



Annual Report 2019

*Chemistry
research
that matters*

Van 't Hoff Institute
for Molecular Sciences

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Executive summary

The HIMS annual report showcases our scientific highlights and key publications of the year 2019. Here we provide an anthology to give you an overall impression of the van 't Hoff Institute's performance in a few minutes of reading.

In 2019 the 'Connecting science' proposal of the Faculty of Science was granted by the National Sectorplan Bèta & Techniek. The Van 't Hoff Institute for Molecular Sciences received 7 new staff positions that are aimed to connect our strong disciplinary research themes. On top of this substantial budget, and the numerous new projects that were acquired (including an NWO VIDI grant for Dr Ning Yan and an ERC Proof of Concept grant for Prof. Joost Reek) the budget for the Research Priority Area Sustainable Chemistry was renewed by the UvA board.

People



HIMS director Prof. Peter Bolhuis: "With the help of the Sectorplan, HIMS has attracted talented staff to kickstart new, exciting and cross disciplinary research lines." Photo by Jan Willem Steenmeijer.

Four talented young scientists started on a tenure track position at the Van 't Hoff Institute. In January, Veni-laureate Dr Andrea Gargano started, in April Dr Bob Pirok, in June Vidi-laureate dr. Annemieke Petrignani began on a MacGillavry Fellowship and in September Dr Alina Astefanei came over from the Rijksdienst voor het Cultureel Erfgoed. Prof. Herma Cuppen of Radboud University was appointed as a new part-time professor of Computational Chemistry at HIMS. To enforce the collaboration on electrochemistry Dr Klaas Jan Schouten of Avantium was appointed as part-time research

assistant professor in Electrocatalysis and Applied Electrochemistry. In July Prof. Peter Bolhuis succeeded Prof. Peter Schoenmakers as the director of the Van 't Hoff Institute.

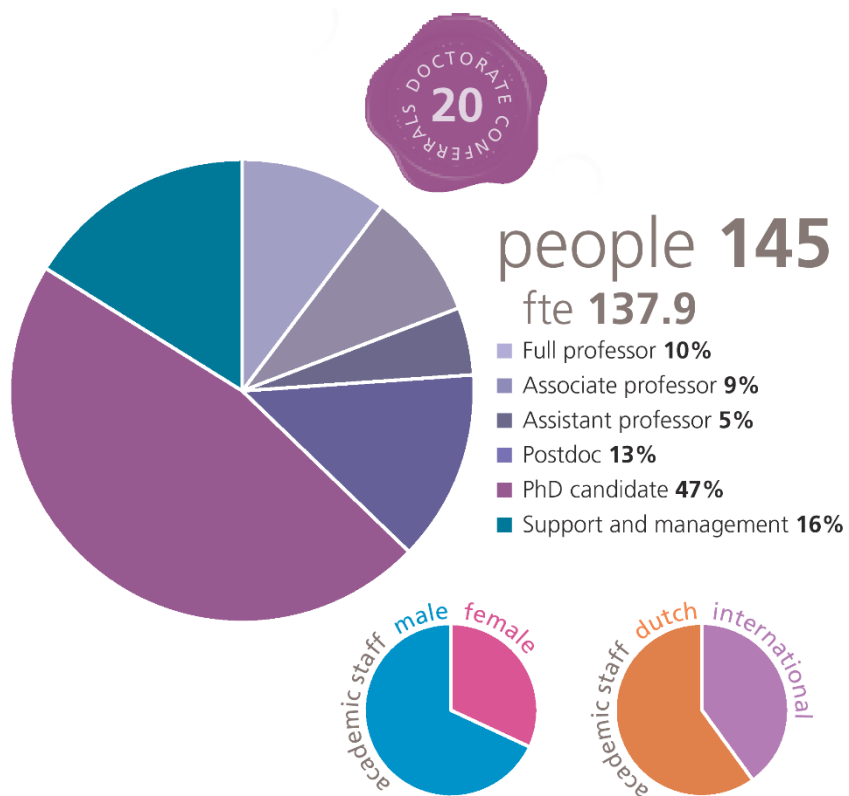
Sadly we also lost a few people that were connected to HIMS for many years. In particular, we commemorate emeritus professors Kees Vrieze and Gerrit Jan Koomen who passed away this year.

New initiatives

Together with the UvA Institutes for Physics and Informatics, the Computational Soft Matter initiative commenced with two additional staff positions. Together with the UvA institutes for Informatics, Life Sciences and Ecology the *AI 4 Science* lab was established with 5 PhD students. Early 2019, the UvA sold its shares based upon a patent on organic synthesis filed in 1998. This gave the Van 't Hoff Institute the opportunity to refurbish and renew equipment used by the Synthetic Organic Chemistry group.

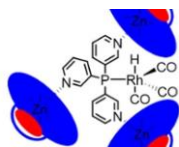
In 2019, spin-off company SusPhos was launched, with the aim to contribute to a circular economy in phosphorus and to establish a sustainable use of this resource. Van 't Hoff Institute's former PhD student Dr Marissa de Boer heads this new company, which in 2019 already received loans for further investments and awards (eg. Amsterdam Science & Innovation Award, NWO Gouden Kiem) that emphasize its great potential. Together with the other founding fathers Dr Chris Slootweg and Bas de Jong and other group members, SusPhos presented a booth at the science program of the Lowlands festival.

HIMS 2019 at a glance:



Scientific Highlights 2019

Cofactor switches catalyst - 16 January 2019



A new catalyst was developed that can be activated by addition of a 'cofactor', in this case a small signalling molecule, resembling processes found in enzymes. PhD-student Lukas Jongkind and professor Joost Reek, affiliated with the UvA research priority area Sustainable Chemistry, reported their findings in *Angewandte Chemie*.

Lukas J. Jongkind, Johannes A.A.W. Elemans, Joost Reek: *Cofactor controlled encapsulation of a rhodium hydroformylation catalyst*. *Angewandte Chemie*, First published: 09 January 2019. DOI: [10.1002/anie.201812610](https://doi.org/10.1002/anie.201812610)

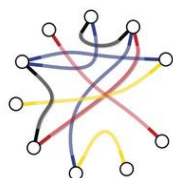
The hidden ingredient in Rembrandt's impasto - 21 January 2019



Rembrandt van Rijn revolutionized painting with a 3D effect using his impasto technique, where thick paint makes a masterpiece protrude from the surface. An international research team with Dr Katrien Keune discovered that Rembrandt's impasto contains an unexpected component: plumbonacrite. This provides insight into the use of paint by the most famous Dutch painter.

Victor Gonzalez, Marine Cotte, Gilles Wallez, Annelies van Loon, Wout de Nolf, Myriam Eveno, Katrien Keune, Petria Noble en Joris Dik: *Rembrandt's impasto deciphered via identification of unusual plumbonacrite by multi-modal Synchrotron X-ray Diffraction*, *Angewandte Chemie International Edition*, online 7 januari 2019
DOI: [10.1002/anie.201813105](https://doi.org/10.1002/anie.201813105)

Multiphysics made easy with random coloured graphs - 31 January 2019



As a result of research performed at the Computational Polymer Chemistry Group, researcher Ivan Kryven proposed a novel theory for representing random structures with multiple types of interactions. In a paper in *Nature Communications*, he shed light on emergent processes in random coloured graphs. What does this bring for chemical research?

I.Kryven "Bond percolation in coloured and multiplex networks", *Nature Communications* 10, 404.
DOI: [10.1038/s41467-018-08009-9](https://doi.org/10.1038/s41467-018-08009-9)

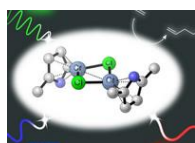
Chris Sloopweg in Nature Chemistry: 'Green Chemistry is an outdated concept' - 21 February 2019



In a commentary published in *Nature Chemistry*, Dr Chris Sloopweg introduced the concept of Circular Chemistry. In analogy to the well-known 12 principles of Green Chemistry, he presented the 12 principles of Circular Chemistry and outlined the paradigm shift that is needed in chemistry in order to establish a circular economy.

