



# Annual Report 2020

*Chemistry  
research  
that matters*

Van 't Hoff Institute  
for Molecular Sciences

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## Executive summary

**This summary gives you a glimpse of our institute's performance. More elaborate listings of our scientific highlights, key publications and other relevant features can be found elsewhere in the annual report 2020.**

The year 2020 was all about our mid-term evaluation. During a 2-day retreat in February in Bergen aan Zee, 32 staff members discussed strategic research lines for the coming years. In particular, the



*HIMS director Prof. Peter Bolhuis: "This COVID-year has been very demanding for everyone. That is why I am even more proud of the great commitment and achievements of our staff - as confirmed by our external mid-term review." Photo by Jan Willem Steenmeijer.*

institute's research focus was clustered into three overarching research topics: Chemistry of Complex Systems and Materials, Chemistry for Sustainability, and Chemistry of Biomolecular Systems.

During the online site-visit in December, our Scientific Advisory Committee concluded that *"the research at the van 't Hoff Institute continues to be of high scientific quality in all four research areas .... it is evident that high quality and innovative research continues to flourish"*. In the coming period we will work further on the implementation of the

overarching research topics, and follow-up on other strategic recommendations, such as improvement of the gender balance, internal procedures and communication, and investment in hardware research data management and storage hardware together with our faculty.

### PhD's, publications and personell

Notwithstanding all the COVID-related problems the Van 't Hoff Institute has really performed remarkably in terms of PhD graduations, this year a whopping 27 PhD graduated. Also, a record number of 246 appealing publications arose, including 29 joint publications from collaborating HIMS groups. 11 publications came from interdisciplinary collaborations involving different HIMS themes.

A farewell party will be organized in 2021 for Prof. Piet Iedema, who is the initiator of the *Science for Arts* activities in our institute. He retired in September 2020, concluding an impressive career in industry and academia. On the other hand, HIMS welcomed quite a few new scientific staff members last year. Within the framework of the national Sectorplan Dr Tristan Bereau, Dr Saer Samanipour and Dr Sonja Pullen were appointed. Dr Amanda Garcia entered via a highly competitive tenure-track grant from the NWO program on electrochemical conversion and materials (ECCM). Prof. Tim Noel came from TU/e to Amsterdam to focus on the fundamentals of flow-chemistry within the research priority Area Sustainable Chemistry.

### New initiatives

The staff at the Van 't Hoff Institute acquired notable grants for new public-private research initiatives, like a NWO TA in Analytical Chemistry and a TTW Open Technology program in Flow-chemistry, as well as curiosity-driven projects and a record number of contract research projects. The institute received a special valorization grant to run an Open Kitchen Lab pilot. This will be a service available in one of the Matrix buildings at the Amsterdam Science Park, where spin-offs can rent a laboratory facility that already has the basic equipment and consumables.

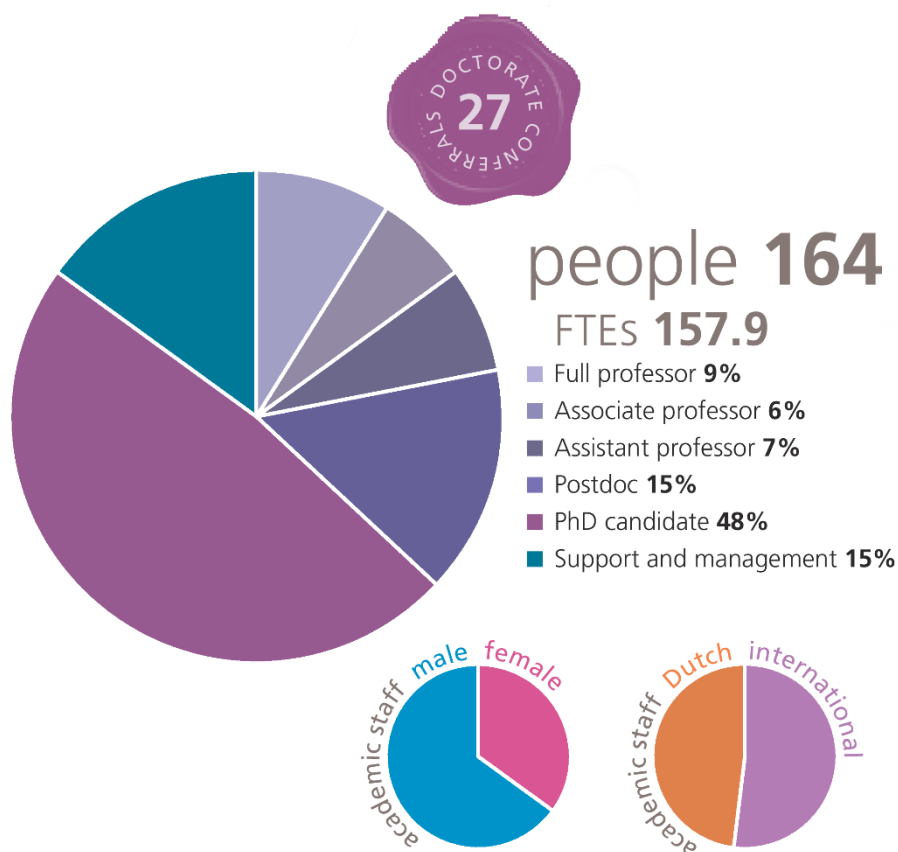
DSM's CTO Dr Marcus Remmers and Director Royal VNCI Manon Bloemer MBA, gave inspiring presentations at the online Amsterdam Chemistry Innovation Day, which attracted over 160

participants from industry and academia. Special attention was given to careers in chemistry and chemical industry in urban development areas.

### Prizes and honours

Several prizes were granted to HIMS researchers. Dr Chris Slootweg and his spin-off SusPhos BV received the NWO Stairway to Impact Award and Rabo Sustainable Innovation Award. Two PhD students were honoured with prizes for their thesis: Dr. Kananat Naksomboon received the KNCV Backer prize, and *cum laude* PhD candidate Dr Mark Koenis received the HRSMC's Dick Stufkens prize. Emeritus professor Rajamani Krishna was again included in the Highly Cited Researchers 2020 list from the Web of Science Group, while a publication by professor Bas de Bruin made it to the top-10 most cited papers of the previous decade by the American Chemical Society.

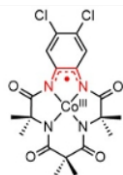
### HIMS at a glance:



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

## Scientific Highlights

### Elucidation of ligand redox non-innocence in Co(TAML) complexes - 21 January 2020



In a paper in the Journal of the American Chemical Society, researchers of the of the Homogeneous, Supramolecular and Bio-Inspired Catalysis group settle the debate on the ligand redox non-innocence in Co(TAML) complexes. Using experiments, spectroscopic research and computer modelling, they show that oxidation and reduction takes place on the ligand while the cobalt ion retains its oxidation state.

Nicolaas P. van Leest, Martijn A. Tepaske, Jean-Pierre H. Oudsen, Bas Venderbosch, Niels R. Rietdijk, Maxime A. Siegler, Moniek Tromp, Jarl Ivar van der Vlugt, Bas de Bruin: *Ligand Redox Noninnocence in [Co<sup>III</sup>(TAML)]<sup>0/-</sup> Complexes Affects Nitrene Formation*. J. Am. Chem. Soc. **2020**, 142, 552-563 DOI: [10.1021/jacs.9b11715](https://doi.org/10.1021/jacs.9b11715)

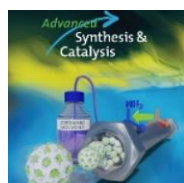
### UvA students look beyond lithium-ion batteries - 19 March 2020



UvA chemistry master students Peter Jungbacker and Tess van Teijlingen, working at the Research Priority Area Sustainable Chemistry, studied the pros and cons of the most promising alternative materials for Li-ion batteries. Their findings, which include both the chemical and socio-economic aspects of batteries, were published as a cover article in the open-access journal 'Materials'.

J. Biemolt, P. Jungbacker, T. van Teijlingen, N. Yan and G. Rothenberg: *Beyond lithium-based batteries*. Materials, **2020**, 13, 425. DOI: [10.3390/ma13020425](https://doi.org/10.3390/ma13020425) (open access)

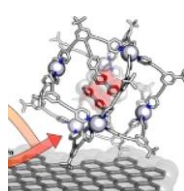
### Synthesis of chiral amines in neat organic solvents using immobilised enzymes in a continuous flow reactor 19 March 2020



Researchers from the Biocatalysis group presented the first account of applying immobilised  $\omega$ -aminotransferase enzymes in neat organic solvents. In a paper in the journal Advanced Synthesis & Catalysis, they describe how they achieve high yields in the synthesis of  $\alpha$ -chiral amines using this enzymatic system in a continuous flow reactor. The paper was designated as a Very Important Publication and featured on the front cover of Advanced Synthesis & Catalysis.

Wesley Böhmer, Alexey Volkov, Karim Engelmark Cassimjee, and Francesco G. Mutti: *Continuous Flow Bioamination of Ketones in Organic Solvents at Controlled Water Activity using Immobilized  $\omega$ -Transaminases*. Advanced Synthesis & Catalysis DOI: [10.1002/adsc.201901274](https://doi.org/10.1002/adsc.201901274)

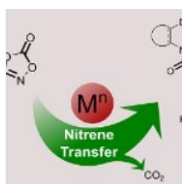
### Controlling the rate of heterogeneous electron transfer across the rim of nanospheres - 20 April 2020



In a paper in the Journal of the American Chemical Society, researchers of the group for Homogeneous, Supramolecular and Bio-Inspired Catalysis explored the redox-chemistry of supramolecular M<sub>6</sub>L<sub>12</sub> and M<sub>12</sub>L<sub>24</sub> cages with different redox-active moieties in their interior. Detailed electrochemical studies allowed the evaluation of the thermodynamics and kinetics of electron transfer from the electrode to the electrochemical probes inside the spheres.

