



Annual Report 2021

*Chemistry
research
that matters*

Van 't Hoff Institute
for Molecular Sciences

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Executive summary

In 2021, we have continued our journey in enhancing cross-disciplinary collaborations and strengthening our institute according to the strategic choices made in the preceding years. As was expressed by the Scientific Advisory Committee (SAC) that presented its mid-term evaluation report in January 2021, it takes time and effort to realize the full potential of the new strategy - even when the starting point is a flourishing institute of high quality and innovative research.



On 1 July 2021, Prof. Wybren Jan Buma became the new director of the institute succeeding Prof. Peter Bolhuis whose term formally ended. Buma: "It is gratifying to see that our Institute's strategic choices have led to a notable expansion and to an impressive growth in successful grant applications at both the fundamental and applied levels." Photo: FNWI.

Specifically under the COVID-conditions that marked most of the year, we observed that bringing everyone on board and building new connections is quite a challenge. Also in other aspects we had to deal with the COVID-pandemic. As chemistry laboratories are very safe working environments we could continue our experimental work, albeit with special precautions. Our special thanks go to the institute's technical support staff and the cooperation of all staff and students.

As a follow-up of the SAC advice we installed a **Diversity and Inclusion committee** with members from all parts of the institute. We are committed to a diverse and inclusive workplace in which everyone is treated with dignity and respect.

The researchers at our institute were very successful in **acquiring external grants**. Among many others are the high-impact personal grants of Dr Chris Slootweg (Vici), Dr Fatemeh Hashemi (Veni) and Dr. Luca Capaldo (Marie Curie Fellowship). There were also large consortia projects (funded by H2020, CBBC, RVO and others), and a number of direct research contracts with industrial partners started. HIMS acquired a project in UvA's new 'Data Science Center' and hosts the new UvA Research Priority Area 'Energy transition through the lens of Sustainable Developments Goals' (Enlens), led by Prof. Bob van der Zwaan. Also two projects were acquired within the Science & Design Zero Waste program of the Faculty of Science.

A total of 21 young researchers **obtained their PhD at our institute**. Dr Thierry Slot, Dr Alberto Pérez de Alba Ortíz and Dr Tessel Bouwens received their doctorate with the distinction 'cum laude'. A number of 313 appealing publications arose, including 21 joint publications from collaborating HIMS groups, often involving interdisciplinary collaborations across the different HIMS themes.

We have seen a number of noteworthy **changes in the HIMS staff**. Prof. Peter Schoenmakers of Analytical Chemistry formally retired in 2021 after a very successful career in both industry and academia. He will stay, however, active in the years to come, guiding his final generation of PhD students and helping the new and young staff in Analytical Chemistry with their teaching duties in the successful Master program Analytical Sciences. Dr Steen Ingemann also formally retired. We -and many students- are happy that he too is continuing his educational activities in the coming year. Dr Tristan Bereau left the institute to pursue a career outside academia. At the same time, HIMS welcomed three new professors by special appointment: Prof. Katrien Keune (main affiliation Rijksmuseum Amsterdam), Prof. Wim Noorduin (main affiliation AMOLF) and Prof. Elizabeth von Hauff (main affiliation VU Amsterdam).



The former Van 't Hoff laboratory at Groenburgwal 44 was named National Chemical Heritage. Photo: Google Street View.

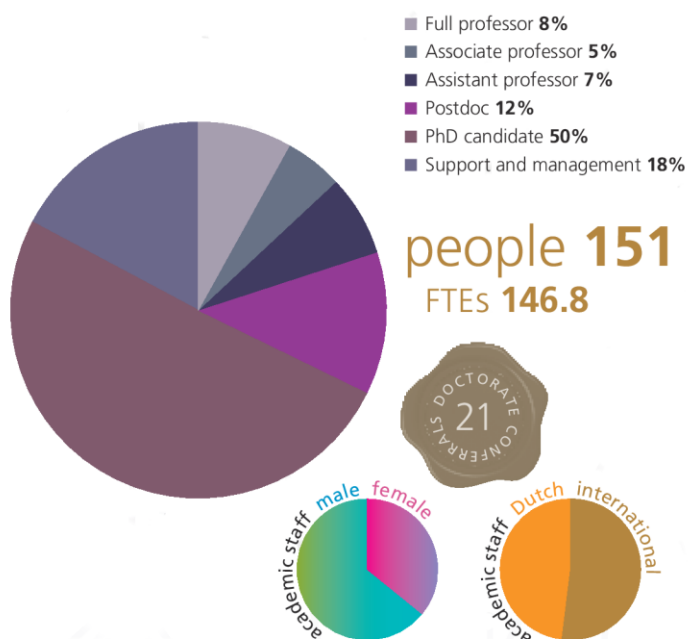
Also in 2021 quite a few prestigious **prizes were granted to HIMS researchers**. Prof. Tim Noël received the Golden Medal of the Royal Netherlands Chemical Society KNCV as well as the IUPAC ThalesNano Prize for Flow Chemistry. Dr Bob Pirok and Prof. Peter Schoenmakers were included in the international Analytical Powerlist. Dr Klaas van Leest received the Dick Stufkens Prize of the Holland Research School of Molecular Chemistry for his PhD thesis and a Rubicon grant from the Dutch Research Council NWO. The 'Sisters in Science' initiative of our

colleagues Lotte Schreuder, Mimi den Uyl and Noor Abdhussain received a lot of attention on national television and social media. In December, they received the NWO Diversity Initiative award.

The **valorisation of HIMS research** and knowledge had several highlights worth sharing. Prof. Joost Reek started a first pilot with Open Kitchen Labs together with Dr Monalisa Goswami of our spin-off company Spark904 . This will be a service at Amsterdam Science Park where spin-offs can rent a laboratory facility with basic equipment and consumables. Unlike already existing services labs, experiments can start here immediately and rental periods can vary from a few days to multiple months. The first online edition of the annual Molecular Simulation course attracted 100 international participants (up from 60 participants in the years before). This year the Amsterdam Centre for Electrochemistry (Amcel) organized a successful first symposium. In the Amcel consortium, academic and industrial partners focus on redox chemistry for a zero-waste economy.

Finally it is nice to mention that the building at Groenburgwal 44 in Amsterdam, where our namesake Prof. Jacobus Van 't Hoff did his Nobel prize winning research in the late 19th century, was named **National Chemical Heritage** by the Royal Netherlands Chemical Society KNCV.

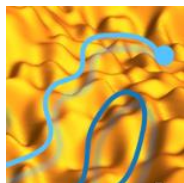
HIMS at a glance:



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

Scientific Highlights

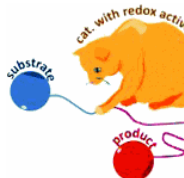
Calibrating a computational microscope - 4 January 2021



A team of computational chemists at HIMS together with colleagues at the Department of Chemistry of the University of Cambridge has developed a new method of seeing molecular motions by incorporating experimental kinetic rate constants into molecular simulations. The results were published in the Proceedings of the National Academy of Sciences.

Brotzakis, Z. F., Vendruscolo, M., & Bolhuis, P. G. (2021): *A method of incorporating rate constants as kinetic constraints in molecular dynamics simulations*. Proceedings of the National Academy of Sciences, 118(2), e2012423118. DOI: [10.1073/pnas.2012423118](https://doi.org/10.1073/pnas.2012423118)

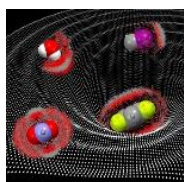
ACS Catalysis paper by Bas de Bruin among the most cited of the previous decade - 5 January 2021



In celebration of its 10th anniversary, ACS Catalysis highlighted impactful papers from across the globe. A 2012 paper by Prof. Bas de Bruin features in the top five of most cited papers with corresponding authors working in Germany and the Netherlands.

Volodymyr Lyaskovskyy and Bas de Bruin: *Redox Non-Innocent Ligands: Versatile New Tools to Control Catalytic Reactions*. ACS Catal. 2012, 2, 2, 270–279. DOI: [10.1021/cs200660v](https://doi.org/10.1021/cs200660v)

Comprehensive evaluation by Tiddo Mooibroek of σ - and π -hole interactions - 25 January 2021



A paper by Dr Tiddo J. Mooibroek was featured on the cover of ChemPhysChem. In his paper, Mooibroek presents a comprehensive and comparative evaluation of different σ - and π -hole interactions present in the IsoStar database. His study is of relevance to the assessment of σ - or π -hole interactions that drive diverse processes such as protein folding, molecular recognition phenomena and crystal engineering.

Tiddo J. Mooibroek: *DFT and IsoStar Analyses to Assess the Utility of σ - and π -Hole Interactions for Crystal Engineering* ChemPhysChem 2021 Vol.22, Issue 2 DOI: [10.1002/cphc.202000927](https://doi.org/10.1002/cphc.202000927)

Video pitch: Recent applications of retention modelling in liquid chromatography - 27 January 2021



In a paper published in the Journal of Separation Science, HIMS PhD student Mimi den Uijl and coworkers provide an overview of recent applications of retention modelling in liquid chromatography. Mimi produced a [video pitch](#) of the paper for the SCM-X 2021 conference that was scheduled to take place in Amsterdam but was held online.

Mimi J. den Uijl, Peter J. Schoenmakers, Bob W.J. Pirok, Maarten R. van Bommel: *Recent applications of retention modelling in liquid chromatography*. JSepSci 2021; 44:88-114. DOI: [10.1002/jssc.202000905](https://doi.org/10.1002/jssc.202000905)

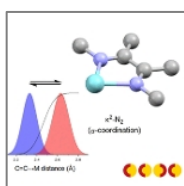
Shedding light on photocatalysis using Bi₂O₃ semiconductor - 10 February 2021



In a paper published in Nature Communications, Prof. Timothy Noël and co-workers at the University of Amsterdam's Van 't Hoff Institute for Molecular Chemistry (HIMS) present the true nature of the catalytically active species in photocatalytic reactions using bismuth oxide semiconductor. Bi₂O₃ is a popular photocatalyst for light-induced organic transformations that provide a sustainable alternative for more traditional synthetic pathways.

Paola Riente, Mauro Fianchini, Patricia Llanes, Miquel Pericàs & Timothy Noël: *Shedding light on the nature of the catalytically active species in photocatalytic reactions using Bi₂O₃ semiconductor*. Nat. Comm. **12**, 625 (2021). DOI: [10.1038/s41467-020-20882-x](https://doi.org/10.1038/s41467-020-20882-x)

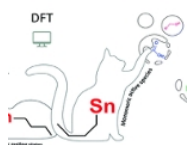
Metrical oxidation states of 1,4-diazadiene derived ligands - 16 February 2021



In a paper in Inorganic Chemistry, PhD student Felix de Zwart from the Heterogeneous, Supramolecular and Bio-inspired Chemistry group together with chemistry bachelor students Anna Laporte and Bente Reus describe the development of an empirical model for the oxidation state of 1,4-diazabutadiene ligands. The model provides fundamental insight into the interplay of coordination chemistry and oxidation states.