Tom Keijer, Vincent Bakker, and J. Chris Sloopweg: *Circular Chemistry to enable a Circular Economy*. *Nature Chemistry*, Volume 11, March 2019., 190-195. DOI: [10.1038/s41557-019-0226-9](https://doi.org/10.1038/s41557-019-0226-9)

UvA chemists shine light on catalyst for industrial plastic production - 22 February 2019



By using a combination of multiple spectroscopic techniques and quantumchemical calculations, PhD-student Bas Venderbosch and colleagues found new details about the formation of the active catalyst in the industrial production of polyethene plastic. They published their results in *ACS Catalysis*.

Bas Venderbosch, Jean-Pierre H. Oudsen, Lukas A. Wolzak, David J. Martin, Ties J. Korstanje and Moniek Tromp: *Spectroscopic Investigation of the Activation of a Chromium-Pyrrolyl Ethene Trimerization Catalyst* *ACS Catal.* 2019, 9, 1197–1210 DOI: [10.1021/acscatal.8b0341](https://doi.org/10.1021/acscatal.8b0341)

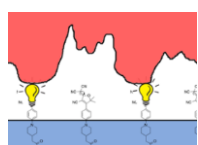
And the secret ingredient is... the network - 25 February 2019



In a recent publication in Scientific Reports, PhD student Verena Schamboeck and supervisors Piet Iedema and Ivan Kryven showed how the mathematical theory of random graphs is vital for rational material design. They investigated the properties of multiplex networks and were able to link these to the mechanical properties of polymers.

Schamboeck, Verena, Iedema, Piet D. and Kryven, Ivan "Dynamic Networks that Drive the Process of Irreversible Step-Growth Polymerization", Scientific Reports (2019). DOI: [10.1038/s41598-018-37942-4](https://doi.org/10.1038/s41598-018-37942-4)

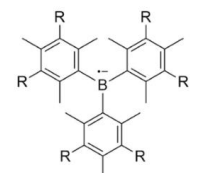
Experimental visualisation of friction reduction - 8 April 2019



A team of physicists and chemists led by Fred Brouwer (HIMS) and Daniel Bonn (IOP) experimentally visualized the mechanism behind friction reduction. The results were published in the journal Science Advances.

Frictional weakening of slip interfaces, B. Weber, T. Suhina, A. M. Brouwer and D. Bonn. *Sci. Adv.* **2019**, Vol. 5, no. 4, eaav7603. DOI: [10.1126/sciadv.aav7603](https://doi.org/10.1126/sciadv.aav7603)

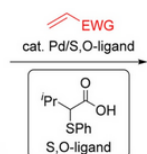
A new mode of chemical reactivity - 16 April 2019



Together with colleagues from the University of East Anglia and Imperial College, Dr Chris Slootweg and Dr Andreas Ehlers published a paper in Angewandte Chemie on the use of boranes in dihydrogen splitting. They describe a new mode of chemical reactivity for metal-free hydrogen activation by Lewis acidic boranes.

Elliot L. Bennett, Elliot J. Lawrence, Robin J. Blagg, Anna S. Mullen, Fraser MacMillan, Andreas W. Ehlers, Daniel J. Scott, Joshua S. Sapsford, Andrew E. Ashley, Gregory G. Wildgoose, and J. Chris Slootweg: *A New Mode of Chemical Reactivity for Metal-Free Hydrogen Activation by Lewis Acidic Boranes*. Angewandte Chemie Int. Ed., First published: 09 April 2019. DOI: [10.1002/anie.201900861](https://doi.org/10.1002/anie.201900861)

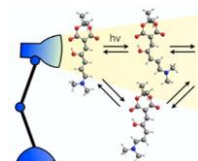
Efficient alternative for multistep synthesis of aniline-based drug precursors - 18 April 2019



Researchers led by associate professor Tati Fernández Ibáñez of the Synthetic Organic Chemistry group developed the first general para-selective C–H olefination of aniline derivatives by Pd/S,O-ligand catalysis. Their results were published online by the Journal of the American Chemical Society (JACS).

Kananat Naksomboon, Jordi Poater, F. Matthias Bickelhaupt, and M. Ángeles Fernández-Ibáñez: *para-Selective C–H Olefination of Aniline Derivatives via Pd/S,O-Ligand Catalysis*. J. Am. Chem. Soc., Article ASAP DOI: [10.1021/jacs.9b01908](https://doi.org/10.1021/jacs.9b01908)

Novel molecular multi-step photoswitches caught in the act - 8 May 2019



Scientists at HIMS, together with collaborators from the University of Groningen, the University of Twente and the European Laboratory for Non-Linear Spectroscopy in Italy, were the first to follow the entire sequence of structural transformations in a new class of molecular switches. The results were published in the Journal of the American Chemical Society.

Habiburrahman Zulfikri, Mark A.J. Koenis, Michael M. Lerch, Mariangela Di Donato, Wiktor Szymański, Claudia Filippi, Ben L. Feringa, Wybren Jan Buma: *Taming the complexity of donor-acceptor Stenhouse adducts: IR movies of the complete switching pathway*. J. Am. Chem. Soc. 2019, 141, 7376–7384; DOI: [10.1021/jacs.9b0034](https://doi.org/10.1021/jacs.9b0034)

Versatile and fast all-visible-light molecular switch achieves breakthrough in molecular photocontrol - 3 June 2019

An international consortium of scientists including Michiel Hilbers and Wybren Jan Buma of the HIMS



Molecular Photonics group developed an entirely new class of molecular photoswitches. These meet many 'holy grail' requirements thought to be impossible to achieve. The results were published in Nature Communications.

Mark W.H. Hoorens, Miroslav Medved', Adèle D. Laurent, Mariangela Di Donato, Samuele Fanetti, Laura Slappendel, Michiel Hilbers, Ben L. Feringa, Wybren Jan Buma & Wiktor Szymanski: *Iminothioindoxyl as a molecular photoswitch with 100 nm band separation in the visible range* Nature Communications **10**, Article number: 2390 (2019); DOI [10.1038/s41467-019-10251-8](https://doi.org/10.1038/s41467-019-10251-8)

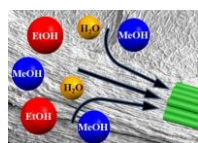
Researchers unravel important feature of the molecular structure of oil paint - 25 June 2019



In 'Science Advances' researchers of HIMS and Rijksmuseum describe the role of zinc ions in the molecular network of oil paint. Their studies could explain why paintings made with zinc white pigment are so sensitive to high humidity conditions. The research also yielded important insights in the world of plastics.

Joen Hermans, Lambert Baij, Mark Koenis, Katrien Keune, Piet Iedema, Sander Woutersen: '2D-IR spectroscopy for oil paint conservation: Elucidating the water-sensitive structure of zinc carboxylate clusters in ionomers', in: *Science Advances* 5, eaaw3592 (21 June 2019).

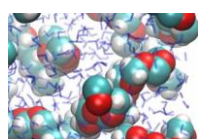
Looking at leaves: enhancing the performance of MOF materials - 26 June 2019



Researchers at the group of Dr Stefania Grecea at the Research Priority Sustainable Chemistry devised a way to enhance the practical performance of Metal-Organic Frameworks (MOFs) by using leaves from the black poplar as a template. In ACS Applied Materials & Interfaces they demonstrate the unique adsorption and separation properties of their bio-inspired design.

Yiwen Tang, David Dubbeldam, Xingmei Guo, Gadi Rothenberg, Stefania Tanase: Efficient Separation of Ethanol–Methanol and Ethanol–Water Mixtures Using ZIF-8 Supported on a Hierarchical Porous Mixed-Oxide Substrate. ACS Appl. Mater. Interfaces 2019, 11, 23, 21126–21136. DOI: [10.1021/acsami.9b02325](https://doi.org/10.1021/acsami.9b02325).

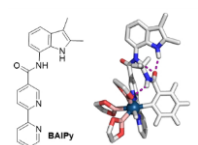
Solubility mystery solved - 30 June 2019



Polyether molecules tend to dissolve better in water as they contain more oxygen and fewer carbon atoms. But there are very counter-intuitive exceptions. The widely used plastic POM has the highest possible oxygen/carbon ratio but is completely insoluble. In Nature Communications, researchers from HIMS and the Max Planck Institute for Polymer Research in Mainz put forth a definitive explanation.

