



# Annual Report 2018

*Chemistry  
research  
that matters*

Van 't Hoff Institute  
for Molecular Sciences

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Van 't Hoff Institute for Molecular Sciences  
P.O. Box 94157, 1090 GD Amsterdam  
Science Park 904, 1098 XH Amsterdam  
The Netherlands

Phone: +31 20 525 5265

Website: [hims.uva.nl](https://hims.uva.nl)

## Executive summary

The year 2018 was a special year; many new projects were acquired and we underpinned our international position with appealing publications in renowned scientific journals. With the Dutch national coordinator Prof. Bert Meijer, HIMS contributed to the national 'Sectorbeeld' of academic science and engineering research. This overview of focus areas is the basis for a request for additional funds from the Dutch government.

The HIMS annual report 2018 showcases many scientific highlights and key publications. Below some highlights are spotlighted.



*HIMS director Prof. Peter Schoenmakers.*

HIMS welcomed new academic staff. Dr Andrew Jupp and Dr Joen Hermans came with their personal Veni-grant. Prof. Arian van Asten expanded his part-time professorship to a full-time appointment on a chair sponsored by the Netherlands Forensic Institute (NFI) and Dr Katrien Keune started as part-time Associate Professor next to her appointment as head of research at the Rijksmuseum. Other staff made successful moves outside our institute. We are proud that Dr Moniek Tromp was appointed as full professor at Groningen University and Dr Michelle Camenzuli accepted an

offer at a UK-based pharmaceutical company. Prof. Henk Hiemstra and Dr Wim Kok retired after successful careers at HIMS. Dr Colet te Grotenhuis was awarded an NWO Rubicon grant to work at MIT.

### Education

HIMS staff is involved in the joint degree chemistry bachelor and master programs together with VU University and in other programs that involve molecular aspects. Within the framework of origins of life, HIMS contributed actively to the new honours course 'How to build an alien', with lectures on life sciences, astronomy, ecology, and chemistry.

### Valorisation

In 2018 many new public-private research projects were granted. Among others, the new CBBC-membership led to three PhD projects. Partners in all new PPP's are Avantium, Lego, Merck, DSM, AkzoNobel, BASF, Shell, Booking.com and an international consortium with Biolitec Research, Germany; Selvita, Poland; PorphyChem, France and BET-Solutions, Greece. Furthermore, new collaborations started with Amsterdam UMC and the Rijksmuseum.

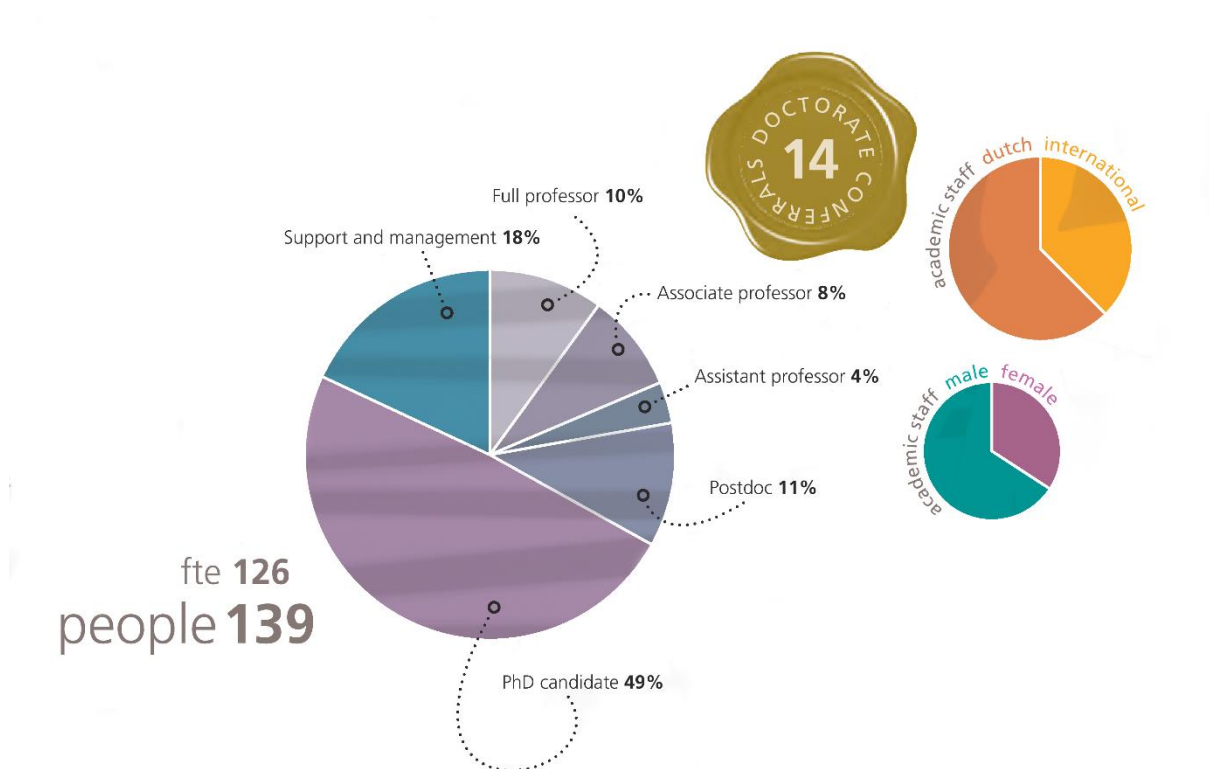
After an incubation project funded by the research priority Area Sustainable Chemistry, in May a spin-off company Spark904, led by former HIMS PhD student Dr Monalisa Goswami was launched at the Startup Village at Amsterdam Science Park. Spark904 provides access to the state-of-the-art and routine analysis equipment of universities and premier institutes, for outsider scientists who so far had no access - at least not on a day-to-day basis.

The Royal Association of the Dutch Chemical Industry VNCI celebrated its 100<sup>th</sup> anniversary together with HIMS in a joint event at Amsterdam Science Park on 19 October that attracted 180 participants,

ranging from students to researchers and captains of industry. VNCI chairman Bernard Wientjes concluded by emphasizing the importance of chemistry for the sustainability of our society and the transition to a circular economy.

A team of computational chemists including HIMS' David Dubbeldam launched a freely available, sophisticated app for molecular visualizations. iRASPA is a visualization package with editing capabilities aimed at materials science. It produces high-quality images of complex molecules, metals, metal oxides, ceramics, biomaterials, zeolites, clays, and metal-organic frameworks. A commenter in the app store writes: 'A must-have for any scientist working with porous materials.'

### **HIMS at a glance:**

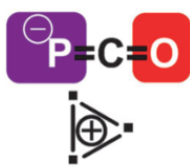


*(more data in the Facts & Figures section of this annual report)*



## Scientific Highlights

### Towards pericyclic organophosphorus chemistry - 29 January 2018



Organic chemists at the group of Dr Chris Slootweg have successfully expanded the field of pericyclic organophosphorus chemistry for the development of sustainable synthetic procedures. They reported in *Angewandte Chemie* on the synthesis of the phosphorus analogues of cyclopentadienone, tricyclopentanone, and housene that have the potential to be used as building blocks for novel catalysts.

