



# Annual Report 2017

*Chemistry  
research  
that matters*

Van 't Hoff Institute  
for Molecular Sciences

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## Executive summary

2017 was a successful year for HIMS, in which new projects were acquired and we underpinned our international position with even more appealing publications in renowned scientific journals. It was also a year in which the research quality at HIMS was evaluated to be of very high calibre, resulting in the highest possible ranking as 'world-leading/excellent'. According to HIMS director Prof. Peter Schoenmakers: "In some ways, HIMS scientists are as diverse as molecules. And many different molecules together may form something beautiful. The Annual Report 2017 demonstrates just that."

HIMS received funding for 16 new projects in a broad field of applications from basic chemistry to solar energy, healthcare, arts and astronomy with a total value of over six million euros. Ten projects were (co-)financed by companies (AkzoNobel, Avantium, BASF, Brite Solar, Da Vinci, Gensonic, KWR, PWN, Shell, Skytree) and other parties (UMC's, Van Gogh museum, RCE). Five new patent applications were filed and a multinational company built a pilot for removing cyanide from the wastewater of steel mills based upon a HIMS patent.

## Acknowledgements



*Per January prof. Peter Schoenmakers was appointed as the new director of HIMS, succeeding Prof. Joost Reek, who stepped down after three years. The latter continues to serve as successful group leader within HIMS and as the figurehead of the UvA research*

Per January prof. Peter Schoenmakers was appointed as the new director of HIMS, succeeding Prof. Joost Reek, who stepped down after three years. The latter continues to serve as successful group leader within HIMS and as the figurehead of the UvA research priority area Sustainable Chemistry in his new role as distinguished research professor at the UvA Faculty of Science. Photo by Jan Willem Steenmeijer.

In 2017, HIMS researchers were acknowledged for their achievements via several grants and prizes. Prof. Fred Brouwer received the Honda-Fujishima Lectureship Award of the Japanese Photochemistry Association, Prof.em. Sjoerd van der Wal was awarded the second ever 'SCM Lifetime

Achievement Award', Dr Moniek Tromp received the NWO Athena Award. Prof. Rajamani Krishna featured in the 2017 list of the world's 'Most Influential Scientific Minds' compiled by Clarivate Analytics. He was the only Dutch researcher in the chemistry category.

Dr Joen Hermans received his PhD cum laude. Prof. Wybren Jan Buma became professor by special appointment of Spectroscopy of Photoactive Molecules and Materials at Radboud University Nijmegen, and Prof. Gadi Rothenberg was appointed Senior Visiting Scholar at Fudan University in Shanghai.

Prof. Bas de Bruin, Prof. Joost Reek and Dr Moniek Tromp were elected as members of the 'Advanced Research Center Chemical Building Blocks Consortium' (ARC-CBBC), the Dutch national research consortium in the area of sustainability and catalysis.




## Positive evaluation

In November, a group of highly esteemed chemistry, biology and earth science experts evaluated the corresponding institutes at UvA and VU universities. The committee concluded that the research quality at HIMS is of very high calibre, which was thus rated in the highest category *world-leading/excellent*: "HIMS has seen a very positive development and exhibits today a significantly

more coherent framework for chemistry at UvA than in the past. The panel has been very impressed by the strong commitment of the individual PIs to their themes within HIMS as an overarching structure. The research topics and the scientific profile holds potential to foster this development and to continue with a strategic planning for the expansion of strengths, and to overcome weaknesses.”

In the meantime, HIMS has started initiatives in line with the recommendations of the committee that aim to drastically improve the gender balance of the staff and to further strengthen the connections between HIMS’ four research themes.

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

Staff		FTEs
Full professors		14
Associate professors		10
Assistant professors		9
Postdocs		27
PhD candidates		72
Support and management staff		26
<hr/>		
Doctorate conferrals		16
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Publications		268

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

## Scientific highlights

Chemistry is an interdisciplinary science focused on design, synthesis and analysis of molecules. The core objective of the Van 't Hoff Institute is to understand and predict the behaviour of molecules in increasingly complex processes and systems. In our research three distinct focus areas can be distinguished:

- **Chemistry of Complex Systems and Materials**

The world around us is complex. Materials are rarely pure and often consist of many components, the environment contains mixtures of many chemical substances, industrial products exist of carefully optimized complex mixtures, often with emergent properties. Elucidating, characterizing, predicting, and eventually designing and controlling such systems and their properties provides a large challenge for chemistry in the next decade. At the Van 't Hoff Institute, several groups work on investigating such complex systems, with application in forensic science, the chemistry of artworks (paintings), complex soft matter and smart materials, and system catalysis.

- **Chemistry for Sustainability**

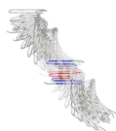
The energy transition, the climate crisis and the environmental problems all call for a sustainable society. Chemistry provides new solutions to these problems. With efficient chemical processes and catalysts using earth-abundant, cheap and non-toxic materials. With investigations into chemical recycling and how materials age and degrade, making the circular society a reality. With solutions for the energy transition, such as solar fuels, using electrochemistry and electrocatalysis. Our research groups are working in all these areas to create tomorrow's sustainable society.

- **Chemistry of Biomolecular Systems**

The living world is an endless source of inspiration for chemistry research. At the Van 't Hoff Institute, chemists make and understand bioinspired, biological and prebiotic molecular systems. For instance, using biocatalysts to make highly specific molecules. Or by developing the synthesis, analysis, design and understanding of biochemical reactions, bioactive molecules and biomaterials, even leading to new processes for medical diagnostics and treatments. Last but not least, our researchers are also studying the origin of life.

More on these focus areas [can be found online](#). Below is a chronological overview of the scientific highlights of 2018 in all three areas.

### **Formation of amyloid fibrils highly susceptible to salt concentration** - 6 February 2017

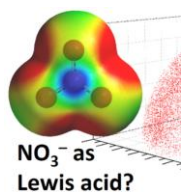


By combining two-dimensional infrared spectroscopy and atomic force microscopy, Amsterdam researchers have established that the spatial structure of amyloid fibrils related to Parkinson's disease is highly dependent on salt concentration during protein aggregation. The results, published recently in Nature's open access journal 'Scientific Reports', can contribute to an explanation of observed differences in fibril-related pathologies.

Steven J. Roeters, Aditya Iyer, Galja Pletikapić, Vladimir Kogan, Vinod Subramaniam & Sander Woutersen: *Evidence for Intramolecular Antiparallel Beta-Sheet Structure in Alpha-Synuclein Fibrils from a Combination of Two-Dimensional Infrared Spectroscopy and Atomic Force Microscopy*. Scientific Reports 7, Article number: 41051 (2017) [doi:10.1038/srep41051](https://doi.org/10.1038/srep41051)



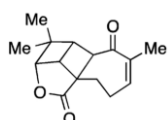
### **The unexpected supramolecular chemistry of nitrate anions** - 21 February 2017



A team of researchers with Dr Tiddo J. Mooibroek of the University of Amsterdam's Van 't Hoff Institute of Molecular Sciences (HIMS) argue that the nitrate anion (NO<sub>3</sub><sup>-</sup>) can display a counterintuitive Lewis acidity. Their findings, reported this week in Nature Communications, may serve as a (retrospective) guide to interpret data involving the chemical behaviour of nitrate anions, which are ubiquitous in Nature.

Antonio Bauzá, Antonio Frontera and Tiddo J. Mooibroek: *NO<sub>3</sub><sup>-</sup> anions can act as Lewis acid in the solid state*. Nature Communications, published online 21 February 2017, DOI: [10.1038/NCOMMS14522](https://doi.org/10.1038/NCOMMS14522)

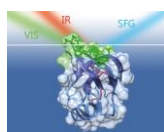
### **Amsterdam aquatolide synthesis enables Science publication on NMR** - 11 April 2017



A sample of the natural compound aquatolide, synthesized in the Synthetic Organic Chemistry laboratory of professor Henk Hiemstra at the Van 't Hoff Institute for Molecular Sciences, played a pivotal role in American NMR research published in this week's issue of Science.