Riccardo Zaffaroni, Eduard O. Bobylev, Raoul Plessius, Jarl Ivar van der Vlugt, and Joost N. H. Reek: *How to Control the Rate of Heterogeneous Electron Transfer across the Rim of M<sub>6</sub>L<sub>12</sub> and M<sub>12</sub>L<sub>24</sub> Nanospheres* J. Am. Chem. Soc. **2020**, 142, 19, 8837–8847 DOI: [10.1021/jacs.0c01869](https://doi.org/10.1021/jacs.0c01869)

### **The use of dioxazolones for the catalytic transfer of acyl nitrenes** - 23 April 2020



Although dioxazolones were discovered nearly 70 years ago, these substrates have recently gained attention in the field of transition-metal catalysis. In a paper in ACS Catalysis, PhD student Kaj van Vliet from the Bio-inspired Sustainable Catalysis group led by Prof. Bas de Bruin reviewed the use of dioxazolones as an important class of acyl nitrene transfer agents.

Kaj M. van Vliet, Lara H. Polak, Maxime A. Siegler, Jarl Ivar van der Vlugt, Célia Fonseca Guerra, Bas de Bruin: *Efficient Copper-Catalyzed Multicomponent Synthesis of N-Acyl Amidines via Acyl Nitrenes*. J. Am. Chem. Soc. 2019, 141, 38, 15240-15249 DOI: [10.1021/jacs.9b07140](https://doi.org/10.1021/jacs.9b07140)

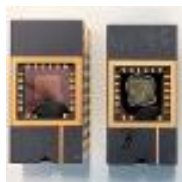
### **New method for constructing 8-membered ring compounds** - 24 April 2020



In a paper in Angewandte Chemie, researchers at the research group Homogeneous, Supramolecular and Bio-Inspired Catalysis presented a new method for the generation of 8-membered ring compounds based on metalloradical catalysis. Their novel procedure provides an efficient and broadly applicable solution for the synthesis of medium-sized ring structures. It features mild reaction conditions and enables asymmetric synthesis and scale-up, thus providing a powerful strategy for the synthesis of pharmaceutical molecules and novel chemicals with medium-sized cyclic structures.

Minghui Zhou, Marianne Lankelma, Jarl Ivar van der Vlugt, Bas de Bruin: *Catalytic Synthesis of 8-Membered Ring Compounds via Cobalt(III)-Carbene Radicals*. Angew. Chem. Int. Ed. **2020**, 142, 552–563 DOI: [10.1002/anie.202002674](https://doi.org/10.1002/anie.202002674)

### **Measuring CO<sub>2</sub> concentrations at ambient conditions with metal-organic frameworks** - 24 April 2020



In a collaboration with the Holst Centre (imec), the Functional Materials group of Dr Stefania Grecea demonstrated that metal-organic frameworks (MOFs) can be used as effective sensing layers for effective CO<sub>2</sub> level monitoring. These materials have the advantage that can be processed and integrated easily into inexpensive impedance sensors. The paper describing the research is part of a collection of papers on 'Molecular Systems for Sensing' of the RSC journal Molecular Systems Design & Engineering.

Bohui Ye, Andreea Gheorghe, Roy van Hal, Marcel Zevenbergen, Stefania Tanase: *Zn-MOF-74 as sensing material for effective CO<sub>2</sub> detection*. Molecular Systems Design & Engineering, 2020, **5**, 1071-1076 DOI: [10.1039/D0ME00004C](https://doi.org/10.1039/D0ME00004C)

### **Think small, learn fast might be the way to go for novel energy technologies** - 24 April 2020



In a paper published in the journal Joule, scientists led by Prof. Bob van der Zwaan presented an analysis of learning curves in energy technology and conclude that a focus on smaller unit size could facilitate faster cost reduction. According to Van der Zwaan, professor of Sustainable Energy Technology, this is particularly relevant for devices and processes capable of generating solar fuels, such as hydrogen, that may become essential elements of future energy systems.

Bart Sweerts, Remko J. Detz, Bob van der Zwaan: *Evaluating the Role of Unit Size in Learning-by-Doing of Energy Technologies*. Joule, Published April 24, 2020. DOI: [10.1016/j.joule.2020.03.010](https://doi.org/10.1016/j.joule.2020.03.010)

### **The surprising viscosity of entangled worms** - 26 May 2020

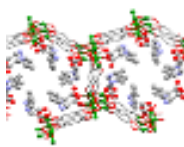


By performing experiments on Tubifex worms bought at the local pet shop, professors Sander Woutersen (HIMS) and Daniel Bonn (IOP) together with postdoc researcher Antoine Deblais (IOP) discovered that the wiggling motion of living worms gives rise to surprising physics. The way the worms spontaneously organise themselves into a blob turns out to be different from the aggregation of randomly moving particles that is well-known to physicists. Furthermore, the worm-blob behaves like a liquid, with a viscosity that depends on the applied shear force in a unique manner. The research was published in two papers in Physical Review Letters.

A. Deblais, S. Woutersen, and D. Bonn: “*Rheology of Entangled Active Polymer-Like T. Tubifex Worms*”, Physical Review Letters **124**, 188002 (2020). DOI: [10.1103/PhysRevLett.124.188002](https://doi.org/10.1103/PhysRevLett.124.188002)

A. Deblais, A. C. Maggs, D. Bonn, and S. Woutersen: “*Phase Separation by Entanglement of Active Polymerlike Worms*”, Physical Review Letters **124**, 208006 (2020). DOI: [10.1103/PhysRevLett.124.208006](https://doi.org/10.1103/PhysRevLett.124.208006)

### **Synthesis of chiral metal-organic frameworks by post-synthetic modification** - 27 May 2020



Using a combination of synthetic, spectroscopic and theoretical approaches, a team of HIMS researchers from various groups demonstrated that the post-synthetic modification of MOFs is an effective approach for the synthesis of chiral materials. The study was carried out in collaboration with the group of Prof. Sharon Ashbrook at the University St Andrews.

Andreea Gheorghe, Benjamin Strudwick, Sander Woutersen, David Dubbeldam, Stefania Tanase: *Synthesis of chiral MOF-74 frameworks using post-synthetic modification by an amino acid*. Chemistry - A European Journal, Accepted 27 May 2020, DOI: [10.1002/chem.202002293](https://doi.org/10.1002/chem.202002293).

### **Evidence for the catalytic properties of ultramarine pigment** - 2 June 2020



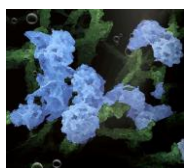
Researchers at the Rijksmuseum, the University of Amsterdam and VU Amsterdam established the catalytical activity of ultramarine pigment in experiments where methanol was dehydrated to dimethyl ether. They expect the catalytic activity of the pigment to also speed up the oxidation of the oil component in paints used by old masters. The research was published in the Journal of Cultural Heritage, featured in Chemistry World and was highlighted in a Nature Briefing.

Kokkie Schnetz, Alessa A. Gambardella, Roe Ivan Elsas, Joost Rosier, Edgar E. Steenwinkel, Arie Wallert, Pieter D. Iedema, Katrien Keune: *Evidence for the catalytic properties of ultramarine pigment*. Journal of Cultural Heritage, online 12 May 2020. DOI: [10.1016/j.culher.2020.04.002](https://doi.org/10.1016/j.culher.2020.04.002)

Chemistry World: [Luxury blue paint pigment catalyses its own ‘disease’](#).

Nature Briefing: [How paintings got the blues — and lost them](#).

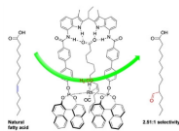
### **Harvesting hydrogen from nanogardens** - 2 July 2020



Easily produced, nature-like nanostructures of cobalt phosphide are highly effective catalysts for the electrolysis of water, according to research performed by Dr Ning Yan and his team together with co-workers from the School of Physics and Technology at Wuhan University, China. In a 'hot paper' featured on the front cover of the Journal of Materials Chemistry A, they describe how relatively straightforward electrochemical deposition methods yield grass-, leave- and flower-like nanostructures that carry the promise of efficient hydrogen generation.

Xiaoyu Yan, Yang Zhao, Jasper Biemolt, Kai Zhao, Petrus C. M. Laan, Xiaojuan Cao and Ning Yan: "Nano-garden cultivation" for electrocatalysis: controlled synthesis of Nature-inspired hierarchical nanostructures. *J. Mater. Chem. A*, 2020, 8, 7626 DOI: [10.1039/d0ta00870b](https://doi.org/10.1039/d0ta00870b)

### **Hot Paper on regioselective hydroformylation via remote supramolecular control** - 3 July 2020



A paper on 'Regioselective Hydroformylation of Internal and Terminal Alkenes via Remote Supramolecular Control' was published as a 'Hot Paper' by Chemistry, a European Journal. The work is the result of joined research between HIMS spin-off company InCatT and the research group for Homogeneous, Supramolecular and Bio-Inspired Catalysis led by Prof. Joost Reek. For the first time, fatty acids could be hydroformylated regioselectively.

Pim R. Linnebank, Stephan Falcão Ferreira, Alexander M. Kluwer, Joost N. H. Reek: *Regioselective Hydroformylation of Internal and Terminal Alkenes via Remote Supramolecular Control* *Chem. Eur. J.* Volume 26, Issue 37, 8214-8219 DOI: [10.1002/chem.202000620](https://doi.org/10.1002/chem.202000620)

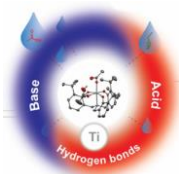
### **Intricate nanospheres containing hydrogenase mimics for proton reduction catalysis** - 15 July 2020



A paper on 'Hydrogenase mimics in M12L24 nano-spheres to control overpotential and activity in proton reduction catalysis' was published in *Angewandte Chemie*. It describes research on nature-inspired molecular systems for proton reduction catalysis led by Prof. Joost Reek at the research group Homogeneous, Supramolecular and Bio-Inspired Catalysis.