Bernd Ensing, Ambuj Tiwari, Martijn Tros, Johannes Hunger, Sérgio R. Domingos, Cristóbal Pérez, Gertien Smits, Mischa Bonn, Daniel Bonn and Sander Woutersen. *On the origin of the extremely different solubilities of polyethers in water*. Nature Communications (2019) 10:2893 DOI: [10.1038/s41467-019-10783-z](https://doi.org/10.1038/s41467-019-10783-z)

Supramolecular substrate organization makes for a selective H borylation catalyst - 16 July 2019



By applying the concept of supramolecular organization of organic molecules to an iridium-based catalyst, researchers led by Prof. Joost Reek were able to selectively functionalize CH bonds in amide-containing molecules. The new strategy, published in Angewandte Chemie, will enable more efficient and sustainable synthesis of complex organic molecules typically found in medicinal applications and the fine chemicals industry.

Shaotao Bai, Charles Bheeter and Joost N. H. Reek: *Hydrogen bond directed ortho-selective C-H borylation of secondary aromatic amides*. *Angewandte Chemie International Edition*, accepted.

DOI: [10.1002/anie.201907366](https://doi.org/10.1002/anie.201907366)

New amine dehydrogenases with unprecedented catalytic properties for the synthesis of drug intermediates - 16 August 2019

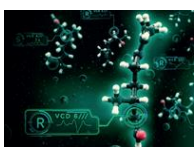


By means of structural-guided protein engineering, researchers from the Biocatalysis group created a new family of amine dehydrogenase enzymes (AmDHs) with unprecedented catalytic properties. The new enzymes, presented in *Nature Communications*, are an important addition to the current enzyme toolbox for the synthesis of chiral amines. They are particularly relevant for the synthesis of key intermediates in the production of important pharmaceuticals, rendering their production more chemically efficient and sustainable.

Joseline A. Houwman, Tanja Knaus, Magda Costa and Francesco G. Mutti, *Efficient synthesis of enantiopure amines from alcohols using resting E. coli cells and ammonia*, *Green Chem.*, **2019**,21, 3846-3857.

DOI: [10.1039/c9gc01059a](https://doi.org/10.1039/c9gc01059a)

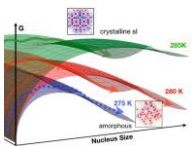
Left or right? Novel algorithm takes chirality determination to the next level - 30 August 2019



Molecular Photonics researchers significantly improved the experimental determination of the chirality of molecules using vibrational circular dichroism (VCD) spectroscopy. By employing a genetic algorithm they were able to 'tame' major uncertainties in VCD analysis. Their improvement, published in *Chemical Science*, could see VCD applied on a large scale, for instance as a tool for high-throughput screening of pharmaceutical compounds or real-time monitoring of (bio)chemical processes.

Mark A. J. Koenis, Yiyin Xia, Sérgio R. Domingos, Lucas Visscher, Wybren Jan Buma and Valentin P. Nicu: *Taming conformational heterogeneity in and with vibrational circular dichroism spectroscopy* *Chem. Sci.* 2019, 10, 7680-7689 DOI: [10.1039/C9SC02866H](https://doi.org/10.1039/C9SC02866H)

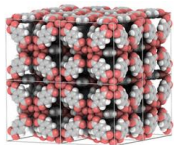
Molecular dynamics simulation sheds new light on methane hydrate formation - 10 September 2019



In a paper in *PNAS*, researchers at the Computational Chemistry group and the Amsterdam Center for Multiscale Modeling provide atomistic insight in the formation of methane hydrates. On the basis of molecular dynamics simulations they explain how selection between competing methane hydrate polymorphs occurs, and how this might be generalized to other hydrates and molecular crystal formation.

Arjun, Thom A. Berendsen, and Peter G. Bolhuis: Unbiased atomistic insight in the competing nucleation mechanisms of methane hydrates. *PNAS* first published September 9, 2019, DOI: [10.1073/pnas.1906502116](https://doi.org/10.1073/pnas.1906502116)

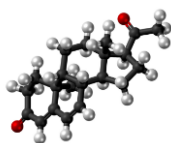
Negative thermal expansion design strategies in metal-organic frameworks - 24 September 2019



In a study published in *Advanced Functional Materials*, a team of American and Dutch researchers present design strategies for adjusting the thermal expansion behaviour of microporous Metal-Organic Frameworks (MOFs). Dr David Dubbeldam and Dr Jurn Heinen contributed to the research, that included both experimental work and computer simulation.

Nicholas C. Burtch, Samuel J. Baxter, Jurn Heinen, Ashley Bird, Andreas Schneemann, David Dubbeldam, Angus P. Wilkinson: Negative Thermal Expansion Design Strategies in a Diverse Series of Metal-Organic Frameworks. *Advanced Functional Materials*, first published: 18 September 2019. DOI: [10.1002/adfm.201904669](https://doi.org/10.1002/adfm.201904669).

University of Amsterdam improves method for determining the structure of complex molecules in medicines - 17 October 2019



Researchers at the Molecular Photonics group improved vibrational circular dichroism (VCD) analysis so that a single measurement suffices to determine the absolute configuration of many-centre chiral molecules that are often used as active ingredients in medicines. The same VCD measurement also provides insight into contamination levels and is therefore also suitable for quality control in pharmaceutical production.

Mark A.J.Koenis, Eveline H.Tiekink, Davita M.E.van Raamsdonk, Nadav U. Joosten, Susanne A.Gooijer, Valentin P.Nicu, Lucas Visscher, and Wybren J.Buma: *Analytical chemistry on many-center chiral compounds based on vibrational circular dichroism: Absolute configuration assignments and determination of contaminant levels*. *Analytica Chimica Acta*, in press, published online 14 September 2019. DOI: 10.1016/j.aca.2019.09.021

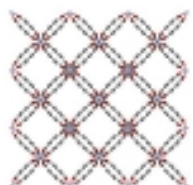
Novel single-atom catalyst for efficient water oxidation - 18 October 2019



Researchers at the research priority area Sustainable Chemistry developed a strategy for creating hybrid materials with superior properties in electrocatalytic water oxidation. In the *Journal of Materials Chemistry A* they report how their 'single-atom' catalyst achieves sufficient conversion rates at a low overpotential, which is of crucial importance to splitting water and storing renewable energy.

Ning Yan, Remko J. Detz, Nitish Govindarajan, Jacobus M. Koelewijn, Bin Hua, Peng Li, Evert Jan Meijer and Joost N. H. Reek: Selective surface functionalization generating site-isolated Ir on a MnO_x/N-doped carbon composite for robust electrocatalytic water oxidation. *J. Mater. Chem. A*, 2019,7, 23098-23104. DOI: 10.1039/C9TA08447A

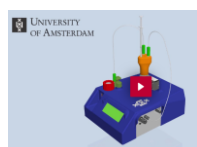
Novel advanced MOF/polymer composite allows for tuneable separation and low cost regeneration - 21 October 2019



Researchers at HIMS and the research priority area Sustainable Chemistry developed a rational design of metal-organic framework (MOF) composites with enhanced water-alcohol separation properties. In *ACS Applied Materials & Interfaces* they demonstrate that loading MOF pores with amide polymers allows for tuneable separation and low cost regeneration.

Yiwen Tang, David Dubbeldam, Stefania Tanase: *Water-ethanol and methanol-ethanol separations using in situ confined polymer chains in a metal-organic framework*. *ACS Appl. Mater. Interfaces*. Published online: 10 October 2019. DOI: 10.1021/acsami.9b1436

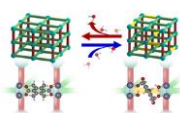
New simple device greatly improves analysis of reaction kinetics - 4 November 2019



PhD student Thierry Slot developed a new device for measuring the kinetics of gas-producing reactions. The simple benchtop device, of which the details are publicly available, costs less than € 250 and weighs only 1500 grams. Yet it gives accurate reaction profiles with over 3000 measurements. It is also programmable for running temperature profiles, providing Arrhenius plots with hundreds of data points from a single experiment. This enables quick and efficient analysis of both kinetics and thermodynamics.