Jordy M. Saya, Klaas Vos, Roel A. Kleinnijenhuis, Jan H. van Maarseveen, Steen Ingemann, and Henk Hiemstra: *Total synthesis of Aquatolide*. Org. Lett., 2015, 17 (15), pp 3892–3894  
DOI: [10.1021/acs.orglett.5b01888](https://doi.org/10.1021/acs.orglett.5b01888)

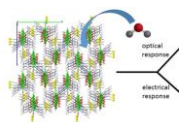
### **Unravelling the secrets of a fungal 'raincoat'** - 14 April 2017



Using advanced interfacial spectroscopy combined with spectral calculations, Amsterdam researchers have determined essential properties of extremely water repelling natural hydrophobin films at the molecular level. Their findings could pave the way towards novel designer microfilms of industrial relevance.

Konrad Meister, Steven J. Roeters, Arja Paananen, Sander Woutersen, Jan Versluis, Géza R. Szilvay, and Huib J. Bakker, *Observation of Ph-induced protein reorientation at the water surface*, Journal of Physical Chemistry Letters, DOI: [10.1021/acs.jpcllett.7b00394](https://doi.org/10.1021/acs.jpcllett.7b00394)

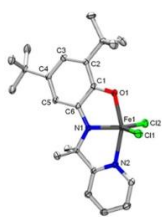
### **Smart materials design leads to new dual-mode humidity sensing** - 17 April 2017



Dr Stefania Tanase Grecea and co-researchers at the University of Amsterdam's Research Priority Area Sustainable Chemistry have demonstrated the first dual-mode humidity sensing material. Based on a lanthanide-based metal organic framework it can sense water both optically and electrically. The research was recently published in the journal Chemical Communications.

Yuan Gao, Pengtao Jing, Ning Yan, Michiel Hilbers, Hong Zhang, Gadi Rothenberg and Stefania Tanase: Dual-mode humidity detection using a lanthanide-based metal–organic framework: towards multifunctional humidity sensors. *Chem. Commun.*, 2017, *Advance Article*. DOI: [10.1039/C7CC01122A](https://doi.org/10.1039/C7CC01122A)

### **Record breaking reactivity of new iron catalyst for synthesis of cyclic amines** - 20 April 2017

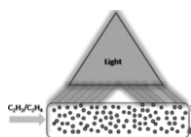


Chemists at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) have developed a very efficient way to selectively produce amines, which are prevalent as a functional group in both bulk and fine chemicals. Using a catalyst based on the earth-abundant element iron, they established a record breaking reactivity in preparing cyclic amines via an atom-efficient C-H amination protocol, inserting a nitrogen atom into an unactivated C-H bond.

B. Bagh, D.L.J. Broere, V. Sinha, P.T. Kuipers, N.P. van Leest, B. de Bruin, S. Demeshko, M. A. Siegler, J.I. van der Vlugt, *Catalytic Synthesis of N-Heterocycles via Direct C(sp<sup>3</sup>)-H Amination Using an Air-Stable Iron(III) Species with a Redox-Active Ligand* *J. Am. Chem. Soc.*, 2017, 139 (14), pp 5117–5124

DOI: [10.1021/jacs.7b00270](https://doi.org/10.1021/jacs.7b00270)

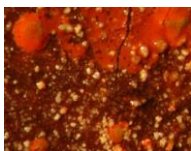
### **Temperature- and light-responsive switch for acetylene/ethylene separation** – 25 April 2017



Following previous work on metal-organic framework (MOF), professor Rajamani Krishna of the Van 't Hoff Institute for Molecular Sciences (HIMS) contributed to an international study on a novel temperature- and light-responsive MOF, published this week in *Angewandte Chemie International Edition*.

C.B. Fan, L.L. Gong, L. Huang, F. Luo, R. Krishna, X.F. Yi, A.M. Zheng, L. Zhang, S.Z. Pu, X.F. Feng, M.B. Luo, G.C. Guo, *Significant Enhancement of C<sub>2</sub>H<sub>2</sub>/C<sub>2</sub>H<sub>4</sub> Separation by a Photochromic Diarylethene Unit: A Temperature- and Light-Responsive Separation Switch*, *Angew. Chem. Int. Ed*, 24 April 2017. DOI: [10.1002/anie.201702484](https://doi.org/10.1002/anie.201702484)

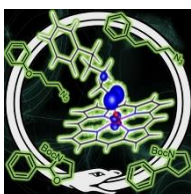
### **Simulation and study of the behaviour of old paints** – 30 April 2017



Oil paintings are subject to slow changes affecting both their external appearance and internal structure. HIMS PhD student Joen Hermans has managed to recreate the molecular structure of old oil paints. He will obtain his doctorate at the University of Amsterdam on Tuesday 9 May.

J.J. Hermans: *Metal Soaps in Oil Paint*. PhD supervisor: Prof. P.D. Iedema. Co-supervisor: Dr. K. Keune. [Read or download this thesis.](#)

### **New cobalt catalyst for highly selective synthesis of cyclic amines** – 8 May 2017



Researchers of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) have developed a cobalt-based catalyst for the direct synthesis of various N-heterocycles from aliphatic azides by means of intramolecular ring-closing C-H bond amination. Their result has just been published online by 'Chemistry, a European Journal', as a Very Important Paper.

Kuijpers, P. F., Tiekink, M. J., Breukelaar, W. B., Broere, D. L. J., van Leest, N. P., van der Vlugt, J. I., Reek, J. N. H. and de Bruin, B.: *Cobalt-Porphyrin-Catalysed Intramolecular Ring-Closing C-H Amination of Aliphatic Azides: A Nitrene-Radical Approach to Saturated Heterocycles*. *Chem. Eur. J.* (2017),23, 1–9

DOI:[10.1002/chem.201700358](https://doi.org/10.1002/chem.201700358)

### **Enzymatic dissolution of lignin in water** – 15 May 2017



Researchers of the University of Amsterdam's Research Priority Area Sustainable Chemistry have developed a new approach to dissolving lignin in water. They used a simple and effective enzymatic process under ambient conditions, paving the way towards industrial application of this abundant natural resource of aromatics. The results, published online in 'ChemSusChem', were recently featured in

'Chemical & Engineering News (C&EN)'.

Pepijn Prinsen, Anand Narani, Aloysius F. Hartog, Ron Wever, and Gadi Rothenberg: *Dissolving Lignin in Water through Enzymatic Sulfation with Aryl Sulfotransferase*. ChemSusChem 2017, DOI: [10.1002/cssc.201700376](https://doi.org/10.1002/cssc.201700376)

### **Amsterdam chemists synthesize molecular pretzels** - 25 May 2017



Chemists at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences have discovered a new class of molecules. This week they report in Nature Communications on their synthesis method leading to 'quasi[1]catenanes': pretzel-like molecules consisting of two molecular rings 'oppositely' coupled at a central carbon atom. The discovery is an important step towards synthesis of lasso peptides; new molecules with a potential use as medicines.

Luuk Steemers, Martin J. Wanner, Martin Lutz, Henk Hiemstra & Jan H. van Maarseveen: Synthesis of spiro quasi[1]catenanes and quasi[1]rotaxanes via a templated backfolding strategy. Nature Communications, published online 25 May 2017. DOI: [10.1038/ncomms15392](https://doi.org/10.1038/ncomms15392)

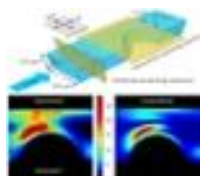
### **Sustainable Chemistry students print their way to new and powerful supercapacitors** – 13 June 2017



Students at the University of Amsterdam's Research Priority Area Sustainable Chemistry have tripled the specific capacitance of nitrogen-doped carbons: new materials with potential applications in fast energy storage (e.g. for regenerative braking or fast charging of cellphones). Their experiments required new pieces of equipment which were designed and produced in the lab using 3D printing.