Riccardo Zaffaroni, Nicole Orth, Ivana Ivanović-Burmazović, Joost Reek: *Hydrogenase mimics in M12L24 nano-spheres to control overpotential and activity in proton reduction catalysis* *Angewandte Chemie International Edition*, First published: 02 July 2020. DOI: [10.1002/anie.202008298](https://doi.org/10.1002/anie.202008298)

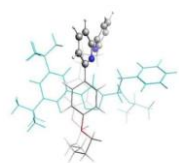
### **Titanium-catalyzed esterification reactions: beyond Lewis acidity** - 27 July 2020



In a paper in *ChemCatChem*, HIMS researchers show that the amphoteric nature of titanium aminotriphenolate complexes (combining a Lewis acidic metal centre with a Brønsted basic ligand site), in combination with preorganization via hydrogen bonding interactions, is essential for their catalytic activity in esterification reactions. Experimental and computational findings of the research, carried out in collaboration with AkzoNobel within the ARC CBBC consortium, demonstrate that Lewis acidity is not the only key factor for catalytic activity, contrary to what often is assumed in literature.

Lukas A. Wolzak, Jarl Ivar van der Vlugt, Keimpe J. van den Berg, Joost N.H. Reek, Moniek Tromp, Ties J. Korstanje: *Titanium-catalyzed esterification reactions: beyond Lewis acidity*. *ChemCatChem*, first published 13 July 2020. DOI: [10.1002/cctc.202000931](https://doi.org/10.1002/cctc.202000931)

### **Vibrational Circular Dichroism spectroscopy for probing the expression of chirality in mechanically planar chiral rotaxanes** - 29 July 2020



In a paper in the RSC flagship journal *Chemical Science*, researchers of the Molecular Photonics group presented a first in-depth VCD study of mechanically planar chiral rotaxanes as prototypical examples of mechanically chiral molecules. They demonstrate that a combined computational/experimental approach can provide detailed insight into the molecular aspects determining the spectroscopical manifestation of the stereochemistry of these molecules. By demonstrating the



power of VCD in these specific examples, they pave the way for its application to mechanically chiral rotaxanes and catenanes more generally.

M.A.J. Koenis, C. Chibueze, M. Jinks, V. Nicu, L. Visscher, S. Goldup and W.J. Buma: *Vibrational Circular Dichroism Spectroscopy for Probing the Expression of Chirality in Mechanically Planar Chiral Rotaxanes*, Chem. Sci., 2020, DOI: [10.1039/D0SC02485F](https://doi.org/10.1039/D0SC02485F).

### **3D-printing of column housings using Fused Deposition Modeling** - 3 August 2020



Researchers at the Analytical Chemistry group successfully developed 3D-printed channels for chromatographical separation of small molecules. The applied fused-deposition modelling (FDM) print technology can be used to produce columns in-house, for a fraction of the cost, with the ability to specify bespoke (on-demand) column dimensions. Their method was reported in a paper in the Journal of Chromatography A.

Noor Abdulhussain, Suhas Nawada, Sinéad Currivan, Marta Passamonti, Peter Schoenmakers: *Fabrication of polymer monoliths within the confines of non-transparent 3D-printed polymer housings*. J. Chromatogr. A, Vol. 1623, 19 July 2020, 461159 DOI: [10.1016/j.chroma.2020.461159](https://doi.org/10.1016/j.chroma.2020.461159)

### **Analysis of municipal wastewater as a predictor for population socioeconomics** - 4 August 2020

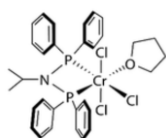


In a paper published in Environmental Science & Technology Letters, Dr Saer Samanipour of the Analytical Chemistry group reported on the chemical analysis of municipal wastewater as a predictor for population socioeconomics. The study attracted worldwide attention after an article in the Science & Technology section of The Economist.

Phil M. Choi, Jake W. O'Brien, Ben J. Tschärke, Jochen F. Mueller, Kevin V. Thomas, and Saer Samanipour: *Population Socioeconomics Predicted Using Wastewater*. Environ. Sci. Technol. Lett. 2020, published online 26 June. DOI: [10.1021/acs.estlett.0c00392](https://doi.org/10.1021/acs.estlett.0c00392)

The Economist, 18 July 2020: [Analysing waste water may assist census takers](https://www.economist.com/science-and-technology/2020/07/18/analysing-waste-water-may-assist-census-takers)

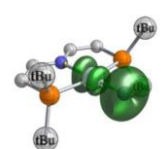
### **Spectroscopic investigations of selective Cr–PNP ethene tri- and tetramerization catalysts** - 17 August 2020



In a study published in Catalysis Science & Technology, HIMS researchers shed light on two important aspects of selective ethene oligomerization catalysts: the nature of the active species (e.g. neutral or cationic), and the role of the ligand in the formation of the active species.

Bas Venderbosch, Lukas A. Wolzak, Jean-Pierre H. Oudsen, Bas de Bruin, Ties J. Korstanje, and Moniek Tromp: *Role of the ligand and activator in selective Cr–PNP ethene tri- and tetramerization catalysts – a spectroscopic study*. Catal. Sci. Technol., 2020, first published 11 August 2020 DOI: [10.1039/d0cy01168a](https://doi.org/10.1039/d0cy01168a)

### **A Platinum(II) Metallonitrene with a Triplet Ground State** - 24 August 2020



Prof. Bas de Bruin contributed to a German study on the electronic structure of a platinum(II) metallonitrene that was published in Nature Chemistry. The study shows that - in contrast to intuition - neither the subvalent character nor the open-shell nature of the ground state of metallonitrenes are reliable predictors for nitrogen atom transfer reactivity.

Sven Schneider, Jian Sun, Josh Abbenseth, Hendrik Verplancke, Martin Diefenbach, Bas de Bruin, David Hunger, Christian Würtele, Joris van Slageren, Max C. Holthausen: *A Platinum(II) Metallonitrene with a Triplet Ground State*. Nature Chemistry, 24 August 2020, DOI: [10.1038/s41557-020-0522-4](https://doi.org/10.1038/s41557-020-0522-4)

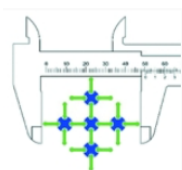
### **Strategies for circular waste management in an urban environment** - 10 September 2020



There's serious room for improvement in managing the waste of the city of Amsterdam. Many waste flows in the city are linear and unsustainable, and the recycling rate of organic waste is quite low. An open-access paper in the journal *Advanced Sustainable Systems* contained the first results of a case study by a joint team from the University of Amsterdam's Faculty of Science and the Amsterdam Business School, in the perspective of designing urban waste management strategies for a sustainable society.

L. Viva, F. Ciulli, A. Kolk and G. Rothenberg: *Designing Circular Waste Management Strategies: The Case of Organic Waste in Amsterdam*. *Adv. Sustainable Syst.*, **2020**, published online. DOI: [10.1002/adsu.202000023](https://doi.org/10.1002/adsu.202000023) (open access).

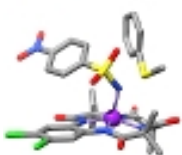
### **Designable catalytic materials combine the best of both worlds** - 14 September 2020



HIMS researchers published a new concept for designing and producing active, selective and stable catalytic materials that enable the use of bio-based feedstocks. These new polymers, which can be tailor-made to specific sizes and functions, can catalyze a variety of reactions. They are also highly stable and scalable, opening opportunities for real-life industrial applications.

I.M. Denekamp, C. Deacon-Price, Z. Zhang and G. Rothenberg: *Covalent structured catalytic materials containing single-atom metal sites with controllable spatial and chemical properties: concept and application*, *Catal. Sci. Technol.*, **2020**, published online. DOI: [10.1039/D0CY01299H](https://doi.org/10.1039/D0CY01299H) (Open Access).

### **Catalytic chemoselective sulfimidation with an electrophilic nitrene radical complex** - 21 September 2020



In a publication in *Chemistry, A European Journal*, researchers at the group for Homogeneous, Supramolecular and Bio-Inspired Catalysis reported on catalytic sulfimidation using a highly active and selective catalyst. The interplay between the redox-active ligand, substrate and cobalt as the metal centre was found to be a key factor in the observed reactivity. The developed protocol holds promise for late-stage functionalization of (drug-like) molecules.

Nicolaas P. van Leest, Jarl Ivar van der Vlugt, Bas de Bruin: *Catalytic Chemoselective Sulfimidation with an Electrophilic [Co<sup>III</sup>(TAML)]-Nitrene Radical Complex*. *Chem. Eur. J.*, accepted article, first published 18 August 2020. DOI: [10.1002/chem.202003566](https://doi.org/10.1002/chem.202003566)

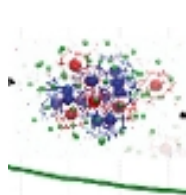
### **Redox-mediated alcohol oxidation coupled to hydrogen formation in a dye-sensitized photosynthesis cell** - 22 September 2020



In a paper in *Chemistry, A European Journal*, HIMS researchers presented a dye-sensitized photoelectrochemical cell that combines light-driven hydrogen production with chemical oxidation of an organic compound (benzyl alcohol). The cell was designed to enable in situ reaction monitoring of substrates and products for screening of organic reactions. Its performance approaches quantitative Faradaic efficiency.

Didjay F. Bruggeman, Tijmen M. A. Bakker, Simon Mathew and Joost Reek: *Redox-Mediated Alcohol Oxidation Coupled to Hydrogen Gas Formation in a Dye-Sensitized Photosynthesis Cell*. *Chem. Eur. J.*, First published 09 September 2020. DOI: [10.1002/chem.202003306](https://doi.org/10.1002/chem.202003306)

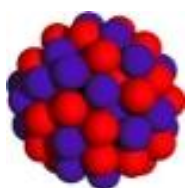
### **Rate prediction for homogeneous nucleation of methane hydrate** - 23 September 2020



Methane hydrates are the single biggest source of fossil fuel on planet earth and play a role in climate change. The molecular process of their formation is not known and heavily debated. In a paper in the Journal of Physical Chemistry B, HIMS Computational Chemistry researchers provide insight in methane hydrate formation. They performed atomistic scale molecular simulations that help establish the key thermodynamic and kinetic properties.

