Study Group Structure and Reactivity (Chemical Sciences, Netherlands Science Foundation)
- Member of Editorial Board European Journal of Organic Chemistry
- Member of board John van Geuns Fonds
- Organizer of Summer School Photochemistry, Holland Research School of Molecular Chemistry, Maastricht, September 2016
- Organizer of workshop Low Energy Electrons, Lithography, Imaging and Soft matter, A'dam 2016.
- Member Int. Advisory Committee "IUPAC Symposium on Photochemistry", Dublin, 2018
- Chair of the IUPAC Symposium on Photochemistry, Amsterdam, 2020

**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, W. Szymanski, B. Feringa (all RUG), A.G.M.M. Tielens (RUL), H. Overkleeft (RUL), S. Amirjalayer (University of Münster), F. Zerbetto (University of Bologna), L. Nafie and R. Dukor (BioTools)
- 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.

**A. Petrignani**

- Collaborations with J. Oomens and J. Bakker (RU), A.G.M.M. Tielens and A. Candian (UL), and T. Lee (NASA Ames)
- Editor "AstroPAH" newsletter.
- SOC member, Workshop AstroPAH & James Webb Space Telescope.
- Awarding of FELIX beam time for spectroscopy measurements of PAHs.

**R.M. Williams**

- Collaborations with: P. Hudhomme (Angers, France) on fulleropyrrolidine-perylenemonoimide dyads, S. Leroy-Lhez (Limoges, France) on photoactive porphyrines for medical applications, J.N.H. Reek (UvA) on water-oxidation (within Biosolar Fuels), R.A.J. Janssen (TU/e) on solar cell materials.
- Member of the Board of Examiners of the Forensic Science Master (UvA).
- Member of the FNWI Library Committee (UvA).
- Member of the Board of Studies (Chemistry UvA).
- Member of the Editorial Advisory Board of "The Scientific World Journal".

**S. Woutersen**

- Collaborations with Prof. M. Bonn (Max Planck Instituut, Mainz), Dr. G. 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 CO2 reduction; Profs. G. Knoer (Universiteit van Linz), J.N.H. Reek and B. de Bruin (UvA) on foto-catalytic H2 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) to be held in September 2017
- Member of the Program Advisory Committee (PAC) of the free-electron laser FELIX
- Proposal-referee for de Velux Foundation (Denmark)

**H. Zhang**

- Collaborations with A. Chan (Percuros b.v.), L. Cruz (LUMC), T. Gregorkiewicz (IoP (UvA)), P. Prosposito (Univ Rome "Tor Vergata"), M. Kubinyi (Univ. Budapest Univ Tech. & Econ.) Y. Mely (Univ. Strasbourg), K. Kong (CIOMP/CAS), H.J. Zhang (CIAC/CAS), Y. Liu (NENU), A. Szemik-Hojniak (Univ Wroclaw), X. Wang (Univ. Georgia South.) , C. Lowik ( Erasmus Med. Cen.), Z. Cui (AHNU), J. Reek, G. Rothenberg, S. Grecea (HIMS/UvA).
- Member of international advisory committee of "the 4th International Symposium on Rare Earth Resource Utilization and the 7th International Symposium on Functional Materials" 2016.
- Managing editor of Journal of Rare Earths.
- Member of academic committee of rare earth society / luminescence branch of China.
- 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.

**Dissertations**

14-01-2016 Hung-Cheng Chen (prof. dr. A.M. Brouwer, prof.dr. J.N.H. Reek, dr. R.M. Williams)
24-11-2016 Wilbert Smit (prof. dr. H.J. Bakker, prof. dr. M. Bonn)
21-12-2016 Simona Strazdaite (prof. dr. H.J. Bakker)

**Grants**

| | |
|---|---|
| Title | Redox Mediators in Dye-sensitized Photoelectrochemical Cells for $CO_2$-reduction |
| Applicants | Prof. dr. Reek, Dr. Koch, Dr. Detz, Prof. dr. Brouwer, Prof. dr. Sinke, Dr. Garnett |
| Grant from | NWO Solar to Products |
| Amount | k€ 557 |

| | |
|---|---|
| Title | ELENA Low energy electron driven chemistry for the advantage of emerging nano-fabrication methods |
| Applicants | ELENA Consortium. A.M. Brouwer member |
| Grant from | European Commission, HORIZON 2020 program, |
| Amount | k€ 1067 (1 PhD student at ARCNL) |

**Prizes**

**H. Zhang**

Award of "the 4th International Symposium on Rare Earth Resource Utilization and the 7th International Symposium on Functional Materials"

**Invited lectures**

**A.M. Brouwer**

- *Minisymposium ''Photochemistry", TU Delft, May 2, 2016.*
  "Fluorescence in confinement: molecules detect mechanical contact"
- *1st International Symposium on Photosynergetics (Grant-in-Aid for Scientific Research on Innovative Areas, MEXT, Japan), Osaka University in June 2nd-4th, 2016.*
  "Fluorescence in confinement: molecules detect mechanical contact"
- *NAMB Constanta, Romania, September 2016.*
  "Fluorescence in confinement: molecular photophysics and contact mechanics"
- *2nd International Symposium on Innovative Material Sciences Based on Supramolecules, Kanazawa, Japan, October 27, 2016.*
  "Fluorescent molecular probes reveal contact and friction"
- *Symposium of Promoting International Joint Research, Shinshu University, Ueda, Japan, October 28, 2016.*
  "Fluorescent molecular probes reveal contact and friction"
- *International Conference on Functional Polymers and Materials, Daejeon, Korea October 31 - November 4, 2016*
  "Extreme Ultraviolet Photoresist Chemistry"

**W.J. Buma**

- *FYSICA 2016, April 8, 2016, Radboud University.*
  "Light on photoactive molecules: electrons and nuclei at work".
- *Multi-Responive Photochromes, Nantes, France, April 25-28, 2016.*
  "Fast photodynamics probed by slow spectroscopy".
- *CHAINS 2016, Veldhoven, December 6-8, 2016.*
  "High-resolution laser spectroscopy of photoactive materials: light on the dark side of the force".

