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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 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 100th 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:**

![HIMS at a glance](image)

(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.

DOI: 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.


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.


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.

**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.


**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.


**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.


**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 CO2. 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 CO2 from power plant emissions.

Selective CO2 adsorption in water-stable alkaline-earth based metal-organic frameworks.

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

Competetive 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.


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.


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.

**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.


**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.


**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.


**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.

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 HIMS, 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. Nurttila  
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 Nanoplatforms**

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
Promotors: 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
Promotors: J.G.M. Janssen, P. Schoenmakers
Co-promotors: 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-promotors: 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-promoters: 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.

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**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 β-Lactam Formation**  
Bas de Bruin was interviewed in ChemistryViews on his paper reporting a one-pot route to β-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 Emerce and Folia about his app iRaspa for designing molecules.  
► Folia, 29 March (in Dutch).  
► Emerce, 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).

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<tr>
<td>Total</td>
<td>31</td>
<td>83</td>
<td>71</td>
<td>117</td>
<td>-17</td>
<td></td>
<td>285</td>
</tr>
</tbody>
</table>

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

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

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.

<table>
<thead>
<tr>
<th>Year</th>
<th>Enrolment</th>
<th>Success rates of graduation in years (t) after start</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>m/f</td>
<td>t ≤ 4</td>
<td>t ≤ 5</td>
</tr>
<tr>
<td>2010</td>
<td>6/9</td>
<td>15</td>
<td>0</td>
</tr>
<tr>
<td>2011</td>
<td>7/8</td>
<td>15</td>
<td>0</td>
</tr>
<tr>
<td>2012</td>
<td>10/5</td>
<td>15</td>
<td>0</td>
</tr>
<tr>
<td>2013</td>
<td>11/10</td>
<td>21</td>
<td>0</td>
</tr>
<tr>
<td>2014</td>
<td>14/7</td>
<td>21</td>
<td>1</td>
</tr>
<tr>
<td>Total</td>
<td>48/39</td>
<td>87</td>
<td>4</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th></th>
<th>AC</th>
<th>CC</th>
<th>MP</th>
<th>SC</th>
<th>Other</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HC</td>
<td>RFT</td>
<td>HC</td>
<td>RFT</td>
<td>HC</td>
<td>RFT</td>
</tr>
<tr>
<td>Scientific staff (1)</td>
<td>39</td>
<td>15.4</td>
<td>40</td>
<td>15,5</td>
<td>40</td>
<td>14,9</td>
</tr>
<tr>
<td>Post-docs (2)</td>
<td>29</td>
<td>25.8</td>
<td>28</td>
<td>23,0</td>
<td>29</td>
<td>24.3</td>
</tr>
<tr>
<td>PhD students (3)</td>
<td>67</td>
<td>49.9</td>
<td>77</td>
<td>56.5</td>
<td>73</td>
<td>53.5</td>
</tr>
<tr>
<td><strong>Total research staff</strong></td>
<td><strong>135</strong></td>
<td><strong>91.2</strong></td>
<td><strong>145</strong></td>
<td><strong>95.0</strong></td>
<td><strong>142</strong></td>
<td><strong>92.8</strong></td>
</tr>
<tr>
<td>Technicians (4)</td>
<td>23</td>
<td>21.2</td>
<td>23</td>
<td>21,0</td>
<td>21</td>
<td>19.7</td>
</tr>
<tr>
<td>Visiting fellows</td>
<td>10</td>
<td>9.4</td>
<td>11</td>
<td>11,0</td>
<td>13</td>
<td>12.4</td>
</tr>
<tr>
<td>Support staff (4)</td>
<td>9</td>
<td>5.7</td>
<td>10</td>
<td>6.5</td>
<td>7</td>
<td>4.9</td>
</tr>
<tr>
<td><strong>Total staff</strong></td>
<td><strong>177</strong></td>
<td><strong>127.4</strong></td>
<td><strong>189</strong></td>
<td><strong>133.5</strong></td>
<td><strong>183</strong></td>
<td><strong>129.8</strong></td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Age bracket</th>
<th>Number</th>
<th>Male</th>
<th>Female</th>
<th>Dutch</th>
<th>Other EU</th>
<th>Other</th>
</tr>
</thead>
<tbody>
<tr>
<td>30-40</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>40-50</td>
<td>11</td>
<td>7</td>
<td>4</td>
<td>8</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>50-60</td>
<td>12</td>
<td>12</td>
<td>0</td>
<td>10</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>60+</td>
<td>5</td>
<td>5</td>
<td>0</td>
<td>4</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Total</td>
<td>30</td>
<td>26 (87%)</td>
<td>4 (13%)</td>
<td>22 (73%)</td>
<td>5 (17%)</td>
<td>3 (10%)</td>
</tr>
</tbody>
</table>