A. Arjun and P. G. Bolhuis: Rate Prediction for Homogeneous Nucleation of Methane Hydrate at Moderate Supersaturation Using Transition Interface Sampling. *J. Phys. Chem. B* 2020, 124, 37, 8099–8109 DOI: [10.1021/acs.jpcc.0c04582](https://doi.org/10.1021/acs.jpcc.0c04582)

### **Quantum dots for electrocatalytic oxidation** - 30 September 2020



In a paper in ACS Applied Nanomaterials, HIMS researchers reported on the straightforward, cheap and clean assembly of nanoclusters as catalysts for electro-oxidation purposes with applications in fuel cells, biosensors and in the industrial process of electroless copper deposition. Containing a combination of palladium and cheap cuprous oxide these catalysts outperform materials based solely on palladium.

Jasper Biemolt, Dylan van Noordenne, Jian-Wen Liu, Elise Antonetti, Manon Leconte, Stefan van Vliet, Roland Bliem, Gadi Rothenberg, Xian-Zhu Fu and Ning Yan: *Assembling Palladium and Cuprous Oxide Nanoclusters into Single Quantum Dots for Electrocatalytic Oxidation of Formaldehyde, Ethanol, and Glucose*. *ACS Appl. Nano Mater.* 2020, Published 27 September 2020. DOI: [10.1021/acsnm.0c02162](https://doi.org/10.1021/acsnm.0c02162)

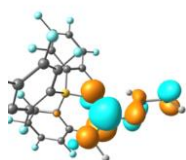
### **Surfing the microwave oven learning curve** - 1 October 2020



In a publication in the Journal of Cleaner Production, Prof. Bob van der Zwaan presented the first example of a learning curve for microwave ovens, which follows a learning rate of around 20%. The paper discusses opportunities for possible microwave heating applications in households and industry, that can contribute to sustainable development. Rapidly reducing prices could lead to a meaningful role of microwave technology in the energy transition.

Remko J. Detz, Bob van der Zwaan: *Surfing the microwave oven learning curve*. *Journal of Cleaner Production*, Volume 271, 20 October 2020, 122278 DOI: [10.1016/j.jclepro.2020.122278](https://doi.org/10.1016/j.jclepro.2020.122278)

### **Single-electron transfer in frustrated Lewis pair chemistry** - 7 October 2020



In a publication designated as 'hot paper' in *Angewandte Chemie*, HIMS researchers shed new light on the mechanism of reactions involving frustrated Lewis pairs (FLPs). They demonstrate that within FLP chemistry, both polar and radical pathways can be accessed. Their paper, which was also highlighted in *ChemistryViews*, describes how the latter generally proceeds via Lewis acid coordination to the substrate prior to radical formation.

Flip Holtrop, Andy Jupp, Bastiaan Kooij, Klaas van Leest, Bas de Bruin, Chris Slootweg: *Single-electron Transfer in Frustrated Lewis Pair Chemistry*, *Angew. Chem. Int. Ed.* 2020. DOI: [10.1002/anie.202009717](https://doi.org/10.1002/anie.202009717)

ChemistryViews highlight: [Frustrated Lewis Pair Radical Chemistry](#)

### **Assessing the future of plastics** - 28 October 2020



Biodegradable plastics have an important role to play in the greening of our society and in the transition to a circular economy. But according to Dr. Layla Filiciotto and Prof. Gadi Rothenberg there's still a long way to go. In a critical review in *ChemSusChem*, they provide a perspective by examining the socio-economic and environmental impacts of biodegradable and bio-based plastics. They also provide a hands-on approach on assessing biodegradability.

L. Filiciotto and G. Rothenberg: *Biodegradable Plastics: Standards, Policies, and Impacts*. *ChemSusChem*, **2020**, EarlyView. DOI: [10.1002/cssc.202002044](https://doi.org/10.1002/cssc.202002044)

### **Molecular confinement solves century-old puzzle** - 30 October 2020



HIMS researchers demystified one of the fuzziest parameters in heterogeneous catalysis: the Arrhenius pre-exponential factor. Using clever catalyst design and a special measurement device constructed in-house, they isolated the kinetics of molecules traveling across catalyst surfaces. The results were published in an open-access paper in *Chemical Science*.

T.K. Slot, N. Riley, N.R. Shiju, J.W. Medlin and G. Rothenberg: *An experimental approach for controlling confinement effects at catalyst interfaces*. *Chem. Sci.*, **2020**, 11, 11024–11029. DOI: [10.1039/D0SC04118A](https://doi.org/10.1039/D0SC04118A)

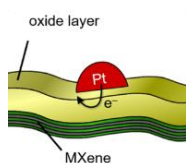
### **New catalysts for converting CO<sub>2</sub> to useful chemicals** - 2 November 2020



A collaboration between the Catalysis Engineering and Heterogeneous Catalysis & Sustainable Chemistry groups led to new layered materials with advanced catalytic properties, addressing one of the key challenges related to climate change. The new catalysts were presented in a paper as part of a special issue on “Green Carbon Science: CO<sub>2</sub> Capture and Conversion” of the international journal *ChemSusChem*.

M. Ronda-Lloret, V. S. Marakatti, W. G. Sloof, J. J. Delgado, A. Sepúlveda-Escribano, E. V. Ramos-Fernandez, G. Rothenberg, N. R. Shiju: *Butane Dry Reforming Catalyzed by Cobalt Oxide Supported on Ti<sub>2</sub>AlC MAX Phase*, *ChemSusChem* **2020**, 13, EarlyView. DOI: [10.1002/cssc.202001633](https://doi.org/10.1002/cssc.202001633)

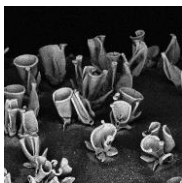
### **Improving hydrogen storage with MXene materials** - 27 November 2020



Researchers from the Catalysis Engineering and Heterogeneous Catalysis and Sustainable Chemistry groups, together with their international collaborators, found a nifty way to improve catalyst performance in on-demand hydrogen generation. Their results were published as an open-access paper in the international journal *2D Materials*.

T.K. Slot, F. Yue, H. Xu, E.V. Ramos-Fernandez, A. Sepúlveda-Escribano, Z. Sofer, G. Rothenberg, N.R. Shiju: *Surface oxidation of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> enhances the catalytic activity of supported platinum nanoparticles in ammonia borane hydrolysis*. *2D Mater.* **2020**, 8, 015001. DOI: [10.1088/2053-1583/ababef](https://doi.org/10.1088/2053-1583/ababef)

**UvA and AMOLF researchers work together towards CO<sub>2</sub> valorisation** - 4 December 2020



A collaboration between researchers of the Catalysis Engineering group and the Self-Organizing Matter group at AMOLF led to the first catalytic application of nickel-based coral-like architectures for CO<sub>2</sub> conversion at relatively low temperatures. The results were published in the journal *Advanced Materials* and highlighted in *Nature* and *Nature Reviews Materials*.

Hans C. Hendrikse, Arno van der Weijden, Maria Ronda-Lloret, Ting Yang, Roland Bliem, N. Raveendran Shiju, Martin van Hecke, Ling Li, and Willem L. Noorduin: *Shape-Preserving Chemical Conversion of Architected Nanocomposites*, *Adv. Mater.*, **2020**, 2003999. DOI: [10.1002/adma.202003999](https://doi.org/10.1002/adma.202003999)

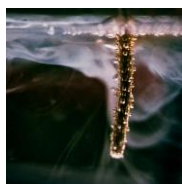
Highlight in *Nature*: [Presto chango: tiny particles get a chemical makeover but keep their shape](#)

*Nature Reviews Materials*: [Nanocomposites keep in shape](#)

## Prizes and honours

The quality of HIMS scientists is reflected in the prizes and honours they receive. Noteworthy examples are the instalment of Prof. Bas de Bruin as Chemistry Europe Fellow and the 2019 Backer-KNCV Prize for the PhD thesis of Kananat Naksomboon. Below is a list of news items reporting on these and other HIMS staff members and students.

### Eric Schuler wins national chemistry photo contest - 6 January 2020



With the photo "Chrysopoeia - electrified golden tin clouds" HIMS PhD student Eric Schuler won the 2019 photo contest of the Royal Netherlands Chemical Society KNCV. The prize was awarded to him during the national chemistry conference CHAINS. The photo shows the cathodic corrosion of a highly pure tin wire in alkaline solution, where the electrochemical potential causes the metal to form nanoparticles in solution.

### Prof. Bas de Bruin named Chemistry Europe Fellow - 6 April 2020



In recognition of his scientific contributions, Chemistry Europe named Prof. Bas de Bruin one of its Fellows. De Bruin's research focus is on the development of new tools in homogeneous catalysis, using metals in unconventional oxidation states and unconventional ligands, specifically aiming at the development of new catalytic reactions.

### Mimi den Uijl competes for 'Spotlight' prize at national 'Evening of Chemistry' - 28 September 2020



PhD candidate Mimi den Uijl presented her research at the Dutch national 'Evening of Chemistry' (Avond van de Chemie). During this annual meeting, organized by chemistry association KNCV, she competed for the 'Spotlight' prize of Young KNCV. Den Uijl won her participation with a self-produced YouTube video.