**H. Zhang**

- *19th International Conference on Dynamical Processes in Excited States of Solids (DPC'16), 17-21 July 2016, Paris, France*.
  "Migration Upconversion in Spatially Separated Doping Nanostructures"
- *1st International conference on upconversion (UPCON2016), 23-25 May 2016, Wroclaw, Poland*
  "Optimization of energy transfer in functional upconversion nanoplatforms"
- *The 4th International Symposium on Rare Earth Resource Utilization and The 7th International Symposium on Functional Materials*, August 16-19, Changchun, China.
  "Luminescence Upconversion Mechanism in Spatially Confined Systems: Revisit and Application"
- *Symposium, 21 August 2016, Minzu University of China.*
  "Biomedical application of photonic Nanomaterials"
- *Symposium, 10 August 2016, Anhui Normal University.*
  "Photonic nanomaterials"
- Dispute chair, Third KNAW NWO PhD event, 24 November 2016, Amsterdam.
- Chair KNAW-CAS joint research "Immunoassay application of upconversion nanomaterials" kick-off meeting, 3-4 May Changchun, China

**S. Woutersen**

- *8th International Conference on Coherent Multi-dimensional spectroscopy, Groningen, 29 juni-1 juli 2016.*
  "Liquid-liquid transitions in aqueous solutions: the Good, the Bad, and the Spectroscopy".
- *WaterX: Exotic properties of water under extreme conditions, Nice, 13-16 July 2016.*
  "Liquid-liquid transitions in aqueous solutions: probing the changes in hydrogen-bond structure with infrared spectroscopy".
- *International Conference on Charge Carrier Dynamics at the Nanoscale, Berlin, 12-13 Sept 2016*
  "Extreme slowing down of proton-charge mobility in water nanodots".
- *Advanced Spectroscopy of Biomolecules, IMM afternoon symposium, Nijmegen, 4 Nov 2016.*
  "Multidimensional infrared spectroscopy of biomolecules".

**Outreach**

**A.M. Brouwer**

- Popular lecture "*Moleculen in beweging door licht*", Rotterdamse Chemische Kring, Rotterdam, 21 November 2016.

**R.M. Williams**

- Meeloop-dag, April 22, 2016, Heleen Mulder, 6 VWO, Hyperion College (Amsterdam).
- Profielwerkstuk *Luminol*, November 18, 2016, Heleen Mulder, 6 VWO, Hyperion College (Amsterdam).

**Joint publications (with other HIMS themes)**

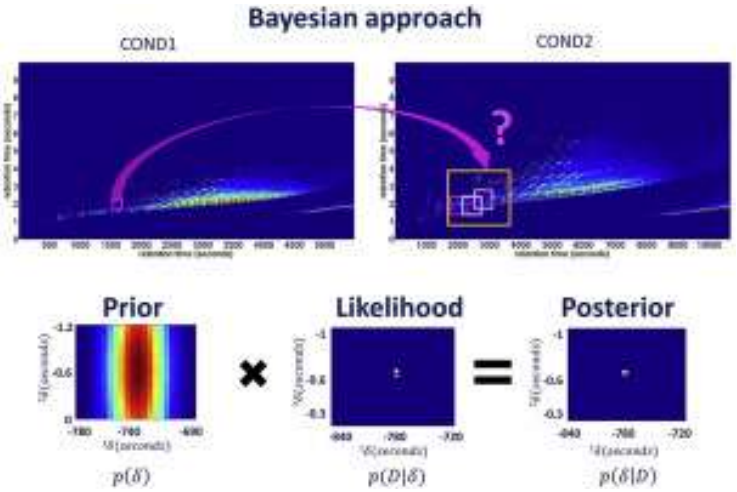
1. Chen, H.-C.; Williams, R. M.; Reek, J. N. H.; Brouwer, A. M. Robust Benzo[Ghi]Perylenetriimide Dye-Sensitized Electrodes in Air-Saturated Aqueous Buffer Solution. *Chem. Eur. J.* **2016**, *22*, 5489-5493.
2. Chen, H-C., Reek, J. N. H., Williams, R. M., & Brouwer, A. M. Halogenated earth abundant metalloporphyrins as photostable sensitizers for visible-light-driven water oxidation in a neutral phosphate buffer solution. *Phys. Chem. Chem. Phys.* **2016**, *18*(22), 15191-15198.
3. Becker, R.; Amirjalayer, A.; Li, P.; Woutersen, S.; Reek, J.N.H. An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media, *Sci. Adv.* **2016**, 2, e1501014.