J. Biemolt, I.M. Denekamp, T.K. Slot, G. Rothenberg and D. Eisenberg: *Boosting the supercapacitance of nitrogen-doped carbon by tuning surface functionalities*. ChemSusChem, 2017, published online 6 June 2017, DOI: [10.1002/cssc.201700902](https://doi.org/10.1002/cssc.201700902)

### **Using photoluminescent nanorods as ultimate probes of fluid flow** – 19 June 2017



A Franco-Dutch international collaboration involving researchers from the laboratories of Condensed Matter Physics and Hydrodynamics at Paris-Saclay University and the Van't Hoff Institute for Molecular Sciences at the University of Amsterdam has resulted in a new method for very precise determination of fluid flow in capillary networks in realtime. Their proof-of-principle is published in this week's edition of Nature Nanotechnology.

JW Kim, S. Michelin, M. Hilbers, L. Martinelli, E. Chaudan, G. Amselem, E. Fradet, JP. Boilot, A.M. Brouwer, C. N. Baroud, J. Peretti, T. Gacoin: *Monitoring the orientation of rare-earth doped nanorods for flow shear tomography* Nature Nanotechnology, published online 19 June 2017. DOI: [10.1038/NNANO.2017.111](https://doi.org/10.1038/NNANO.2017.111)



### **Microwave spectroscopy reveals structural details of motor molecule** – 5 September 2017



A team of scientists including professor Wybren Jan Buma of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) has published a study unravelling the exact structure of the tiny molecular motor of chemistry Nobel laureate Ben Feringa. Using rotational spectroscopy the team reveals just how the individual parts of the motor are constructed and arranged with respect to each other.

Sérgio R. Domingos, Arjen Cnossen, Wybren J. Buma, Wesley R. Browne, Ben L. Feringa and Melanie Schnell; *Cold snapshot of a molecular rotary motor captured by high-resolution rotational spectroscopy*; *Angewandte Chemie International Edition*, 2017; DOI: [10.1002/anie.201704221](https://doi.org/10.1002/anie.201704221)

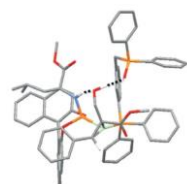
### **From hydrogen sulfide waste to sustainable hydrogen and sulfur** – 8 September 2017



In a collaborative project of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) with the State Key Laboratory of Fine Chemicals in Dalian (China), researchers have succeeded in the sustainable conversion of hydrogen sulfide. Using a light-driven process they are able to convert this chemical waste product into molecular hydrogen and solid sulfur. Their results have been published as a VIP paper in *Angewandte Chemie*.

Jing, X., Yang, Y., He, C., Chang, Z., Reek, J. N. H. and Duan, C. (2017), *Control of Redox Events by Dye Encapsulation Applied to Light-Driven Splitting of Hydrogen Sulfide*. *Angew. Chem. Int. Ed.* DOI: [10.1002/anie.201704327](https://doi.org/10.1002/anie.201704327)

### **Rational optimization of catalysts for asymmetric hydrogenation** - 25 September 2017



A team of chemists led by professors Joost Reek and Bas de Bruin at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences has developed a strategy to optimise catalyst design through computational modelling. In *Angewandte Chemie* they report the enhanced performance of a supramolecular rhodium catalyst for asymmetric hydrogenation, as a result of such 'in silico' optimization.

Daubignard, J., Detz, R. J., Jans, A. C. H., de Bruin, B. and Reek, J. N. H. (2017), *Rational Optimization of Supramolecular Catalysts for the Rhodium-Catalyzed Asymmetric Hydrogenation Reaction*. *Angew. Chem. Int. Ed.* DOI: [10.1002/anie.201707670](https://doi.org/10.1002/anie.201707670)

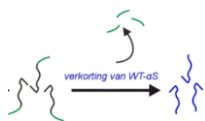
### **First UvA manuscript on new ChemRxiv preprint server** - 24 October 2017



A team of researchers and students of the Molecular Photonics research group at the Van 't Hoff Institute for Molecular Sciences (HIMS) have published their research manuscript regarding perovskite materials on the new ChemRxiv preprint server. ChemRxiv has been initiated to share early results with the chemical community ahead of formal peer review and publication.

Loreta A. Muscarella, Dina Petrova, Rebecca Jorge Cervasio, Aram Farawar, Olivier Lugier, Charlotte McLure, Martin J. Slaman, Junke Wang, Elizabeth von Hauff and René M. Williams: *Enhanced Grain-boundary Emission Lifetime and Additive Induced Crystal Orientation in One-Step Spin-Coated Mixed Cationic (FA/MA) Lead Perovskite Thin Films Stabilized by Zinc Iodide Doping*. DOI: [10.26434/chemrxiv.5484073](https://doi.org/10.26434/chemrxiv.5484073)

### **A stronger twist to cytotoxic amyloid fibrils** - 24 October 2017



Researchers from Amsterdam and Enschede have for the first time performed a structural comparison of two types of amyloid fibrils that have been associated with Parkinson's disease. Using a combination of experimental methods they show that a cytotoxic C-terminal truncated form of the alpha-synuclein protein that is abundant in vivo, aggregates into more strongly twisted fibrils that are more exposed to water. The results have been published in the Journal of the American Chemical Society.

Aditya Iyer, Steven J. Roeters, Vladimir Kogan, Sander Woutersen, Mireille M. A. E. Claessens, and Vinod Subramaniam: *C-terminal truncated  $\alpha$ -synuclein fibrils contain strongly twisted  $\beta$ -sheets*. J. Am. Chem. Soc., Publication Date (Web): 02 Oct 2017 [DOI: 10.1021/jacs.7b07403](https://doi.org/10.1021/jacs.7b07403)

### **Art science innovation aids forensic criminal investigation** - 13 November 2017



Based upon a technique originally developed for imaging chemical elements in paintings and other works of art, Dutch researchers have established a new method for detecting 'hard to find' and concealed forensic traces. The method, resulting from a special collaboration between the University of Amsterdam (UvA), the Netherlands Forensic Institute (NFI), TU Delft and the Rijksmuseum, has recently been published in Nature's open access journal Scientific Reports.

Kirsten Langstraat, Alwin Knijnenberg, Gerda Edelman, Linda van de Merwe, Annelies van Loon, Joris Dik & Arian van Asten: *Large area imaging of forensic evidence with MA-XRF* Scientific Reports, published online 08 November 2017. DOI:10.1038/s41598-017-15468-5

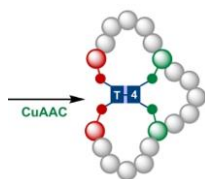
### **UvA researchers report first MAX phase catalysis** - 27 November 2017



International research has shown that a new class of materials, which are neither metallic nor ceramic, can efficiently catalyse the partial oxidation of butane. The results of the project, headed by Dr Shiju Raveendran, have just been published by Angewandte Chemie. It involved researchers from six institutes in four countries.

Ng, W., Gnanakumar, E., Rothenberg, G., Batyrev, E., Sharma, S., Pujari, P., Greer, H., Zhou, W., Sakidja, R., Barsoum, M. and Shiju, N. R.,  $Ti_3AlC_2$  MAX-phase as an efficient catalyst for oxidative dehydrogenation of n-butane. Angew. Chem. Int. Ed., 2017. DOI: [10.1002/anie.201702196](https://doi.org/10.1002/anie.201702196)

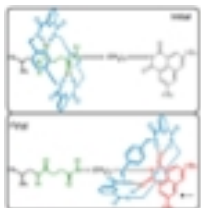
### **Simple one-pot synthesis of druggable tricyclic peptides** - 18 December 2017



A research team of chemists at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) and Pepscan (Lelystad) have developed a new methodology for locking linear peptides into highly rigidified tricyclic structures with pharmaceutical potential. Their findings have just been reported as an Angewandte Chemie 'Hot Paper'.

Richelle, G. J. J., Ori, S., Hiemstra, H., van Maarseveen, J. H. and Timmerman, P. (2017), *General and Facile Route to Isomerically Pure Tricyclic Peptides Based on Templated Tandem CLIPS/CuAAC Cyclizations*. Angew. Chem. Int. Ed.. doi:10.1002/anie.201709127

**Study reveals new details of molecular machine in motion** - 22 December 2017



Researchers of the Molecular Photonics group at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) report new details on the motion of a molecular shuttle. In *Nature Communications* they show that two-dimensional infrared spectroscopy (T2DIR) can be used to directly monitor the position and conformational changes of the shuttle during its operation.