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 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)

<table>
<thead>
<tr>
<th>HIMS Themes</th>
<th>Research</th>
<th>Total</th>
<th>%</th>
<th>Support</th>
<th>Total</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AC</td>
<td>CC</td>
<td>MP</td>
<td>SC</td>
<td>Other</td>
<td></td>
</tr>
<tr>
<td>Direct funding</td>
<td>6.7</td>
<td>7.8</td>
<td>4.6</td>
<td>16.9</td>
<td>0.7</td>
<td>36.7</td>
</tr>
<tr>
<td>Research grants</td>
<td>7.8</td>
<td>10.5</td>
<td>8.9</td>
<td>27.5</td>
<td>-</td>
<td>54.7</td>
</tr>
<tr>
<td>Contract research</td>
<td>2.2</td>
<td>1.5</td>
<td>2.0</td>
<td>14.3</td>
<td>-</td>
<td>20.0</td>
</tr>
<tr>
<td>Other</td>
<td>0.8</td>
<td>0.3</td>
<td>1.5</td>
<td>6.5</td>
<td>9.1</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>17.5</td>
<td>20.2</td>
<td>17.0</td>
<td>65.2</td>
<td>0.7</td>
<td>120.6</td>
</tr>
</tbody>
</table>

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.

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

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.

<table>
<thead>
<tr>
<th>2018</th>
<th>Direct</th>
<th>NWO</th>
<th>EU &amp; Contract research</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>HIMS Base Budget</td>
<td>2.640</td>
<td>-</td>
<td>-</td>
<td>2.640</td>
</tr>
<tr>
<td>Budget (variable)</td>
<td>-4.003</td>
<td>3.794</td>
<td>2.652</td>
<td>10.479</td>
</tr>
<tr>
<td>Other income 2</td>
<td>2.270</td>
<td>12</td>
<td>-</td>
<td>2.322</td>
</tr>
<tr>
<td>Matching contract research</td>
<td>-3.016</td>
<td>3.047</td>
<td>805</td>
<td>-</td>
</tr>
<tr>
<td>Percentage</td>
<td>37%</td>
<td>42%</td>
<td>22%</td>
<td>100%</td>
</tr>
<tr>
<td>Personal costs</td>
<td>-3.865</td>
<td>-2.879</td>
<td>-1.486</td>
<td>-8.330</td>
</tr>
<tr>
<td>Other costs (projects)</td>
<td>-3.483</td>
<td>-859</td>
<td>-824</td>
<td>-7.094</td>
</tr>
<tr>
<td>Overheads 3</td>
<td>1.949</td>
<td>-3.114</td>
<td>-1.200</td>
<td>-2.425</td>
</tr>
<tr>
<td>Costs total</td>
<td>-5.399</td>
<td>-6.852</td>
<td>-3.620</td>
<td>-15.871</td>
</tr>
<tr>
<td>Percentage</td>
<td>34%</td>
<td>43%</td>
<td>23%</td>
<td>100%</td>
</tr>
</tbody>
</table>

HIMS Result 2018: 607 1433 -42 566


Costs total: Direct -5.399 NWO -6.852 EU & Contract research -3.620 Total -15.871

HIMS Result: 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.