T. Krachko, A. W. Ehlers, M. Nieger, M. Lutz, J. C. Slootweg: *Synthesis and Reactivity of the Phosphorus Analogues of Cyclopentadienone, Tricyclopentanone, and Housene*, *Angew. Chem. Int. Ed.* 2018, 57, 1683. DOI: [10.1002/anie.201711838](https://doi.org/10.1002/anie.201711838)

### Precisely tailoring the dynamics of upconversion luminescence - 31 January 2018



A team of researchers led by Professors Hong Zhang (photonic nanochemistry) and Evert Jan Meijer (computational chemistry) has significantly improved the fundamental understanding of photon upconversion in nanoparticles. Through the collaborative approach of advanced spectroscopy and theoretical modelling they were able to establish that the migration of excitation energy greatly affects the upconversion dynamics. In *Angewandte Chemie* the researchers describe how 'dopant ions spatially separated' (DISS) nanostructures can be used for tailoring the upconversion dynamics.

Jing Zuo, Dapeng Sun, Langping Tu, Yanni Wu, Yinghui Cao, Bin Xue, Youlin Zhang, Yulei Chang, Xiaomin Liu, Xianggui Kong, Wybren Jan Buma, Evert Jan Meijer, and Hong Zhang: *Precisely Tailoring Upconversion Dynamics via Energy Migration in Core-Shell Nanostructures* *Angewandte Chemie International Edition*, accepted 24 January 2018 DOI: [10.1002/anie.201711606](https://doi.org/10.1002/anie.201711606) and [10.1002/ange.201711606](https://doi.org/10.1002/ange.201711606)

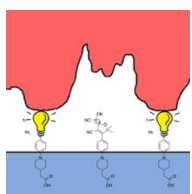
### Amsterdam chemists make bicycle-like molecular drive - 7 February 2018



A team including professors Sander Woutersen and Wybren Jan Buma together with co-workers at the University of Murcia have synthesized molecules that operate like the pedals of a bicycle. Fueled by light, the molecules can be used as molecular switches that pave the way for the design of functional molecular systems effective under severe spatial restrictions.

Saeed Amirjalayer, Alberto Martinez-Cuezva, Jose Berna, Sander Woutersen, and Wybren Jan Buma: *Photo-induced pedalo-type motion in an azodicarboxamide-based molecular switch*. *Angewandte Chemie International Edition*, 2018, 57, 1792; DOI: [10.1002/anie.201709666](https://doi.org/10.1002/anie.201709666)

### Luminescent molecules help reveal new insights in friction - 4 March 2018



The proportionality of friction to normal force, first discovered by Leonardo da Vinci, is nowadays still being used extensively. However, a team of researchers including professor Fred Brouwer show that Da Vinci's relation does not always accurately describe reality. Their results were published in *Nature Communications*.

B. Weber, T. Suhina, T. Junge, L. Pastewka, A. M. Brouwer and D. Bonn: *Molecular probes reveal deviations from Amontons' law in multi-asperity frictional contacts*, *Nature Communications* volume 9, 888 (2018). DOI: [10.1038/s41467-018-02981-y](https://doi.org/10.1038/s41467-018-02981-y)

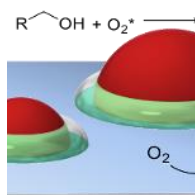
### **Indication of the existence of two kinds of supercooled water** - 10 March 2018



Although predicted already 25 years ago, the existence of two different states of liquid water - at extremely low temperature and high pressure - has never been confirmed experimentally. HIMS researchers together with researchers from Arizona State University have now changed this. In *Science*, they describe how they prevent water from freezing by adding a special type of antifreeze, and how they observed a transition between two different liquid states of water at about 80 degrees C below zero.

Sander Woutersen, Michiel Hilbers, Bernd Ensing, Zhaofeng Zhao & Austen Angell, *A liquid-liquid transition in supercooled aqueous solution related to the HDA-LDA transition*, *Science* 09 Mar 2018, Vol 359, Issue 6380 pp. 1127. DOI:10.1126/science.aao7049

### **UvA chemists shed light on intermediate steps in cascade reactions** - 19 March 2018



PhD student Thierry Slot presents a theoretical concept that describes tandem reactions for active particles on active surfaces. The research, supervised by professor Gadi Rothenberg and part of the university's Research Priority Area Sustainable Chemistry, was published as an open-access concept paper in the international journal *ChemCatChem*.

Cooperative surface-particle catalysis: the role of the "active doughnut" in catalytic oxidation. T.K. Slot, D. Eisenberg and G. Rothenberg, *ChemCatChem*, 2018, *EarlyView*. DOI: [10.1002/cctc.201701819](https://doi.org/10.1002/cctc.201701819)

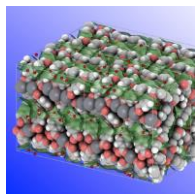
### **Oil paint from the lab offers insight into ageing of Old Masters** - 30 March 2018



A team of chemists of the Rijksmuseum and the Van 't Hoff Institute for Molecular Sciences has uncovered new details about the ageing processes in oil paintings. A specially developed model paint was rapidly aged, while the process was continuously followed with infrared spectroscopy. The experiments showed that 'metal soaps', a class of compounds that are often associated with paint degradation, form rather easily if an oil paint contains free fatty acids. Additionally, the exposure of oil paint to water or organic solvents seems to influence the ageing of paint.

Lambert Baij, Joen J. Hermans, Katrien Keune, Piet Iedema: *Time-Dependent ATR-FTIR Spectroscopic Studies on Fatty Acid Diffusion and the Formation of Metal Soaps in Oil Paint Model Systems*, *Angewandte Chemie*, published online 9 March 2018, DOI [10.1002/anie.201712751](https://doi.org/10.1002/anie.201712751)

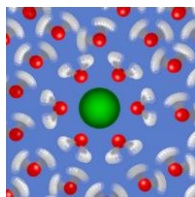
### **Novel, water-stable metal-organic framework for selective CO2 adsorption** - 17 April 2018



Researchers of the Research Priority Area Sustainable Chemistry have developed a novel porous material capable of selectively adsorbing CO<sub>2</sub>. In the journal *Inorganic Chemistry Frontiers* they present their design of a water-stable metal-organic framework (MOF) that according to team leader Dr Stefania Grecea can pave the way to cost-effective separation of CO<sub>2</sub> from power plant emissions.

Selective CO<sub>2</sub> adsorption in water-stable alkaline-earth based metal-organic frameworks. Y. Tang, A. Kourtellaris, A.J. Tasiopoulos, S.J. Teat, D. Dubbeldam, G. Rothenberg and S. Tanase, *Inorg. Chem. Front.*, 2018, 5, 541-549. DOI: [10.1039/C7QI00734E](https://doi.org/10.1039/C7QI00734E)

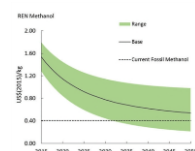
### **Isotope effect reveals non-cooperative water dynamics in salt solutions** - 23 May 2018



Water molecules surrounding ions behave in a much less cooperative way than they do in bulk water. This follows from a study on the isotope-dependent dielectric response of salt solutions, which has just been published in *Physical Review Letters* by researchers from the Amsterdam research institutes HIMS and AMOLF. Their results lead to an update of Nobel-laureate Onsager's 40-year old theory for the response of salt solutions to electric fields, and enables a reliable determination of hydration numbers that play a key role in chemistry and biophysics.