Felix J. de Zwart, Bente Reus, Annechien A.H. Laporte, Vivek Sinha and Bas de Bruin: *Metrical oxidation states of 1,4-diazadiene (DAD) derived ligands*. Inorganic Chemistry, publication date February 15, 2021. DOI: [10.1021/acs.inorgchem.0c03685](https://doi.org/10.1021/acs.inorgchem.0c03685) (preprint repository: [10.26434/chemrxiv.13378967.v1](https://doi.org/10.26434/chemrxiv.13378967.v1))

Mechanistic elucidation of monoalkyltin(IV)-catalyzed esterification - 24 February 2021



In a paper in the RSC journal Catalysis Science & Technology, HIMS researchers report on the mechanistic investigation of esterification catalyzed by mono-n-butyltin(IV) species, a class of catalysts that has been used since decades by the chemical industry to make polyesters. The researchers analysed the working of these catalysts under catalytically relevant conditions with a variety of spectroscopic techniques complemented with DFT calculations. They propose a mononuclear mechanism where carbon–oxygen bond breaking is the rate-determining step.

Lukas A. Wolzak, Joen J. Hermans, Folkert de Vries, Keimpe J. van den Berg, Joost N. H. Reek, Moniek Tromp and Ties J. Korstanje: *Mechanistic elucidation of monoalkyltin(IV)-catalyzed esterification*. *Catal. Sci. Technol.*, 2021, Advance Article. DOI: [10.1039/D1CY00184A](https://doi.org/10.1039/D1CY00184A)

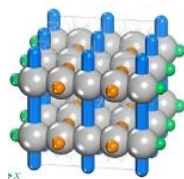
Hot Paper on 'alcohol aminase' enzymes - 11 March 2021



Research of the Biocatalysis research group led by HIMS associate professor Francesco Mutti featured on the cover of Chemistry—A European Journal. The 'Hot Paper' reports on the generation of oxidoreductases that possess both alcohol dehydrogenase and amine dehydrogenase activity. This opens up new opportunities in biocatalytic organic synthesis.

Vasilis Tseliou, Don Schilder, Marcelo F. Masman, Tanja Knaus, Francesco G. Mutti: *Generation of Oxidoreductases with Dual Alcohol Dehydrogenase and Amine Dehydrogenase Activity* Chem. Eur. J. 10/2021. DOI: [10.1002/chem.202003140](https://doi.org/10.1002/chem.202003140) (paper) [10.1002/chem.202004194](https://doi.org/10.1002/chem.202004194) (cover feature)

Synergetic enhancement between sorption and diffusion in zeolites with continuum intersecting channels - 12 March 2021



In a paper published in *Science Advances*, researchers report synergetic enhancement between sorption and diffusion in zeolites with continuum intersecting channels. The research was performed by a Chinese research team led by Prof. Anmin Zheng at the Wuhan Institute of Physics and Mathematics. HIMS Prof. em. Rajamani Krishna, along with Dr Jasper van Baten (formerly at HIMS) assisted with molecular simulations, data analysis and interpretation.

Zhiqiang Liu, Jiamin Yuan, Jasper M. van Baten, Jian Zhou, Xiaomin Tang, Chao Zhao, Wei Chen, Xianfeng Yi, Rajamani Krishna, German Sastre, Anmin Zheng: *Synergistically enhance confined diffusion by continuum intersecting channels in zeolites* *Sci. Adv.* 2021; 7, eabf0775 (2021). DOI: [10.1126/sciadv.abf0775](https://doi.org/10.1126/sciadv.abf0775)

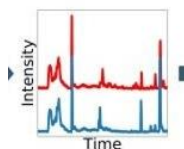
Paper on monomers from carbon dioxide as cover feature of ChemSusChem - 25 March 2021



Eric Schuler, a PhD candidate working with Prof. Gert-Jan M. Gruter and Dr Shiju Raveendran, helped to develop a process to turn CO₂ into polymers. In a publication in *ChemSusChem*, the researchers reported the first major improvements of the 175-year-old formate-to-oxalate coupling reaction using superbases as catalysts. This reaction is an incremental step in the route from CO₂ to polymers.

E. Schuler, P. A. Ermolich, N. R. Shiju, G.-J. M. Gruter, *Monomers from CO₂: Superbases as Catalysts for Formate-to-Oxalate Coupling*, *ChemSusChem* 6/2021,14, 1517-1523.
DOI: [10.1002/cssc.202002725](https://doi.org/10.1002/cssc.202002725) (paper) [10.1002/cssc.202100327](https://doi.org/10.1002/cssc.202100327) (cover feature)

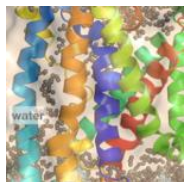
Chemical attribution of fentanyl: The effect of human metabolism - 29 March 2021



A paper in *Forensic Chemistry* reported the result of a study by HIMS researchers in cooperation with TNO on the chemical profiling of fentanyl in biological samples. The work demonstrates for the first time the possibility of chemical attribution of drugs through the analysis of metabolic trace levels in biological samples. This can be very valuable for forensic casework and intelligence purposes.

Mirjam de Bruin-Hoegée, Djarah Kleiweg, Daan Noort, Arian C. van Asten: *Chemical attribution of fentanyl: The effect of human metabolism*. *Forensic Chemistry*, Vol 24, June 2021 DOI: [10.1016/j.forc.2021.100330](https://doi.org/10.1016/j.forc.2021.100330)

Predicting structure and dynamics of membrane protein GerAB from *Bacillus subtilis* - 12 April 2021



Dr Jocelyne Vreede of the research group Computational Chemistry worked together with researchers at the UvA's Swammerdam Institute for Life Sciences (SILS) to elucidate the structure and dynamics of the spore membrane protein GerAB from the bacterium *Bacillus subtilis*. The study contributes to a better understanding of the germination of *B. subtilis* spores, a model organism for bacterial spore formers associated with food spoilage and foodborne diseases.

Blinker, S.; Vreede, J.; Setlow, P.; Brul, S. *Predicting the Structure and Dynamics of Membrane Protein GerAB from Bacillus subtilis*. *Int. J. Mol. Sci.* **2021**, 22, 3793. DOI: [10.3390/ijms22073793](https://doi.org/10.3390/ijms22073793)

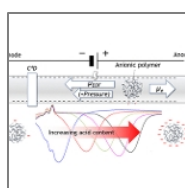
Researchers paint portrait of Marie Curie in semiconductor - 13 April 2021



Amsterdam researchers developed a novel technique for spatially controlled patterning of semiconductors with tuneable optoelectronic properties. As a proof of principle, Lukas Helmbrecht and Wim Noorduin 'painted' a portrait of Marie Curie in a perovskite semiconductor layer. Both researchers work at the AMOLF research institute at Amsterdam Science Park. Noorduin is professor of Self-Organising Matter at HIMS and Lukas Helmbrecht obtained his PhD under Noorduin's supervision. The results of their research were published in 'Advanced Materials'.

L. Helmbrecht, M.H. Futscher, L.A. Muscarella, B. Ehrler, W.L. Noorduin: *Ion Exchange Lithography: Localized Ion Exchange Reactions for Spatial Patterning of Perovskite Semiconductors and Insulators*, *Advanced Materials* (2021). DOI: [10.1002/adma.202005291](https://doi.org/10.1002/adma.202005291)

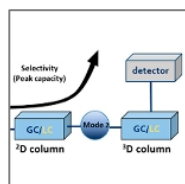
Charge-based separation of acid-functional polymers - 21 April 2021



Water-borne polymers continue to gain ground in the field of environmentally friendly coating solutions. There is a strong need for methods allowing characterization of the polymers and polymer particles. In a paper in *Analytical Chemistry*, PhD student Ton Brooijmans describes a method for charge-based separation of acid-functional polymers by non-aqueous capillary electrophoresis, employing deprotonation and heteroconjugation approaches.

Ton Brooijmans, Pascal Breuer, Aniek Schreuders, Myrthe van Tilburg, Peter J. Schoenmakers, and Ron A.H. Peters: *Charge-Based Separation of Acid-Functional Polymers by Non-aqueous Capillary Electrophoresis Employing Deprotonation and Heteroconjugation Approaches*. *Analytical Chemistry* 2021, 93, 14, 5924-5930. DOI: [10.1021/acs.analchem.1c00311](https://doi.org/10.1021/acs.analchem.1c00311)

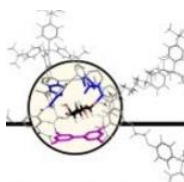
Review on three-dimensional separations in chromatography - 22 April 2021



In a paper published in *Chemical Reviews*, Noor Abdulhussain, Suhas Nawada and Peter Schoenmakers of the research group Analytical Chemistry provide an overview of current and future developments in three-dimensional separations which are crucial for the analysis of highly complex mixtures. The article is part of the 'Frontiers of Analytical Science' special issue of *Chemical Reviews*.

Noor Abdulhussain, Suhas Nawada, and Peter Schoenmakers: *Latest Trends on the Future of Three-Dimensional Separations in Chromatography*. *Chem. Rev.* 2021, Publication Date April 20, 2021. DOI: [10.1021/acs.chemrev.0c01244](https://doi.org/10.1021/acs.chemrev.0c01244)

First synthetic galectin mimic as a platform for carbohydrate binding molecules - 11 May 2021



In a paper in *Angewandte Chemie*, research assistant professor Tiddo Mooibroek and co-workers present the first synthetic mimic of a class of carbohydrate binding proteins called galectins. Their research provides a platform for preparing a new family of carbohydrate binding molecules, opening up novel chemical pathways for carbohydrate recognition and functionalisation.

Tiddo Jonathan Mooibroek, Brian Timmer, Xander Schaapkens and Arjaan Kooijma: *A synthetic galectin mimic*. *Angew. Chem. Int. Ed.* First published: 08 May 2021. DOI: [10.1002/anie.202104924](https://doi.org/10.1002/anie.202104924)

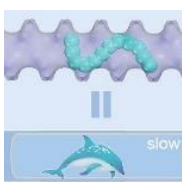
Micrometre-size molecular modelling kit shows real chemical reactions - 17 May 2021



A team of researchers from the University of Amsterdam and New York University built a 'molecular modelling kit' using micrometre-sized 'patchy particles'. The kit allows for a much more direct study of molecular dynamics and can even model certain chemical reactions. Hannah Jonas, Peter Bolhuis and Sander Woutersen of contributed to the research that was published in Nature Communications.

P. J. M. Swinkels, S. G. Stuij, Z. Gong, H. Jonas, N. Ruffino, B. van der Linden, P. G. Bolhuis, S. Sacanna, S. Woutersen and P. Schall: *Revealing pseudorotation and ring-opening reactions in colloidal organic molecules*. Nat Commun 12, 2810 (2021). DOI: [10.1038/s41467-021-23144-6](https://doi.org/10.1038/s41467-021-23144-6)

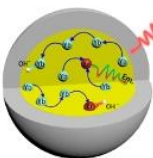
Anomalous diffusion of confined long-chain molecules: the thermal resistance effect - 17 May 2021



In a paper in PNAS researchers describe for the first time a counter-intuitive diffusion behaviour of linear-chain hydrocarbon molecules under confinement in nanoscale channels. The work provides a new perspective for a fundamental understanding of the diffusion process. Prof. Rajamani Krishna contributed with ab initio molecular dynamics (MD) simulations that clearly established the connection between the molecular structure and anomalous diffusion.