T.K. Slot, N.R. Shiju and G. Rothenberg: *A simple and efficient device and method for measuring the kinetics of gas-producing reactions*. *Angew. Chem. Int. Ed.*, 2019, EarlyView. DOI: [10.1002/anie.20191100](https://doi.org/10.1002/anie.20191100)

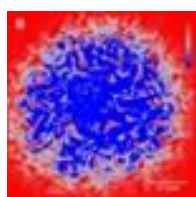
Loading-dependent water effects on the properties of water stable MOFs - 2 December 2019



According to a team of American and Dutch researchers, the structure of water-stable Metal-Organic Frameworks is less static than it might appear. In *Nature Chemistry* they presented data on hydrolytic MOF stability, resulting from in situ experiments and computational methods. The observations were explained by a dynamic structural change in response to water guest molecules. Computational chemists Jurn Heinen and David Dubbeldam contributed to the research.

Nicholas C. Burtch, Ian M. Walton, Julian T. Hungerford, Cody R. Morelock, Yang Jiao, Jurn Heinen, Yu-Sheng Chen, Andrey A. Yakovenko, Wenqian Xu, David Dubbeldam, Krista S. Walton: *In-situ visualization of loading-dependent water effects in a stable metal-organic framework*. *Nature Chemistry*, DOI: [10.1038/s41557-019-0374-y](https://doi.org/10.1038/s41557-019-0374-y)

Slippery when wet: how does lubrication work? - 12 December 2019



In a paper in *Science Advances*, researchers including Prof. Fred Brouwer presented new experimental insight into how lubrication works. They developed a new method using fluorescent molecules to directly observe nanometric lubrication films with a sensitivity of a single molecular layer. Their quantitative description of the relation between topography, contact pressure and lubrication provides a deeper understanding of lubrication.

Dina Petrova, Bart Weber, Clémence Allain, Pierre Audebert, Cees H. Venner, Albert M. Brouwer, and Daniel Bonn: *Fluorescence microscopy visualization of the roughness-induced transition between lubrication regimes*. *Science Advances* 06 Dec 2019: Vol. 5, no. 12, eaaw4761 DOI: [10.1126/sciadv.aaw4761](https://doi.org/10.1126/sciadv.aaw4761)

The world's fastest molecular shuttle - 16 December 2019



Thanks to a clever chemical design, HIMS researchers succeeded in making a very fast molecular machine. The moving parts shift more than one nanometre relative to each other in a record-breaking time of 30 billionths of a second. The results were published in *The Journal of the American Chemical Society*.

Tatu Kumpulainen, Matthijs R. Panman, Bert H. Bakker, Michiel Hilbers, Sander Woutersen, and Albert M. Brouwer: *Accelerating the Shuttling in Hydrogen-Bonded Rotaxanes: Active Role of the Axle and the End Station* *Journal of the American Chemical Society* 2019 141 (48), 19118-19129 DOI: [10.1021/jacs.9b10005](https://doi.org/10.1021/jacs.9b10005)

Prizes and honours

The quality of HIMS scientists is reflected in the prizes and honours they receive. Noteworthy examples are the Dal Nogare Award for Peter Schoenmakers, the NWO Vidi grant for Ning Yan and the appointment of Annemieke Petrignani as MacGillavry Fellow. Below is a list of news items reporting on these and other HIMS staff members and students.

Francesco Mutti listed among research talents by journal ChemBioChem - 26 March 2019



The board members of the Wiley journal ChemBioChem have included Dr Francesco Mutti in their selection of emerging young scientists that 'will shape the future of research at the interface of chemistry and biology'. Mutti leads the Biocatalysis research group.

Dieuwertje Modder wins poster competition at national student symposium - 26 March 2019



At the national chemistry student 'PAC symposium' held 7 March at Vrije Universiteit, chemistry master student Dieuwertje Modder won the first prize in the 'Young KNCV' poster competition. With her poster, Modder presented her research project at the research group for Homogeneous, Supramolecular and Bio-inspired Catalysis.

Joen Hermans nominated for Dutch New Scientist talent awards - 25 April 2019



HIMS researcher Joen Hermans was among the nominees for the Science Talent Award 2019 issued by the Dutch edition of the magazine New Scientist. Hermans' research focuses on chemical changes in the paint of old oil paintings. In 2017 he was also a finalist in the Dutch final of the science pitch competition FameLab.

Vidi grant for Ning Yan - 24 May 2019



The Netherlands Organisation for Scientific Research (NWO) awarded a Vidi grant to Dr Ning Yan of the Research Priority Area Sustainable Chemistry. The grant of 800,000 euro enables him to form his own research group and develop innovative research in the field of bi-atom catalysis.

Amsterdam analytical chemists heap up the awards at HPLC 2019 in Milan - 10 July 2019



Young researchers of the Analytical Chemistry research group earned a total of five awards at the 48th International Symposium on High-Performance Liquid Phase Separations and Related Techniques.

Annemieke Petrignani appointed as MacGillavry fellow - 18 July 2019



Dr Annemieke Petrignani was appointed as MacGillavry Fellow in the Molecular Photonics group as a result of a recruitment programme for talented women, named after the groundbreaking crystallographer professor Carolina MacGillavry. Petrignani's research focuses on organic chemistry from space to the origins of life.

Prestigious international catalysis award for Piet van Leeuwen - 22 July 2019



Former HIMS professor Piet van Leeuwen was awarded the Alwin Mittasch Prize 2019, in honour of his groundbreaking contributions to the molecular understanding of catalysis using organometallic complexes and their transfer into industrial hydroformylation.

Marie Brands nominated for KNCV Golden Master Award 2019 - 24 July 2019



Marie Brands, a PhD student at the research group for Homogeneous, Supramolecular and Bio-Inspired Catalysis was nominated for the 'Golden Master Award' of the Royal Netherlands Chemical Society KNCV. She competed for the award at the 'Avond van de Chemie 2019' on 3 October 2019 in Theater Odeon, Zwolle.

Chris Slootweg competes for Amsterdam Science & Innovation Award - 30 October 2019



Dr Chris Slootweg was one of nine finalists for the Amsterdam Science & Innovation Award 2019. He was nominated for his idea "Circular phosphate economy: Pioneers in closing the phosphorus cycle". The AMSIA finalists pitched their innovative ideas during a festive award ceremony in NEMO Science Centre on Tuesday 26 November.

Poster prize for Klaas van Leest at HRSMC 25th anniversary symposium - 18 November 2019



PhD researcher Klaas van Leest was awarded the poster prize at the 25th anniversary symposium of the Holland Research School of Molecular Chemistry (HRSMC). On Friday 15 November, the prize was handed to Van Leest by Prof. Luc Visscher, chairman of the jury.

Amsterdam Science & Innovation Award 2019 for SusPhos team - 28 November 2019



The SusPhos process developed at HIMS was one of the winners of an Amsterdam Science & Innovation Award 2019. On 27 November Marissa de Boer, CEO of the spin-off company of the same name, received the award certificate and a 7,500 euro cheque for further development.

SusPhos startup team wins Gouden KIEM 2019 - 13 December 2019



SusPhos won the 'Gouden KIEM' for best Dutch startup in chemistry issued by the Dutch science foundation NWO and Holland Chemistry. The award was presented Tuesday 10 December at the Dutch national chemistry conference CHAINS. It consists of 25,000 euros for a research project and a sculpture.

Unilever Research Prize 2019 for Steven Beijer - 15 December 2019



Steven Beijer, PhD candidate at the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences (HIMS), won a Unilever Research Prize 2019. On Thursday 12 December, he received his prize during the award ceremony at Unilever's new Foods Innovation Centre in Wageningen.

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.

Vidi grant for Ning Yan - 24 May 2019



The Netherlands Organisation for Scientific Research (NWO) awarded a Vidi grant to Dr Ning Yan of the Research Priority Area Sustainable Chemistry. The grant of 800,000 euro enables him to form his own research group and develop innovative research in the field of bi-atom catalysis.