## 2.4 Analytical Chemistry

| Group | Analytical Chemistry | | |
|---|---|---|---|
| Groupleader | Prof.dr.ir. P.J. Schoenmakers | | |
| Academic staff | Prof.dr. G.L. Corthals<br>Prof.dr. M.R. van Bommel (0,2 FTE)<br>Dr. W.Th. Kok<br>Dr. G.I. Vivo Truyols<br>Dr. M. Camenzuli | | |
| Associated academic staff | Prof.dr.ir. J.G.M. Janssen (BHL)<br>Prof.dr. A.C. van Asten (BHL)<br>Prof.dr. R.A.H. Peters (BHL)<br>Prof.dr. S. van der Wal (em. BHL) | | |
| Temporary staff | | Start date | (foreseen) end date |
| Postdocs | Dr. A. Astefanei | 15-09-2015 | 15-09-2017 |
| | Dr. I. Dapic | 01-11-2015 | 30-09-2017 |
| | Dr. A.F.G. Gargano | 01-09-2013 | 31-01-2017 |
| | Dr. B. Wouters | 01-11-2015 | 31-10-2017 |
| PhD students | Ir. K.D.B. Bezemer | 01-10-2015 | 31-03-2017 |
| | F.T. van Beek, MSc. | 01-04-2016 | 31-03-2020 |
| | A.R. Garcia Cicourel, MSc. | 01-03-2016 | 28-02-2020 |
| | Drs. G. Groeneveld | 01-09-2016 | 31-08-2020 |
| | Drs. B.W.J. Pirok | 01-04-2015 | 30-03-2019 |
| | Drs. H. Cornelisson van de Ven | 01-10-2012 | 30-09-2016 |
| | Drs. M.G.Gerritsen | 01-05-2014 | 30-04-2016 |
| | Drs. A.A.S. Sampat | 01-02-2012 | 31-01-2016 |
| | Drs. M. Woldegebriel | 01-04-2013 | 31-03-2017 |
| | Drs. M.Pacheco Bothelho Mourao | 01-09-2013 | 31-08-2017 |
| | Drs. A.A. Baglai | 01-10-2012 | 30-09-2016 |
| | Drs. Barcaru | 01-04-2013 | 31-03-2017 |
| | L.R. Roca, MSc. | 01-09-2016 | 31-08-2020 |

**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.

**Highlight**




Great progress was made at the interfaces between chemistry and mathematics ("chemometrics") and between chemometrics and forensics ("forensimetrics"). Often in collaboration with the Korteweg-de-Vries Institute for Mathematics (Prof. M. Sjerps). A novel peak-tracking method based on Bayesian statistics has been proposed. The method consists of assigning (*i.e.* tracking) peaks from two GC×GC-FID data sets of the same sample recorded under different conditions. Opposed to traditional (*i.e.* deterministic) peak-tracking algorithms, in which the assignment problem is solved with a unique solution, the proposed algorithm is probabilistic. In other words, the uncertainty of matching two peaks is quantified without excluding other possible candidates, ranking the possible peak assignments regarding their posterior probability. This represents a significant advantage over existing deterministic methods. Two algorithms are presented, the blind-peak-tracking algorithm (BPTA) and the peak-table-matching algorithm (PTMA). The PTMA method was able to assign correctly 78% of a selection of peaks in a GC×GC-FID chromatogram of a diesel sample and proved to be extremely fast. (A. Barcaru, E. Derks and G. Vivó-Truyols, Anal. Chim. Acta 940 (2016) 46-55)

**Dr. Michelle Camenzuli**

- Nominated again for the LCGC Emerging Scientist Award for my contributions to LC column technology and 2DLC
- Successfully obtained EU (ERC-ADG-2015) funding as a co-applicant for STAMP: Separation Technology for A Million Peaks (2499k€)
- PhD candidate/student has commenced research within the STAMP project under my supervision (Liana Roca)
- Three invitations to publish in a peer-reviewed journal and a popular analytical chemistry magazine

Top-3 key publications

1. A. Astefanei, I. Dapic, M. Camenzuli, Different stationary phase selectivities and morphologies for Intact Protein Separations, Chromatographia (2016). doi:10.1007/s10337-016-3168-z.
2. F. Canals, F. Elortza, A. Paradela, G.L. Corthals, M. Camenzuli, The EuPA Standardization Initiative, EuPA Open Proteomics, 11 (2016) 31-32
3. A. Jones, S. Pravadali-Cekic, S. Hua, D. Kocic, M. Camenzuli, G. Dennis, R.A. Shalliker, Post column derivatization using reaction flow high performance liquid chromatography columns, JoVE, 110 (2016) e53462

**Dissertation**

30-06-2016 Martin Lopatka (prof.dr. M.J. Sjerps, dr. G. Vivo Truyols)
administrated at Korteweg de Vries institute UvA

**Grants**

Title Chemistry of Light-Induced Degradation (COLD)
Applicants prof.dr. Peter Schoenmakers, prof.dr. Maarten van Bommel

| | |
|---|---|
| Partner | Unilever |
| Grant from | TKI Chemie, TKI Toeslag |
| Amount | k€ 40 |

| | |
|---|---|
| Title | Separation Technology for A Million Peaks (STAMP) |
| Applicant | prof.dr. Peter Schoenmakers |
| Grant from | ERC Advanced Grant |
| Amount | k€ 2,500 |

| | |
|---|---|
| Title | HOSAna |
| Applicant | Prof.dr. Peter Schoenmakers, prof.dr. Govert Somsen (VU) |
| Partners | VU, DSM, Postnova, Bruker |
| Grant from | NWO / PTA-COAST |
| Amount | k€ 557 (1 PhD student for HIMS) |

| | |
|---|---|
| Title | Gamification of participatory science for training and education purposes -GAPARS |
| Applicant | Prof.dr. Garry Corthals |
| Partners | Consortium of eight European research institutes and companies |
| Grant from | EU - H2020 |
| Amount | k€ 240 |

**Prizes**

| | |
|---|---|
| Fleur van Beek | Poster prize at national chemistry conference CHAINS |
| Bert Wouters | 2016 Solvay Prize for his PhD research on groundbreaking research on the development of a microfluidic chip for spatial three-dimensional liquid chromatography. |

**Patents and utilization**

| | |
|---|---|
| Topic | Reflectron Modulation Interface (ReMI) - Making the incompatible compatible in analytical chemistry |
| Staff member | H. Cornelisson van de Ven M.Sc. |
| Activities | Finalist of Amsterdam Science & Innovation Award 2016. As follow up several discussions with companies that may be interested to apply the technology. |

| | |
|---|---|
| Topic | A handheld device for the diagnosis of tuberculosis (AMSIA finalist) |
| Staff member | Dr. A. Kolk and M. Mourao M.Sc. |
| Activities | Finalist of Amsterdam Science & Innovation Award 2016. As follow up several discussions with companies that may be interested to apply the technology. |