Jiamin Yuan, Zhiqiang Liu, Yimo Wu, Jingfeng Han, Xiaomin Tang, Chengbin Li, Wei Chen, Xianfeng Yi, Jian Zhou, Rajamani Krishna, German Sastre, Anmin Zheng: *Thermal resistance effect on anomalous diffusion of molecules under confinement*. PNAS May 17, 2021 DOI: [10.1073/pnas.2102097118](https://doi.org/10.1073/pnas.2102097118)

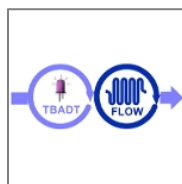
Quantitatively understanding defects in phosphors from a nano perspective - 21 May 2021



Researchers led by Prof. Hong Zhang obtained insight into the microscopic dynamics of energy transfer and conversion in doped phosphors. Using dedicated nanostructures and computer modelling they were able to quantitatively determine the mechanism of interaction between hydroxyl impurities and luminescence centres inside lanthanide-doped phosphors. Their findings were published by the Nature journal 'Light: Science and Applications'.

Yansong Feng, Zhi Li, Qiqing Li, Jun Yuan, Langping Tu, Lixin Ning, Hong Zhang: *Internal OH⁻ Induced Cascade Quenching of Upconversion Luminescence in NaYF₄:Yb/Er Nanocrystals*. Light: Science & Applications 10 (2021) 150). DOI: [10.1038/s41377-021-00550-5](https://doi.org/10.1038/s41377-021-00550-5)

Convenient methodology to forge C–N bonds - 8 June 2021



In a paper in Angewandte Chemie, researchers of the Flow Chemistry group presented a convenient methodology to forge C(sp³)–N bonds. Featuring mild reaction conditions, their protocol is amenable both to early and late-stage functionalization of organic molecules. As such, this synthetic method is valuable for the synthesis of medicinal and agrochemical intermediates.

Ting Wan, Luca Capaldo, Gabriele Laudadio, Alexander Nychev, Juan Rincon, Pablo Garcia-Losada, Carlos Mateos Gutierrez, Michael O. Frederick, Manuel Nuno, and Timothy Noel: *Decatungstate-mediated C(sp³)–H Heteroarylation via Radical-Polar Crossover in Batch and Flow*. Angew. Chem. Int. just accepted. DOI: [10.1002/anie.202104682](https://doi.org/10.1002/anie.202104682)

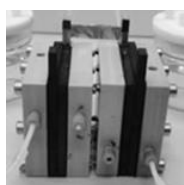
Selective formation of nanospheres featured on front cover of Chemical Science - 10 June 2021



Research at the Homogeneous, Supramolecular and Bio-Inspired Catalysis group was featured on the cover of Chemical Science. In their paper, Eduard Bobylev, David Poole, Bas de Bruin and Joost Reek report on the selective formation of supramolecular nanospheres by carefully tuning the ligand design. They present a systematic study on the selective formation of platinum-based spheres using a combination of experimental and theoretical approaches in a paper that was also showcased as a HOT Chemical Science article.

Eduard Bobylev, David Poole, Bas de Bruin, and Joost Reek: *Selective formation of Pt₁₂L₂₄ nanospheres by ligand design*. Chem. Sci., 2021,12, 7696-7705. DOI: [10.1039/D1SC01295A](https://doi.org/10.1039/D1SC01295A) (paper) [10.1039/D1SC90123K](https://doi.org/10.1039/D1SC90123K) (cover)

Novel electrolyser for hydrogen production - 14 July 2021



In a Nature Communications paper, a group of researchers led by Dr Ning Yan showcases a practical membrane-free approach to water electrolysis using earth-abundant catalysts. The new electrolyser concept offers significant advantages over electrolyzers that are currently being developed for large-scale hydrogen production.

Xiaoyu Yan, Jasper Biemolt, Kai Zhao, Yang Zhao, Xiaojuan Cao, Ying Yang, Xiaoyu Wu, Gadi Rothenberg & Ning Yan: *A membrane-free flow electrolyzer operating at high current density using earth-abundant catalysts for water splitting*. Nat Commun 12, 4143 (2021). DOI: [10.1038/s41467-021-24284-5](https://doi.org/10.1038/s41467-021-24284-5)

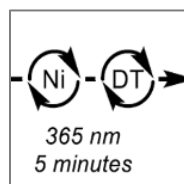
Investments in solar and wind power generation need to increase fast if goals of Paris Agreement are to be met - 16 July 2021



To meet the Paris Agreement to keep global warming below 2 °C, society has to increase investments in low-carbon power generation, especially for solar and wind technologies. This follows from a multi-model scenario study of the international ENGAGE consortium that was recently published in Environmental Research Letters. According to Prof. Bob van der Zwaan of Sustainable Energy Technology who participated in the study, this decade is going to be critical: "If we don't step up our actions now, we will fall behind in mitigating global warming".

Christoph Bertram, Keywan Riahi, Jérôme Hilaire, et.al.: *Energy system developments and investments in the decisive decade for the Paris Agreement goals*. Environ. Res. Lett. 16 (2021) 074020. DOI: [10.1088/1748-9326/ac09ae](https://doi.org/10.1088/1748-9326/ac09ae)

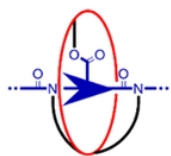
Photocatalytic acylation and arylation of alkylic C-H bonds in a flow system - 16 August 2021



In a paper in Angewandte Chemie, Prof. Timothy Noël and coworkers at the Flow Chemistry group presented a photocatalytic procedure that enables the acylation/arylation of unfunctionalized alkyl derivatives. Owing to the intensified conditions of the flow chemistry set-up, they were able to reduce reaction times from 12-48 hours to only 5-15 minutes.

Daniele Mazzarella, Antonio Pulcinella, Loïc Bovy, Rémy Broersma, and Timothy Noël: *Rapid and Direct Photocatalytic C(sp³)-H Acylation and Arylation in Flow* Angewandte Chemie, First published: 30 July 2021, DOI: [10.1002/anie.202108987](https://doi.org/10.1002/anie.202108987)

A novel approach to the synthesis of mechanically interlocked peptidic products - 17 August 2021



Researchers of the research group Synthetic Organic Chemistry developed a novel approach to the synthesis of mechanically interlocked peptidic products. In a paper in ACS Organic&Inorganic, they present an ester-functionalized, aromatic δ -amino acid as a versatile central covalent templating unit, and show how this is capable of producing a catenane and a rotaxane from the same multimacrocylic intermediate.

Simone Pilon, Steen Ingemann Jørgensen, and Jan H. van Maarseveen: *Covalent [2]Catenane and [2]Rotaxane Synthesis via a δ -Amino Acid Template*. ACS Org. Inorg. Au Publication Date: August 11, 2021, DOI: [10.1021/acscorginorgau.1c00017](https://doi.org/10.1021/acscorginorgau.1c00017)

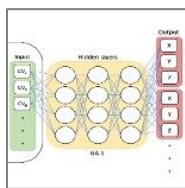
A perspective on tying peptide ropes - 26 August 2021



Prof. Jan van Maarseveen of Bio-inspired Synthetic Chemistry was invited by Nature Chemistry to provide a perspective on creating interlocked molecules by tying peptide ropes, using a chemical as well as a biological toolbox.

Van Maarseveen, J.H.: *Tying peptide ropes*. Nat. Chem. (2021) 23 August 2021. DOI: [10.1038/s41557-021-00771-6](https://doi.org/10.1038/s41557-021-00771-6)

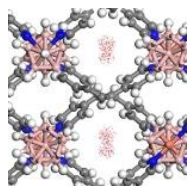
Unraveling reaction mechanisms via machine learning - 21 September 2021



Researchers at the Computational Chemistry group developed a machine learning framework to automatically find, from simulation data, the set of collective variables that best describe the reaction coordinate of complex reactions and molecular transitions. They demonstrated their method, named FABULOUS, amongst others for describing a biologically relevant transition in DNA. It was published in a paper in the Journal of Chemical Theory and Computation

Ferry Hooft, Alberto Pérez de Alba Ortíz, and Bernd Ensing: *Discovering Collective Variables of Molecular Transitions via Genetic Algorithms and Neural Networks*. J. Chem. Theory Comput. 17, 4, 2294–2306 (2021) DOI: [10.1021/acs.jctc.0c00981](https://doi.org/10.1021/acs.jctc.0c00981)

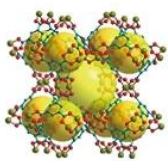
Benchmark purification of acetylene from carbon dioxide - 7 October 2021



Professor Rajamani Krishna contributed to research published in a 'hot paper' in Angewandte Chemie. He performed modelling and simulations on the C_2H_2/CO_2 separation performance of a symmetrically interpenetrated dodecaborate pillared MOF (ZNU-1). The paper presents benchmark selective separation results, reporting a high C_2H_2 capacity and a record in C_2H_2/CO_2 selectivity.

Lingyao Wang, Wanqi Sun et al.: Yuanbin Zhang, Nuo Xu, Rajamani Krishna, Jianbo Hu, Yunjia Jiang, Yabing He, and Huabin Xing: *Interpenetration Symmetry Control Within Ultramicroporous Robust Boron Cluster Hybrid MOFs for Benchmark Purification of Acetylene from Carbon Dioxide*. Angew. Chem. Int. Ed. 2021, 60, 22865–22870. DOI: [10.1002/anie.202107963](https://doi.org/10.1002/anie.202107963)

Microporous crystalline physisorbents for propyne/propadiene separation - 8 October 2021



In a paper in *Nature Communications* an international team of researchers present a convenient and energy-efficient method for separating propyne/propadiene mixtures. They take a physisorptive approach using microporous metal-organic frameworks (MOFs). Professor Rajamani Krishna contributed to the research with his expertise on modelling and simulation of the separation performance.

Yun-Lei Peng, Ting Wang, Chaonan Jin, Cheng-Hua Deng, Yanming Zhao, Wansheng Liu, Katherine A. Forrest, Rajamani Krishna, Yao Chen, Tony Pham, Brian Space, Peng Cheng, Michael J. Zaworotko & Zhenjie Zhang: *Efficient propyne/propadiene separation by microporous crystalline physisorbents*. *Nat Commun* 12, 5768 (2021). DOI: [10.1038/s41467-021-25980-y](https://doi.org/10.1038/s41467-021-25980-y)

A partnership between Europe and North Africa for electricity and hydrogen - 11 October 2021



In a paper in *Energy Policy*, Prof. Bob van der Zwaan and co-workers at TNO present detailed model calculations confirming that Europe and North Africa could turn into each other's trading partners when it comes to energy. By focusing on two main energy carriers, electricity and hydrogen, the researchers describe what the technology impacts and cost implications of such a partnership could look like.