### Kaj van Vliet is first candidate to obtain PhD in HRSMC excellence track - 2 October 2020



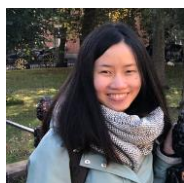
In September, Dr. Kaj van Vliet received his PhD certificate from Prof. Bas de Bruin. This was a remarkable moment, not only because pandemic times had delayed the presentation, but also because Van Vliet was the first PhD to graduate on a personally drafted research proposal prepared during the Excellence Master 'Sustainability: the Molecular Approach' of the Holland Research School of Molecular Chemistry.

### Klaas Jan Schouten becomes member of ECCM - 30 October 2020



Dr. Klaas Jan Schouten was appointed member of the Electrochemical Conversion and Materials (ECCM) committee. This aims to develop a joint R&D agenda for the Netherlands with a focus on the long target of CO<sub>2</sub> neutrality in 2050, bringing together national experts from industry, government and academia.

**Kananat Naksomboon wins the Backer-KNCV Prize 2019** - 17 November 2020



Kananat Naksomboon won the Backer-KNCV Prize for her PhD-thesis 'Bidentate ligand-promoted Palladium-catalyzed C-H olefination of aromatic compounds' supervised by associate professor M.A. Fernández-Ibáñez. The prize is awarded annually to the best PhD thesis in the field of organic chemistry defended in The Netherlands.

**Rajamani Krishna among world's highly cited chemists** - 19 November 2020



Professor Rajamani Krishna was included in the Highly Cited Researchers 2020 list compiled based on data and analysis performed by bibliometric experts from the Institute for Scientific Information at the Web of Science Group (part of Clarivate Analytics). The list contains scientists who have been most frequently cited by their peers over the last decade.

## Grants and funding

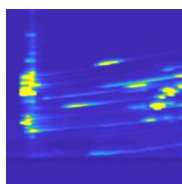
Below is an overview of news item on grants and funding obtained by HIMS scientists. More on the financial aspects of the institute can be found in the Facts & Figures section of this annual report.

### Novel chemistry for utilizing methane as a feedstock for high-value chemicals - 20 January 2020



The Dutch science foundation NWO funded research into new chemistry for the utilization of methane, building upon a recent discovery in the group of associate professor Dr Chris Sloopweg. The novel chemical activation and functionalisation of methane can contribute to using this abundantly available gas for the synthesis of valuable chemicals.

### PARADISE: bringing analytical science to the next level - 17 February 2020



Together with the Netherlands Forensic Institute and the companies Genentech, Shell and DSM, analytical chemists from HIMS and Vrije Universiteit Amsterdam started the PARADISE project to develop robust, automated methodologies that allow multidimensional characterization of the most challenging man-made and natural products. The project was awarded funding of almost a million euros from the Science PPP Fund of the Netherlands Organisation for Scientific Research NWO.

### How universal are life's building blocks? - 25 February 2020



Astrochemist and MacGillavry Fellow Dr Annemieke Petrignani was awarded funding of € 280,000 through the Planetary and Exoplanetary Science programme (PEPSci) of NWO. The focus of this research, carried out in cooperation with Dr Helen King from Utrecht University, will be on polymerization processes as a selection mechanism between potential terrestrial and extra-terrestrial building blocks of life.

### How does the accessibility of DNA affect the expression of genes? - 9 March 2020



Dr Jocelyne Vreede of the Computational Chemistry group received an NWO KLEIN-2 grant for a four-year project investigating how the shape and compactness of DNA affect the expression of genes. In cooperation with Prof. Willem Kegel, professor of Self-organizing Systems at Utrecht University, experimental, theoretical and computational approaches will be developed to provide quantitative and detailed insights into this as of yet unknown aspect of DNA transcription.

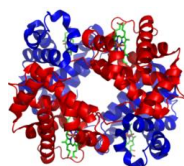
### Amanda Garcia joins HIMS with NWO-ECCM tenure-track grant - 30 March 2020



Dr Amanda Garcia was awarded a highly competitive tenure-track grant of 950,000 euros from the NWO program on electrochemical conversion and materials (ECCM). Focussing on electrocatalysis and electro-organic synthesis, she joined HIMS and the growing group of interdisciplinary researchers collaborating in the Amsterdam Centre for Electrochemistry (Amcel).



### **The role of metal-ions on protein aggregation** - 12 June 2020



Dr Jocelyne Vreede (Computational Chemistry) and Dr Alina Astefanei (Analytical Chemistry) received an NWO grant for a public-private partnership with DSM to investigate the role of ions on the shape and aggregation of metalloproteins. Metalloproteins are of great industrial interest as they can be used as food enzymes. DSM is one of the largest producers of food enzymes in the world.

### **Idea Generator funding for Sander Woutersen** - 3 July 2020



HIMS professor Sander Woutersen was awarded funding through the 'Idea Generator' programme of the Dutch Research Agenda. He received 50,000 euros for research into 'How Nature prevents protein aggregation in cells'. This is important for understanding the origins of life, but also for understanding and preventing diseases such as Alzheimer's and Parkinson's.

### **Erasmus + Strategic Partnership grant awarded** - 25 August 2020



A team of HIMS lecturers together with the Teaching and Learning Centre of the Faculty of Science and five international partners started a three-year project to promote the importance of Continuous Professional Development (CPD) at European universities. Together the partners received almost half a million euro from the European Union.

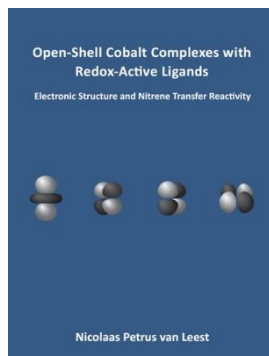
### **Funding for research into enzymatic depolymerisation of synthetic polymers** - 27 November 2020



The Biocatalysis and Analytical Chemistry research groups were granted € 265,000 by TKI Chemie / Holland Chemistry for joint research into the enzymatic depolymerisation of synthetic polymers. They will collaborate with industrial partners DSM Coating Resins and InnoSyn. Project PIs are associate professor Francesco Mutti of Biocatalysis and assistant professor Andrea Gargano of Analytical Chemistry.

## Dissertations

Of the 27 students that received their PhD at HIMS in 2020, three were granted the distinction 'cum laude': Mark Koenis, Vasilis Tseliou and Klaas van Leest. All theses are listed below; a link is provided to download each thesis from the UvA repository.



3 December 2020

### Open-shell cobalt complexes with redox-active ligands - Electronic structure and nitrene transfer reactivity

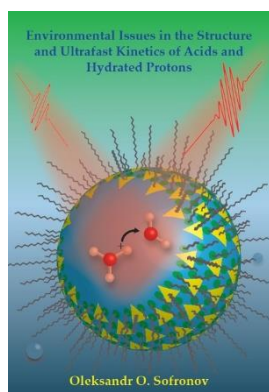
Author: N. (Klaas) P. van Leest

Supervisor: B. de Bruin

Co-supervisor: J.I van der Vlugt

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



27 November 2020

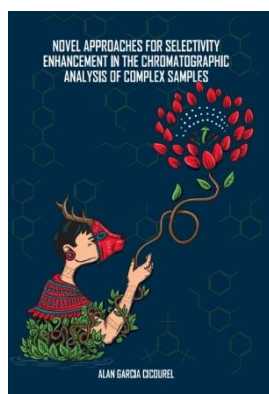
### Environmental issues in the structure and ultrafast kinetics of acids and hydrated protons

Author: O. (Oleksandr) O. Sofronov

Supervisor: H.J. Bakker

Group: Molecular Photonics

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



20 November 2020

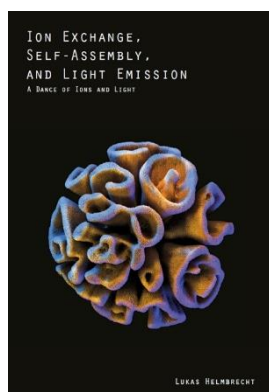
### Novel approaches for selectivity enhancement in the chromatographic analysis of complex samples

Author: A. (Alan) R. García Cicourel

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

Group: Analytical Chemistry

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



20 November 2020

### Ion exchange, self-assembly, and light emission

#### A dance of ions and light

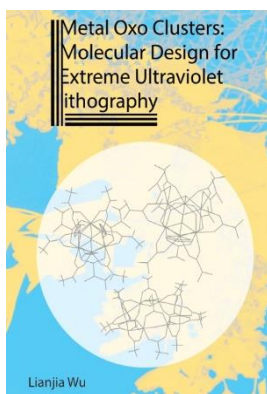
Author: L. (Lukas) Helmbrecht

Supervisors: H.J. Bakker

Co-supervisor: W.L. Noorduin

Group: Molecular Photonics

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



18 November 2020

**Metal oxo clusters: molecular design for extreme ultraviolet lithography**

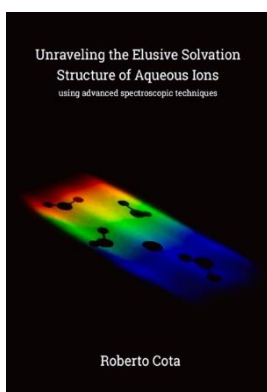
Author: L. (Lianjia) Wu  
Supervisors: A.M. Brouwer  
Co-supervisor: S. Castellanos Ortega  
Group: Molecular Photonics  
Link: [Read or download this thesis](#)



13 November 2020

**Into the deep waters of emulsions and hydrogels**

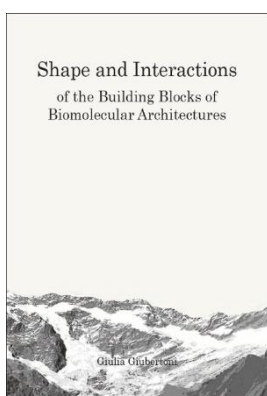
Author: E. (Eliane) P. van Dam  
Supervisor: H.J. Bakker  
Group: Molecular Photonics  
Link: [Read or download this thesis](#)