**Joint publications**

1. F. Canals, F. Elortza, A. Paradela**, G.L. Corthals**, **M. Camenzuli**, The EuPA Standardization Initiative, EuPA Open Proteomics, 11 (2016) 31-32

# 3. Evaluation

After the mid-term evaluation in 2013, there were only light assessments by the Scientific Advisory Board (WAR) of HIMS in the years after. The committee gathered 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>The Composition of the WAR ultimo 2016 is:</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. Floris Rutjes, Radboud University
Prof. dr. Michel Nielen, Wageningen University

# 4. Valorisation

HIMS researchers explore a wide range of subjects; from pure basic scientific inspired quests to application inspired fundamental research projects. HIMS received funding for 15 research proposals (see section 1.4.4). As much as 13 of these projects were inspired by future applications and 9 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 2016 four 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. In general the institute does not apply for patents for exploration by itself.


On 28 October 2016, HIMS organised together with Innovation Lab Chemistry Amsterdam (ILCA) and the Amsterdam Green Campus the Amsterdam Chemistry Innovation Day (ACID 2016). About 60 representatives from companies (from Amsterdam SMEs to multinationals) and academic groups gathered at the HIMS laboratories. The day started with an inspiring lecture by Mike Dingemans, Director New Business R&D at FUJIFILM Manufacturing Europe. PhD students and postdocs of HIMS took the opportunity to meet potential employers outside academia and interactive workshops and a poster session were used to discuss opportunities for research collaborations. The RPA Sustainable Chemistry discussed valorisation and possibilities for cooperation with its Industrial Advisory Board on 28 October 2016 too.

ACID illustrates the growing collaboration between HIMS and ILCA. 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 2016 HIMS published its analytical infrastructure online to make it better accessible to ILCA members and other companies. Via ILCA HIMS became member of the Amsterdam Chemie Café where chemists from the Metropolitan area.

Together with ACE Venture Lab an intensive Sustainable Chemistry bootcamp week was organised in November 2016. The jury was pleasantly surprised by the quality and viability of the proposals and decided to award *Simon Mathew, Marissa de Boer and Monalisa Goswami each* financial support and mentoring during the start-up of their chemistry-based businesses.

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 trains (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.

**Patents and utilization**

| | |
|---|---|
| Topic | Catalysts and Processes for Producing Aldehydes |
| Staff members | Prof.dr. Joost Reek, together with dr. Xiaowu Wang and dr. Jody Rodgers (Eastman). |
| Activities | Patent filed on June 24, 2016 by Eastman |

| | |
|---|---|
| Topic | Redox self-sufficient biocatalytic amination of alcohols |
| Staff members | Dr. F. Mutti and dr. T. Knaus |
| Activities | Patent application filed by BASF: PCT Int. Appl. (2016), WO 2016001362 A1 20160107; Eur. Pat. Appl. (2016), EP 2963121 A1 20160106. |

| | |
|---|---|
| Topic | Reflectron Modulation Interface (ReMI) - Making the incompatible compatible in analytical chemistry |
| Staff member | H. Cornelisson van de Ven M.Sc. |
| Activities | Finalist of Amsterdam Science & Innovation Award 2016. As follow up several discussions with companies that may be interested to apply the technology. |

| | |
|---|---|
| Topic | A handheld device for the diagnosis of tuberculosis (AMSIA finalist) |
| Staff member | Dr. A. Kolk and M. Mourao M.Sc. |
| Activities | Finalist of Amsterdam Science & Innovation Award 2016. As follow up several discussions with companies that may be interested to apply the technology. |

| | |
|---|---|
| Topic | A novel porous material in supercapacitors |
| Staff members | Dr. D. Eisenberg, Prof.dr. G. Rothenberg |
| Activities | Applied for patent: Eur. Pat. Appl. (2016) EP16171357,05. |

| | |
|---|---|
| Topic | Special funnel |
| Staff member | Dr. T.J. Mooibroek |
| Activities | Patentability checked upon invention. |

| | |
|---|---|
| Topic | ExSPect |
| Staff member | M. Goswami M.Sc. |
| Activities | Winner of ACE Venture lab Sustainable chemistry bootcamp. Investigation of possibilities for spin-off company that focusses on spectroscopy tools for third parties. |

| | |
|---|---|
| Topic | Dye-sensitized solar cells |
| Staff member | Dr. S. Mathew |
| Activities | Winner of ACE Venture lab Sustainable chemistry bootcamp. Investigation of possibilities for spin-off company that focusses on synthesis of dyes for coloured solar cells. |

| | |
|---|---|
| Topic | Multicyclic CLIPS Peptides |
| Staff Members | Prof.dr. JH. van Maarseveen, Drs. G. Richelle, Drs. D. Streefkerk, Prof.dr. P. Timmerman |
| Activities | Applied for patent. |

| | |
|---|---|
| Topic | Efficient conversion of $CO_2$ to CO |
| Staff Members | Dr. N.R. Shiju, Dr. E. Solomon Raja |
| Activities | Preparations for patent application. |

| | |
|---|---|
| Topic: | New carbon-based materials for advanced chromatography. |
| Staff members: | Prof.dr. G. Rothenberg, S. Koot , Dr. M. Camenzuli |
| Activities: | Preparations for patent application on invention of new column material. |

| | |
|---|---|
| Topic: | Cyanide removal from industrial wastewater streams |
| Staff members: | Dr. N.R. Shiju, prof.dr. G. Rothenberg. |
| Activities: | Industrial pilot plant under construction with partners. |

# 5. Organisation

In 2016 prof.dr. Joost Reek was scientific director of the institute. The leaders of the four HIMS themes and education are represented in management team. Until 31 December 2016 the management team consists of:

Prof.dr. Joost Reek (chair)
Drs. Marcel Bartels (institute manager)
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 2016 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 2016 (from left to right on the picture):
Dongdong Zhang (Molecular Photonics)
Marta Pacheco Botelho Mourao (Analytical Chemistry)
Ambuj Tiwari (Computational Chemistry)
Sandra Nurttila (Sustainable Chemistry)

The council has undertaken the following activities in 2016:

- Contribution to the HIMS PhD-brochure
- Feedback at several MT meetings on the subject of courses, evaluations and the PhD track
- Organisation of social activities for HIMS PhDs and postdocs
- Initiated the discussion on work pressure within 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. Currently Prof.dr. Wybren Jan Buma (HIMS, UvA) is the scientific director. The research school was accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW) and is currently in its fourth accreditation period.