Matthijs R. Panman, Chris N. van Dijk, Adriana Huerta-Viga, Hans J. Sanders, Bert H. Bakker, David A. Leigh, Albert M. Brouwer, Wybren Jan Buma & Sander Woutersen: *Transient two-dimensional vibrational spectroscopy of an operating molecular machine*. *Nature Communications* (2017) Published online 20 December 2017 DOI: [10.1038/s41467-017-02278-6](https://doi.org/10.1038/s41467-017-02278-6)

## Prizes and honours

The quality of HIMS scientists is reflected in the prizes and honours they receive. Noteworthy examples are the Emerging Investigator award for Shiju Raveendran, the Csaba Horváth Young Scientist Award for Bob Pirok, the Fujishima Lectureship for Fred Brouwer and the Athena Prize for Moniek Tromp. Below is a list of news items reporting on these and other HIMS staff members and students.

### Angewandte Chemie profiles Jarl Ivar van der Vlugt - 6 February 2017



The current issue of Angewandte Chemie, one of the top journals in the chemistry domain, contains a profile of Jarl Ivar van der Vlugt, assistant professor at the research group for Homogeneous, Supramolecular and Bio-Inspired Catalysis of the Van 't Hoff Institute for Molecular Sciences (HIMS).

### Lifetime achievement award for Sjoerd van der Wal - 6 February 2017



Sjoerd van der Wal, emeritus professor of Bioterials Analysis at the Van 't Hoff Institute for Molecular Sciences, has been awarded the second ever 'SCM Lifetime Achievement Award' for his outstanding achievements in separation science. The award was presented to him at the Eighth International Symposium on the Separation and Characterization of Natural and Synthetic Macromolecules, held earlier this month in Amsterdam.

### Emerging Investigator Award for chemist Shiju Raveendran - 27 February 2017



The International Conference on Nanostructured Materials and Nanocomposites (ICNM) has awarded an Emerging Investigator Award to associate professor Dr Shiju Raveendran of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS). The award recognises scientists and engineers working in the field of nanoscience and technology.

### Tom Keijer wins poster competition at national student symposium - 6 March 2017



At the national chemistry student 'PAC symposium' held 2 March at Utrecht University, UvA master student Tom Keijer has won the first prize in the 'Young KNCV' poster competition. With his poster Keijer presented his research project at the Homogeneous, Supramolecular and Bio-inspired catalysis group (HOMKAT) of the Van 't Hoff Institute for Molecular Sciences (HIMS).

### Colet te Grotenhuis runner up in best lecture competition - 13 March 2017



At the Dutch national catalysis conference NCCC held 6-8 March in Noordwijkerhout, PhD student Colet te Grotenhuis of the Van 't Hoff Institute for Molecular Sciences finished second in the best lecture competition sponsored by graduate school NIOK. Colet won 250 euros and a certificate.

### **René Williams is 'Outstanding Reviewer'** - 14 March 2017



Dr René Williams of the Molecular Photonics research group at the Van 't Hoff Institute for Molecular Sciences (HIMS) has been recognized as one of ten 'Outstanding Reviewers' of 2016 for Photochemical & Photobiological Sciences, a publication of the Royal Society of Chemistry (UK).

### **Gaston Richelle wins a SciFinder Future Leaders Award** - 24 April 2017



PhD student Gaston Richelle of the Van 't Hoff Institute for Molecular Sciences has been selected by the American Chemical Society as one of the SciFinder Future Leaders of 2017.

### **Chemistry PhD student Joen Hermans graduates cum laude** - 11 May 2017



On Tuesday 9 May 2017 Joen Hermans of the research group Computational Polymer Chemistry and Science for Arts successfully defended his thesis 'Metal Soaps in Oil Paint – Structure, Mechanisms and Dynamics'. Because of his pioneering work in the multidisciplinary area of art related research, combined with his high productivity, Hermans was granted the distinction 'Cum Laude'.

### **Tiddo Mooibroek nominated for New Scientist talent award** - 23 May 2017

**NewScientist**



Tiddo Mooibroek (1982)  
Scheikunde

Chemist Tiddo Mooibroek of the Van 't Hoff Institute for Molecular Sciences (HIMS) is among the 25 young scientists nominated for the 2017 'Wetenschapstalent' award of the Dutch edition of New Scientist. After scrutiny by a jury and a public vote the winner will be announced by Nobel laureate Ben Feringa on 22 June. Voting starts today on the [newschemist.nl](http://newschemist.nl) website.

### **Young Scientist Challenge prize for iCARE project led by Fleur Van Beek** - 29 May 2017



At the Forum for Analytical Science and Technology (FAST) held 16-17 May in Veldhoven, the iCARE project led by PhD student Fleur van Beek of the Van 't Hoff Institute for Molecular Sciences (HIMS) was awarded 5600 euros, to be used for a feasibility study.

### **Bob Pirok wins Csaba Horváth Young Scientist Award 2017** - 27 June 2017



At the HPLC2017 international symposium on high performance liquid-phase separations, held 18-22 June in Prague, PhD researcher Bob Pirok of the Van 't Hoff Institute for Molecular Sciences has won the Csaba Horváth Young Scientist Award, an important prize in the field of Analytical Chemistry.

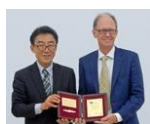


#### **Ning Yan selected as 'Emerging Investigator' in Green Chemistry** - 9 July 2017



Dr Ning Yan of the University of Amsterdam's Research Priority Area Sustainable Chemistry has been chosen as one of the emerging investigators by Green Chemistry, the leading international journal in the area of sustainable chemistry with an impact factor of 9.1.

#### **Fred Brouwer receives Japanese photochemistry award** - 18 September 2017



The Japanese Photochemistry Association (JPA) has awarded its prestigious Honda-Fujishima Lectureship Award to professor Fred Brouwer of the Van 't Hoff Institute for Molecular Sciences (HIMS) at the University of Amsterdam (UvA). Brouwer, who also heads the Nanophotochemistry research group at ARCNL, received the award for his significant contributions to the photochemistry research field.

#### **Praise for Peter Schoenmakers again puts him on 'Power List'** - 31 October 2017



The 2017 edition of the Power List compiled by the magazine The Analytical Scientist features ten categories. Peter Schoenmakers of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) is listed in two of these 'Magnificent Tens'. As runner up in the separation scientists category and at third place in the leaders section he continues his strong performance in this bi-annual international listing of academic relevance.

#### **Moniek Tromp awarded Athena Prize 2017** - 28 November 2017



Dr Moniek Tromp of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences has been awarded the Athena Prize 2017 by the Netherlands Organisation for Scientific Research (NWO). The prize honours her as a top female scientist in the field of chemistry.

#### **Unilever Research Prize for Ilse Denekamp** - 11 December 2017



Ilse Denekamp, PhD candidate at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences, has won the Unilever Research Prize for her MSc project on new supercapacitor materials.

#### **Moniek Tromp elected member of the European Academy of Sciences** - 18 December 2017

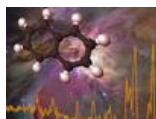


Dr Moniek Tromp of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences has been elected member of the European Academy of Sciences (EurASc).

## 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.

### NWO funding for research into fingerprints of interstellar molecules - 17 January 2017



Together with two new PhD students Dr Annemieke Petrignani and Prof. Wybren Jan Buma of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS) will determine the 'fingerprints' of PAH molecules, and their formation and decomposition in space. The researchers of the HIMS theme 'Molecular Photonics' will receive funding by the Netherlands Organisation for Scientific Research NWO as part of the Dutch Astrochemical Network (DAN) II.

### European grant for cooperation in research on novel cancer approach - 10 July 2017



Researchers of 5 European countries have recently been granted 2.5 million Euro for the project 'Immunotherapy Approaches To Improving Cancer Outcome and Quality of Life' (CANCER). Associate professor Dr Hong Zhang of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences participates in the project, which is funded through the European programme for Research and Innovation Staff Exchange (RISE).