Funding for circular chemistry research - 8 October 2019



Dr Chris Sloopweg has obtained funding for two projects in the field of circular chemistry. NWO supported his research into the synthesis of acetic acid from methane and carbon dioxide through the Dutch Research Agenda (NWA). Sloopweg also received a KIEM-GoChem grant for his work on phosphate reuse, funded by the NWO domain Science (ENW) and the SIA Taskforce for Applied Research.

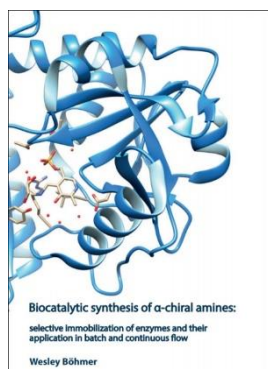
Funding for nanomaterials in cancer treatment - 11 November 2019



The Biophotonics group of Prof. Hong Zhang was part of the Dutch Medical Photonics (MEDPHOT) consortium that received 5.4 million euros from the 'Perspectief' Programme of the Netherlands Organization for Scientific Research (NWO). The consortium wants to better visualize the effectiveness of medicines in the treatment of diseases such as cancer.

Dissertations

In 2019, twenty candidates received their PhD at HIMS, one of them - Dr Bob Pirok - with the distinction cum laude. All theses are listed below; a link is provided to download each thesis from the UvA repository.



19 December 2019

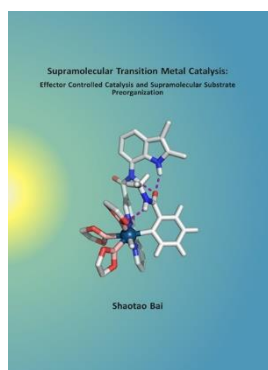
Biocatalytic synthesis of α -chiral amines - Selective immobilization of enzymes and their application in batch and continuous flow

Author: W. (Wesley) Böhmer

Supervisors: F. Mutti, J.H. van Maarseveen

Group: Biocatalysis

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



16 December 2019

Supramolecular Transition Metal Catalysis - Effector controlled catalysis and supramolecular substrate preorganization

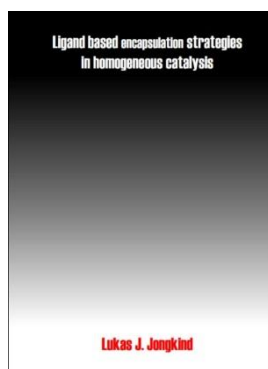
Author: S. (Shaotao) Bai

Supervisor: J.N.H. Reek

Co-supervisor: A.M. Kluwer

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



10 December 2019

Author: L. (Lukas) J. Jongkind

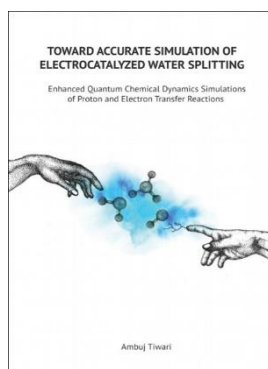
Ligand based encapsulation strategies in homogeneous catalysis

Supervisor: J.N.H. Reek

Co-supervisor: J.I. van der Vlugt

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



3 December 2019

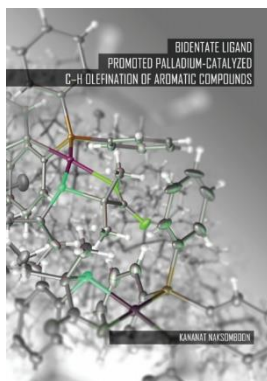
Toward accurate simulation of electrocatalyzed water splitting - Enhanced quantum chemical dynamics simulations of proton and electron transfer reactions

Author: A. (Ambuj) Tiwari

Supervisors: B. Ensing, P.G. Bolhuis

Group: Computational Chemistry

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

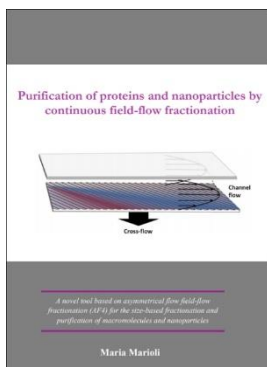


10 October 2019

Author: K. (Kananat) Naksomboon

Bidentate ligand promoted palladium-catalyzed C–H olefination of aromatic compounds

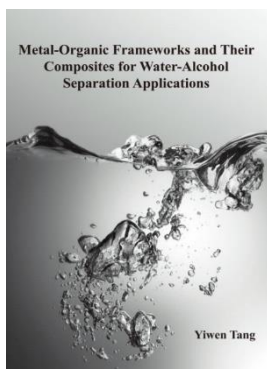
Supervisor: M.A. Fernández Ibáñez
Co-supervisor: J.H. van Maarseveen
Group: Synthetic Organic Chemistry
Link: [Read or download this thesis](#)



27 September 2019

Purification of proteins and nanoparticles by continuous field-flow fractionation

Author: M. (Maria) Marioli
Supervisor: P.J. Schoenmakers
Co-supervisor: W. Kok
Group: Analytical Chemistry
Link: [Read or download this thesis](#)

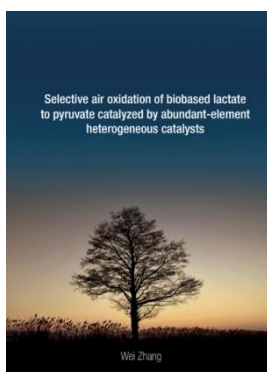


18 September 2019

Author: Y. (Yiwen) Tang

Metal-organic frameworks and their composites for water-alcohol separation applications

Supervisors: S. Grecea, G. Rothenberg.
Group: Heterogeneous Catalysis and Sustainable Chemistry
Link: [Read or download this thesis](#)

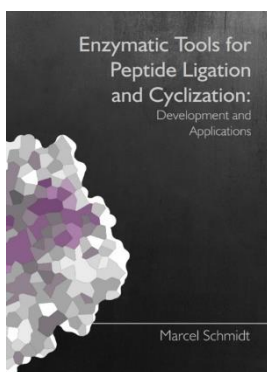


6 September 2019

Author: W. (Wei) Zhang

Selective Air Oxidation of Biobased Lactate to Pyruvate Catalyzed by Abundant-Element Heterogeneous Catalysts

Supervisors: G. Rothenberg, N.R. Shiju.
Group: Heterogeneous Catalysis and Sustainable Chemistry
Link: [Read or download this thesis](#)



5 July 2019

Author: M. (Marcel) Schmidt

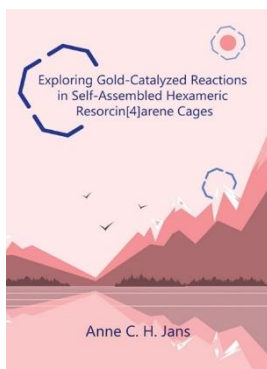
Enzymatic Tools for Peptide Ligation and Cyclization - Development and Applications

Supervisors: J.H. van Maarseveen, T.N. Grossmann.

Co-supervisor: F. Mutti.