Formally, the HRSMC comprises research groups of the University of Amsterdam (UvA), VU University (VU) and Leiden University (UL). In 2016, two research groups of the Radboud University (RU) became an (unofficial) *associated* member upon their request. 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. 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 2016, the HRSMC has granted one proposal for PhD research written by MSc chemistry student Tessel Bouwens (appointed at the UvA).
Furthermore, in 2016 nine applications were awarded within the HRSMC Fellowship Programme. This programme 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 2016**

- The annual HRSMC symposium for all UvA, VU, UL and RU HRSMC members, organized at Leiden University (17 November 2016; attended by ca. 190 scientists). At this symposium, the annual Dick Stufkens prize for the best thesis within the HRSMC was awarded to Dr. Lando Wolters.
- The two weeks HRSMC Course *'Molecular Simulation'*, organized under the auspices of CECAM (4-15 January 2016, UvA)
- The HRSMC Lab visit at the LaserLaB VU for the UvA/UL groups (22 April 2016)
- The HRSMC Course *'Molecular Modeling'* (6-17 June, 2016, VU)
- The HRSMC introduction meeting for new PhD members of the HRSMC (10 June 2016, VU)
- The HRSMC social activity for all PhD members and postdocs of the HRSMC (10 June 2016)

- The HRSMC Summer School *'Photochemistry, Fundamentals and Applications'* (27 – 31 August, 2016, Kasteel Vaeshartel, Maastricht)
- The HRSMC – HIMS Sustainability workshop (23 September 2016, Amsterdam, WCW)

### 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.

### 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). Named after the Amsterdam pioneer in forensic science, 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 2016 the center welcomed Amsterdam University of Applied Sciences (HvA) as its first primary partner and the Engineering faculty of Delft University of Technology (3mE, TU Delft) as it first secondary partner.

In 2013-2016 a total of 11 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 40 PhD students published 200+ peer reviewed publications in forensic science together with their supervisors in the various FNWI institutes and AMC and NFI teams. Currently within the realm of the CLHC 8 special chairs in forensic science have been realized in the areas of forensic statistics and mathematics, forensic data science, forensic biophysics, forensic biology, forensic radiology, forensic medicine, forensic analytical chemistry and criminalistics. On June 1st 2016 prof dr Christianne de Poot was appointed on a special chair in criminalistics at VU university and on September 22nd prof Udo (forensic medicine, AMC/GGD) gave his inaugural speech.


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 of Forensic Science. In 2016 in total 4 Frontiers sessions were organized respectively on forensic biometrics (March 11, Science Park, UvA), forensic statistics and criminalistics (June 10, Science Park), epigenetics (September 23, O2 building, VU) and explosives (November 25, Science Park). The sessions were well attended (80+) by the students but also by scientists, forensic experts and legal representatives from the Dutch criminal justice system. Invited speakers included prof Bruce McCord from Florida International University, prof Didier Meuwly from Twente University/NFI, prof Charles Berger from Leiden University/NFI, prof van der Heijden from Delft University/TNO and prof Miranda de Meijer from the faculty of Law of the UvA and the Public Prosecution Office. CLHC scientists and PhD students provided 4 presentations during the sessions. The CLHC organizes an annual forensic PhD symposium at CWI's conference center at Science Park. The 2016 session was organized on October 28, was well attended (100+) and focused on the value of interdisciplinary collaboration in forensic science.

Although the CLHC is an FNWI-AMC-NFI-HvA 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 were involved in forensic science as part of their broader 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. Within HIMS in 2016 in total 2 PhD students were fully (FEXIN and COMFOR project) and 2 PhD students were partly (Chromametrics project) involved in forensic research. HIMS associated scientists and forensic professors published in total 16 forensic publications in peer reviewed international scientific journals. In 2016 for the first time two project submissions were completed within the H2020 program of the EU (Secure Societies and Marie Curie Individual Fellowships).

In 2017 the main priority of the CLHC is to further develop itself as an internationally recognized forensic science center including internationally funded projects, international collaborations with academic institutes, forensic laboratories and police forces and international student exchange programs. To this end the CLHC will present its bid to host the IAFS (International Association of Forensic Sciences) conference of 2020 in Amsterdam.

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.

# 6. Facts and figures

## 6.1 Personnel

The following tables total the complete HIMS staff as full time equivalents (fte) per employment type. The first table per research group, the second per research theme.