30 October 2020

**Unraveling the elusive solvation structure of aqueous ions - using advanced spectroscopic techniques**

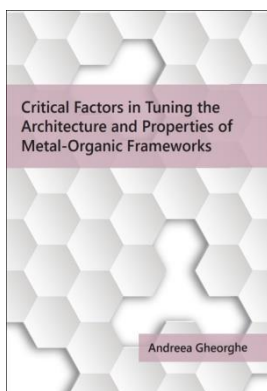
Author: R. (Roberto) O. Cota  
Supervisors: S. Woutersen, H.J. Bakker  
Group: Molecular Photonics  
Link: [Read or download this thesis](#)



16 October 2020

**Shape and interactions of the building blocks of biomolecular architectures**

Author: G. (Giulia) Giubertoni  
Supervisors: H.J. Bakker, G.H. Koenderink  
Group: Molecular Photonics  
Link: [Read or download this thesis](#)



8 October 2020

**Critical factors in tuning the architecture and properties of metal-organic frameworks**

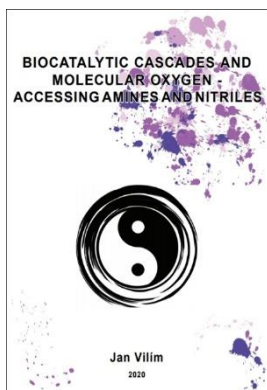
Author: A. (Andreea) Gheorghe

Supervisor: S. Grecea

Co-supervisor: G. Rothenberg

Group: Heterogeneous Catalysis and Sustainable Chemistry

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



07 October 2020

**Bio-catalytic cascades and molecular oxygen-accessing amines and nitriles**

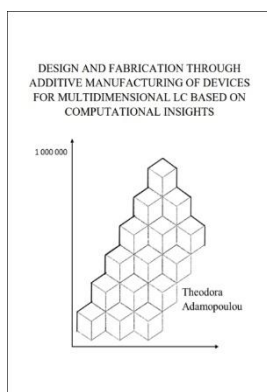
Author: J. (Jan) Vilím

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

Co-supervisor: M.A. Fernández Ibáñez

Group: Biocatalysis

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



30 September 2020

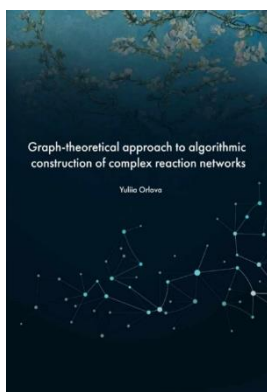
**Design and fabrication through additive manufacturing of devices for multidimensional LC based on computational insights**

Author: T. (Theodora) Adamopoulou

Supervisors: P.J. Schoenmakers, G.E. Desmet

Group: Analytical Chemistry

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



24 September 2020

**Graph-theoretical approach to algorithmic construction of complex reaction networks**

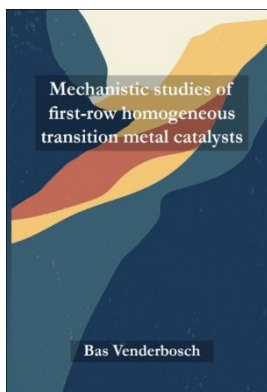
Author: Y. (Yuliia) Orlova

Supervisor: P.D. Iedema

Co-supervisor: I. Kryven

Group: Computational Polymer Chemistry

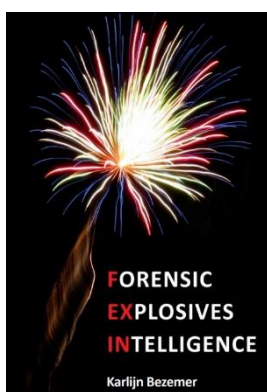
Link: [Read or download this thesis](#)



07 September 2020

### **Mechanistic studies of first-row homogeneous transition metal catalysts**

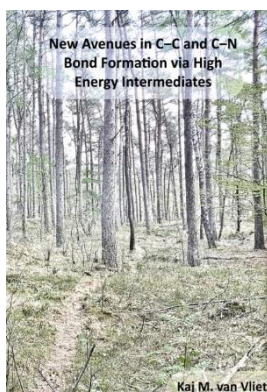
Author: B. (Bas) Venderbosch  
Supervisors: M. Tromp, J.N.H. Reek  
Co-supervisor: T.J. Korstanje  
Link: [Read or download this thesis](#)



02 September 2020

### **Forensic explosives intelligence**

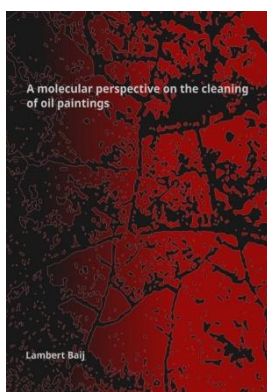
Author: K. (Karlijn) D.B. Bezemer  
Supervisors: A.C. van Asten, P.J. Schoenmakers  
Group: Analytical Chemistry  
Link: [Read or download this thesis](#)



03 July 2020

### **New avenues in C-C and C-N bond formation via high energy intermediates**

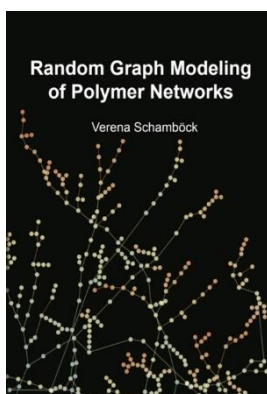
Author: K. (Kay) M. van Vliet  
Supervisor: B. de Bruin  
Co-supervisor: A.M. Brouwer  
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis  
Link: [Read or download this thesis](#)



02 July 2020

### **A molecular perspective on the cleaning of oil paintings**

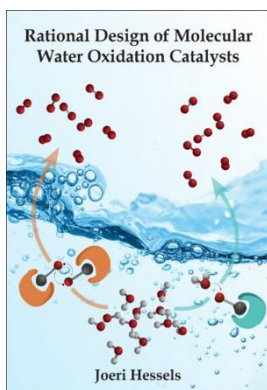
Author: C.L. (Lambert) M. Baij  
Supervisor: K. Keune  
Co-supervisors: P.D. Iedema, J.J. Hermans  
Group: Computational Polymer Chemistry  
Link: [Read or download this thesis](#)



01 July 2020

### Random graph modeling of polymer networks

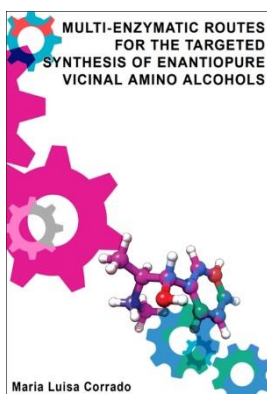
Author: V. (Verena) Schamböck  
Supervisors: P.D. Iedema, I. Kryven  
Group: Computational Polymer Chemistry  
Link: [Read or download this thesis](#)



29 June 2020

### Rational design of molecular water oxidation catalysts

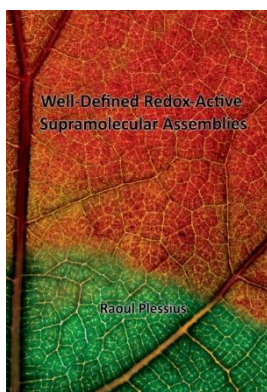
Author: J. (Joen) Hessels  
Supervisor: J.N.H. Reek  
Co-supervisor: R.J. Detz  
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis  
Link: [Read or download this thesis](#)



24 June 2020

### Multi-enzymatic routes for the targeted synthesis of enantiopure vicinal amino alcohols

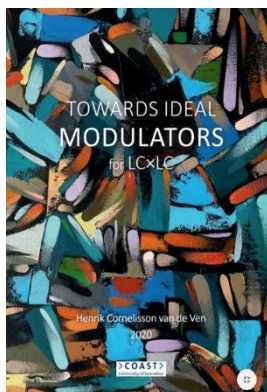
Author: M. (Maria) Luisa Corrado  
Supervisors: F. Mutti, J.H. van Maarseveen  
Group: Biocatalysis  
Link: [Read or download this thesis](#)



16 June 2020

### Well-defined redox-active supramolecular assemblies

Author: R. (Raoul) Plessius  
Supervisor: J.I. van der Vlugt, J.N.H. Reek  
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis  
Link: [Read or download this thesis](#)



5 June 2020

### **Towards ideal modulators for LCxLC**

Author: H. (Henrik) Cornelisson van de Ven

Supervisor: P.J. Schoenmakers

Co-supervisor: S. van der Wal

Group: Analytical Chemistry

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



3 June 2020

### **Exciting tin-oxo cages**

#### **Light-induced chemistry for nanopatterning**

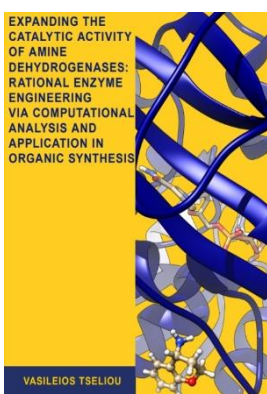
Author: J. (Jarich) Haitjema

Supervisor: A.M. Brouwer

Co-supervisor: S. Castellanos Ortega

Group: Molecular Photonics

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



12 May 2020

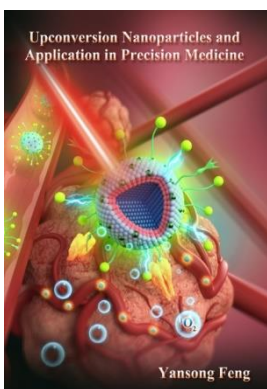
### **Expanding the catalytic activity of amine dehydrogenases**