Roberto Cota, Niklas Ottosson, Huib J. Bakker, and Sander Woutersen: *Evidence for Reduced Hydrogen-Bond Cooperativity in Ionic Solvation Shells from Isotope-Dependent Dielectric Relaxation* *Physical Review Letters* 120, 216001 – Published 22 May 2018 DOI: [10.1103/PhysRevLett.120.216001](https://doi.org/10.1103/PhysRevLett.120.216001)

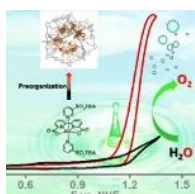
### **Competitive solar fuels within two decades** - 8 July 2018



According to a techno-economic analysis by researchers from the UvA research priority area Sustainable Chemistry and TNO, the industrial synthesis of renewable hydrogen, syngas, methanol and diesel could become competitive with respect to their fossil counterparts within the next two decades.

R. J. Detz, J. N. H. Reek and B. C. C. van der Zwaan: *The future of solar fuels: when could they become competitive?* *Energy & Environmental Science*, DOI: [10.1039/C8EE00111A](https://doi.org/10.1039/C8EE00111A)

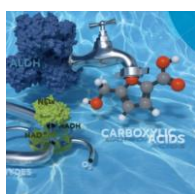
### **Supramolecular nanoconcentrators boost performance of water oxidation catalyst** - 12 July 2018



By applying their 'nanoconcentrator' concept of functionalized self-assembled nanospheres to a ruthenium-based water oxidation catalyst, HIMS researchers have been able to enhance the catalyst's rate by two orders of magnitude. The team led by Professor Joost Reek expects this new strategy to enable more efficient devices for artificial photosynthesis. The results were published by the journal *Angewandte Chemie International Edition*.

Fengshou Yu, David Poole III, Simon Mathew, Ning Yan, Joeri Hessels, Nicole Orth, Ivana Ivanović-Burmazović and Joost N. H. Reek: *Control over Electrochemical Water Oxidation Catalysis by Preorganization of Molecular Ruthenium Catalysts in Self-Assembled Nanospheres*. *Angewandte Chemie International Edition*, accepted. DOI: [10.1002/anie.201805244](https://doi.org/10.1002/anie.201805244)

### **Sustainable and very selective biocatalytic conversion of aldehydes to carboxylic acids** - 30 August



The Biocatalysis research group led by Dr Francesco Mutti has developed the first viable biocatalytic 'green' process for the chemoselective oxidation of aldehydes into carboxylic acids. The paper describing the research was published by the journal *Green Chemistry*.

Knaus, Tanja & Tseliou, Vasilis & D Humphreys, Luke & Scrutton, Nigel & Mutti, Francesco. (2018). *A biocatalytic method for the chemoselective aerobic oxidation of aldehydes to carboxylic acids*. *Green Chemistry*. DOI: [10.1039/C8GC01381K](https://doi.org/10.1039/C8GC01381K)

### **Colourant study offers mechanistic insight in Lewis acid-base coupling** - 17 September 2018



Associate professor Chris Slootweg and co-workers developed the synthesis of a unique set of arylazophosphonium salts with easily tuneable colourant properties. In a publication in *Angewandte Chemie* they report detailed mechanistic studies of the synthesis revealing that simple diazonium salts can be used as N-based Lewis acids in the reaction with phosphine donor ligands. This paves the way for the metal-free functionalisation of dinitrogen.

Evi R. M. Habraken Nicolaas P. van Leest Pim Hooijschuur Prof. Dr. Bas de Bruin Dr. Andreas W. Ehlers Dr. Martin Lutz Assoc. Prof. J. Chris Slootweg: *Aryldiazonium Salts as Nitrogen-Based Lewis Acids: Facile Synthesis of Tuneable Azophosphonium Salts*. *Angewandte Chemie International Edition* Volume 57, Issue 37. DOI: [10.1002/anie.201806913](https://doi.org/10.1002/anie.201806913)

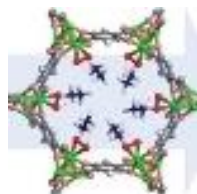
### **Promiscuous enzyme enables efficient and benign synthesis of nitriles** - 28 September 2018



Researchers of the Biocatalysis group discovered an unexpected catalytic promiscuity of the enzyme galactose oxidase. They utilized this to develop a one-pot enzymatic transformation of alcohols into nitriles under mild, cyanide-free conditions. A patent was applied for and their results were published in the renowned journal *Angewandte Chemie*.

Jan Vilím, Tanja Knaus, Francesco Mutti: *Catalytic Promiscuity of Galactose Oxidase: A Mild Synthesis of Nitriles from Alcohols, Air and Ammonia*. *Angewandte Chemie International Edition*. DOI: [10.1002/anie.201809411](https://doi.org/10.1002/anie.201809411)

### **New metal-organic framework for highly efficient separation of ethane from ethylene** - 29 October



Industrial production of ethylene, the key ingredient in the most common form of plastic, requires its separation from ethane in a process that consumes large amounts of energy. An alternative would be differential sorption in microporous materials. In *Science*, a Chinese-American research team presents a metal-organic framework (MOF) that can bind ethane more strongly than ethylene. Professor Rajamani Krishna contributed to the research with calculations and simulations of the MOF performance, demonstrating its potential for the industrial separation of the gases at ambient conditions.

Libo Li, Rui-Biao Lin, Rajamani Krishna, Hao Li, Shengchang Xiang, Hui Wu, Jinping Li, Wei Zhou, Banglin Chen: Ethane/ethylene separation in a metal-organic framework with iron-peroxo sites. *Science* 26 Oct 2018 Vol. 362, Issue 6413, pp. 443-446. DOI: [10.1126/science.aat0586](https://doi.org/10.1126/science.aat0586)

### **Rigid metal-organic framework as a molecular sieve for ethylene** - 9 November 2018



A Chinese-American research team developed an ultra microporous rigid metal-organic framework that can act as a molecular sieve for the separation of ethylene/ethane mixtures. The results were published by *Nature Materials*. Professor Rajamani Krishna contributed to the research with simulations of the MOF performance.

Rui-Biao Lin, Libo Li, Hao-Long Zhou, Hui Wu, Chaohui He, Shun Li, Rajamani Krishna, Jinping Li, Wei Zhou, Banglin Chen: *Molecular sieving of ethylene from ethane using a rigid metal-organic framework*. *Nature Materials* (2018), published online 05 November 2018 DOI: [10.1038/s41563-018-0206-2](https://doi.org/10.1038/s41563-018-0206-2)



**UvA researchers advocate mitigation of stationary NOx emissions in Europe** - 15 November 2018



Working at the Research Priority Area Sustainable Chemistry, MSc student Cedric Koolen and Prof. Gadi Rothenberg have made an analysis of air pollution in Europe. In a concept article published by ChemSusChem they present recommendations for mitigation of the most common pollutants including a cost/benefit analysis. They conclude that mitigation of NOx emissions by the stationary combustion sector (including public heating) would reap the most gains in lifespan and reduction of healthcare costs.