Research- and supporting staff 2016 of HIMS and the HIMS groups, per employment type (fte)[a]

| HIMS Groups | GC | PS | PI | PB | EJM | FB | WJB | FM | GR | JR | MT | JvM | Other | Total |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Tenured staff | 1,0 | 3,2 | 1,0 | 3,0 | 3,0 | 1,6 | 3,0 | | 3,0 | 3,0 | 1,0 | 2,8 | 0,7 | 26,3 |
| Non-tenured staff | 3,0 | 1,1 | 2,0 | 0,9 | 1,6 | | 5,0 | 2,0 | 4,4 | 7,4 | 1,8 | 2,7 | | 31,9 |
| PhD candidates | | 9,2 | 2,1 | 4,2 | 2,0 | 2,0 | 5,4 | 3,9 | 4,5 | 20,8 | 2,9 | 3,9 | | 61,0 |
| **Total research staff** | **4,0** | **13,5** | **5,1** | **8,1** | **6,7** | **3,6** | **13,4** | **5,9** | **12,0** | **31,2** | **5,7** | **9,4** | **0,7** | **119,2** |
| Technicians [b] | 1,0 | 2,4 | | | | 2,0 | 0,9 | 0,9 | 2,0 | 2,8 | 0,8 | 3,0 | 1,0 | 16,8 |
| Visiting fellows [c] | | | | | 0,3 | | | 0,7 | | 0,3 | | | | 1,3 |
| **Total research** | **5,0** | **15,8** | **5,1** | **8,1** | **7,0** | **5,6** | **14,3** | **7,5** | **14,0** | **34,3** | **6,6** | **12,4** | **1,7** | **137,4** |
| Supporting staff | | | | | | | | | | | 0,0 | 0,0 | 5,9 | 5,9 |
| **Total staff** | **5,0** | **15,8** | **5,1** | **8,1** | **7,0** | **5,6** | **14,3** | **7,5** | **14,0** | **34,3** | **6,6** | **12,4** | **7,6** | **143,3** |

Research groups: GC = group Corthals; PS = group Schoenmakers; PI: group Iedema; PB = group Bolhuis; EJM = group Meijer; FB: group Brouwer WJB = group Buma/Woutersen; FM = group Mutti; GR = group Rothenberg; JR = group Reek/de Bruin; MT = group Tromp; JVM = group Van Maarseveen/Hiemstra; Other = Elsevier who focusses only on education, from September 2016 onwards.

| HIMS Themes | AC | CC | MP | SC | Other | Total |
|---|---|---|---|---|---|---|
| Tenured staff | 4,2 | 7,0 | 4,6 | 9,8 | 0,7 | 26,3 |
| Non-tenured staff | 4,1 | 4,5 | 5,0 | 18,3 | | 31,9 |
| PhD candidates | 9,2 | 8,4 | 7,4 | 36,1 | | 61,0 |
| **Total research staff** | **17,5** | **19,9** | **17,0** | **64,2** | **0,7** | **119,2** |
| Technicians [b] | 3,4 | | 2,9 | 9,6 | 1,0 | 16,8 |
| Visiting fellows [c] | | 0,3 | | 1,0 | | 1,3 |
| **Total research** | **20,8** | **20,2** | **19,9** | **74,7** | **1,7** | **137,4** |
| Supporting staff | | | | | 5,9 | 5,9 |
| **Total staff** | **20,8** | **20,2** | **19,9** | **74,7** | **7,6** | **143,3** |

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Sustainable Chemistry.

In the following table the research input of the HIMS staff members (net time available for research) is presented as full time equivalents (fte) per employment type. Since these numbers exclude education activities the total does not amount to the above mentioned total amount of HIMS employees. The numbers are based on an input of 0.5 fte per fte tenured staff, 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.

| HIMS Themes | AC | CC | MP | SC | Other | Total |
|---|---|---|---|---|---|---|
| Tenured staff | 2,1 | 3,5 | 2,3 | 4,9 | 0,3 | 13,1 |
| Non-tenured staff | 3,7 | 4,1 | 4,5 | 16,5 | | 28,7 |
| PhD candidates | 6,9 | 6,3 | 5,6 | 27,1 | | 45,8 |
| **Total research staff** | **12,7** | **13,9** | **12,3** | **48,5** | **0,3** | **87,6** |
| Technicians | 3,4 | | 2,9 | 9,6 | 1,0 | 16,8 |
| Visiting fellows | | 0,2 | | 0,5 | | 0,6 |
| **Total research** | **16,0** | **14,0** | **15,2** | **58,5** | **1,3** | **105,1** |
| Supporting staff | | | | | 5,9 | 5,9 |
| **Total staff** | **16,0** | **14,0** | **15,2** | **58,5** | **7,3** | **111,0** |

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Sustainable Chemistry.

## 6.2 Research

### 6.2.1 Research input of the HIMS themes

The HIMS institute is financed via different funding streams: Direct funding (*eerste geldstroom*) is the funding HIMS receives from the university to cover to main costs for permanent staff, support, building and overheads. The RPA Sustainable Chemistry is also funded by this channel. The university may grant strategic project funding. The most research grants (*tweede geldstroom*) are funded by national or European funding or research agencies like NWO, FOM, STW and KNAW. A third funding component is contract research (*derde geldstroom*), directly paid by companies, governments, European Research Council or other third parties.
Last but not least HIMS welcomes a group of guest researchers. These are usually PhD students with a scholarship (*bursalen*) or senior researchers employed elsewhere having a sabbatical. The tables below give an insight in the distribution of funds and the funding of staff salaries.

Research- and supporting staff 2016 of HIMS per funding type (fte)

| **HIMS Themes** | **Research** | | | | | **Total** | **%** | **Support** | **Total** | **%** |
|---|---|---|---|---|---|---|---|---|---|---|
| | AC | CC | MP | SC | Other | | | | | |
| Direct funding | 6.7 | 7.8 | 4.6 | 16.9 | 0.7 | 36.7 | 30% | 22.6 | 59.3 | 41% |
| Research grants | 7.8 | 10.5 | 8.9 | 27.5 | - | 54.7 | 45% | | 54.7 | 38% |
| Contract research | 2.2 | 1.5 | 2.0 | 14.3 | - | 20.0 | 17% | 0.1 | 20.1 | 14% |
| Other | 0.8 | 0.3 | 1.5 | 6.5 | - | 9.1 | 8% | | 9.1 | 6% |
| **Total** | **17.5** | **20.2** | **17.0** | **65.2** | **0.7** | **120.6** | **100%** | **22.7** | **143.3** | **100%** |