Group: Synthetic Organic Chemistry

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



3 July 2019

Author: A. (Anne) C.H. Jans

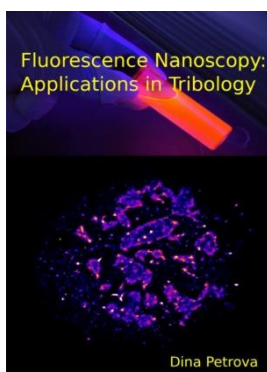
Exploring Gold-Catalyzed Reactions in Self-Assembled Hexameric Resorcin [4] arene Cages

Supervisor: J.N.H. Reek

Co-supervisor: J.I. van der Vlugt

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



26 June 2019

Author: D. (Dina) Petrova

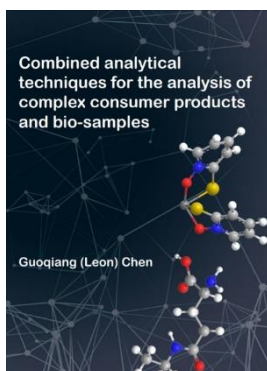
Fluorescence nanoscopy - Applications in tribology

Supervisor: A.M. Brouwer

Co-supervisor: D. Bonn

Group: Molecular Photonics

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



5 June 2019

Combined analytical techniques for the analysis of complex consumer products and bio-samples

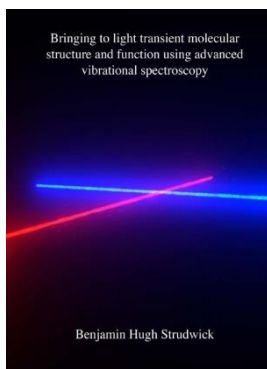
Author: G. (Guiqiang aka Leon) Chen

Supervisor: J.G.M. Janssen

Co-supervisor: P.J. Schoenmakers

Group: Analytical Chemistry

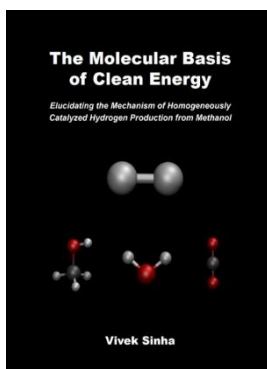
Link: [Read or download this thesis](#)



24 May 2019

Bringing to light transient molecular structure and function using advanced vibrational spectroscopy

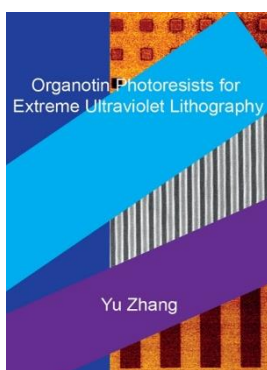
Author: B. (Benjamin) H. Strudwick
Supervisors: S. Woutersen, W.J. Buma
Group: Molecular Photonics
Link: [Read or download this thesis](#)



23 April 2019

The Molecular Basis of Clean Energy - Elucidating the Mechanism of Homogeneously Catalyzed Hydrogen Production from Methanol

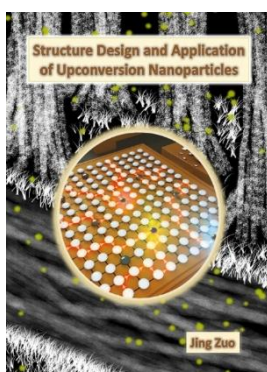
Author: V. (Vivek) Sinha
Supervisor: B. de Bruin
Co-supervisor: H. Grützmacher
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: [Read or download this thesis](#)



11 April 2019

Organotin Photoresists for Extreme Ultraviolet Lithography

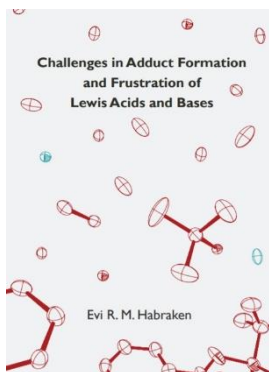
Author: Y. (Yu) Zhang
Supervisor: A.M. Brouwer
Co-supervisors: P.C.M. Planken, S. Castellanos Ortega
Group: Molecular Photonics
Link: [Read or download this thesis](#)



2 April 2019

Structure design and applications of upconversion nanoparticles

Author: J. (Jing) Zuo
Supervisor: H. Zhang
Co-supervisor: W.J. Buma
Group: Molecular Photonics
Link: [Read or download this thesis](#)



28 March 2019

Challenges in adduct formation and frustration of Lewis acids and bases

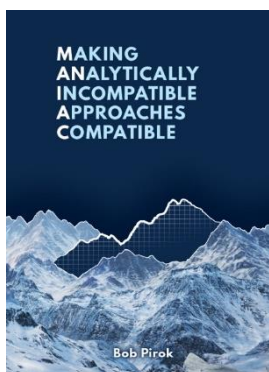
Author: E. (Evi) R.M. Habraken

Supervisor: J.C. Slootweg

Co-supervisors: A.W. Ehlers, A.R. Jupp

Group: Synthetic Organic Chemistry

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



22 March 2019

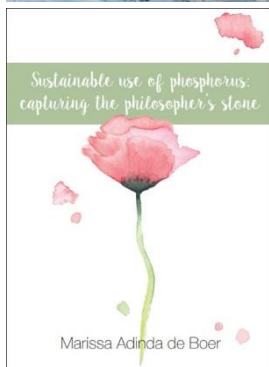
Making ANalytically Incompatible Approaches Compatible

Author: B. (Bob) W.J. Pirok

Supervisors: P.J. Schoenmakers, R.A.H. Peters

Group: Analytical Chemistry

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



25 January 2019

Sustainable use of phosphorus - Capturing the philosopher's stone

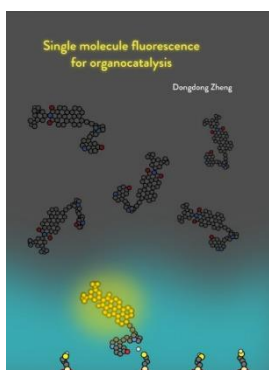
Author: M. (Marissa) A. de Boer

Supervisor: J.C. Slootweg

Co-supervisor: J.H. van Maarseveen

Group: Synthetic Organic Chemistry

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



18 January 2019

Single molecule fluorescence for organocatalysis

Author: D. (Dongdong) Zheng

Supervisor: A.M. Brouwer

Co-supervisor: R.M. Williams

Group: Molecular Photonics

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

Valorisation

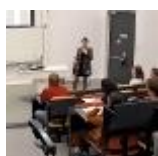
Knowledge transfer to industry and society is in the DNA of our institute. We are always looking for partnerships with industry to identify research questions that matter, transfer our knowledge and turn innovative ideas into reality. Below is an overview of valorisation results in 2019.

Successful International Winter School MolSim-2019 - 23 January 2019



More than 70 PhD researchers from all over the world participated in 2019 edition of the 2-week winter school 'Understanding Molecular Simulations' (MolSim). Scientists from the Computational Chemistry group of HIMS provided a varied program of lectures and hands-on lab courses.

Fruitful explorations of the circular economy during joint sustainability workshop - 15 April 2019



On Thursday 4 April, the University of Amsterdam's Roeterseiland campus hosted the joint workshop 'Towards a Circular Economy' of the Holland Research School of Molecular Chemistry (HRSMC) and the Van 't Hoff Institute for Molecular Sciences (HIMS).

Researchers unravel important feature of the molecular structure of oil paint - 25 June 2019



In 'Science Advances', researchers of HIMS and Rijksmuseum described the role of zinc ions in the molecular network of oil paint. This could give the explanation why paintings made with zinc white pigment are so sensitive to high humidity conditions. The research also yielded important insights in the world of plastics.

HIMS researchers collect urine at Lowlands festival - 29 August 2019



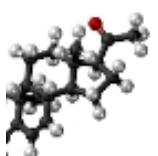
At the Dutch summer festival Lowlands, Chris Slootweg, Bas de Jong and Steven Beijer collected the urine of visitors to see whether residual products from pharmaceuticals and chemicals end up in the recovered phosphate. This struvite can be used as a renewable resource for high-value phosphate products such as flame retardants.

New joint initiative: AI4Science lab - 20 September 2019



The UvA institutes for astronomy (API), biology (IBED), chemistry (HIMS), informatics (IVI), life sciences (SILS) and physics (IoP) initiated a new 'AI4Science' lab that aims to solve scientific data problems with modern machine learning approaches. Dr Bernd Ensing of Computational Chemistry is scientific director, together with Prof. Joris Mooij (Informatics Institute).

Improved method for determining the structure of complex molecules in medicines - 17 October 2019



Spectroscopy based on 'vibrational circular dichroism' (VCD) can significantly improve the practical determination of the structure of chiral molecules. HIMS researchers have improved VCD so that a single measurement suffices to determine the absolute configuration of many-centre chiral molecules that are often used as active ingredients in medicines.

New simple device greatly improves analysis of reaction kinetics - 4 November 2019



HIMS Researchers developed a new device for measuring the kinetics of gas-producing reactions. This simple benchtop device, of which the details are publicly available, costs less than € 250, weighs only 1500 grams yet gives accurate reaction profiles with over 3000 measurements.