### Sino-Dutch grant for research into flexible printed circuit boards - 28 August 2017



Dr Ning Yan and Prof. Gadi Rothenberg of the University of Amsterdam's Sustainable Chemistry research priority area have been awarded a joint grant to research and develop new catalysts and processes for making the next generation of printed-circuit electronic boards in a project with Chinese academic and industrial partners.

### NWO-KIEM grant for enhancing Amsterdam Piezo Valve - 28 August 2017



Wybren Jan Buma of the Van 't Hoff Institute for Molecular Sciences has recently been awarded a KIEM grant by the Netherlands Organisation for Scientific Research (NWO) within the programme High Tech Systems and Materials. Together with the Dutch company MassSpecpecD Buma will develop an enhanced version of the Amsterdam Piezo Valve, a device for generating high frequency pulsed atomic and molecular beams.

### Towards a natural conservation of healthy fats in food - 19 September 2017



Dutch universities and companies have joined forces to find ways to prevent the decay of fatty acids in food. The Innovation Fund for Chemistry supports this research which is led by Wageningen University. The research group for Analytical Chemistry at the Van 't Hoff Institute for Molecular Sciences (University of Amsterdam), headed by professor Peter Schoenmakers, contributes with crucial expertise in advanced analytical separation technology.

**TooCOLD: A toolbox for studying the chemistry of light-induced degradation** - 23 November 2017



A multidisciplinary research team coordinated by Prof. Maarten van Bommel has been awarded a NWO grant to develop a 'Toolbox for studying the Chemistry Of Light-induced Degradation'. The so-called 'TooCOLD' project will provide new insights to protect works of art, to improve water purification systems and to ensure the quality and safety of food.

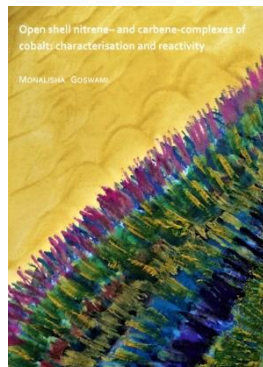
**NWO-ECHO grant for Jan van Maarseveen** - 18 December 2017



The Netherlands Organisation for Scientific Research (NWO) has awarded Jan van Maarseveen of the Van 't Hoff Institute for Molecular Sciences an ECHO project grant of 260,000 euro. He will use the grant to continue his research on the synthesis of so-called lasso peptides.

## Dissertations

In 2017, seventeen students received their PhD at HIMS, one of them - Dr Joen Hermans - with the distinction *cum laude*. All theses are listed below; a link is provided to download each thesis from the UvA repository.



### Open shell nitrene- and carbene-complexes of cobalt: characterisation and reactivity

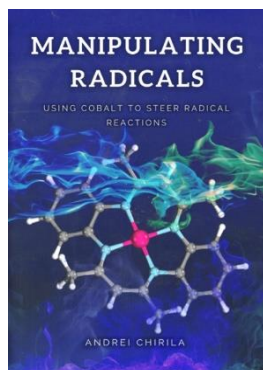
10 November 2017

Author: M. (Monalisa) Goswami

Promotors: B. de Bruin, J.N.H. Reek

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



### Manipulating radicals. Using cobalt to steer radical reactions

02 November 2017

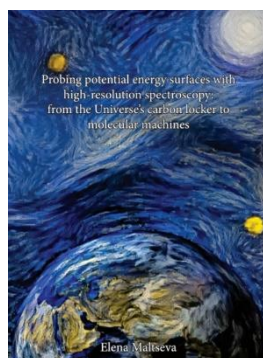
Author: A. (Andrei) Chirila

Promotor: B. de Bruin

Co-promotor: W.I. Dzik

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



### Probing Potential Energy Surfaces with High-Resolution Spectroscopy

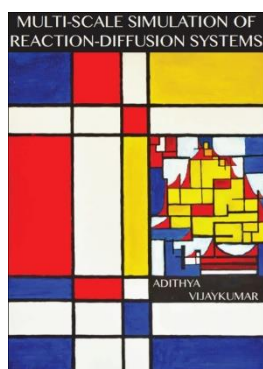
25 October 2017

Author: E. (Elena) O. Maltseva

Promotors: W.J. Buma, J. Oomens

Group: Molecular Photonics

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



### Multi-scale simulation of reaction-diffusion systems

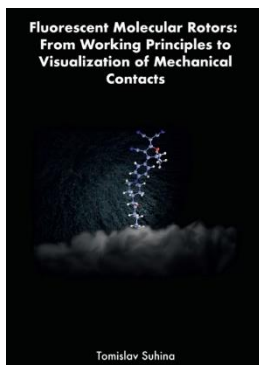
24 October 2017

Author: A. (Adithya) Vijaykumar

Promotors: P.G. Bolhuis, P.R. ten Wolde

Group: Computational Chemistry

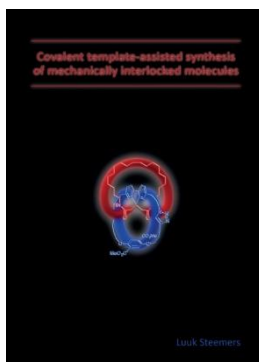
Link: [Read or download this thesis](#)



### Fluorescent molecular rotors

10 October 2017

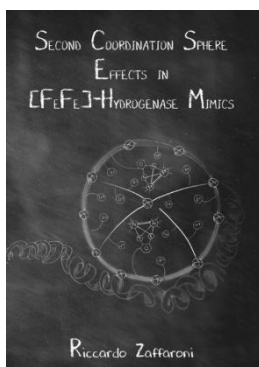
Author: T. (Tomislav) Suhina  
Promotors: A.M. Brouwer, D. Bonn  
Group: Molecular Photonics  
Link: [Read or download this thesis](#)



### Covalent template-assisted synthesis of mechanically interlocked molecules

03 October 2017

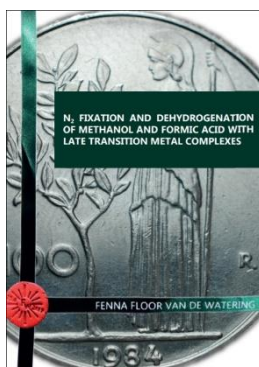
Author: L. (Luuk) Steemers  
Promotors: J.H. van Maarseveen, H. Hiemstra  
Group: Synthetic Organic Chemistry  
Link: [Read or download this thesis](#)



### Second coordination sphere effects in [FeFe]-Hydrogenase mimics

22 June 2017

Author: R. (Riccardo) Zaffaroni  
Promotor: J.N.H. Reek  
Co-promotors: B. de Bruin, R.J. Detz  
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis  
Link: [Read or download this thesis](#)



### N<sub>2</sub> fixation and dehydrogenation of methanol and formic acid with late transition metal complexes

15 June 2017

Author: F. (Fenna) F. van de Watering  
Promotors: J.N.H. Reek, B. de Bruin  
Co-promotor: W.I. Dzik  
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis  
Link: [Read or download this thesis](#)

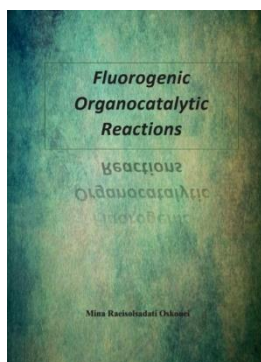


### Metal soaps in paint

09 May 2017

Author: J. (Joen) J. Hermans  
Promotor: P.D. Iedema  
Co-Promotor: K. Keune  
Group: Computational Polymer Chemistry  
Link: [Read or download this thesis](#)