C.D. Koolen and G. Rothenberg, *Air Pollution in Europe*, ChemSusChem, **2018**, published online. Open Access. DOI: [10.1002/cssc.201802292](https://doi.org/10.1002/cssc.201802292)

## Prizes and honours

The quality of HIMS scientists is reflected in the prizes and honours they receive. Noteworthy examples are the Fritz-Pregl Medal for Peter Schoenmakers and the Journal of Chromatography A Young Scientist Award for Bob Pirok. Below is a list of news items reporting on these and other HIMS staff members and students.

### Humboldt Research Fellowship for Chris Slootweg - 1 February 2018



Dr Chris Slootweg, associate professor at the Van 't Hoff Institute for Molecular Sciences, was awarded a Humboldt Research Fellowship for experienced researchers. Organic chemist Slootweg will be a guest researcher at the University of Regensburg (Germany) with professors Manfred Scheer and Robert Wolf.

### Makoto Fujita Winner of Wolf Prize in Chemistry 2018 - 20 February 2018



The 2018 Wolf Foundation Prize for Chemistry was awarded to Makoto Fujita of the University of Tokyo for his achievements in the field of supramolecular chemistry. At the time, Fujita was a visiting professor via the Research Priority Area sustainable chemistry.

### Amsterdam chemistry students excel at national student symposium - 13 March 2018



The 'Young KNCV' poster competition at the national chemistry student 'PAC symposium', held 8 March at Utrecht University, was dominated by students from the joint Master's programme of the two Amsterdam universities (UvA and VU). Wowa Stroek took home the first prize, Stephan Falcao Ferreira was runner-up, and Brendan Horst secured the third prize.

### Veni grants for Joen Hermans and Andrew Jupp - 21 August 2018



Dr Joen Hermans and Dr Andrew Jupp were awarded NWO Veni grants to perform research at the Van 't Hoff Institute for Molecular Sciences. The grants of € 250.000 each provide them with the opportunity to further elaborate their own research ideas over a three-year period.

### Cum Laude for chemistry PhD graduate Gaston Richelle - 4 December 2018



On 30 November 2018 Gaston Richelle of the Synthetic Organic Chemistry group successfully defended his PhD thesis on 'Multicyclic peptides manufactured via scaffold-assisted CLIPS/CuAAC technology'. He received his PhD with the distinction 'cum laude', honouring his novel and original research that resulted in landmark papers and has potential for application in combatting infectious diseases.

## Grants and funding

Below is an overview of news item on grants and funding obtained by HIMS scientists. More on the financial aspects of the institute can be found in the Facts & Figures section of this annual report.

### Funding for HIMS researchers in NWO Mat4Sus programme - 24 January 2018



HIMS researchers received contributions from the NWO 'Materials for Sustainability' programme (Mat4Sus). Mat4Sus encourages interdisciplinary material research to facilitate a smooth transition from fossil fuels to sustainable energy sources. The nature of the projects is both public-private and fundamental.

### New projects in the study and conservation of art - 30 January 2018



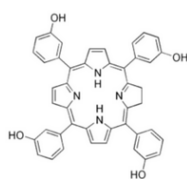
Three new projects involving HIMS researchers Dr Katrien Keune, Dr Moniek Tromp and Prof. Maarten van Bommel obtained funding through the Netherlands Institute for Conservation, Art and Science (NICAS). The focus in this call was on data science.

### Humboldt Research Fellowship for Chris Slootweg - 1 February 2018



Dr Chris Slootweg, associate professor at the Van 't Hoff Institute for Molecular Sciences, was awarded a Humboldt Research Fellowship for experienced researchers. Organic chemist Slootweg will be a guest researcher at the University of Regensburg (Germany) with professors Manfred Scheer and Robert Wolf.

### Light-activated molecules to fight cancer and infection - 12 March 2018



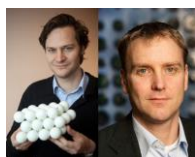
HIMS researchers at the Molecular Photonics group are involved in a new European research project for the optimized design of molecules to fight cancer and infections. A unique feature of the molecules is their activation upon exposure to light, leading to innovative applications in treatments against skin tumours, first-aid bandages and self-sterilising devices.

### Research into sustainable chemistry awarded with 1.2 million euros - 29 June 2018



The Advanced Research Center for Chemical Building Blocks Consortium awarded three research projects to professors Joost Reek and Bas de Bruin. Three new PhD students will be collaborating with industrial partners to investigate the synthesis of catalytic nanoparticles, the photoelectrochemical production of sustainable fuels, and new catalysts for the drying of paint.

**Peter Bolhuis and Peter Schall receive 'NWO Projectruimte' grant** - 25 July 2018



Professors Peter Bolhuis (HIMS) and professor Peter Schall (Institute of Physics) received an NWO 'Projectruimte grant' for research into 'Activating viscoelastic colloidal architectures'. They perform the first systematic studies on active solids towards fundamental insights into biology and novel biomaterials and biomedical applications.

**Veni grants for Joen Hermans and Andrew Jupp** - 21 August 2018



Dr Joen Hermans and Dr Andrew Jupp were awarded NWO Veni grants of € 250.000 each. The grants provide them with the opportunity to further elaborate their own research ideas over a three-year period.

**Colet te Grotenhuis receives NWO Rubicon grant** - 24 August 2018



Dr Colet te Grotenhuis obtained her PhD with professors Bas de Bruin and Joost Reek and subsequently received an NWO Rubicon grant. This provided her with the opportunity to gain international research experience at the Massachusetts Institute of Technology (Cambridge, USA).

**Funding for promising research to improve cold-stress tolerance of plants** - 29 September 2018



Professor Wybren Jan Buma of the Molecular Photonics research group, together with associate professor Teun Munnik of the Swammerdam Institute for Life Sciences, has found a way to improve the resilience of plants to low-temperature stress. The agricultural sector has already expressed its interest. For the further development of their method, the researchers received a grant from the Physics2Market Fund of Innovation Exchange Amsterdam (IXA).

**'Boostcrop' consortium receives millions to increase agricultural and horticultural yields** - 29 October 2018



The European 'Boostcrop' consortium with HIMS professors Wybren Jan Buma and Jos Oomens has been awarded nearly 5 million euros from the European 'Future and Emerging Technologies' programme. Boostcrop aims to increase yields in agri- and horticulture with a new approach based on the development and application of molecular temperature controllers.



**Booking.com supports research into renewable jet fuel from waste** - 18 December 2018



Dr Shiju Raveendran of the UvA's research priority area Sustainable Chemistry has acquired a 150,000 euro grant from Booking.com for research into the manufacture of renewable jet fuel from food waste and other organic residue.