Collaboration on Sustainable Innovation with China gets a boost - 5 November 2019



HIMS signed a formal agreement on research collaboration with the Shanghai Institute for Cleantech Innovation and the Shanghai Advanced Research Institute (SARI) of the Chinese Academy of Sciences (CAS). The agreement is a platform for joint research, valorisation and education as well as the exchange of researchers and students.

Innovation Fund Noord-Holland invests in SusPhos technology - 14 November 2019



Startup company SusPhos has received a convertible loan of € 300,000 from the Innovation Fund Noord-Holland. The loan enables SusPhos to bring technology to market that upgrades phosphate from waste streams into high purity products. SusPhos is led by Dr Marissa de Boer who obtained her PhD at HIMS.

Amsterdam Science & Innovation Award 2019 for SusPhos team - 28 November 2019



The SusPhos process developed at HIMS is one of the winners of an Amsterdam Science & Innovation Award 2019. On 27 November Marissa de Boer, CEO of the spin-off company of the same name, received the award certificate and a 7,500 euro cheque for further development.

SusPhos startup team wins Gouden KIEM 2019 - 13 December 2019



UvA startup SusPhos won the 'Gouden KIEM' for best Dutch startup in chemistry. The award, issued by the Dutch science foundation NWO and Holland Chemistry, was presented Tuesday 10 December at the Dutch national chemistry conference CHAINS. It consists of 25,000 euros for a research project and a sculpture.

Outreach

Lectures and other contributions in 2019

For the general public

- Kun je Blauw bloed hebben? En lusten vampieren dat dan? Expedition Next (NWA) Lecture, NEMO middaglezing, Nationale Jeugd-Museum (MJU) lezing (Bas de Bruin)
- Achieving the 2°C target of the Paris Agreement: energy technology requirements and beyond. Professional lecture at TNO Hoogleraren- en Lectorendag (Bob van der Zwaan)
- The Energy Transition and the Paris Agreement: an energy technology perspective, and beyond, lecture at Rotary Minerva (Bob van der Zwaan)
- Hoe kun je zeldzame schatten bewaren? Kinderlezing Universiteitsdag Amsterdam (Maarten van Bommel)
- Waarom komt er uitlaatgas uit je mond? Vondelparktheater kinderlezing i.s.m. NEMO (Jan van Maarseveen)
- Ge(s)laagd multidisciplinair onderzoek bij een gezonken schip bij Texel. Lecture at Koninklijke Industriële Groote Club (Maarten van Bommel)

For high school students and teachers

- Steunpunt scheikunde: grenzen aan de chemie / Vaksteunpunt samen met steunpunt biologie: chemie in de biologie / Vaksteunpunt: Scheikunde didactiek. Lectures for (secondary school) teachers (Bernd Ensing)
- Chemie in Amsterdam, lectures and workshops for upper secondary school teachers and students (Bernd Ensing)
- Koolstof en zijn burenen. Lecture at Woudschoten Chemieconferentie for secondary school teachers (Jan van Maarseveen)
- Werken als scheikundig onderzoeker, Lecture for secondary school students (Jocelyne Vreede)

TV and radio broadcast contributions

- DWDD TV talk show on nitrogen, following the current discussion about Dutch nitrogen policy (Jan van Maarseveen).
▶ [De Wereld Draait Door](#), 4 October.
- Radio Swammerdam broadcast on the theme "Sustainable with raw materials" (Gert-Jan Gruter).
▶ [Radio Swammerdam](#), 8 September.
- TV science programme 'De Kennis van Nu', episode on illegal fireworks (Karlijn Bezemer and Arian van Asten).
▶ [De Kennis van Nu](#), 4 September.

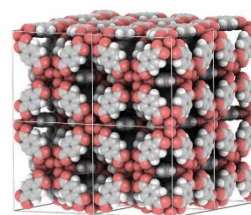


- Katrien Keune contributed to the national TV news in an item on 'Operation Nightwatch' and featured in two other programmes. In the broadcast 'Het geheim van de Meester' a painting by Adriaen Coorte was analysed in the HIMS lab. A broadcast restoration of paintings also features Katrien and the lab.
 - ▶ [NOS journaal](#), 8 July (item at 17:38).
 - ▶ Het geheim van de Meester, 8 January
 - ▶ Het Klokhuis, 9 January
- Amsterdam TV station AT5 on different power plant fuels, in response to unrest about a new biomass plant at Diemen (Ties Korstanje).
 - ▶ [TV 5](#), 30 March.



HIMS researchers in the media in 2019

- **Illegal fireworks**
In the Dutch newspaper Financieele Dagblad, Arian van Asten explains how criminals blowing up ATMs obtain their explosive material from illegal fireworks.
 - ▶ [Financieele Dagblad, 11 December \(login required\)](#).
- **Handy new device for kinetics analysis**
Dutch chemistry bi-weekly C2W has an article about the handy new kinetics analysis device developed by Thierry Slot, Raveendran Shiju and Gadi Rothenberg.
 - ▶ [C2W article](#) (11 November).
- **Predictive chemistry**
Dutch newspaper Financieele Dagblad reports on simulation models that can predict the chemical properties of consumer products. The contribution of Gadi Rothenberg puts this trend into perspective.
 - ▶ [Financieele Dagblad, 18 October \(login required\)](#)
- **Negative thermal expansion in MOFs**
Research of David Dubbeldam and Jurn Heinen was reported at various science news websites.
 - ▶ [Phys.org](#), 25 September.
 - ▶ LongRoom news, 28 September.
- **Artificial Intelligence in chemical synthesis**
Dutch chemistry bi-weekly C2W reports on artificial intelligence in synthesis robots and poses the question whether synthetic organic chemists will eventually become superfluous. Jan van Maarseveen is among the chemists reflecting on this matter.
 - ▶ [C2W](#), 18 September.
- **Determining chirality**
Dutch chemistry bi-weekly C2W reports on research by Mark Koenis and Wybren Jan Buma who improved the VCD technique, enabling a substantially more accurate determination of the chirality of molecules. The news was also reported on by Phys.org.
 - ▶ [C2W](#), 11 September.
 - ▶ [Phys.org](#), 8 September.



- **Collecting urine at a music festival**

Dutch popular science website Kennislink and Folia magazine report on the research of Chris Slootweg, Steven Beijer and others, who are collecting the urine of visitors at the Lowlands festival and investigate whether drug use is of influence on extracting struviet from the urine as a phosphate fertilizer.

▶ [Kennislink](#), 19 August.

▶ [Folia](#), 21 June.

- **Art conservation**

2019 saw much attention for HIMS research in the field of art conservation.

Katrien Keune featured in an article in the Analytical Scientist on 'New Tools for Old Masters'

▶ [The Analytical Scientist](#), 30 July.

In the TV broadcast 'Het geheim van de Meester' a painting by Adriaen Coorte was analysed in the HIMS lab.

▶ Het geheim van de Meester, 8 January

A broadcast of the educational TV programme 'Het Klokhuis' about the restoration of paintings also features the lab

▶ Het Klokhuis, 9 January

The Rijkmuseum's 'Operation Nightwatch' induced many media reports with a contribution by Katrien Keune:

▶ [NOS journaal](#), 8 July (item at 17:38).

▶ [Podcast of PODNL](#), 8 July

▶ [Video by Folia](#), 19 July

▶ [Article in newspaper De Volkskrant](#), 8 January

PhD student Mimi den Uijl featured in a 'Weer iets geleerd' video by Metro Nederland (on the colours of Van Gogh) and an episode of the "Makkelijk Praten" podcast (on light degradation and fading colours).

▶ [MetroNederland/YouTube](#), 17 July

▶ [Makkelijk praten](#), 27 June



- **Solving a solvability mystery**

Various chemistry media reported on the research by Sander Woutersen (HIMS), Bernd Ensing (HIMS) and Daniel Bonn (IoP) into the question why of two types of commonly used polyethers one is water-soluble and the other is not.