### **Fluorogenic organocatalytic reactions**

*25 April 2017*

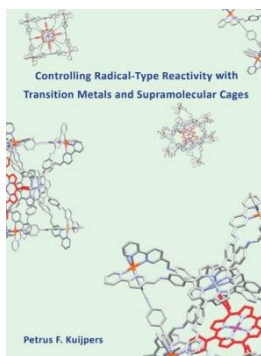
Author: M. (Mina) Raeisolsadati Oskouei

Promotor: A.M. Brouwer

Co-Promotor: H. Hiemstra

Group: Molecular Photonics

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



### **Controlling radical-type reactivity with transition metals and supramolecular cages**

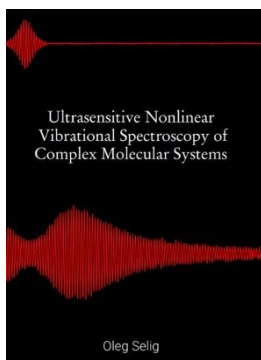
*19 April 2017*

Author: P. (Paul) F. Kuijpers

Promotors: B. de Bruin, J.N.H. Reek

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



### **Ultrasensitive nonlinear vibrational spectroscopy of complex molecular systems**

*30 March 2017*

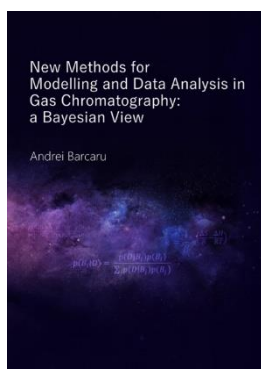
Author: O. (Oleg) Selig

Promotor: H.J. Bakker

Co-Promotor: Y.A. Rezus

Group: Molecular Photonics

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



### **New methods for modelling and data analysis in gas chromatography: a Bayesian view**

*29 March 2017*

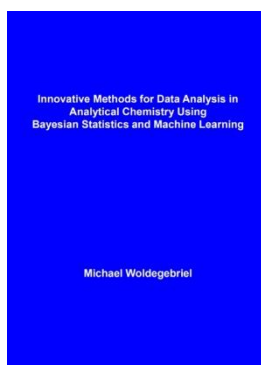
Author: A. (Andrei) Barcaru

Promotor: P.J. Schoenmakers

Co-promotor: G.Vivo Truyols

Group: Analytical Chemistry

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



### **Innovative methods for data analysis in analytical chemistry using bayesian statistics and machine learning**

*29 March 2017*

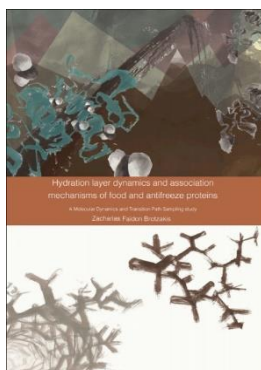
Author: M. (Michael) T. Woldegebriel

Promotor: P.J. Schoenmakers

Co-promotor: G.Vivo Truyols

Group: Analytical Chemistry

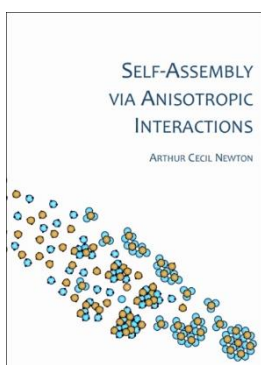
Link: [Read or download this thesis](#)



### **Hydration Layer Dynamics and Association Mechanisms of Food and Antifreeze Proteins**

*07 March 2017*

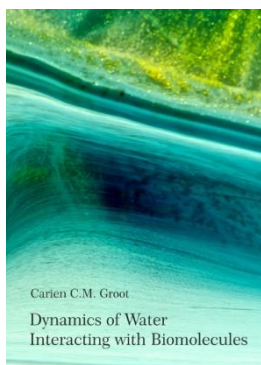
Author: Z. (Zacharias) F. Brotzakis  
Promotor: P.G. Bolhuis  
Group: Computational Chemistry  
Link: [Read or download this thesis](#)



*26 January 2017*

### **Self-assembly via Anisotropic Interactions**

Author: A. (Arthur) C. Newton  
Promotor: P.G. Bolhuis  
Co-promotor: P. Schall  
Group: Computational Chemistry  
Link: [Read or download this thesis](#)



*13 January 2017*

### **Dynamics of Water Interacting with Biomolecules**

Author: C. (Carien) C.C. Groot  
Promotor: H.J. Bakker  
Group: Molecular Photonics  
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. In 2017, HIMS received funding for 16 research proposals of which as many as 12 were inspired by future applications. Furthermore, 10 of these projects involve companies participating and co-financing. On top of all that, two new contract research projects were started directly for the benefit of companies.**

In 2017, four new patent applications were filed, in collaboration with research consortia or companies. In case results of HIMS research may have future commercial value, HIMS follows an active approach to find industrial partners to collaborate with. The technology transfer office IXA supports HIMS scientists with contracts and IP affairs, and advises on funding (grants). Where appropriate HIMS protects its intellectual property. Usually, industrial partners, that are the potential users of the knowledge, will be involved in an early stage. In general, the institute does not apply for patents for exploration by itself.

### Amsterdam Chemistry Innovation Day

On 20 October 2017, HIMS organised together with Innovation Lab Chemistry Amsterdam (ILCA) and the Amsterdam Green Campus the Amsterdam Chemistry Innovation Day (ACID 2017). Over 95 representatives from companies (from Amsterdam SMEs to multinationals) and academic groups gathered at the HIMS laboratories.



The day started with an inspiring lecture by Nelleke van der Puil, Vice President of Materials at The LEGO Group. PhD students and postdocs of HIMS took the opportunity to meet potential employers outside academia and interactive workshops and a poster session were used to discuss opportunities for research collaborations. The RPA Sustainable Chemistry discussed valorisation and possibilities for cooperation with its Industrial Advisory Board on 20 October 2017 too.

ACID illustrates the growing collaboration between HIMS and ILCA. Several companies housing in the Matrix buildings at the Science Park Amsterdam visit HIMS on a regularly base to collect NMR spectra or perform other measurements. Prof.dr. Gert-Jan Gruter initiated a close collaboration between HIMS and the company Avantium where he is CTO.

### Training and collaboration

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

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

## Patents and utilization

- **Novel nickel-based complex and use thereof in a method for the oligomerisation of olefins**  
Prof.dr. Joost Reek, dr. Pierre Boulens, dr. H. Olivier-bourbigou (IFP), dr. P.-A. Breuil (IFP).  
*Patent application filed by IFP Energies Nouvelles was granted by EU patent office on 3 May 2017, under number EP3013841.*
- **Catalysts and Processes for Producing Aldehydes**  
Prof.dr. Joost Reek, dr. X. Wang and dr. J. Rodgers (Eastman).  
*Patent application filed by Eastman Corp. was granted by US patent office on 16 May 2017, under number US 9649625 B1.*
- **Use of a nitrogen-doped porous carbon material for enriching phosphorylated proteins or peptides**  
Prof.dr. Gadi Rothenberg, dr. Michelle Camenzuli.  
*Patent application filed at EPO.*
- **Multicyclic peptides and methods for their Preparation**  
prof.dr. Jan van Maarseveen, Gaston Richelle, Dieuwertje Streefkerk, prof.dr. Peter Timmerman.  
*Patent application filed at EPO: Eur. Pat. Appl. EP16202466.*
- **Molecular heaters**  
Prof.dr. Wybren Jan Buma, prof. V. Stavros (U. Warwick), prof. M. Ashfold (U. Bristol).  
*Patent application filed at UK PO.*
- **Supercapacitor and porous material**  
Prof.dr. Gadi Rothenberg.  
*Patent application abandoned.*
- **Method for removing cyanide compounds from waste water**  
Prof.dr. Gadi Rothenberg, dr. N.R. Shiju.  
*Patent application abandoned.*
- **Design of a smart inlet /outlet**  
Dr. S. Nawada, prof.dr. Peter Schoenmakers.  
*Evaluated, no follow-up.*
- **XASPECT - benchtop Xray absorption spectrometer**  
Dr. Moniek Tromp.  
*Possibilities for start-up evaluated.*
- **HPBandage - Hydrophobic bandage**  
Dr. Tomislav Suhina.  
*AMSIA application, no follow-up.*
- **Electrochemical Methane Reforming**  
Dr. Ning Yan.  
*Under Evaluation.*
- **Production of Perovskite materials**  
Dr. René Williams.  
*Under Evaluation.*