Author: V. (Vasileios) Tseliou

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

Group: Biocatalysis

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



22 April 2020

### **Upconversion nanoparticles and application in precision medicine**

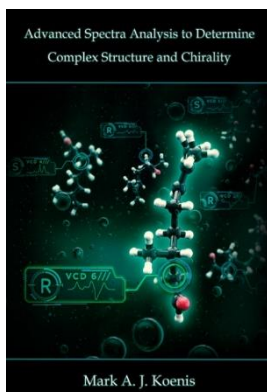
Author: Y. (Yansong) Feng

Supervisor: H. Zhang

Co-supervisor: W.J. Buma

Group: Molecular Photonics

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



15 April 2020

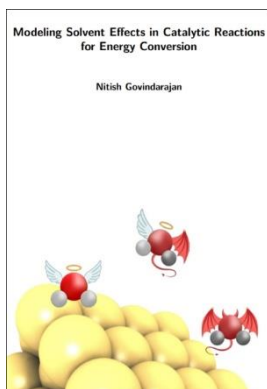
**Advanced x-ray absorption spectroscopy - Analyzing electronic structures of catalysts**

Author: J.P. (Jean-Pierre) H. Oudsen

Supervisors: M. Tromp, J.N.H. Reek

Co-supervisor: T.J. Korstanje

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



14 April 2020

**Modeling solvent effects in catalytic reactions for energy conversion**

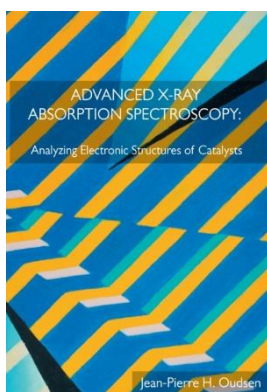
Author: N. (Nitish) Govindarajan

Supervisor: E.J. Meijer

Co-supervisor: P.G. Bolhuis

Group: Computational Chemistry

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



21 February 2020

**Advanced spectra analysis to determine complex structure and chirality**

Author: M. (Mark) A.J. Koenis

Supervisors: W.J. Buma, L. Visscher

Co-supervisor: V.P. Nicu

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.

### Amsterdam Chemistry Innovation Day

Because of the COVID-19 pandemic, the Amsterdam Chemistry Innovation Day 2020 was held fully online on 30 October. It featured keynote contributions from, amongst others, Victor Everhardt (Vice Mayor of Economic Affairs and the Amsterdam Harbour, City of Amsterdam), Marcus Remmers (CTO DSM) and Manon Bloemer (Director Royal VNCI). HIMS scientists hosted sessions on diverse subjects such as Careers in chemistry; Chemistry and Artificial Intelligence, and Valorisation of Life Sciences.

### Patent applications:

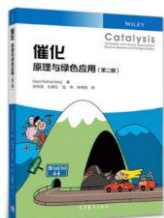
Mutti, F., Tseliou, V., Knaus, T., & Masman, M. F. (2020). *L-Lysine epsilon-dehydrogenase variants and uses thereof*. (Patent No. WO 2020165417 A1 20200130).

Munnik, T., Buma, W. J., Stavros, V., Ashfold, M., & Franklin, K. (2020). *Molecular Heaters: To protect plants against cold stress and boost growth at lower temperatures*. (Patent No. WO2020/053580 A1).

Mutti, F., Vilím, J., & Knaus, T. (2020). *Process for the manufacture of nitrile compounds*. (Patent No. WO 2020020844 A1 20200130).

### Valorisation news items:

#### Chinese edition of popular catalysis textbook published - 23 June 2020



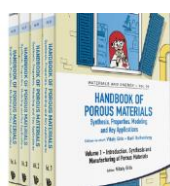
The second edition of 'Catalysis: Concepts & Green Applications', the popular undergraduate textbook written by Prof. Gadi Rothenberg of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences, was translated in Chinese. A low-cost paperback edition available to Chinese students was published by 'Higher Education Press', the publishing house of the Chinese Ministry of Education.

#### Patented 'molecular heaters' to increase crop yield - 23 September 2020



Prof. Wybren Jan Buma of Molecular Photonics (HIMS) and Dr Teun Munnik of Plant Cell Biology (SILS) developed a novel class of molecules capable of raising the temperature of plants, in a cooperation with researchers from the universities of Warwick and Bristol. Application of such 'molecular heaters' allows crops to grow at lower environmental temperatures. This can extend the growth season, increase the availability of arable land, and facilitate speed breeding programs for new crop varieties. After having been awarded a patent, the researchers started looking for partners to further develop feasible applications of the molecular heaters.

#### UvA researchers collaborate on new Handbook of Porous Materials - 30 September 2020



A group of authors including researchers and alumni from the Van 't Hoff Institute for Molecular Sciences (HIMS) completed a four-volume reference work covering the fundamentals and key applications of porous materials. This "Handbook of Porous Materials" was published by World Scientific Publishers in a digital and a print edition.

**Physics2market grant for pilot Open Kitchen Labs** - 14 December 2020



Professor Joost Reek (HIMS) and Dr Monalisa Goswami (Spark904) received a grant to run a first pilot with Open Kitchen Lab. This will be a service available in one of the Matrix buildings at Amsterdam Science Park, where spin-offs can rent a laboratory facility that already has the basic equipment and consumables.

## Outreach

### Lectures and other contributions in 2020

#### *For the general public*

- Paintings research [Pint of Science](#) 23/09/20 (Katrien Keune)
- The future of plastics, Spui 25-lecture 28/02/20 (Gert Jan Gruter)

#### *For highschool students and teachers*

- Chemistry in Amsterdam (16/11/20 → 20/11/20): [How research in chemistry contributes to making the food industry more sustainable](#) Wybren Jan Buma talks about his research on molecules that can be used to increase yields in agriculture.
- Coordination chemistry to make small cavities: Lecture for HBO students, January 2020 (Tiddo Mooibroek)
- Guiding research projects (profielwerkstuk) on sustainability-related topics, Centrum Jongeren Communicatie Chemie (Stefania Grecea)
- Profielwerkstuk support Atheneum College Hageveld Heemstede: Analytical Science in Operation Nightwatch (Katrien Keune)
- Profielwerkstuk support Keizer Karel College Amstelveen: Lead white in paintings (Katrien Keune)

### HIMS researchers in the media in 2020

#### ***Unsuccessful UvA experiment did result in 100% vegetable plastic***

Ten years ago UvA scientists made a discovery, now there is the first product in the form of a plant-based chair. Gadi Rothenberg obtained a lot of media attention with the story about how his accidental “sticky mess” led to a 100% natural bioplastic.

▶ [25 December, Nu.nl](#)

▶ [24 November, RTV Drenthe](#)

▶ [YouTube: The most sustainable chair ever!](#)



#### ***How Algorithms Are Revolutionizing Liquid Chromatography***

Bob Pirok and his team use informatics techniques to make LC more automated and pain-free. *Technology Networks* recently spoke to Pirok to find out more about his innovative algorithms.

▶ [17 December, Technology Networks](#)

#### ***Opinion: climate change more of a problem than a life threatening virus***

In an op-ed article in *De Volkskrant* Jan van Maarseveen gives his opinion about the approach of combatting the climate change.

▶ [7 December, De Volkskrant](#)

#### ***Isotopes make the bomb***

UvA chemist Karlijn Bezemer (HIMS) investigates whether the chemical fingerprint of illegal explosives could help trace the culprit. *C2W* has a news item about her work

▶ [4 December, C2W](#).

### **Powder letters**

Powder letters were sent to various Dutch companies and institutions. How do you find out the sender of this type of threatening letter? Chemist Arian van Asten (UvA-HIMS) explains it in De Telegraaf and on the RTL Nieuws website.

▶ [20 november, De Telegraaf \(via LexisNexis\)](#)

▶ [20 november, RTL Nieuws](#)

### **"As far as the climate is concerned, it is one second to twelve"**

For decades, Jan van Maarseveen built ring-shaped molecules as part of drug research. Now he is trying to develop sustainable technology with molecules of this kind that should put a stop to the climate crisis.

▶ [19 November, NewScientist](#)



### **Climate crisis**

Jan van Maarseveen talks to AD about new technology to stop the climate crisis.

▶ [15 November, AD](#)

### **Chemical Science article featured in C2W**

C2W published an item about the [paper](#) of Thierry Slot and master student Nathan Riley (in Dutch)

▶ [6 November, C2W](#)

### **Circular chemistry**

Chris Slootweg drew up the '12 principles of circular chemistry' in 2019. MVO Nederland has an interview with him about this.

▶ [16 October, MVO Nederland](#)

### **Hydrogen peroxide against corona**

Many dentists currently recommend rinsing your mouth with highly diluted hydrogen peroxide to kill the coronavirus. Does this work? RTL Nieuws asked UvA chemist Bas de Bruin (HIMS).

▶ [9 October, RTL Nieuws](#)

### **"Molecular heaters" of plants**

The technology developed by Wybren Jan Buma (UvA-HIMS) and Teun Munnik (UvA-SILS) to increase the temperature of plants via special molecules, which has recently been patented, is picked up by the specialized press. AgriHolland, Food & Agri Business and Greenity, among others, report about it.

▶ [AgriHolland, 23 September](#)

▶ [Food & Agri Business, 23 September 2020](#)

▶ [Greenity, 25 September 2020](#)

### **Can the climate problem be solved with nuclear energy?**

In an interview with Nu.nl Bob van der Zwaan gives his opinion on this question.

▶ [Nu.nl, 23 September 2020](#)

### **Three-Dimensional Thinking**

Noor Abdulhussain was interviewed by The Column (issued by Chromatography online) on her recently published [article](#) and the latest developments in 3D-printing for separation science. The interview was featured on the cover

▶ [The Column](#)

▶ [11 September, C2W](#)



### **PhD research of Karlijn Bezemer**

▶ [31 August, De Ingenieur](#)

### **Flames at the Shell oil refineries**

Bas de Bruin explains at EditieNL (RTL Nieuws) how this happens.

▶ [EditieNL 13 August](#)

### **Beirut explosion**

In an item for EditieNL (RTL Nieuws), Bas de Bruin provided background on fertilizer explosions and the colour of the smoke cloud.