**ECHO grants for HIMS researchers** - 18 December 2018



With the awarding of three ECHO grants, the Netherlands Organisation for Scientific Research (NWO) supported fundamental chemical research at HIMS into signalling molecules, molecular fluorescence, and organic chemistry.

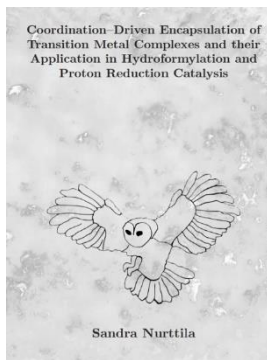
**Sander Woutersen receives 'Physics Projectruimte' grant** - 23 December 2018



Professor Sander Woutersen received funding for his research into supercooled water together with professor Daniel Bonn of the Institute of Physics. The proposal was awarded a grant from the 'Physics Projectruimte' by the NWO Domain Science (ENW).

## Dissertations

In 2018, fourteen students received their PhD at HIMB, one of them - Dr Gaston Richelle - with the distinction cum laude. All theses are listed below; a link is provided to download each thesis from the UvA repository.



19 December 2018

**Coordination-driven encapsulation of transition metal complexes in molecular capsules and their application in hydroformylation and proton reduction catalysis**

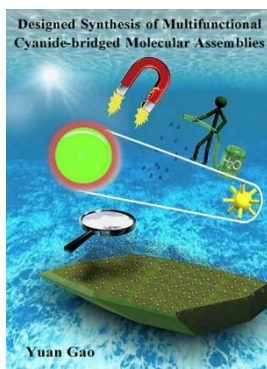
Author: S. (Sandra) S. Nurttala

Promotor: J.N.H. Reek

Co-promotor: T.J. Mooibroek

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

Link: [Read or download this thesis](#)



14 December 2018

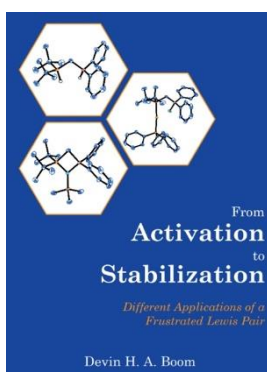
**Designed synthesis of multifunctional cyanide-bridged molecular assemblies**

Author: Y. (Yuan) Gao

Promotor: G. Rothenberg, S. Grecea

Group: Heterogeneous Catalysis and Sustainable Chemistry

Link: [Read or download this thesis](#)



7 December 2018

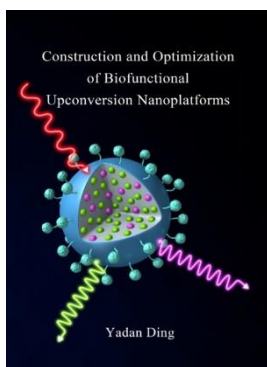
**From activation to stabilization - Different applications of a frustrated Lewis pair**

Author: D. (Devin) H.A. Boom

Promotors: J.C. Slootweg, A.W. Ehlers

Group: Synthetic Organic Chemistry

Link: [Read or download this thesis](#)



6 December 2018

**Construction and Optimization of Biofunctional Upconversion Nanoplatfoms**

Author: Y. (Yadan) Ding

Promotor: W.J. Buma, H. Zhang

Group: Molecular Photonics

Link: [Read or download this thesis](#)



30 November 2018

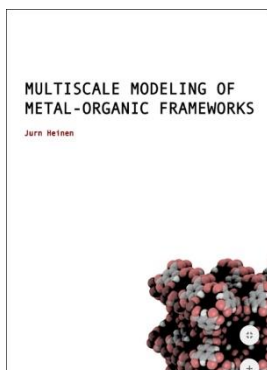
### **Multicyclic peptides manufactured via scaffold-assisted CLIPS/CuAAC technology**

Author: G. (Gaston) J.J. Richelle

Promoters: P. Timmerman, J.H. van Maarseveen

Group: Synthetic Organic Chemistry

Link: [Read or download this thesis](#)



16 October 2018

### **Multiscale modeling of metal-organic frameworks**

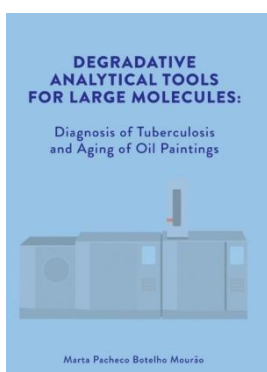
Author: J. (Jurn) Heinen

Promotor: E.J. Meijer

Co-promotor: D. Dubbeldam

Group: Computational Chemistry

Link: [Read or download this thesis](#)



12 October 2018

### **Degradative analytical tools for large molecules: Diagnosis of tuberculosis and aging of oil paintings**

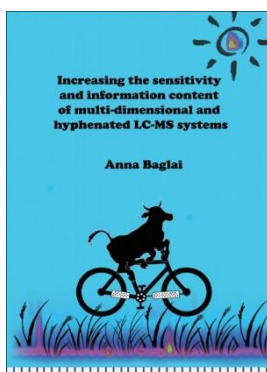
Author: M. (Marta) Pacheco Botelho Mourão

Promoters: J.G.M. Janssen, P. Schoenmakers

Co-promoters: A.H.J. Kolk, W.T. Kok

Group: Analytical Chemistry

Link: [Read or download this thesis](#)



7 September 2018

### **Increasing the sensitivity and information content of multi-dimensional and hyphenated LC-MS systems**

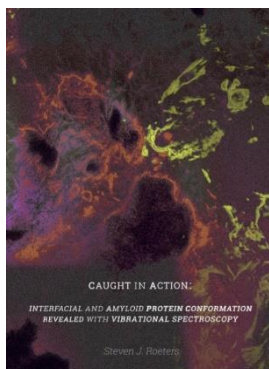
Author: A. (Anna) Baglai

Promotor: P. Schoenmakers

Co-promoters: S. van der Wal

Group: Analytical Chemistry

Link: [Read or download this thesis](#)



5 September 2018

**Caught in action: interfacial and amyloid protein conformation revealed with vibrational spectroscopy**

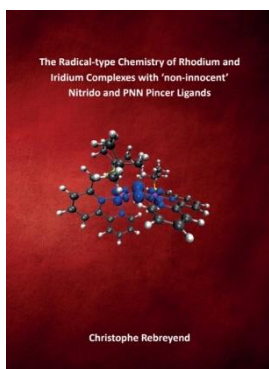
Author: S. (Steven) J. Roeters

Promotor: S. Woutersen

Co-promotors: V. Subramaniam

Group: Molecular Photonics

Link: [Read or download this thesis](#)



22 June 2018

**The radical-type chemistry of rhodium and iridium complexes with 'non-innocent' nitrido and PNN pincer ...**

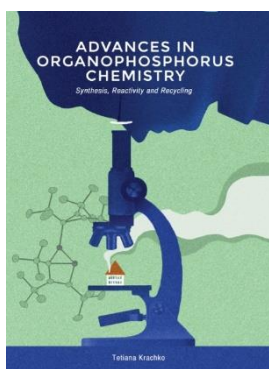
Author: C. (Christophe) Rebreyend

Promotor: B. de Bruin

Co-promotor: J.L. Van der Vlugt

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

Link: [Read or download this thesis](#)