- **Surface Acoustic Wave Nebulisation Mass Spectrometry (SAWN) as a service**  
Prof.dr. Garry Corthals.  
*Possibilities for start-up, under evaluation.*
- **New organic pigment**  
Dr. Chris Sloomweg, Evi Habraken M.Sc..  
*IDF under evaluation for patent application.*



## Outreach

### Lectures and other contributions

#### *For the general public*

- Spui 25 lecture for Bèta in de Binnenstad: *Aantrekkingskracht op moleculair niveau*' (Joost Reek)
- Lecture for members leden IVN Woerden: *'Hoe werkt een spinnendraad en andere vormen van chemische oorlogsvoering in de wereld van insecten'* (Bas de Bruin).
- Lecture for VOLA (Vereniging van Oud-leden van het ACD): *"Mooie Moleculen Maken: Studeren en Werken aan de Universiteit van 1970–2017"* (Henk Hiemstra).
- Associate Editor of the magazine *'Amsterdam Science'*, a platform for communicating the latest and most interesting findings of Amsterdam universities and research institutes to Dutch society (Francesco Mutti).
- Presentation about the restoration of colour to 18th-century furniture by using light, at the 'Bessensap' conference for science and media (Maarten van Bommel).
- Pop-up lecture *'Hoe schoon is varen?'* on a ferry in the Amsterdam harbour, in the honour of the University of Amsterdam's lustrum (385 years) (Moniek Tromp).
- Spiegelbeeld VHTO (Landelijk expertisebureau meisjes/vrouwen en beta/techniek), setting up an outreach science program for girls (6-10 years), in collaboration with VHTO (Moniek Tromp).
- Lecture for children (Kinderlezing): *'Hoe weet ik of iets waar is?'* at Science Center NEMO (Jocelyne Vreede).



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

- General and inorganic chemistry lectures for the students representing the Netherlands at the 49th International Chemistry Olympiad (Stefania Grecea).
- Lecture *Hoe trek je een moleculaire draad door een ring? Op weg naar de lasso peptiden*, Woudschoten conference for highschool chemistry teachers (Jan van Maarseveen).
- Lecturer in the final training of the Dutch students that were selected for the International Chemistry Olympics 2017 (Steen Ingemann Jørgensen).


#### *For other students*

- Lecture *'Op weg naar de synthese van lasso peptiden. Hoe leg je een knoop in een lineair molecuul?'*, Fontys University of Applied Sciences, Eindhoven (Jan van Maarseveen).

#### *TV and radio broadcast contributions*

- Klokhuis TV broadcast *'Fireworks'* (Bas de Bruin).  
▶ [Klokhuis](#).
- TV programme *'Proefkeuken'*, on fireworks (Moniek Tromp)  
▶ [Proefkeuken VPRO](#).

## HIMS researchers in the media

- ***'I pursue the unknown particle'***  
An interview with Moniek Tromp for Kennislink after winning the Athena price for excellent female researchers in chemistry.  
▶ [Kennislink, 11 December 2017.](#)
- ***Painting scanner to solve crimes***  
Arian van Asten in various media about new research which shows that the X-Ray Fluorescence scanner used in the Rijksmuseum can also trace hard to find evidence on e.g. clothing of victims and perpetrators of crimes.  
▶ [Volkskrant, 12 November.](#)  
▶ Nederlands Dagblad, 14 November.  
▶ [AT5, 13 November.](#)
- ***From toilet to electric socket***  
Gadi Rothenberg and other UvA chemists in het Parool, Magazine of the Royal Geographical Society and the Leeuwarder Courant about winning energy out of toilet paper.  
▶ [Magazine of the Royal Geographical Society](#) (PDF).  
▶ [Leeuwarder Courant, 28 October](#) (PDF).  
▶ [Parool, 21 October](#) (PDF).  

- ***Biological water is simply water***  
Sander Woutersen and others in C2W about their research on the behaviour of 'biological water' in living cells.  
▶ [C2W, 12 October.](#)
- ***Cooperation with ECN on electricity from used toilet paper***  
Research of Bob van der Zwaan on the first techno-economic analysis of this waste recycling concept in Groene Courant.  
▶ Groene Courant, 26 September.
- ***Used toilet paper converted in electricity***  
The research project of Gadi Rothenberg and Bob van der Zwaan appeared on Phys.org and Energienieuws.  
▶ [Phys.org., 12 September.](#)  
▶ [Energienieuws, 19 September.](#)
- ***More than 6 billion tons of plastic pollutes our earth***  
Gert-Jan Gruter in a NOS article about the problem of the accumulation of plastic waste.  
▶ [NOS op 3, 20 July.](#)
- ***Maarten van Bommel at Bessensap***  
On 16 June, NWO Bessensap, a meeting organized by NWO and VWN (Vereniging voor Wetenschappsjournalistiek en -communicatie Nederland) was held in De Rode Hoed in Amsterdam. Here journalists, press officers and researchers were gathered, and [Maarten van Bommel](#) was one of the speakers. He gave a presentation about the restoration of color to 18<sup>th</sup> century furniture by using light.  
▶ [Kennislink, 29 June 2017.](#)
- ***Dutch inventors conquer the world***  
Gert-Jan Gruter is nominated for the European Inventor Awards 2017. In the radio

programme 'Langs de Lijn En Omstreken', he and colleague inventor Hans Clevers are interviewed.

▶ [NPO Radio 1, 7 June.](#)

- ***The harmful effect of metal soaps on oil paintings***

An interview in NRC with Joen Hermans who recently completed his PhD on the chemical process of metal soap formation in paintings.

▶ [NRC, 2 June.](#)



- ***Useful CO<sub>2</sub>***

Gert-Jan Gruter in an article of Kennislink about using CO<sub>2</sub> for making useful products.

▶ [Kennislink 17 May.](#)

- ***New catalyst developed by Shiju Raveendran in various media***

Shiju Raveendran and his colleagues recently discovered a new catalyst which can efficiently convert Carbon dioxide(CO<sub>2</sub>) to Carbon monoxide(CO). The news appeared in various (international) science magazines.

▶ [The Science Times, 11 April.](#)

▶ [Phys.org, 7 April.](#)

▶ [Science Daily, 6 April.](#)

## Facts & Figures

### Research

#### Research output

Research output 2017 per type of publication (source: PURE).

HIMS themes	AC	CC	MP	SC	Other	Joint	Total
Refereed articles	24	54	53	96		-8	219
Non-refereed articles		1		1	1		2
Book (authored)				1			1
Book (edited)	1						1
Book (chapter)s	1		1	2			4
PhD-theses	2	4	5	6			17
Non-refereed conference publications	1				1		1
Not eligible			4				4
Refereed conference publications		1	3		2		4
Other conference contrib. (poster, abstract)		4	5	11	1		20
Patents	1			1		-1	1
<b>Total</b>	<b>30</b>	<b>64</b>	<b>71</b>	<b>118</b>	<b>5</b>	<b>-9</b>	<b>279</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		6	4	10	11			31
Other honourable achievements		1	2	2	7			12
Key note lectures		2	33	36	40	11		122
Media coverage		4	3	3	14	1		25
Outreach activities	Organizing an event		4	21	9			34
	Lectures for general or professional public		1	1				2
<b>Total</b>		<b>13</b>	<b>47</b>	<b>73</b>	<b>81</b>	<b>12</b>		<b>226</b>