Bob van der Zwaan, Sam Lamboo, Francesco Dalla Longa: *Timmermans' dream: An electricity and hydrogen partnership between Europe and North Africa* *Energy Policy* 159 (2021) 112613.
DOI: [10.1016/j.enpol.2021.112613](https://doi.org/10.1016/j.enpol.2021.112613)

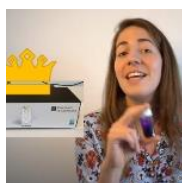
Novel sustainable molecular heaters for boosting crop production - 10 November 2021



With the aim of addressing frost damage in plants and increasing crop yields, an international team of researchers including Prof. Wybren Jan Buma synthesised and characterized novel non-toxic phenolic barbiturics with optimal photothermal properties. In a paper published as 'Pick of the Week' in the RSC journal *Chemical Science*, they reveal how these molecules very effectively convert absorbed UV-light into heat and offer great potential for use in foliar sprays to boost crop production.

T.T. Abiola, B. Rioux et. al.: Towards developing novel and sustainable molecular light-to-heat converters. *Chemical Science*, 10 November 2021, DOI: [10.1039/D1SC05077J](https://doi.org/10.1039/D1SC05077J)

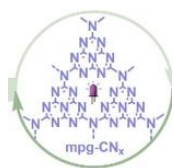
A novel method to study the photodegradation of organic colourants - 23 November 2021



In a paper in *Dyes & Pigments*, researchers from the TooCOLD project at HIMS and the Centre for Analytical Sciences Amsterdam report on a novel method to study the degradation of colourants that are of relevance to cultural heritage. PhD student Mimi den Uyl explained the research in a [video](#) posted on YouTube.

Mimi J. den Uijl, Anika Lokker, Bob van Dooren, Peter J. Schoenmakers, Bob W.J. Pirok, Maarten R. van Bommel: *Comparing different light-degradation approaches for the degradation of crystal violet and eosin Y*, *Dyes and Pigments*, Volume 197, 2022, 109882, DOI: [j.dyepig.2021.109882](https://doi.org/10.1016/j.dyepig.2021.109882)

Photocatalytic azolation of arenes using heterogeneous carbon nitride - 24 November 2021



An article by researchers from the Flow Chemistry research group was showcased as 'pick of the week' by Chemistry Europe. Together with researchers from the University of Cambridge, they report on the photocatalytic C(sp²)-H azolation of arenes using heterogeneous carbon nitride in batch and flow processes.

Zhenghui Wen, Ting Wan, Arjun Vijeta, Carla Casadevall, Laura Buglioni, Erwin Reisner, Timothy Noël: Photocatalytic c-h azolation of arenes using heterogeneous carbon nitride in batch and flow. ChemSusChem, First published: 16 September 2021 DOI: [10.1002/cssc.202101767](https://doi.org/10.1002/cssc.202101767)

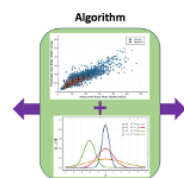
Net zero-emission pathways for reducing the risks of climate change - 29 November 2021



An international team of researchers including Prof. Bob van der Zwaan explored the physical and macroeconomic impacts associated with climate mitigation pathways with different levels of temperature overshoot. The results published in Nature Climate Change underpin the need to include climate risk analysis in developing mitigation pathways.

Laurent Drouet et.al.: *Net zero-emission pathways reduce the physical and economic risks of climate change*. 2021, Nature Climate Change, DOI: [10.1038/s41558-021-01218-z](https://doi.org/10.1038/s41558-021-01218-z)

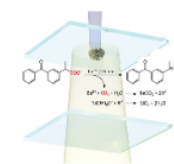
Machine learning for prediction of peak width in HRMS data - 14 December 2021



In a paper in Analytical Chemistry, assistant professors Saer Samanipour and Bob Pirok of the Analytical Chemistry research group presented a novel approach for the seamless interconversion of centroided data and profile data from LC-HRMS acquired with QToF mass analyzers. For this, they developed new algorithms in cooperation with researchers at the University of Queensland and the Norwegian Institute for Water Research.

Saer Samanipour, Phil Choi, Jake W. O'Brien, Bob W. J. Pirok, Malcolm J. Reid, and Kevin V. Thomas: *From Centroided to Profile Mode: Machine Learning for Prediction of Peak Width in HRMS Data*. Anal. Chem, November 29, 2021, DOI: [10.1021/acs.analchem.1c03755](https://doi.org/10.1021/acs.analchem.1c03755)

Controlled nucleation and shaping of self-assembling nanocomposites using light - 20 December 2021



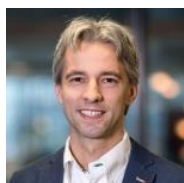
An article in Advanced Materials describes the light-controlled nucleation and growth of self-assembling composites according to precise user-defined designs. The research was carried out by PhD student Marloes Bistervels at the Self-Organizing Matter research group at AMOLF under the supervision of HIMS professors Wim Noorduyn and Fred Brouwer.

Marloes H. Bistervels, Marko Kamp, Hinc Schoenmakers, Albert M. Brouwer and Willem L. Noorduyn, *Light-controlled nucleation and shaping of self-assembling nanocomposites*, Advanced Materials (2021), doi.org/10.1002/adma.202107843

Prizes and honours

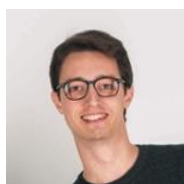
The quality of HIMS scientists is reflected in the prizes and honours they receive. Noteworthy examples are the KNCV Gold Medal for Prof. Timothy Noël; the Dick Stufkens Prize 2021 for Dr Klaas van Leest ; and the NWO Diversity Initiative Award 2021 for the 'Sisters in Science' Mimi den Uijl, Lotte Schreuders and Noor Abdulhussein. Below is a list of news items reporting on these and other HIMS staff members and students.

Timothy Noël is awarded the 2020 IUPAC-ThalesNano prize for Flow Chemistry - 27 January 2021



The 2020 IUPAC-ThalesNano prize for Flow Chemistry has been awarded to Professor Timothy Noël of the University of Amsterdam's Van 't Hoff Institute for Molecular Sciences. The prize, consisting of an award of \$ 7500, honours outstanding contributions in the field of flow chemistry, microfluidics, micro fabrication, and micro systems engineering.

Luca Capaldo receives Marie Curie Fellowship - 17 February 2021



HIMS researcher Luca Capaldo has been awarded a Marie Skłodowska-Curie Individual Fellowship by the European Commission. He receives approximately €175,000 for research into net-oxidative C-H to C-C bond conversion by means of hydrogen atom transfer using flow-photo-electrocatalysis. Capaldo aims to open new avenues in organic synthesis, in particular in realizing cross-dehydrogenative couplings, functionalization of alkenes and the dehydrogenation of alkanes.

Chris Slootweg receives Vici grant - 14 April 2021



Associate professor Dr Chris Slootweg has been awarded an NWO Vici grant of 1.5 million euros to develop novel chemical routes for establishing circularity in phosphorus. As one of the largest personal academic grants i.... As one of the largest personal academic grants in the Netherlands, the Vici grant allows scientists to further develop their line of research and strengthen their research group.

Thierry Slot obtains PhD with distinction 'cum laude' - 20 April 2021



Dr Thierry Slot successfully defended his PhD thesis titled 'Understanding confinement effects and nanostructuring in heterogeneous catalysis', obtaining his doctorate with the distinction cum laude. He will pursue his career further at the Technion in Haifa, Israel, for which he obtained an Azrieli Fellowship.

Francesco Mutti becomes Fellow of the Royal Society of Chemistry - 28 April 2021



Associate professor Dr Francesco Mutti of the research group Biocatalysis has been admitted as a Fellow of the Royal Society of Chemistry (RSC). Mutti has been a member of the RSC since 2019. Achieving Fellow status in the chemical profession denotes to the wider community a high level of accomplishment as a professional chemist.

Timothy Noël receives KNCV Gold Medal 2021 - 12 July 2021



The KNCV Gold Medal 2021, the highest Dutch award for top chemical talent, has been awarded to Prof. Timothy Noël of Flow Chemistry at the Van 't Hoff Institute for Molecular Sciences of the University of Amsterdam. Noël will receive the coveted prize at the national chemistry conference CHAINS, which is expected to take place 'live' in Veldhoven in December this year.

SusPhos is Frisian Startup of the Year 2021 - 16 September 2021



UvA spin-off company SusPhos, based at the WaterCampus in Leeuwarden, was voted last week as Frisian Startup of the Year 2021. This young company focuses on upcycling phosphate-rich waste streams into valuable products such as fertilizer and flame retardants. The seed of one of these techniques was sown at HIMS, in research by Dr Chris Slootweg, Dr Marissa de Boer and Ing. Bas de Jong.

Cum Laude PhD in chemistry for Tessel Bouwens - 20 September 2021



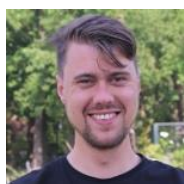
On 15 September, Tessel Bouwens successfully defended her PhD thesis on 'Pseudorotaxane Strategies for Guiding Self-Assembly and the Application of Molecular Machinery in Photoelectrochemical Devices'. She received her doctorate with the distinction 'cum laude' in recognition of her novel and original research performed at the Homogeneous, Supramolecular and Bio-Inspired Catalysis group

Cum Laude for chemistry PhD graduate Alberto Pérez de Alba Ortíz - 27 September 2021



On 22 September, Alberto Pérez de Alba Ortíz successfully defended his PhD thesis entitled 'Traversing the free-energy pathways of intricate biomolecular processes – enhanced simulation development and applications'. He was awarded the distinction 'cum laude' for remarkable research leading to new understanding of various biomolecular processes.

Klaas van Leest receives Dick Stufkens Prijs 2021 - 15 October 2021



The Dick Stufkens Prize 2021 for the best PhD thesis of the Holland Research School of Molecular Chemistry (HRSMC) has been awarded to Dr Nicolaas Petrus (Klaas) van Leest for his thesis 'Open-Shell Cobalt Complexes with Redox-Active Ligands; Electronic Structure and Nitrene Transfer Reactivity'. Van Leest obtained his doctorate with the qualification 'cum laude' at the end of 2020.

Two UvA analytical scientists in worldwide 'Power List' - 1 November 2021



The 2021 edition of the 'Power List' compiled by the magazine The Analytical Scientist features two analytical chemists of HIMS : Dr Bob Pirok and Prof. Peter Schoenmakers. The Power List presents the 100 world's most influential analytical scientists as an inspiration to their fellows.

Hannah Flerlage wins Student Recycling Award 2021 - 22 November 2021



UvA chemistry student Hannah Flerlage has won the Student Recycling Award from the Dutch industry association BRBS Recycling. She beat three co-finalists with her Master's thesis on the synthesis of high quality, sustainable and biodegradable phosphorus compounds from waste. Flerlage continues her research as a PhD student with Dr Chris Sootweg.