▶ [EditieNL, 5 August.](#)

### **Radical reactions**

Interview with Bas de Bruin

▶ [16 June, C2W](#)

### **Cooperation with Chinese universities**

Folia magazine interviewed Gadi Rothenberg on the pros en cons of cooperation with Chinese universities

▶ [Folia, 7 May.](#)

### **Disinfection of face masks**

Fred Brouwer contributed to an item of Edition NL (RTL Nieuws) on disinfecting face masks using UV-light

▶ [Edition NL, 27 March.](#)

### **Rembrandt van Rijn's paint**

Katrien Keune contributed to the TV programme 'Historisch bewijs' about a box with paint bags supposedly used by Rembrandt van Rijn. In an additional online edition of the programme she provides insight into the use of XRF scanning and X-ray methods.

▶ [Historisch bewijs, 12 February.](#)

▶ [Historisch bewijs extra, 12 February.](#)



## Facts and figures

### Research

#### Research output

Research output 2020 per type of publication (source: PURE)

HIMS themes	AC	CC	MP	SC	Other <sup>1</sup>	Joint <sup>2</sup>	Total
Refereed articles (academic)	28	60	43	99	10	24	240
Non-refereed articles	1			1	1		3
Book - Authored				1			1
Book (chapter)s	6			2			8
PhD-theses	4	4	9	10			27
Patent			1	2			3
Other research output	5	2	1	2			7

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

<sup>1</sup> e.g. AMOLF, ARCNL, Avantium.

<sup>2</sup> The number of joint results obtained from collaborations between different research groups. The total number of 24 joint publications includes 34 collaborations.

#### Other output and honours

HIMS themes	AC	CC	MP	SC	Other	Joint	Total
Keynote lectures	9	10	3	26			48
Hosting a conference		1	1	2			4
Lecture for general public, media coverage		3	1	1			5
Prizes/awards	6	3	5	13			27

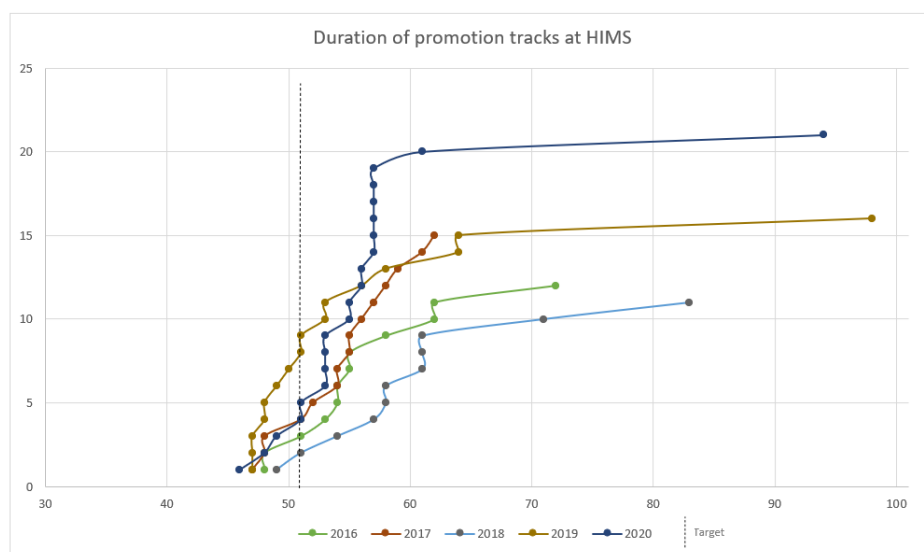
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis.

#### 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		
			#	%	#	%	#	%	#	%	#	%	#	%	#	%	
2012	13	6	19	2	11	9	47	5	26	1	5	17	89	-	-	2	11
2013	7	8	15	3	20	6	40	5	33	-	-	14	93	-	-	1	7
2014	6	7	13	1	8	8	62	2	15	-	-	11	85	-	-	2	15
2015	19	4	23	3	13	14	61	2	9	-	-	19	83	3	13	1	4
2016	18	13	31	1	3	10	32	-	-	-	-	10	32	18	58	2	6
<b>Total</b>	<b>63</b>	<b>38</b>	<b>101</b>	<b>10</b>	<b>10</b>	<b>47</b>	<b>47</b>	<b>14</b>	<b>14</b>	<b>1</b>	<b>1</b>	<b>71</b>	<b>70</b>	<b>21</b>	<b>21</b>	<b>8</b>	<b>8</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

This table presents the HIMS staff numbers (average head count in 2018) and in Research FTE. Research FTE means net time available for research as full time equivalents (FTE) per employment type. The numbers are based on an input of 0.5 FTE per FTE Scientific staff, 0.9 FTE per FTE Post-docs, 0.75 FTE per FTE PhD students and 1.0 FTE per FTE Technicians, Visiting Fellows and Support staff. Detailed information on these numbers is available as supporting information. 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)	6,1	3,0	8,1	4,1	5,1	2,5	13,2	6,6	0,0	0,0	32,5	16,2
Post-docs (2)	3,6	3,2	0,4	0,3	4,4	4,0	12,2	11,0	0,0	0,0	20,6	18,5
PhD students (3)	12,1	9,1	7,5	5,6	11,0	8,2	41,3	31,0	0,0	0,0	71,9	53,9
<b>Total research staff</b>	<b>21,8</b>	<b>15,3</b>	<b>16,0</b>	<b>10,0</b>	<b>20,5</b>	<b>14,7</b>	<b>66,7</b>	<b>48,6</b>	<b>0,0</b>	<b>0,0</b>	<b>125,0</b>	<b>88,6</b>
Technicians (4)	3,6	3,6	0,1	0,1	3,2	3,2	11,2	11,2	0,0	0,0	18,1	18,1
Visiting fellows	0,0	0,0	0,0	0,0	0,3	0,3	0,0	0,0	0,0	0,0	0,3	0,3
Support staff (4)	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	5,7	5,7	5,7	5,7
<b>Total staff</b>	<b>25,4</b>	<b>18,9</b>	<b>16,1</b>	<b>10,1</b>	<b>23,7</b>	<b>18,2</b>	<b>78,2</b>	<b>59,8</b>	<b>5,7</b>	<b>5,7</b>	<b>149,1</b>	<b>112,7</b>

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

Note 1: Comparable with WOPI categories professor, associate professor and assistant professor; tenured and nontenured staff.

Note 2: Comparable with WOPI category researcher, or non-tenured staff.

Note 3: Standard PhD (employed) and contract PhDs (externally or internally funded but not employed).

Note 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 2020.

Age bracket	Number	%-age	Male	Female	Dutch	Other EU	Other
30-40	12	28%	9	3	4	5	3
40-50	13	30%	8	5	9	3	1
50-60	13	30%	13	0	12	0	1
60+	5	12%	5	0	4	1	0
<b>Total</b>	<b>43</b>	<b>100%</b>	<b>35</b>	<b>8</b>	<b>29</b>	<b>9</b>	<b>5</b>

## 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 2020 of HIMS per funding type (fte)

HIMS Themes	Research					Total	%	Support	Total	%
	AC	CC	MP	SC	Other					
Direct funding	-	-	-	-	-	60	36%	14,9	74,9	40%
Research grants	7,25	3,51	8,81	36,61	-	49,6	40%	3,2	52,8	36%
Contract research	7,23	1	3,15	13,43	-	30,2	24%		30,2	20%
Other	-	-	-	0,4	2,9	3,3	0%	5,7	9	4%
<b>Total</b>	<b>14,4</b>	<b>9,6</b>	<b>9,5</b>	<b>46,3</b>	<b>2,9</b>	<b>143,1</b>	<b>100%</b>	<b>23,8</b>	<b>151,45</b>	<b>100%</b>

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 2020 (mln €) per funding type

HIMS themes	AC	CC	MP	SC	Other	Total <sup>1</sup>
Direct funding	0	0	0,36	0	0	<b>0,36</b>
Research grants	0	0	0,33	2,14	0	<b>2,47</b>
Contract research	0	0	0	2,47	0	<b>2,47</b>
<b>Total</b>	<b>0</b>	<b>0</b>	<b>0,69</b>	<b>2,14</b>	<b>0</b>	<b>5,3</b>

Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis. Other includes the institute's office. Note 1: Budgets were obtained for (in FTE)10 PhD's, 7,7 PD and 2,7 staff.

## HIMS result 2020 (k€)

The HIMS result for 2020 amounts to +1.6 Mio€. These concern reservations from past budgets for costs in the framework of the *Sectorplan Natuur- en Scheikunde* and the RPA Sustainable Chemistry foreseen. Due to the pandemic travel restrictions many new hires arrived later than budgeted. Spending, especially on congresses and travel was lower than in usual years. The institutes is required to have a reserve of minimal 10% of its annual revenue to which the surplus is counted in part as well.

2020	EU & Contract research			Total
	Direct	NWO		
HIMS Base Budget	3.622	-	-	3.622
Budget (variable1)	6.764	3.792	2.417	12.973
Other income 2	2.034	19	23	2.076
Matching contract research	-4.164	3.296	868	-
<b>Budget total</b>	<b>8.256</b>	<b>7.107</b>	<b>3.308</b>	<b>18.671</b>
<i>Percentage</i>	<i>44%</i>	<i>38%</i>	<i>18%</i>	<i>100%</i>
Personal costs	-4.972	-3.286	-1.385	-9.643
Other costs (projects)	-3.686	-676	-810	-5.172
Overheads 3	1.876	-3.158	-1.105	-2.387
<b>Costs total</b>	<b>-6.782</b>	<b>-7.120</b>	<b>-3.300</b>	<b>-17.202</b>
<i>Percentage</i>	<i>39%</i>	<i>41%</i>	<i>19%</i>	<i>100%</i>
<b>HIMS Result 2020</b>	<b>1.474</b>	<b>-13</b>	<b>8</b>	<b>1.469</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.