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Sustainable Chemistry.

| **HIMS Groups** | GC | PS | PI | PB | EJM | FB | WJB | FM | GR | JR | MT | JvM | Other | **Total** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Direct funding | 4.0 | 2.7 | 1.0 | 3.0 | 3.8 | 1.6 | 3.0 | 1.2 | 5.8 | 5.4 | 1.7 | 2.8 | 0.7 | 36.7 |
| Research grants | - | 7.8 | 4.1 | 3.6 | 2.8 | 1.0 | 7.9 | 0.9 | 2.5 | 14. | 3.8 | 6.3 | - | 54.7 |
| Contract research | - | 2.2 | - | 1.5 | - | - | 2.0 | 3.8 | 0.6 | 9.7 | 0.2 | - | - | 20.0 |
| Other | - | 0.8 | - | - | 0.3 | 1.0 | 0.5 | 0.7 | 3.0 | 2.5 | - | 0.3 | - | 9.1 |
| **Total** | **4.0** | **13.5** | **5.1** | **8.1** | **6.9** | **3.6** | **13.4** | **6.6** | **11.9** | **31.5** | **5.7** | **9.4** | **0.7** | **120.6** |

Research groups: GC = group Corthals; PS = group Schoenmakers; PI: group Iedema; PB = group Bolhuis; EJM = group Meijer; FB: group Brouwer WJB = group Buma/Woutersen; FM = group Mutti; GR = group Rothenberg; JR = group Reek/de Bruin; MT = group Tromp; JVM = group Van Maarseveen/Hiemstra; Other = Elsevier who focusses only on education, from September 2016 onwards.

Externally financed projects acquired in 2016 (mln €) per funding type

| **HIMS themes** | AC | CC | MP | SC | Other | **Total [1]** |
|---|---|---|---|---|---|---|
| Direct funding | 0.00 | 0.00 | 0.00 | 0.25 | 0.00 | **0.25** |
| Research grants | 0.11 | 0.09 | 0.43 | 2.30 | 0.00 | **2.93** |
| Contract research | 2.74 | 0.01 | 0.05 | 0.41 | 0.00 | **3.22** |
| **Total** | **2.85** | **0.11** | **0.48** | **2.96** | **0.00** | **6.40** |

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Sustainable Chemistry.

| **HIMS Groups** | GC | PS | PI | PB | EJM | FB | WJB | FM | GR | JR | MT | JvM | Other | **Total [1]** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Direct funding | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.25 | 0.00 | 0.00 | 0.00 | **0.25** |
| Research grants | 0.00 | 0.11 | 0.00 | 0.09 | 0.00 | 0.00 | 0.43 | 0.00 | 0.10 | 1.87 | 0.00 | 0.33 | 0.00 | **2.93** |
| Contract research | 0.24 | 2.50 | 0.00 | 0.00 | 0.01 | 0.00 | 0.05 | 0.00 | 0.12 | 0.03 | 0.00 | 0.27 | 0.00 | **3.22** |
| **Total** | **0.24** | **2.61** | **0.00** | **0.09** | **0.01** | **0.00** | **0.48** | **0.00** | **0.22** | **2.14** | **0.00** | **0.60** | **0.00** | **6.40** |

[1] Budgets were obtained for (in FTE) 14,4 PhD's, 17 PD and 2,5 staff.

## 6.2.2 Research output of the HIMS themes

Research output 2016 per type of publication (source: PURE)

| **HIMS themes** | AC | CC | MP | SC | Other | Joint [1] | **Total** |
|---|---|---|---|---|---|---|---|
| Refereed articles | 41 | 59 | 43 | 91 | | -14 | 220 |
| Non-refereed articles | | | | | | | |
| Books | | | | | | | |
| Book chapters | | | 1 | 4 | | | 5 |
| PhD-theses | 1 | 2 | 3 | 8 | | | 14 |
| Conference papers | | | | | | | |
| Patents | | | | 4 | | | 4 |
| Professional publications | | | | | | | |
| Publications general public | | | | | | | |
| Other research output | 1 | 12 | | 1 | | | 14 |
| **Total** | **43** | **73** | 47 | **108** | | **-15** | **258** |

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Sustainable Chemistry.

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

Number of refereed articles 2016, in ranges of different impact factor (source: PURE)

| **HIMS themes** | AC | CC | MP | SC | Other | Joint | **Total** |
|---|---|---|---|---|---|---|---|
| >15 | 0 | 5 | 0 | 4 | | -1 | 8 |
| 10-15 | 0 | 4 | 2 | 16 | | -2 | 20 |
| 5-10 | 10 | 14 | 13 | 22 | | -4 | 55 |
| <5 | 31 | 36 | 28 | 49 | | -7 | 137 |
| **Total** | **41** | **59** | **43** | **91** | | **-14** | **220** |

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Sustainable Chemistry.

The institute aims to increase the total of joint publications, since this number measures the joint projects within the institute. On average HIMS produced 8 joint publications in the period 2011 – 2015.

## 6.2.3 Efficiency of the doctoral research path

The following tables show the efficiency of the doctoral research path (period of start appointment 2008-2012; planned PhD defence 2012-2016). Note that these numbers are arranged per starting date of the PhD students, while the figure in paragraph 1.4.5 counts the length of the PhD tracks based on PhD defences in each year.