Daniele Mazzarella honoured as early career researcher - 23 November 2021



At the Young Chemists Symposium in Rimini, the Italian Chemical Society and Elsevier announced the winners of the 2021 Reaxys SCI Early Career Researcher Awards. Daniele Mazzarella, a postdoctoral researcher at the Flow Chemistry research group was one of three laureates.

Sisters in Science receive NWO Diversity Initiative Award - 9 December 2021



The 'Sisters in Science' Mimi den Uijl, Lotte Schreuders and Noor Abdulhussain have been awarded the Diversity Initiative Award 2021 by the Dutch Research Council NWO. The three chemists receive a sum of 50,000 euros for their initiative that aims to break stereotypes and show that everyone can be a scientist.

Ning Yan receives award for novel flow-electrolyzer concept to produce hydrogen - 13 December 2021



Assistant professor Dr Ning Yan has been awarded the 2021 Aquila Capital Transformation Award for his Nature Communications paper on 'A membrane-free flow electrolyser operating at high current density using earth-abundant catalysts for water splitting'. The award, recognizing research for mitigating climate change, comes with 20,000 euros.

Sonja Pullen wins Lorentz Center Chemistry competition - 15 December 2021

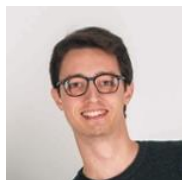


With their proposal for a workshop on the challenges and future perspectives of photocatalysis, Dr Sonja Pullen and co-applicants have won the 2021/22 Chemistry Competition of the Lorentz Center and the Royal Netherlands Chemical Society KNCV. As a result, the Lorentz Center will host the workshop in Leiden in the course of 2022.

Grants and funding

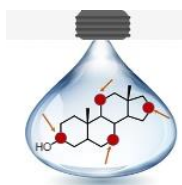
Below is an overview of news item on grants and funding obtained by HIMS scientists. More on the financial aspects of the institute can be found in the Facts & Figures section of this annual report.

Luca Capaldo receives Marie Curie Fellowship - 17 February 2021



HIMS researcher Luca Capaldo has been awarded a Marie Skłodowska-Curie Individual Fellowship by the European Commission. He receives approximately €175,000 for research into net-oxidative C-H to C-C bond conversion by means of hydrogen atom transfer using flow-photo-electrocatalysis. Capaldo aims to open new avenues in organic synthesis, in particular in realizing cross-dehydrogenative couplings, functionalization of alkenes and the dehydrogenation of alkanes.

Joint PhD project on steroid synthesis with the University of Perugia - 1 April 2021



The University of Amsterdam (UvA) and the University of Perugia (UniPG) have signed a 4-year agreement for a joined PhD project in the area of sustainable synthesis of steroids using novel chemo-enzymatic strategies and flow technology. The cooperation harnesses the expertise of the laboratory of Medicinal and Advanced Synthetic Chemistry led by professor Antimo Gioiello at UniPG, and the Biocatalysis lab led by professor Francesco Mutti at HIMS.

Vasilis Tseliou receives Marie Skłodowska-Curie Individual Fellowship - 12 April 2021



Dr Vasilis Tseliou has received a Marie Skłodowska-Curie Individual Fellowship under the Horizon 2020 program of the EU. He will visit the group of Prof. Paolo Melchiorre at ICIQ, Spain for a two year research project. Vasilis obtained his PhD with the distinction cum laude under the supervision of Dr Francesco Mutti of the HIMS Biocatalysis group.

Chris Slootweg receives Vici grant - 14 April 2021



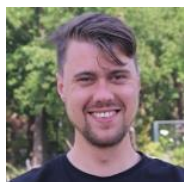
Associate professor Dr Chris Slootweg has been awarded an NWO Vici grant of 1.5 million euros to develop novel chemical routes for establishing circularity in phosphorus. As one of the largest personal academic grants in the Netherlands, the Vici grant allows scientists to further develop their line of research and strengthen their research group.

Mind the gap! - 19 May 2021



Dr. Stefania Grecea, associate professor at HIMS, has received UvA Grassroots funding for her proposal 'Mind the gap! Bridging pre-knowledge gaps using digital concept maps'. She will develop the use of digital concept maps to bridge students' pre-knowledge gaps.

Klaas van Leest receives NWO Rubicon grant - 21 June 2021



Klaas van Leest has been awarded a Rubicon grant by the Dutch Research Council NWO. He will use it to visit the group of Prof. Chi-Ming Che at the University of Hong Kong, where he will conduct postdoctoral research in the field of photoredox catalysis for two years. He hopes to contribute to the development of a sustainable, circular process for ammonia production, using sunlight as the energy resource and nitrate as the nitrogen source.

Three HIMS projects in ARC CBBC program 'New Chemistry for a Sustainable Future' - 1 July 2021



Professors Bas de Bruin, Joost Reek and Peter Bolhuis have been granted their proposals in the new research program of ARC CBBC, the Dutch national chemistry research centre that investigates chemical building blocks for novel sustainable energy and materials. As a result, the institute receives 1,2 million euros to welcome three PhD students for research in the fields of catalysis and computational chemistry.

Carbon capture and utilisation in context - 13 August 2021



Dr Amanda Garcia has been awarded a competitive top-up grant for Responsible Innovation of 325,000 euros, as part of the program on ElectroChemical Conversion and Materials (ECCM) from the Dutch Research Council NWO. It concerns research on 'Carbon capture and utilisation - historical context, technological challenges and societal acceptability' that will be carried out in collaboration with Prof. Gadi Rothenberg (HIMS) and Prof. John Grin (Faculty Social and Behavioural Sciences).

Towards a novel device for ammonia sensing - 16 August 2021



Dr Stefania Grecea will develop a new concept for ammonia sensing that can be implemented in wearable devices to measure ammonia concentrations in farming- and sensitive ecosystem environments. For this, she has been awarded a 50,000 euro grant in the Open Competition XS call of the Dutch Research Council NWO (Domain Science).

Co-electrolysis for efficient electrochemical CO₂ conversion - 23 August 2021



As part of the 7 million euro EU CO₂SMOS project, Dr Ning Yan is developing an efficient co-electrolysis technology that combines the chemical reduction of CO₂ with the production of value-added chemicals. Working closely with the Amsterdam-based company Avantium, Yan sets out to establish the technological, economical and environmental viability of the novel co-electrolysis concept.

Chemical profiling and trace analysis of illegal home-made explosives - 15 September 2021



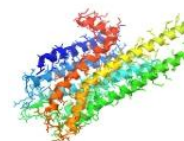
In the European INHERIT consortium under coordination of the Swedish Defence Research Agency (FOI), HIMS researchers will develop advanced analytical methods for the chemical profiling of frequently encountered precursors to illegal explosives. Working together with the FBI, the aim of the consortium is to develop new methods and strategies to disrupt terrorist timelines and prevent attacks with explosives in Europe and the USA.

Two novel sustainable chemistry projects granted at Catalysis Engineering group - 12 October 2021



Dr Shiju Raveendran and Dr Ihsan Amin of the Catalysis Engineering research group have both been awarded 50,000 euros in the Open Competition XS call of the Dutch Research Council NWO (Domain Science). Dr Raveendran will develop a plasma-in-liquid reactor to conduct chemical reactions at low temperature and pressure with renewable electricity. Dr Amin proposes to use borophene, a new emerging graphene-like 2D material, as catalyst to generate hydrogen.

Understanding psychedelics using molecular simulations - 18 November 2021



Psychedelics have, in recent years, re-entered the fields of psychiatry and neuroscience. Peter Bolhuis and Florent Smit have been awarded a 50,000 euro grant in the Open Competition XS call of the Dutch Research Council NWO (Domain Science) for taking on the challenge of studying the activation mechanism of the specific serotonin receptor involved.

Veni grants for Giulia Giubertoni and Fabian Eisenreich - 16 December 2021



The Dutch Research Council NWO has awarded Giulia Giubertoni and Fabian Eisenreich Veni grants to perform research at HIMS. This will provide them with the opportunity to further elaborate their research ideas over a three-year period. The grants of up to € 280,000 confirm the quality and innovative nature of their research and help to further establish themselves in their field.

150,000 euro ECCM grant for Amanda Garcia - 16 December 2021



Dr Amanda Garcia has been awarded a grant of almost € 150,000 from the ECCM Kickstart DE-NL call. This aims to accelerate the electrification of the chemical industry through cross-border cooperation between partners from Germany and the Netherlands. Garcia's project is about imaging oxidation reactions on high surface area anodes for paired electrolysis.

Eva Meeus receives HRSMC mobility funding - 20 December 2021



PhD student Eva Meeus (research group Homogeneous, Supramolecular and Bio-Inspired Catalysis) has received funding from the PhD Mobility Programme of the Holland Research School of Molecular Chemistry. She will visit the group of Prof. Thomas R. Ward at the University of Basel to work on artificial metalloenzymes for a period of three months.

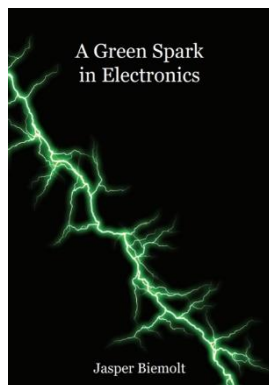
NWO XS grant for Paola Riente Paiva - 21 December 2021



Dr Paola Riente Paiva of the Flow Chemistry group has been awarded a 50,000 euro grant in the Open Competition XS call of the Dutch Research Council NWO (Domain Science). She will use the grant to study the effect of magnetic fields on homogeneous photocatalytic reactions, aiming to enhance conversion efficiencies.

Dissertations

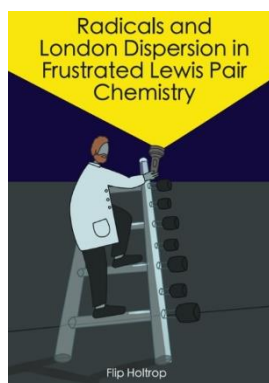
Of the 21 students that received their PhD at HIMS in 2021, four were granted the distinction 'cum laude': Thierry Slot, Tessel Bouwens, Alberto Pérez de Alba Ortíz and Eduard Bobylev. All these are listed below; a link is provided to download each thesis from the UvA repository.