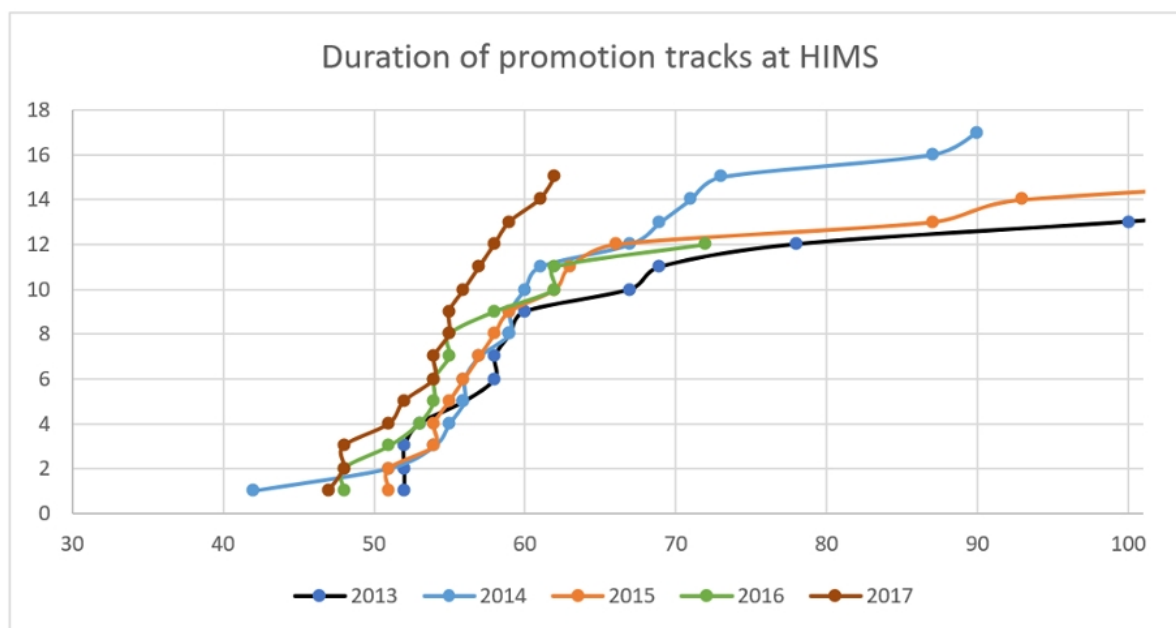
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis.

#### 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 (incl external)			Success rates of graduation in years (t) after start (UvA internal only)										Total				
Start	m	f	Total	t ≤ 4		t ≤ 5		t ≤ 6		t ≤ 7		Graduated		Not yet		Discontinued	
					%		%		%		%		%		%		%
2009	7	8	15	0	0	8	53	3	20	0	0	11	73	0	0	4	27
2010	12	6	18	0	0	6	33	7	0	0	0	16	89	0	0	2	11
2011	11	10	21	3	14	6	29	4	19	2	0	15	71	1	0	5	24
2012	14	7	21	1	5	14	67	3	0	1	0	19	90	1	0	1	5
2013	5	7	12	2	17	5	42	3	25	1	0	11	92	0	0	1	8
<b>Totaal</b>	<b>49</b>	<b>38</b>	<b>87</b>	<b>6</b>	<b>7</b>	<b>39</b>	<b>45</b>	<b>20</b>	<b>23</b>	<b>4</b>	<b>0</b>	<b>72</b>	<b>83</b>	<b>2</b>	<b>0</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 2017) 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)	4,2	2,1	6,4	3,2	6,7	3,4	14,0	7,0	0,2	0,0	31,5	15,7
Post-docs (2)	7,0	6,3	3,9	3,5	3,8	3,4	15,4	13,9	0,0	0,0	30,1	27,1
PhD students (3)	8,4	6,3	13,4	10,1	13,0	9,7	46,6	35,0	0,0	0,0	81,4	61,1
<b>Total research staff</b>	<b>19,6</b>	<b>14,7</b>	<b>23,7</b>	<b>16,8</b>	<b>23,5</b>	<b>16,5</b>	<b>76,0</b>	<b>55,8</b>	<b>0,2</b>	<b>0,0</b>	<b>143,0</b>	<b>103,8</b>
Technicians (4)	3,0	3,0	0,0	0,0	2,8	2,8	9,6	9,6	1,0	1,0	16,4	16,4
Visiting fellows	0,0	0,0	1,0	0,5	0,0	0,0	1,0	0,5	0	0,0	2,0	1,0
Support staff (4)	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	6,4	6,4	6,4	6,4
<b>Total staff</b>	<b>22,6</b>	<b>17,7</b>	<b>24,7</b>	<b>17,3</b>	<b>26,3</b>	<b>19,3</b>	<b>86,7</b>	<b>66,0</b>	<b>7,6</b>	<b>7,4</b>	<b>167,8</b>	<b>127,6</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 2017.

Age bracket	Number	Male	Female	Dutch	Other EU	Other
30-40	5 (16%)	3	2	2	1	2
40-50	10 (31%)	7	3	7	2	1
50-60	10 (31%)	10	0	8	1	1
60+	7 (22%)	7	0	6	1	0
Total	32	27 (84%)	5 (16%)	23 (72%)	5(16%)	4 (12%)

## 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 2017 of HIMS per funding type (fte)

HIMS Themes	Research					Total	%	Support	Total	%
	AC	CC	MP	SC	Other					
Direct funding	10,2	8,6	8,0	33,3	0,4	60,6	43%	5,35	66,0	45%
Research grants	3,9	8,8	8,7	36,8	0,0	58,1	41%		58,1	40%
Contract research	6,3	1,5	1,5	13,1	0,1	22,5	16%	0,1	22,6	15%
<b>Total</b>	<b>20,3</b>	<b>19,0</b>	<b>18,3</b>	<b>83,2</b>	<b>0,5</b>	<b>141,3</b>	<b>100%</b>	<b>22,7</b>	<b>146,7</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 2017 (mln €) per funding type.

HIMS themes	AC	CC	MP	SC	Other	Total <sup>1</sup>
Direct funding	0,00	0,00	0,00	0,00	0,00	<b>0</b>
Research grants	0,80	0,01	0,02	3,76	0,00	<b>4,58</b>
Contract	0,07	0,02	0,34	1,08	0,00	<b>1,49</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>6,07</b>

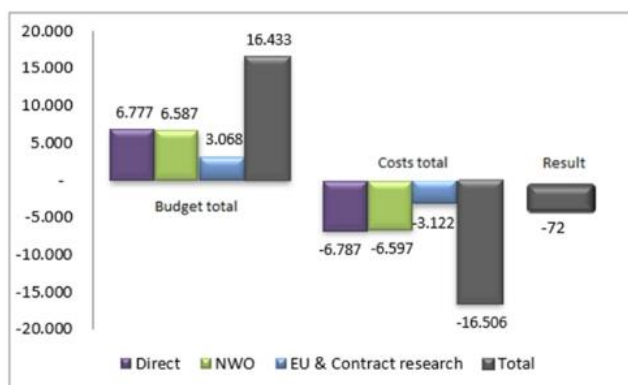
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. Note 1: Budgets were obtained for a total of (in FTE) 15 PhDs, 4,3 PD and 1,2 staff.

## HIMS result 2017 (k€)

The HIMS result of 2017 is a negative -k€ 72, largely due to a loss in EU- and contract research. A larger negative result was budgeted, so the negative result was expected and will be compensated in the following years.

2017	EU & Contract research			Total
	Direct	NWO	research	
HIMS Base Budget	3.765			3.765
Budget (variable1)	684	6.024	2.937	9.645
Other income 2	2.328	563	131	3.022
<b>Budget total</b>	<b>6.777</b>	<b>6.587</b>	<b>3.068</b>	<b>16.433</b>
<i>Percentage</i>	<i>41%</i>	<i>40%</i>	<i>19%</i>	<i>100%</i>
Personal costs	-4.542	-2.688	-1.341	-8.571
Other costs (projects)	-1.673	-974	-587	-3.234
Overheads 3	1.644	-2.935	-1.157	-2.448
<b>Costs total</b>	<b>-6.787</b>	<b>-6.597</b>	<b>-3.122</b>	<b>-16.506</b>
<i>Percentage</i>	<i>41%</i>	<i>40%</i>	<i>19%</i>	<i>100%</i>
<b>HIMS Result 2017</b>	<b>-7</b>	<b>-10</b>	<b>-55</b>	<b>-72</b>

	EU & Contract			Total
	Direct	NWO	research	
Budget total	6.777	6.587	3.068	16.433
Costs total	-6.787	-6.597	-3.122	-16.506
<b>HIMS Result 2017</b>	<b>-7</b>	<b>-10</b>	<b>-55</b>	<b>-72</b>



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.