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** |
| **Analytical Chemistry (AC)** | | | | | | | | | | | |
| **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 |
| **2012** | 2 | 2 | **4** | 0 | 1 | 0 | 0 | 0 | 0 | 3 | 0 |
| **Total** | **5** | **9** | **14** | **1** | **4** | **0** | **1** | **0** | **0** | **5** | **3** |
| **%** | **36** | **64** | **100** | **7** | **29** | **0** | **7** | **0** | **0** | **36** | **21** |
| **Computational Chemistry (CC)** | | | | | | | | | | | |
| **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** | 4 | 1 | **5** | 0 | 2 | 2 | 0 | 0 | 0 | 1 | 0 |
| **2011** | 3 | 0 | **3** | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 2 |
| **2012** | 3 | 1 | **4** | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 1 |
| **Total** | **11** | **6** | **17** | **1** | **5** | **3** | **2** | **0** | **0** | **2** | **4** |
| **%** | **65** | **35** | **100** | **6** | **29** | **18** | **12** | **0** | **0** | **12** | **24** |
| **Molecular Photonics (MP)** | | | | | | | | | | | |
| **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** | 3 | 2 | **5** | 1 | 1 | 1 | 0 | 0 | 0 | 1 | 1 |
| **2012** | 3 | 2 | **5** | 0 | 3 | 0 | 0 | 0 | 0 | 2 | 0 |
| **Total** | **14** | **8** | **22** | **1** | **6** | **6** | **0** | **0** | **4** | **3** | **2** |
| **%** | **64** | **36** | **100** | **5** | **27** | **27** | **0** | **0** | **18** | **14** | **9** |
| **Sustainable Chemistry (SC)** | | | | | | | | | | | |
| **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 | 3 | 3 | 0 | 0 | 0 | 0 | 0 |
| **2012** | 6 | 2 | **8** | 0 | 5 | 0 | 0 | 0 | 0 | 3 | 0 |
| **total** | **21** | **17** | **38** | **1** | **20** | **9** | **1** | **0** | **0** | **3** | **4** |
| **%** | **55** | **45** | **100** | **3** | **53** | **24** | **3** | **0** | **0** | **8** | **11** |

## 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** |
| **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 | 7 | 0 | 0 | 3 | 1 | 1 |
| **2011** | 11 | 10 | **21** | 3 | 6 | 4 | 0 | 0 | 0 | 4 | 4 |
| **2012** | 14 | 7 | **21** | 1 | 11 | 0 | 0 | 0 | 0 | 8 | 1 |
| **Total** | **51** | **40** | **91** | **4** | **35** | **18** | **4** | **0** | **4** | **13** | **13** |
| **Cumulative per theme 2008-2012** | | | | | | | | | | | |
| **AC** | 5 | 9 | **14** | 1 | 4 | 0 | 1 | 0 | 0 | 5 | 3 |
| **CC** | 11 | 6 | **17** | 1 | 5 | 3 | 2 | 0 | 0 | 2 | 4 |
| **MP** | 14 | 8 | **22** | 1 | 6 | 6 | 0 | 0 | 4 | 3 | 2 |
| **SC** | 21 | 17 | **38** | 1 | 20 | 9 | 1 | 0 | 0 | 3 | 4 |
| **Total** | **51** | **40** | **91** | **4** | **35** | **18** | **4** | **0** | **4** | **13** | **13** |
| ***%*** | **56** | **44** | **100** | **4** | **38** | **20** | **4** | **0** | **4** | **14** | **14** |

## 6.3 Finance 2016

The table below shows the HIMS financial result 2016. The HIMS institute is financed via different funding streams: Direct funding (*eerste geldstroom*) is the funding HIMS receives from the university to cover to main costs for permanent staff, support, building and overheads. The RPA Sustainable Chemistry is also funded by this channel. The university may grant strategic project funding. The most Research grants (*tweede geldstroom*) are funded by national or European funding or research agencies like NWO, FOM, STW and KNAW. A third funding component is Contract research (*derde geldstroom*), directly paid by companies, governments, European Research Council or other third parties.

Last but not least HIMS welcomes a group of guest researchers. These are usually PhD students with a scholarship (bursalen) or senior researchers employed elsewhere having a sabbatical. The tables below give an insight in the distribution of funds and the funding of staff salaries.

HIMS result 2016 (k€)

| | Direct | Research grants | Contract research | Total |
|---|---|---|---|---|
| **HIMS Budget** | | | | |
| Budget (fixed) | 3.986 | - | - | **3.986** |
| Budget (variable[1]) | 5.842 | 3.364 | 1.925 | **11.131** |
| Other income [2] | 335 | - | - | **335** |
| Matching contract research | -3.853 | 2.994 | 859 | **0** |
| **Budget total** | **6.310** | **6.358** | **2.784** | **15.452** |
| ***Percentage*** | ***41*** | ***41*** | ***18*** | ***100*** |
| **HIMS Costs** | | | | |
| Personal costs | -4.143 | -2.342 | -1.184 | **-7.669** |
| Other costs (projects) | -2.081 | -948 | -550 | **-3.578** |
| Overhead (central) | 743 | -542 | -201 | **0** |
| Overhead (faculty) | -972 | -1.197 | - 454 | **-2.623** |
| Overhead (institute) | 1.827 | -1.330 | - 497 | **0** |
| Various costs | - | - | - | **-** |
| Other (secundary) costs | -1.597 | - | - | **-1.597** |
| **Costs total** | **-6.223** | **-6.359** | **-2.886** | **-15.468** |
| ***Percentage*** | ***40*** | ***41*** | ***19*** | ***100*** |
| | | | | |
| **HIMS Result 2016** | ***87*** | **-1** | **-102** | **-16** |
| Reservations[3] | 328 | - | - | 328 |
| **Result inclusive reservations** | **415** | **-1** | **-102** | **312** |

[1] Direct funding assigned via allocation model (incl. matching on project funding, *SectorPlan*, RPA Sustainable Chemistry)
[2] Contributions for HRSMC and CLHC.
[3] From reservations (incl. *SectorPlan* and RPA Sustainable Chemistry).

The HIMS result for 2016 amounts to +312k€. This result includes the spending of 328 k€ from reserved budgets. These concern reservations from past budgets for costs in the framework of the *Sectorplan Natuur- en Scheikunde* and the RPA Sustainable Chemistry.