19 June 2018

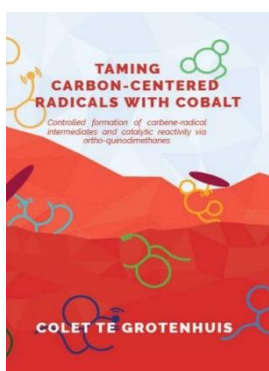
**Advances in organophosphorus chemistry: Synthesis, reactivity and recycling**

Author: R. (Tetiana) Krachko

Promotors: J.C. Slootweg, A.W. Ehlers

Group: Synthetic Organic Chemistry

Link: [Read or download this thesis](#)



01 June 2018

**Taming carbon-centered radicals with cobalt**

Author: C. (Colet) te Grotenhuis

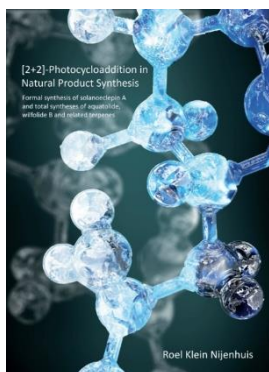
Promotor: B. de Bruin

Co-promotor: J.N.H. Reek

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

Link: [Read or download this thesis](#)





17 May 2018

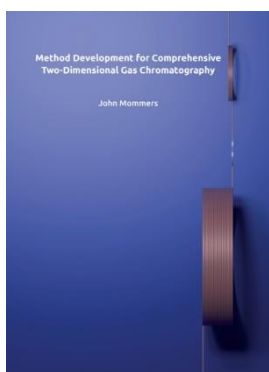
### **[2+2]-Photocycloaddition in natural product synthesis**

Author: R. (Roel) A. Klein Nijenhuis

Promotors: J.H. van Maarseveen, H. Hiemstra

Group: Synthetic Organic Chemistry

Link: [Read or download this thesis](#)



15 March 2018

### **Method Development for Comprehensive Two-Dimensional Gas Chromatography**

Author: J. (John) H.M. Mommers

Promotor: S. van der Wal

Co-promotors: P. Schoenmakers, C.G. de Koster

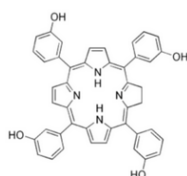
Group: Analytical Chemistry

Link: [Read or download this thesis](#)

## Valorisation

HIMS researchers explore a wide range of subjects; from pure basic scientific inspired quests to application inspired fundamental research projects. Besides scientific output there are many more ways that HIMS researchers try to provide value to society. Valorisation is always on their mind, for instance through public-private collaboration.

### Light-activated molecules to fight cancer and infection - 12 March 2018



HIMS researchers at the Molecular Photonics group are involved in a new European research project for the optimized design of molecules to fight cancer and infections. A unique feature of the molecules is their activation upon exposure to light, leading to innovative applications in treatments against skin tumours, first-aid bandages and self-sterilising devices.

### Funding for promising research to improve cold-stress tolerance of plants - 29 September 2018



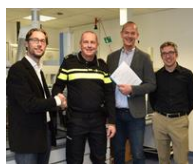
Professor Wybren Jan Buma of the Molecular Photonics research group, together with associate professor Teun Munnik of the Swammerdam Institute for Life Sciences, has found a way to improve the resilience of plants to low-temperature stress. The agricultural sector has already expressed its interest. For the further development of their method, the researchers received a grant from the Physics2Market Fund of Innovation Exchange Amsterdam (IXA).

### 'Boostcrop' consortium receives millions to increase agricultural and horticultural yields - 29 October 2018



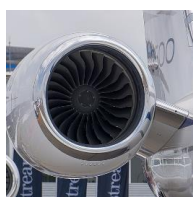
The European 'Boostcrop' consortium with HIMS professors Wybren Jan Buma and Jos Oomens has been awarded nearly 5 million euros from the European 'Future and Emerging Technologies' programme. Boostcrop aims to increase yields in agri- and horticulture with a new approach based on the development and application of molecular temperature controllers.

### Collaboration with forensic experts of the Amsterdam Police - 10 December 2018



HIMS researchers scientists started a collaboration with the forensic experts of the Amsterdam Police. The aim of the collaboration is to provide accurate and valuable chemical information in criminal investigations, provide intelligence on the production of illicit drugs, and offer options for rapid and robust chemical field analysis of drug samples.

### Booking.com supports research into renewable jet fuel from waste - 18 December 2018



Dr Shiju Raveendran of the UvA's research priority area Sustainable Chemistry has acquired a 150,000 euro grant from Booking.com for research into the manufacture of renewable jet fuel from food waste and other organic residue.

## Outreach

### Lectures and other contributions in 2018

#### **For the general public**

- Popular talk to inspire artists for their exposition on Noordwijk, the City of Space, Wat is Sterrenstof? (Annemieke Petrignani)
- NEMO Kinderlezing *Hoe kun je zeldzame schatten bewaren?* (Maarten van Bommel)
- NEMO Kinderlezing *Raakt Energie Nooit Op?* (Moniek Tromp)

#### **For high school students and teachers**

- At *Circulaire Chemie*, a lecture series on sustainable chemistry, Chris Slootweg gives a lecture on *Circulaire chemie als toekomst voor groene chemie* for secondary school teachers
- Bachelor Day, lectures by Sander Woutersen, Célia Fonseca Guerra and Jan van Maarseveen for upper secondary school students
- Speeddate education: Information rounds consisting of an introduction of about 30 minutes and 4 times 15 minutes of speed dating with 'role models' for lower secondary school students (Jocelyne Vreede)
- Trial-studying (proefstuderen) for upper secondary school students and teachers. Lecture/practicum by Evert Jan Meijer
- Chemie in Amsterdam, lectures and labtours for upper secondary school teachers and students (Annemieke Petrignani, Jan van Maarseveen, Raveendran Shiju, Bernd Ensing)
- Formatief evalueren / Redeneren binnen scheikunde (Steunpunt Scheikunde), lectures for (secondary school) teachers (Bernd Ensing)

#### **TV and radio broadcast contributions**

- QMusic radio 'Joost mag het weten', on burning candles (7 March, Jan van Maarseveen)  
▶ [Joost mag het weten](#).
- DWDD TV talkshow, on the restoration of Rembrandt's Nightwatch (16 October, Katrien Keune).  
▶ [De Wereld Draait Door](#).
- BNR news radio, on gender equality in academia (21 December, Moniek Tromp)  
▶ [BNR news radio](#).



### HIMS researchers in the media in 2018

- **Air pollution in Europe**  
An interview with Gadi Rothenberg about air pollution in Europe. 'It's much worse than I expected'.  
▶ [Folia, 27 November \(in Dutch\)](#).
- **New pathways for biocatalytic cascades**  
The European research project Biosusamin and its principal investigator Dr Francesco Mutti

are featured in the summer edition of the magazine 'EU Research'.

▶ [HIMS news item](#).