▶ [Chemistry World](#), 4 July

▶ [C2W](#), 1 July

- **Enhancing the performance of MOF materials**

Dutch chemistry bi-weekly C2W reported on research by Yiwen Tang, Stefania Grecea and others. By using leaves from the black poplar as a template, they produced hierarchical porous structures of mixed-metal oxide materials that can act as support for MOF crystals.

▶ [C2W](#), 2 July

- **Sustainable plastic**

Gert-Jan Gruter is frequently consulted as an expert on issues of plastic and sustainability

- ▶ [Kennislink](#), 2 May
- ▶ [One World](#), 4 March

- **Circular Chemistry**

The commentary of Chris Sloopweg in Nature Chemistry where he introduced the concept of Circular Chemistry received much media attention.

- ▶ [NRC Handelsblad](#), 11 March
- ▶ [De Standaard](#), 12 March
- ▶ [C2W](#), 12 April



- **Open access**

Bas de Bruin was among several professors consulted by NRC Handelsblad about the so-called 'plan S' of European science financiers to introduce open access.

- ▶ [NRC Handelsblad](#), 8 February

- **Decarbonization**

The Energienieuws platform spoke with Bob van der Zwaan about a recently published EU-report about decarbonization to which Van der Zwaan made a significant contribution.

- ▶ [Energienieuws](#), 11 January

Facts and figures

Research

Research output

Research output 2019 per type of publication (source: PURE)

HIMS themes	AC	CC	MP	SC	Other ¹	Joint ²	Total
Refereed articles (academic)	31	63	43	108		28	245
Non-refereed articles		1			1		2
Book (chapter)s	1	1		2	1		5
PhD-theses	3	1	5	11			20
Other research output	6		5	9		1	20

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

¹ AMOLF, ARCNL, Avantium, etc ² The number of joint results obtained from collaborations between different research groups. The total number of 29 joint publications includes 38 collaborations.

Other output and honours

HIMS themes	AC	CC	MP	SC	Other	Joint	Total
Keynote lectures	20	1	13	45			79
Hosting a conference		2	1	3			6
Lecture for general public, media coverage		1	1	1			3
Prizes/awards	6	3	2	22			33

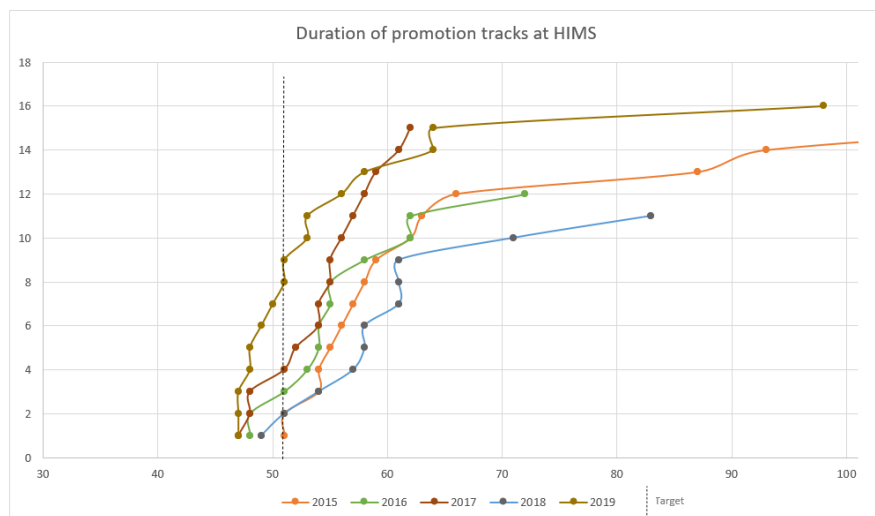
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis.

Efficiency of the doctoral research path

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

Enrolment			Success rates of graduation in years (t) after start								Total						
Start	m / f		Total	t ≤ 4		t ≤ 5		t ≤ 6		t ≤ 7		Graduated		Not yet		Discontinued	
	#	%	#	%	#	%	#	%	#	%	#	%	#	%	#	%	
2011	8	8	16	2	13	6	38	2	13	2	13	12	75	0	-	4	25
2012	13	6	19	2	11	9	47	5	26	1	5	17	89	0	-	2	11
2013	7	8	15	3	20	6	40	5	33	-	-	14	93	0	-	1	7
2014	6	7	13	1	8	8	62	2	15	-	-	11	85	0	-	2	15
2015	19	4	23	3	13	5	22	-	-	-	-	8	35	14	61	1	4
Total	53	33	86	11	13	34	40	14	16	3	3	62	72	14	16	10	12

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

This table presents the HIMS staff numbers (average head count in 2019) 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. The following tables total the complete HIMS staff as full time equivalents (fte) per employment type per research theme.

	AC		CC		MP		SC		Other		Total	
	HC	RFTE	HC	RFTE	HC	RFTE	HC	RFTE	HC	RFTE	HC	RFTE
Scientific staff (1)	4,8	2,4	7,9	4,0	5,5	2,7	13,1	6,6	0,0	0,0	31,3	15,7
Post-docs (2)	2,5	2,3	0,0	0,0	2,6	2,3	8,2	7,4	0,0	0,0	13,3	12,0
PhD students (3)	13,0	9,8	8,3	6,3	11,7	8,8	51,7	38,8	0,0	0,0	84,7	63,7
Total research staff	20,3	14,5	16,2	10,3	19,8	13,8	73,0	52,8	0,0	0,0	129,3	91,4
Technicians (4)	3,0	3,0	0,0	0,0	3,8	3,8	9,7	9,7	0,0	0,0	16,5	16,5
Visiting fellows	0,0	0,0	0,0	0,0	0,3	0,3	0,8	0,8	0,0	0,0	1,1	1,1
Support staff (4)	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	5,5	5,5	5,5	5,5
Total staff	23,3	17,5	16,2	10,3	23,9	17,9	83,5	63,3	5,5	5,5	152,4	114,5

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

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 2019.

Age bracket	Number	%-age	Male	Female	Dutch	Other EU	Other
30-40	8	22%	7	1	4	3	1
40-50	13	35%	8	5	9	3	1
50-60	11	30%	11	0	10	0	1
60+	5	14%	5	0	4	1	0
Total	37	100%	31	6	27	7	3

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 area's, that also count for 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 in the distribution of funds and the funding of staff salaries only.

Research- and supporting staff 2019 of HIMS per funding type (fte)

HIMS Themes	Research					Total	%	Support	Total	%
	AC	CC	MP	SC	Other					
Direct funding						56,9	36%	18,3	75,2	40%
Research grants	6,1	2,8	8,4	28,17	7,89	53,36	40%	3,7	57,06	36%
Contract research	7		1,9	6,54	2,1	17,54	24%		17,54	20%
Other						0	0%		0	4%
Total	13,1	2,8	10,3	34,71	9,99	127,8	100%	22	149,8	100%

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

Externally financed projects acquired in 2019(100k €) per funding type

HIMS themes	AC	CC	MP	SC	Other	Total ¹
Direct funding						
Research grants	844	297	242	1,511		
Contract research	37	31		2,654		
Total	881	328	242	4,165	0	5,616

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. 'Other' includes the institute's office.¹Budgets were obtained for 27 (in FTE), 44 PhD's, 10,6 PD and 3,67 staff.

HIMS result 2019 (k€)

The HIMS result for 2019 amounts to +545k€. This positive result is based on reservations from past budgets for costs in the framework of the *Sectorplan Natuur- en Scheikunde* and the RPA Sustainable Chemistry, not being spend yet and not all vacancies were filled.

2019	EU & Contract research			
	Direct	NWO	research	Total
HIMS Base Budget	3.550	-	-	3.550
Budget (variable1)	4.604	4.110	1.657	10.371
Other income 2	2.722		156	2.878
Matching contract research	-4.257	3.573	683	-
Budget total	6.619	7.683	2.496	16.798
Percentage	39%	46%	15%	100%
Personal costs	-4.175	-3.203	-1.126	-8.504
Other costs (projects)	-3.988	-876	-521	-5.385
Overheads 3	2.161	-3.612	-913	-2.364
Costs total	-6.002	-7.691	-2.560	-16.253
Percentage	37%	47%	16%	100%
HIMS Result 2020	617	-8	-64	545

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