1 December 2021

A green spark in electronics- Electrochemical innovations for a sustainable printed circuit board industry

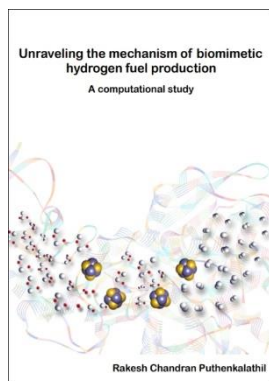
Author: J. (Jasper) Biemolt
Supervisors: G. Rothenberg, N. Yan
Group: Heterogeneous Catalysis and Sustainable Chemistry
Link: [Read or download this thesis](#)



26 November 2021

Radicals and London Dispersion in Frustrated Lewis Pair Chemistry

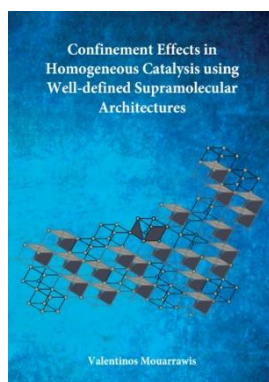
Author: F. (Flip) Holtrop
Supervisor: J.C. Slootweg
Co-supervisor: A.R. Jupp, J.H. van Maarseveen
Group: Synthetic Organic Chemistry
Link: [Read or download this thesis](#)



24 November 2021

Unraveling the mechanism of biomimetic hydrogen fuel production

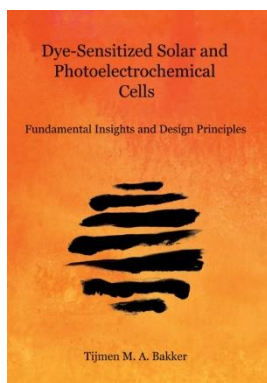
Author: R. (Rakesh) C. Puthenkalathil
Supervisor: B. Ensing, P.G. Bolhuis
Group: Computational Chemistry
Link: [Read or download this thesis](#)



22 October 2021

Confinement effects in homogeneous catalysis using well-defined supramolecular architectures

Author: V. (Valentinos) Mouarrawis
Supervisors: J.N.H. Reek, B. de Bruin
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: [Read or download this thesis](#)



8 October 2021

Dye-sensitized solar and photoelectrochemical cells - Fundamental insights and design principles

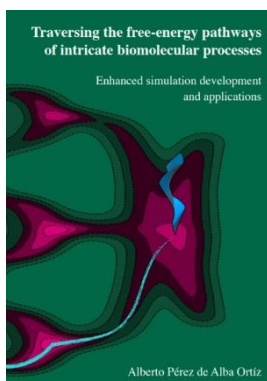
Author: T. (Tijmen) M.A. Bakker

Supervisor: J.N.H. Reek

Co-supervisors: S. Mathew, R. Detz

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



22 September 2021

Traversing the free-energy pathways of intricate biomolecular processes - Enhanced simulation development and applications

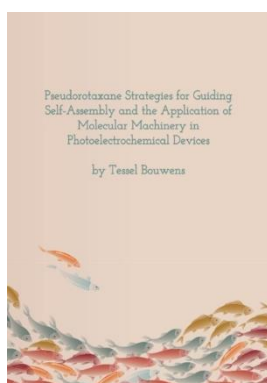
Author: A. (Alberto) Pérez de Alba Ortíz

Supervisor: B. Ensing

Co-supervisor: E.J. Meijer

Group: Computational Chemistry

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



15 September 2021

Pseudorotaxane strategies for guiding self-assembly and the application of molecular machinery in photoelectrochemical devices

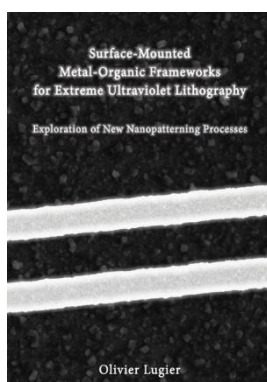
Author: T. (Tessel) Bouwens

Supervisor: J.N.H. Reek

Co-supervisor: S. Mathew

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



3 June 2021

Surface-mounted metal-organic frameworks for extreme ultraviolet lithography - Exploration of new nanopatterning processes

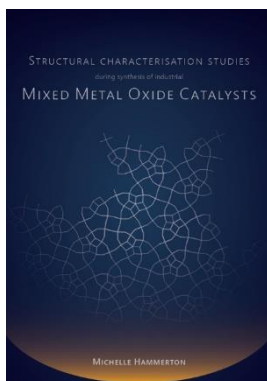
Author: O. (Olivier) C.M. Lugier

Supervisor: A.M. Brouwer

Co-supervisor: S. Castellanos Ortega

Group: Molecular Photonics

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



26 April 2021

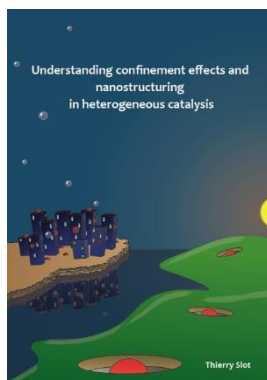
Structural characterisation studies during synthesis of industrial mixed metal oxide catalysts

Author: M. (Michelle) Hammerton

Supervisor: M. Tromp

Co-supervisor: K. Köhler

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



12 April 2021

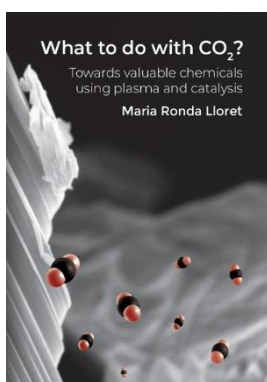
Understanding confinement effects and nano structuring in heterogeneous catalysis

Author: T. (Thierry) K. Slot

Supervisors: G. Rothenberg, N. Shiju

Groups: Heterogeneous Catalysis and Sustainable Chemistry and Catalysis Engineering

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



9 April 2021

What to do with CO₂? Towards valuable chemicals using plasma and catalysis

Author: M. (Maria) Ronda Lloret

Supervisors: N. Shiju, G. Rothenberg

Groups: Heterogeneous Catalysis and Sustainable Chemistry and Catalysis Engineering

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



7 April 2021

Sustainable selective oxidations in confined spaces

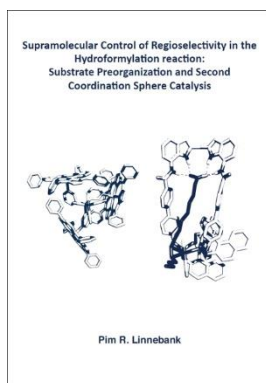
Author: I. (Ilse) M. Denekamp

Supervisors: G. Rothenberg, D. Dubbeldam

Group: Heterogeneous Catalysis and Sustainable Chemistry

Group: Computational Chemistry

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



31 March 2021

Supramolecular control of regioselectivity in the hydroformylation reaction - Substrate preorganization and second coordination sphere catalysis

Author: P. (Pim) Linnebank

Supervisor: J.N.H. Reek

Co-supervisor: A.M. Kluwer

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis

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



17 March 2021

The hidden life of cosmic carbon - Infrared fingerprint spectroscopy and fragmentation chemistry of gas-phase polycyclic aromatic hydrocarbons

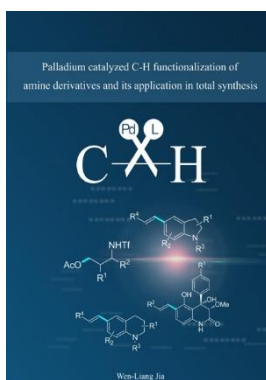
Author: S. (Sandra) Wiersma

Supervisor: W.J. Buma

Co-supervisors: A. Petrigani, J.M. Bakker

Group: Molecular Photonics

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



11 March 2021

Palladium catalyzed C-H functionalization of amine derivatives and its application in total synthesis

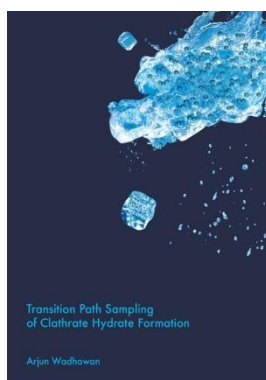
Author: W.-L. (Wen-Liang) Jia

Supervisor: M.Á. Fernández-Ibáñez

Co-supervisor: J.H. van Maarseveen

Group: Synthetic Organic Chemistry

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



9 March 2021

Transition path sampling of clathrate hydrate formation

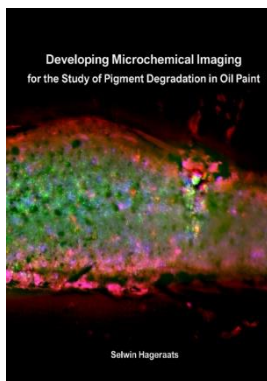
Author: A. (Arjun) Wadhawan

Supervisor: P.G. Bolhuis

Co-supervisor: N. Shahidzadeh

Group: Computational Chemistry

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



03 March 2021

Developing microchemical imaging for the study of pigment degradation in oil paint

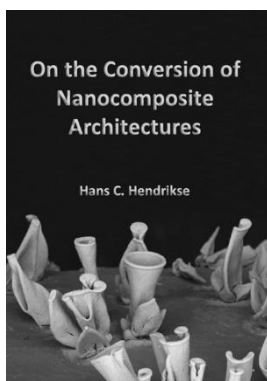
Author: S. (Selwin) Hageraats

Supervisor: K. Keune

Co-supervisor: M. Thoury

Group: Computational Polymer Chemistry

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



26 February 2021

On the conversion of nanocomposite architectures

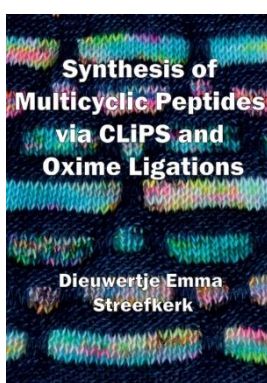
Author: H. (Hans) C. Hendrikse

Supervisor: H.J. Bakker

Co-supervisor: W.L. Noorduin

Group: Molecular Photonics

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



16 February 2021

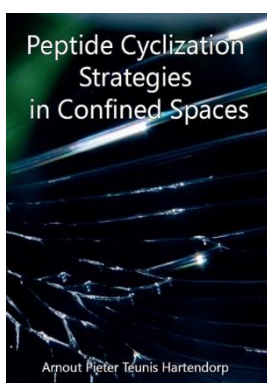
Synthesis of Multicyclic Peptides via CLiPS and Oxime Ligations

Author: D. (Diewertje) E. Streefkerk

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

Group: Synthetic Organic Chemistry

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



9 February 2021

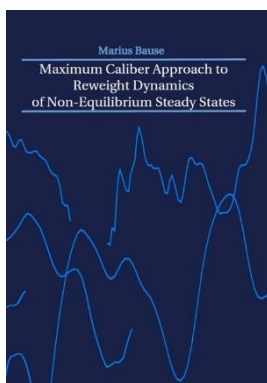
Peptide cyclization strategies in confined spaces

Author: A. (Arnout) P.T. Hartendorp

Supervisors: J.N.H. Reek, J.H. van Maarseveen

Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis and Synthetic Organic Chemistry

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



26 January 2021

Maximum caliber approach to reweight dynamics of non-equilibrium steady states

Author: M. (Marius) Bause

Supervisor: T. Berau

Co-supervisor: E.J. Meijer

Group: Computational Chemistry

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 news items in 2021.

From sticky mess to plant-based chair - 6 January 2021



'Such a thing doesn't exist,' UvA researchers Gadi Rothenberg and Albert Alberts repeatedly heard when they accidentally discovered 100% bioplastic in 2010. Now ten years later, in collaboration with furniture manufacturer VepaDreentea, they have created a chair made entirely from plant-based materials.