▶ [Article in EU Research](#) (PDF).

- **Molecular materials for sustainable applications**

Research of the Inorganic Materials team of the Sustainable Chemistry research priority area, led by Dr Stefania Grecea, was highlighted in SciTech Europa Quarterly, issue 27, 2018.

▶ [Read the article](#) (PDF).

- **The future of solar fuels**

According to a techno-economic analysis by Remko Detz, Joost Reek and Bob van der Zwaan, the industrial synthesis of renewable hydrogen, syngas, methanol and diesel could become competitive with respect to their fossil counterparts within the next two decades. The results were featured in various online magazines.

▶ [Solar Magazine](#), 9 July (in Dutch).

▶ [NH Nieuws](#), 6 July (in Dutch).

▶ [HIMS news item](#).

- **An end to disposable plastic**

Gert-Jan Gruter in Nederlands Dagblad about his search for a sustainable alternative for regular plastic.

▶ [Nederlands Dagblad](#), 29 May (PDF, in Dutch).

- **Cheap and Diastereoselective  $\beta$ -Lactam Formation**

Bas de Bruin was interviewed in ChemistryViews on his paper reporting a one-pot route to  $\beta$ -lactams, amides, and esters.

▶ [ChemistryViews](#), 5 April.

- **Learning from plants about storing solar energy**

Joost Reek featured in an article and video by Folia magazine about his research on converting sunlight into fuel.

▶ [Folia](#), 4 April (Article, in Dutch).

▶ [YouTube](#) (Video, in Dutch).

- **An app for molecular visualisation**

David Dubbeldam in Emerge and Folia about his app iRaspa for designing molecules.

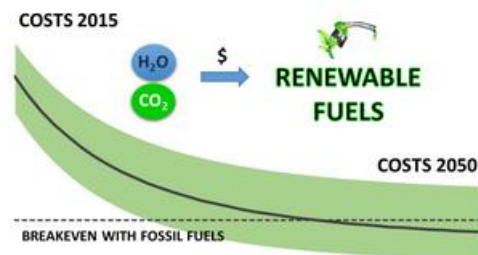
▶ [Folia](#), 29 March (in Dutch).

▶ [Emerge](#), 28 March (in Dutch).

- **Pregnant? Go home!**

An interview with Moniek Tromp in *Algemeen Nijmeegs Studentenblad* about women in top positions in science.

▶ [Algemeen Nijmeegs Studentenblad](#), 8 March (in Dutch).





## Facts & Figures

### Research

#### Research output

Research output 2018 per type of publication (source: PURE).

HIMS themes	AC	CC	MP	SC	Ot	Joint	Total
Refereed articles	22	66	58	95		-12	229
Non-refereed articles		1		1			2
Book (chapter)s		1		1			2
PhD-theses	3	1	2	8			14
Non-refereed conf. publ.	1						1
Other conf. contr. (poster, abstract)	5	14	11	12		-5	37
<b>Total</b>	<b>31</b>	<b>83</b>	<b>71</b>	<b>117</b>		<b>-17</b>	<b>285</b>

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. The 'Joint' column contains the number of joint results from collaborations between research groups.

#### Other output and honours

HIMS themes		AC	CC	MP	SC	Other	Joint	Total
Awards/prizes		5	4	6	24			39
Key note lectures		12	16	21	50		-2	97
Media coverage		2	7	1	24		-2	32
Outreach activities	Organizing an event	1	11	3	8		-3	20
	Popular lectures	1		2	2			5
<b>Total</b>		<b>21</b>	<b>38</b>	<b>33</b>	<b>108</b>		<b>-7</b>	<b>193</b>

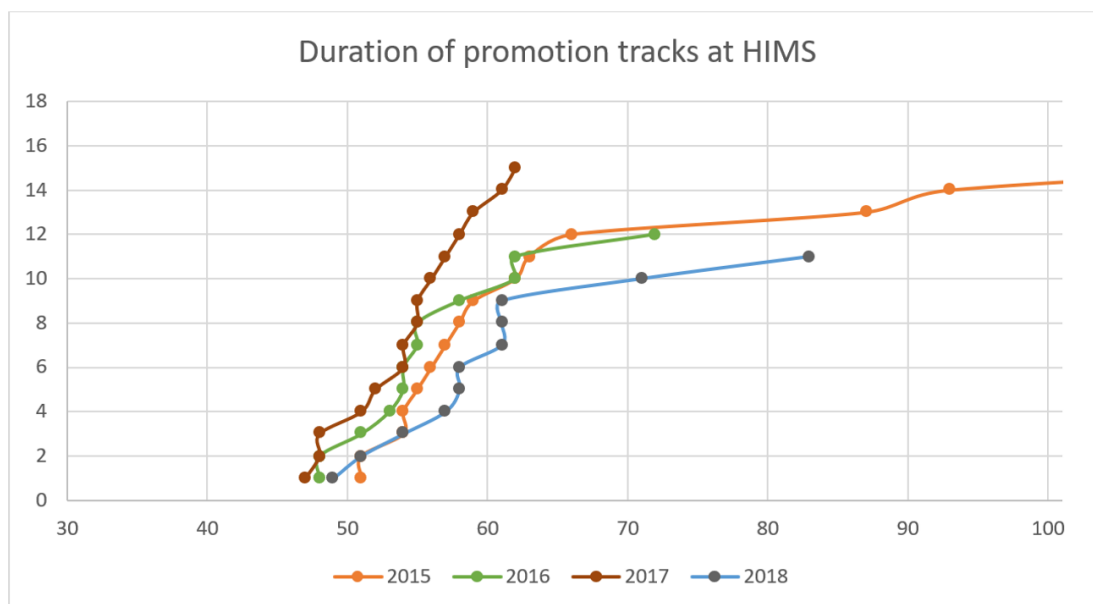
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis.

#### Efficiency of the doctoral research path

All PhD candidates conducting research with the primary aim/obligation of graduating, based on a 0.8-1.0 FTE contract. This includes PhD candidates with employee status and contract PhD candidates without employee status. The second category receives external funding or a university scholarship to conducting research under the authority of the research unit with the primary aim of graduating.

Enrolment				Success rates of graduation in years (t) after start								Total					
Start	m / f		Total	t ≤ 4		t ≤ 5		t ≤ 6		t ≤ 7		Graduated		Not yet		Discontinued	
	#	%	#	#	%	#	%	#	%	#	%	#	%	#	%	#	%
2010	6	9	15	0	-	4	27	8	54	12	80	12	80	0	-	3	20
2011	7	8	15	0	-	8	53	11	73	11	73	11	73	0	-	4	27
2012	10	5	15	0	-	6	40	13	87	13	87	13	87	1	7	1	7
2013	11	10	21	3	14	9	43	13	62	-	-	13	62	4	19	4	19
2014	14	7	21	1	5	12	57	-	-	-	-	12	57	8	38	1	5
<b>Total</b>	<b>48</b>	<b>39</b>	<b>87</b>	<b>4</b>	<b>5</b>	<b>39</b>	<b>45</b>	<b>-</b>	<b>-</b>	<b>-</b>	<b>-</b>	<b>61</b>	<b>70</b>	<b>13</b>	<b>15</b>	<b>13</b>	<b>15</b>

The graph below shows the duration of promotion tracks at HIMS (from start to hora est) in months for the past years. Each dot represents a single PhD. The table below presents the median promotion time in months per year. Externally prepared promotions are not taken into account in these figures.