UvA and AC2T Research sign research collaboration on materials for clean energy - 18 January 2021



The University of Amsterdam (UvA) has signed a long-term collaboration with AC2T Research GmbH, the Austrian Excellence Centre for Tribology. The collaboration in the area of new materials for clean energy will be led by Prof. Gadi Rothenberg (HIMS) and Dr Andreas Pauschitz (AC2T research).

Successful 2021 edition of International Winter School on Molecular Simulation - 19 January 2021



More than 100 PhD researchers, postdocs and other researchers from all over the world participated in the Winter School Understanding Molecular Simulation (MolSim2021) organized by the Computational Chemistry group. The MolSim winter school is part of the scientific training program of [CECAM](#), the European centre for computational research in the field of science and technology.

Novel heterogeneous catalysts explained in Lego-animated manual - 17 March 2021



Ilse Denekamp, a PhD student working under the supervision of Prof. Gadi Rothenberg has 'translated' her PhD research in a short film. The one-minute animation highlights the advantages of novel tailor-made single-site catalytic materials for heterogeneous catalysis.

Important step towards full circularity of SusPhos process - 2 April 2021



HIMS researchers have taken an important step towards full circularity of phosphate recycling in the SusPhos process. In a project financed by a 'Gouden KIEM' grant from NWO and ChemistryNL, they have succeeded at lab scale in recovering the magnesium used as a process additive.

UvA researchers coach finalists of high school chemistry competition - 26 April 2021



Students of Canisius College Nijmegen won the 'profielwerkstuk' competition 'Imagination at Work' of Centrum JongerenCommunicatie Chemie (C3). They investigated the capture of CO₂ using porous materials, coached by Stefania Grecea and Andreea Gheorghe of the Functional Materials research group. All other finalists were also coached by HIMS researchers.

Visiting high school students win prizes as a result of their research at HIMS - 26 May 2021



High school students Chris Kooijman (18) and Max Tiemersma (17) from RSG Simon Vestdijk in Harlingen won a 'profielwerkstuk' prize with their investigation in methanol synthesis from carbon dioxide. They performed part of their research together with Dr Maria Ronda Lloret at the Catalysis Engineering group.

Open Kitchen Labs: an accessible chemistry lab for startups - 16 June 2021



Anyone who wants to turn waste into a resource for new processes and new products will sooner or later run into questions that can only be answered in a laboratory. That's why 'Open Kitchen Labs' at Amsterdam Science Park has been started: accessible, shared laboratory space, including equipment and expert support, at affordable pricing.

Towards a novel device for ammonia sensing - 16 August 2021



Dr Stefania Grecea will develop a new concept for ammonia sensing that can be implemented in wearable devices to measure ammonia concentrations in farming- and sensitive ecosystem environments. For this, she has been awarded a 50,000 euro grant in the Open Competition XS call of the Dutch Research Council NWO (Domain Science).

Chemical profiling and trace analysis of illegal home-made explosives - 15 September 2021



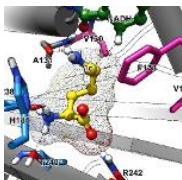
In the European INHERIT consortium under coordination of the Swedish Defence Research Agency (FOI), HIMS researchers will develop advanced analytical methods for the chemical profiling of frequently encountered precursors to illegal explosives. Working together with the FBI, the aim of the consortium is to develop new methods and strategies to disrupt terrorist timelines and prevent attacks with explosives in Europe and the USA.

SusPhos is Frisian Startup of the Year 2021 - 16 September 2021



UvA spin-off company SusPhos, based at the WaterCampus in Leeuwarden, was voted Frisian Startup of the Year 2021. This young company focuses on upcycling phosphate-rich waste streams into valuable products such as fertilizer and flame retardants. The seed of one of these techniques was sown at HIMS research by Dr Chris Slootweg, Dr Marissa de Boer and ing. Bas de Jong.

Biocatalysis group strengthens cooperation with Olon Group and Biosphere - 26 October 2021



The Olon Group, an Italian company producing active pharmaceutical ingredients and intermediates, has announced a partnership with the company Biosphere — an Italian SME specialised in fermentation and industrial biotechnology — and the Biocatalysis Group of HIMS led by Dr Francesco Mutti.

Sonja Pullen wins Lorentz Center Chemistry competition - 15 December 2021



With their proposal for a workshop on the challenges and future perspectives of photocatalysis, Dr Sonja Pullen and co-applicants have won the 2021/22 Chemistry Competition of the Lorentz Center and the Royal Netherlands Chemical Society KNCV. As a result, the Lorentz Center will host the workshop in Leiden in the course of 2022.

Outreach

Lectures and other contributions in 2021

For the general public

- De poederdoos uit het Palmhoutwrak - een lezing over het onderzoek naar de edelmetaalvondsten uit het Palmhoutwrak. In dit inmiddels beroemde scheepswrak zijn tal van bijzondere edelmetalen objecten gevonden (Tonny Beentjes, Janneke van der Stok, Ineke Joosten, Maarten van Bommel)
- Hoe leg je moleculaire knopen? - professional lecture (Jan van Maarseveen)
- 'Highlights van het onderzoek aan de Nachtwacht', Speeddaten Rijksmuseum Amsterdam (Katrien Keune)
- Operation Night Watch, FAST2021, Amersfoort (Katrien Keune)
- Onderzoek en behandeling: een kwestie van timing, Workshop Waardemanagement Prioriteiten voor Collectiemanagement en Conservering voor gemeentelijke archeologische depots (Ineke Joosten, Tonny Beentjes, Maarten van Bommel)
- AMOR - Archeologisch MetaalOppervlak Research, lunch lecture (Janneke van der Stok, Ineke Joosten, Tonny Beentjes, Maarten van Bommel)
- 'Operatie Nachtwacht: hoe staat het ermee?', Lunch Dates Vrienden, Rijksmuseum, Amsterdam (Katrien Keune)
- Taming electrons and covalently made mechanically interlocked molecules, professional lecture (Jan van Maarseveen)
- Organizing biweekly NICAS Colloquium (Katrien Keune)

For high school students and teachers

- *Afval als grondstof voor de chemie - Supervising finalists of the national school chemistry competition at CSG Jan Arentsz Alkmaar (Stefania Grecea, Andreea Gheorghe, Chris Slootweg, Steven Beijer)*
- *Visiting high school students Chris Kooijman and Max Tiemersma from RSG Simon Vestdijk in Harlingen win two profielwerkstuk prizes as a result of their research at HIMS (N. Raveendran Shiju, Maria Ronda Lloret)*
- *Profielwerkstukbegeleiding Atheneum College Hageveld Heemstede: analytische onderzoekstechnieken in Operatie Nachtwacht (Katrien Keune)*
- *Profielwerkstuk begeleiding Keizer Karel College Amstelveen: chemie over loodwit in schilderkunst (Katrien Keune)*

HIMS researchers appearing in the media in 2021

The dream team: the magical top ten chemistry talents

Marie Brands and Lotte Metz appear in this list

▶ [16 December 2021 Change Inc.](#)



Lotte Metz in the talented chemistry dream team as photographed by Change Inc.

Plantics among five fast-growing 'climate tech' companies

Plantics, founded in 2014 by Gadi Rothenberg, is mentioned in FD as one of the fast-growing 'climate tech' companies investors will keep an eye on.

▶ [15 December 2021 FD](#)

Sisters in Science win NWO Diversity Initiative Award

Interview with Mimi, Noor and Lotte in AD

▶ [2 December 2021 AD](#)

Musings from the Power List: Bob Pirok

Interview with Bob Pirok in the Analytical Scientist.

▶ [30 November 2021 The Analytical Scientist](#)

Jan van Maarseveen and Sander Woutersen in Folia

120 years after the famous UvA chemist Jacobus Henricus van 't Hoff won the Nobel Prize in Chemistry in 1901, the Amsterdam laboratory where he worked on his research is declared National Chemical Heritage. Jan van Maarseveen and Sander Woutersen talk about Van 't Hoff to Folia.

▶ [17 November 2021 Folia](#)

Gadi Rothenberg at Wiley: Research and Teaching in the Digital Age

Researchers' top tips have been collected to help others thrive in the learning and teaching digital age.

▶ [8 November 2021 www.wiley.com](#)

Timothy Noël in C2W about his passion for flow chemistry

C2W has an interview with chemist Timothy Noël (UvA-HIMS), who recently won the KNCV Gold Medal. There he talks about his predilection for flow chemistry: synthesis as done by an engineer, not in test tubes but in a miniature version of a chemical factory.

▶ [27 October 2021 C2W](#)

Henk Hiemstra in De Volkskrant about the Nobel Prize in Chemistry for organocatalysis

This year's Nobel Prize in Chemistry goes to Benjamin List and David MacMillan for the discovery of organic catalysts. In De Volkskrant, UvA chemist Henk Hiemstra (HIMS) talks about the importance of organocatalysis.

▶ [6 October 2021 De Volkskrant](#)

Joost Reek at RTL News about getting energy from diapers

A new factory in Gelderland recycles diapers and incontinence material, with part of the material

being processed into reusable raw materials and part converted into energy. Joost Reek (HIMS) explains.

► [20 September 2021 RTL Nieuws](#)

SistersinScience at Anna's Brains

Lotte, Noor and Mimi feature in the scientific television show 'Anna's Brains', a VPRO series of 8 episodes on NPO3 which tries to answer scientific questions.

► [Episode 30 August 2021](#), featuring Mimi: Kan je leven onder water?

► [Episode 6 September 2021](#), featuring Mimi: Kan je praten met dieren?

► [Episode 27 September 2021](#), featuring Lotte: Kan je een zelfrijdende fiets maken?

► [Episode 18 October 2021](#), featuring Noor: Kan je surfen op lucht?

An introduction to the program could be seen at the show of [Humberto](#).



Episode of 'Anna's Brains' on living under water, featuring Mimi den Uyl (left). Photo: NPO.

Article on Susphos: Recycling: SusPhos maakt de fosfaatcirkel rond

Samen met stikstof en kalium is fosfaat nodig om gewassen te laten groeien. Het is dus een belangrijk bestanddeel van kunstmest. Daarnaast heeft fosfaat een brandvertragende werking, wat een tweede toepassingsgebied oplevert. SusPhos wint de grondstof fosfaat terug uit de afvalwaterketen. Het winningsproces werd vier jaar geleden ontwikkeld. Begin volgend jaar wordt een fabriek met een capaciteit van 50.000 ton per jaar gebouwd. CTO Willem Schipper vertelt over deze keuze en over meer stukjes van de puzzel die het bedrijf het komende jaar gaat leggen.

► [July 2021, Chemie Magazine](#)

Jan van Maarseveen in NRC about improved production of gamma-cyclodextrin American chemists have developed a way to simplify the production of gamma-cyclodextrin. One of the things this sugar-like molecule is used for is to make medicines easier to absorb in your body. NRC Handelsblad writes about the discovery and asked Jan van Maarseveen (UvA-HIMS) about his interpretation.

► [30 June 2021, NRC Handelsblad](#)

Gert-Jan Gruter in Algemeen Dagblad about plastic litter

In Eindhoven, a coca-cola bottle dating back at least a quarter of a century was unearthed during work, of which even the plastic cap was still completely intact. Reason for Algemeen Dagblad to ask a number of experts, including Gert-Jan Gruter (UvA-HIMS) about how long plastic objects remain intact if they are thrown away as litter.

► [29 June 2021, Algemeen Dagblad](#)

Joen Hermans about the chemistry of oil paint

Joen Hermans (UvA-HIMS) talks about his research in the chemistry of oil paint, and why Rembrandt was also a brilliant chemist besides a great painter.

► [22 June 2021, NPO Radio 1, Focus](#)

Joen Hermans about master painters and chemistry

The master painters of the golden age also needed chemical knowledge to create their paintings. Joen Hermans talks about the chemical properties of the paint from that time.

▶ [6 June 2021, Algemeen Dagblad](#)

Create mirror image molecules without mess

Some molecules have 'mirror images'. Researchers from Basel University selectively made one of six possible mirror images of a molecule. In this article Joost Reek comments on it.

▶ [2 June 2021, NRC](#)

Joen Hermans lectures at Universiteit van Nederland: Wat maakt Rembrandt een scheikundig wonder?

The Night Watch as it now hangs in the museum is no longer the same as when Rembrandt added the last brushstrokes. The oil and pigments in paintings react with each other and the environment, causing paint to change or sometimes even disappear. Chemist Joen Hermans (University of Amsterdam & Rijksmuseum) shows which chemical reactions all take place on a work of art.

▶ [6 May 2021, Universiteit van Nederland](#)



Joen Hermans presented a video lecture at the 'Universiteit van Nederland'.

Wim Noorduyn and Lukas Helmbrecht in NRC about their chemical painting trick

In NRC Handelsblad PhD candidate Lukas Helmbrecht and his supervisor Wim Noorduyn (both UvA-HIMS and AMOLF) tell about the chemical magic trick with which they can "paint" a fluorescent image. Specialist medium E-Totaal pays attention to the portrait of Marie Curie that the chemists made with their technique. The technique is based on a semiconductor layer of perovskite.

▶ [16 April 2021, NRC](#)

▶ [13 April 2021, E-Totaal](#)

Gadi Rothenberg about his "sticky mess"

Gadi Rothenberg (HIMS) has once again reached multiple media with the story about his "sticky mess", a 100% natural bioplastic discovered by accident.

▶ [9 March 2021, podcast "Bijvangst"](#)

▶ [3 March 2021, InnovationOrigins](#)

Fighting the corona virus with UV-light?

Since the very beginning of the corona crisis, attempts have been made to return to normal life as soon as possible. One of the possible solutions that could help with this: a lamp that switches off the corona virus particles.

Fred Brouwer explains.

▶ [3 March 2021, EenVandaag](#)

Nuclear energy not necessary for climate goals (and expensive)

Bob van der Zwaan at NU.nl about nuclear energy.

▶ [1 March 2021, NU.nl](#)

Shedding light on photocatalysis

C2W featured Tim Noël's Nature Communications paper on the true nature of the catalytically active species in photocatalytic reactions using bismuth oxide semiconductor.

▶ [22 February 2021, C2W](#)

Sisters in Science

Noor Abdulhussain, Mimi den Uijl and Lotte Schreuders founded the Instagram account "[Sisters in Science](#)". Their goal? Breaking stereotypes and showing that it's not only white old men who work in science.



▶ [28 February 2021, De Telegraaf](#)

▶ [26 February 2021, Chemie Magazine](#)

▶ [16 February 2021, Linda.nl](#) (interview with Noor Abdulhussain)

▶ [11 February 2021, RedPers.nl](#)

Unsuccessful UvA experiment did result in 100% vegetable plastic

Ten years ago UvA scientists discovered 100 percent bioplastic, now there is a plant-based chair. Gadi Rothenberg explains to newspaper Het Parool (interview in Dutch).

▶ [12 January 2021, Het Parool](#)

Facts & Figures

Research

Research output

Research output 2021 per type of publication (source: PURE)

HIMS themes	AC	CC	MP	SC	Other	Joint ¹	Total
Refereed articles	48	75	60	113	17	21	313
Book - Edited				4			4
Book (chapter)s	1	2	1	11			15
PhD-theses		4	2	14	1		21
Conference papers							
Other research output	3	7	3	13	18 ³		14

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

¹Joint results obtained from collaborations between different research groups.

The total number of 21 publications include a total number of 38 collaborations.

³e.g. AMOLF, ARCNL, AVANTIUM etc

Other output and honours

HIMS themes	AC	CC	MP	SC	Other	Joint	Total
Keynote lecture	5	9	8	3			25
Hosting a Conference	1	2			1		
Lectures for general public, media coverage		2		4			6
Prizes/awards	6	5	7	26		-4	40
Total	19	37	35	67		-4	154

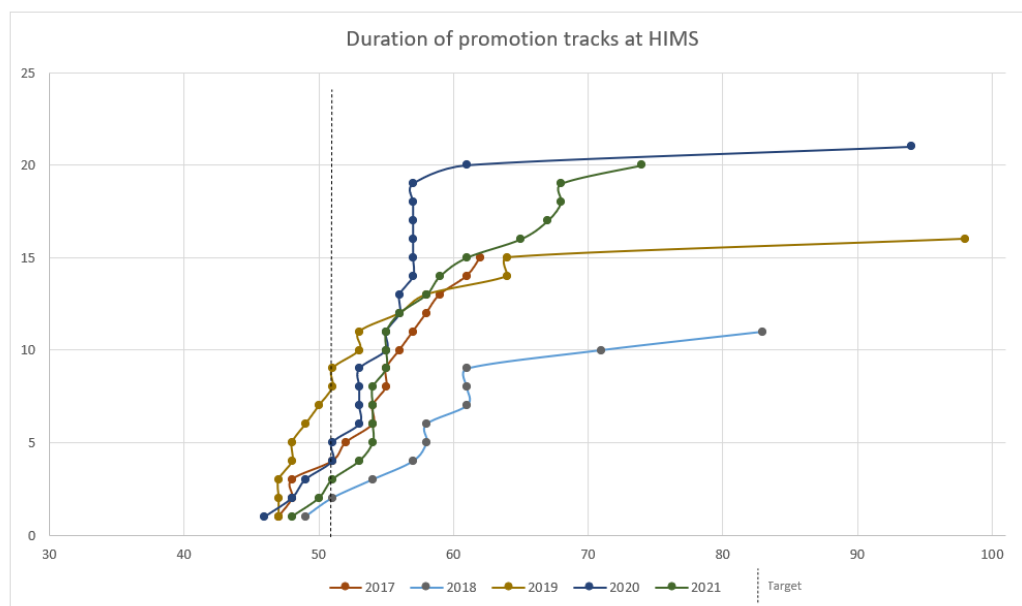
Research themes: AC = Analytical Chemistry; CC = Computational Chemistry; MP = Molecular Photonics; SC = Synthesis & Catalysis.

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	
	#	%	#	#	%	#	%	#	%	#	%	#	%	#	%	#	%
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	3	13	1	4	21	91	1	4	1	4
2016	18	13	31	1	3	22	71	3	10	-	-	26	84	3	10	2	6
2017	13	11	24	-	-	11	46	4	17	-	-	15	63	6	25	3	13
Total	63	43	106	8	8	61	58	17	16	1	1	87	82	10	9	9	8

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. Externally prepared promotions are not taken into account in these figures. In 2021, 8 PhD candidates received a corona delay related extension with an average of 1.8 months pp.



Personnel

FTE numbers

This table presents the HIMS staff numbers head count in 2021 and average FTE for the year. 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)	7,1	3,5	7,1	3,5	5,3	2,6	14,5	7,3	0,0	0,0	34	16,9
Post-docs (2)	1,8	1,7	1,9	1,7	3,1	2,8	12,5	11,2	0,0	0,0	19,3	17,4
PhD students (3)	13,1	9,8	6,4	4,8	10,7	8,0	45,0	33,8	0,0	0,0	75,2	56,4
Total research staff	22,0	15,0	15,4	10,0	19,1	13,4	72,0	52,3	0,0	0,0	128,5	90,7
Technicians (4)	4,2	4,2	0,8	0,8	2,9	2,9	13,0	13,0	0,0	0,0	20,9	20,9
Visiting fellows	0,0	0,0	0,0	0,0	0,0	0,0	1,1	1,1	0,0	0,0	1,1	1,1
Support staff (4)	0,0	0,0	0,0	0,0	0,0	0,0	0,4	0,4	5,9	5,9	6,3	6,3
Total staff	26,2	19,2	16,2	10,8	22,0	16,3	86,5	66,8	5,9	5,9	155,7	119,0

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 2021.

Age bracket	Number	%-age	Male	Female	Dutch	Other EU	Other
30-40	11	30%	7	4	3	6	2
40-50	10	27%	4	6	5	3	2
50-60	12	32%	12	0	11	0	1
60+	4	11%	4	0	4	0	0
Total	37	100%	27	10	23	9	5

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. Other are prizes or awards not suitable for the previous categories.

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 2021 of HIMS per funding type (fte)

HIMS Themes	Research					Total	%	Support	Total	%
	AC	CC	MP	SC	Other					
Direct funding	-	-	-	-	-	44,45	36%	16,65	61,1	40%
Research grants	7,7	8,8	7,4	25,7	-	49,6	40%	4,25	53,85	36%
Contract research	6,7	0,8	2,1	20,6	-	30,2	24%		30,2	20%
Other	-	-	-	-	-	0	0%	6,3	6,3	4%
Total	14,4	9,6	9,5	46,3	0	124,25	100%	27,2	151,45	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 2018 (mln €) per funding type.

HIMS themes	AC	CC	MP	SC	Other	Total ¹
Direct funding	-	120		455	-	575
Research	-	419	327	3.097		3.843
Contract research	715	-	-	1.854	-	2.569
Other				50		0
Total	715	539	327	5.456	-	6.987

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

HIMS result 2021 (k€)

The HIMS result for 2021 amounts to +1.09 Mio€. These concern reservations from past budgets for costs in the framework of the *Sectorplan Natuur- en Scheikunde* and the RPA Sustainable Chemistry foreseen. 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.

2021	EU & Contract research Total			
	Direct	NWO	EU & Contract research	Total
HIMS Base Budget	3.618	-	-	3.618
Budget (variable1)	5.886	3.467	2.589	11.942
Other income 2	2.336	209	55	2.600
Matching contract research	-3.858	2.591	1.267	-
Budget total	7.982	6.267	3.911	18.160
<i>Percentage</i>	<i>44%</i>	<i>35%</i>	<i>22%</i>	<i>100%</i>
Personal costs	-4.803	-2.951	-1.887	-9.641
Other costs (projects)	-3.715	-711	-467	-4.893
Overheads 3	1.596	-2.613	-1.512	-2.529
Costs total	-6.922	-6.275	-3.866	-17.063
<i>Percentage</i>	<i>41%</i>	<i>37%</i>	<i>23%</i>	<i>100%</i>
HIMS Result 2021	1.060	-8	45	1.097

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.