## Personnel

### FTE numbers

The table below presents the HIMS staff numbers (average headcount in 2018) and in Research FTE. Research FTE means net time available for research as full-time equivalents (FTE) per employment type. The numbers are based on an input of 0.5 FTE per FTE Scientific staff, 0.9 FTE per FTE Post-docs, 0.75 FTE per FTE PhD students, and 1.0 FTE per FTE Technicians, Visiting Fellows and Support staff. Detailed information on these numbers is available as supporting information. .

	AC		CC		MP		SC		Other		Total	
	HC	RFTE	HC	RFTE	HC	RFTE	HC	RFTE	HC	RFTE	HC	RFTE
Scientific staff (1)	39	15.4	40	15,5	40	14,9	34	14,9	35	15,5	40	16,6
Post-docs (2)	29	25.8	28	23,0	29	24,3	28	23,0	41	34,6	47	39,6
PhD students (3)	67	49.9	77	56,5	73	53,5	67	49,5	74	53,1	82	58,1
<b>Total research staff</b>	<b>135</b>	<b>91.2</b>	<b>145</b>	<b>95,0</b>	<b>142</b>	<b>92,8</b>	<b>129</b>	<b>87,4</b>	<b>150</b>	<b>103,1</b>	<b>169</b>	<b>114,2</b>
Technicians (4)	23	21.2	23	21,0	21	19,7	22	19,8	21	19,3	21	19,9
Visiting fellows	10	9.4	11	11,0	13	12,4	8	7,6	10	8,5	7	6,2
Support staff (4)	9	5.7	10	6,5	7	4,9	9	6,5	8	6,1	7	5,9
<b>Total staff</b>	<b>177</b>	<b>127.4</b>	<b>189</b>	<b>133,5</b>	<b>183</b>	<b>129,8</b>	<b>168</b>	<b>121,3</b>	<b>189</b>	<b>137,1</b>	<b>204</b>	<b>146,1</b>

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. Notes: 1. Comparable with WOPI categories professor, associate professor and assistant professor; tenured and nontenured staff. 2. Comparable with WOPI category researcher, or non-tenured staff. 3. Standard PhD (employed) and contract PhDs (externally or internally funded but not employed). 4. The Standard Evaluation Protocol combines the Technical support (Technicians) and administrative support (Support staff) in a single category Support.

## Diversity

Age, gender, and nationality distribution of scientific staff of HIMS ultimo 2018.

Age bracket	Number	Male	Female	Dutch	Other EU	Other
30-40	2	2	0	0	1	1
40-50	11	7	4	8	2	1
50-60	12	12	0	10	1	1
60+	5	5	0	4	1	0
Total	30	26 (87%)	4 (13%)	22 (73%)	5 (17%)	3 (10%)

## Finance

### Research project funding

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 university may grant Strategic project funding or Research priority areas, which also count as direct funding category.
- Most research grants (*tweede geldstroom*) are funded by national or European funding or research agencies like NWO 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 into the distribution of funds and the funding of staff salaries only.

### Research- and supporting staff 2018 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%
<b>Total</b>	<b>17.5</b>	<b>20.2</b>	<b>17.0</b>	<b>65.2</b>	<b>0.7</b>	<b>120.6</b>	<b>100%</b>	<b>22.7</b>	<b>143.3</b>	<b>100%</b>

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. The column 'Other' includes the institute's office.

## Externally financed projects acquired in 2018 (mln €) per funding type.

HIMS themes	AC	CC	MP	SC	Other	Total <sup>1</sup>
Direct funding	0.00	0.00	0.00	0.25	0.00	<b>0.25</b>
Research grants	0.11	0.09	0.43	2.30	0.00	<b>2.93</b>
Contract research	2.74	0.01	0.05	0.41	0.00	<b>3.22</b>
<b>Total</b>	<b>2.85</b>	<b>0.11</b>	<b>0.48</b>	<b>2.96</b>	<b>0.00</b>	<b>6.40</b>

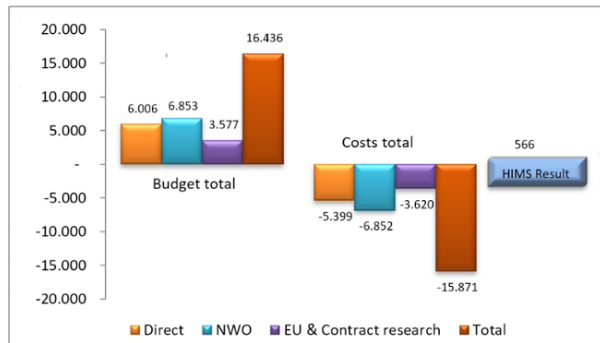
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. Note 1: Budgets were obtained for a total of (in FTE) 14,4 PhDs, 17 PD and 2,5 staff.

## HIMS result 2018 (k€)

The HIMS result of 2018 amounts to +566k€. These concern reservations from past budgets for costs in the framework of the *Sectorplan Natuur- en Scheikunde* and the RPA Sustainable Chemistry foreseen in 2019, as well as budget reserved for replacement of departing staff. The institute is required to have a reserve of minimal 10% of its annual revenue to which the surplus is counted in part as well.

2018	EU & Contract research			Total
	Direct	NWO	Contract research	
HIMS Base Budget	3.649	-	-	3.649
Budget (variable1)	4.003	3.794	2.682	10.479
Other income 2	2.270	12	-	2.282
Matching contract research	-3.916	3.047	895	-
<b>Budget total</b>	<b>6.006</b>	<b>6.853</b>	<b>3.577</b>	<b>16.436</b>
<i>Percentage</i>	<i>37%</i>	<i>42%</i>	<i>22%</i>	<i>100%</i>
Personal costs	-3.865	-2.879	-1.486	-8.230
Other costs (projects)	-3.483	-859	-874	-7.639
Overheads 3	1.949	-3.114	-1.260	-2.425
<b>Costs total</b>	<b>-5.399</b>	<b>-6.852</b>	<b>-3.620</b>	<b>-15.871</b>
<i>Percentage</i>	<i>34%</i>	<i>43%</i>	<i>23%</i>	<i>100%</i>
<b>HIMS Result 2018</b>	<b>607</b>	<b>1433</b>	<b>-42</b>	<b>566</b>

	EU & Contract research			Total
	Direct	NWO	Contract research	
Budget total	6.006	6.853	3.577	16.436
Costs total	-5.399	-6.852	-3.620	-15.871
HIMS Result 2018	607	1.433	-42	566



Notes: 1. Direct funding assigned via allocation model, incl. matching on project funding, SectorPlan, RPA Sustainable Chemistry. 2. Contributions for HRSMC and CLHC, SectorPlan, RPA Sustainable Chemistry and other external contracts. 3. Faculty overhead, institute overhead, central overhead.