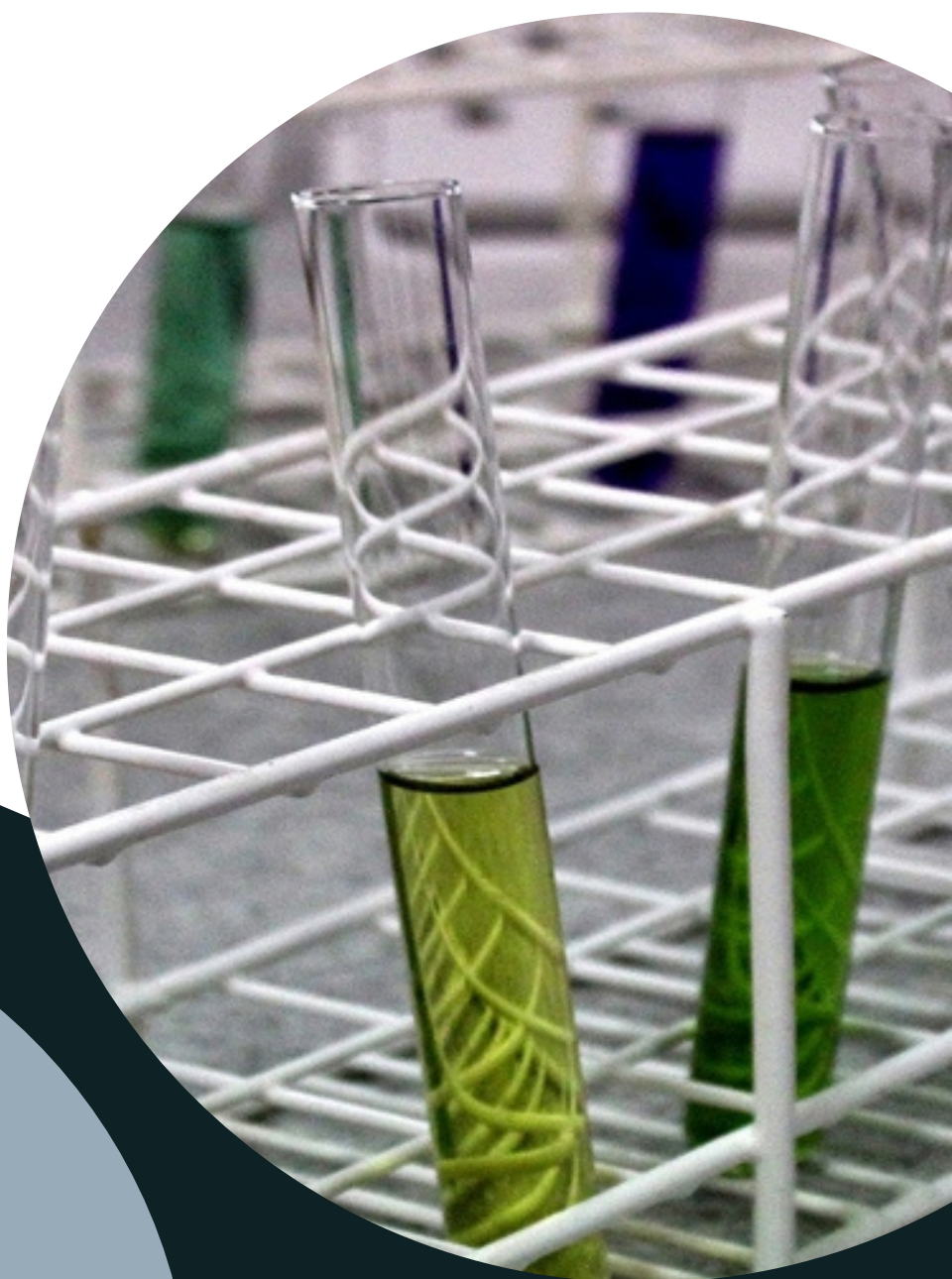


HOLLAND RESEARCH SCHOOL OF MOLECULAR CHEMISTRY



ANNUAL
REPORT

2021

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General

This annual report presents an overview of the research and educational activities of the graduate research school 'Holland Research School of Molecular Chemistry' (HRSMC) during 2021. The University of Amsterdam legally represents the HRSMC. The research school was founded in 1994 and has been re-accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW) in 1999, 2005 and 2012. The HRSMC is now in its fifth period 2019-2024. The HRSMC is a collaboration between top research groups of four Dutch Universities: the University of Amsterdam (UvA), the VU Amsterdam (VU), Leiden University (UL) and the Radboud University (RU).

The HRSMC harbours a powerhouse of expertise in Synthetic, Physical, and Theoretical Chemistry as well as Spectroscopy and Molecular Physics. This multidisciplinary character makes the School unique in the Netherlands and abroad; it allows it to operate in a broad field that addresses fundamental scientific problems but also challenges society currently faces in areas like sustainability, energy, and health.

This annual report presents a survey of the activities and achievements of the HRSMC, both educational and scientific, as well as the scientific achievements of the participating research groups.

As an interuniversity research school, the HRSMC has two main targets:

- A. to promote and facilitate research aimed at the three HRSMC research themes: (1) 'Synthesis, Characterisation, Properties and Reactivity of Molecules', (2) 'Physical Chemistry and Spectroscopy' and (3) 'Theoretical Chemistry'. The HRSMC board strives for coherence in the research activities of its members by promoting collaboration between the research groups and safeguarding complementarities with respect to infrastructure and expertise.
- B. to facilitate and provide a coherent, high-level educational programme to its PhD students, which offers a seamless connection to the Master degree programme. The primary aim is to teach PhD researchers to answer key questions in molecular science and to use their insights in a multidisciplinary approach.

The extensive educational programme (Schools, Courses and Symposia) offered by the HRSMC means that for all practical purposes the school takes care of the educational program of its PhD students and safeguards their progress. Importantly, the educational activities of the HRSMC are also accessible for (advanced) MSc students and thereby seamlessly connect to the undergraduate programs of the participating universities.

Besides organizing several educational activities, the HRSMC organized two application rounds within the Fellowship and PhD Mobility Programme.

Prof. dr. Wybren Jan Buma

Scientific Director of the HRSMC

The Research Programme

The research program of the HRSMC is embedded in top research groups of the VU Amsterdam (VU), the University of Amsterdam (UvA), Leiden University (UL) and the Radboud University (RU). It is organized around three different research themes in molecular chemistry which complement and mutually reinforce each other.

Theme 1: Synthesis, Characterisation, Reactivity and Properties of Molecules

This theme deals, among others, with the design, synthesis and characterization of new compounds, the development of new (bio)catalytic reactions, and the investigation of their mechanisms.



Theme 2: Physical Chemistry and Spectroscopy

Theme 2 addresses the issue of experimentally uncovering the fundamental factors behind molecular properties through the interaction between light and molecular matter. Advanced spectroscopic techniques are employed to probe and utilize fundamental processes such as catalytic events, reaction mechanisms and dynamics, and energy and electron transfer.



Theme 3: Theoretical Chemistry

Research within this theme is fully dedicated to understanding the structure of molecules and their chemistry from first principles. HRSMC's theoretical chemistry groups cover method and software development, computational chemistry, and the development of models and guiding principles for rational design of catalysts and sustainable processes. They are working on a broad range of time and length scales (atomic, molecular, supra-molecular, condensed-phase/membrane processes), naturally leading to a multi-scale approach of fundamental and applied theoretical chemistry.



Overview of the Research Groups in 2021

Theme **Group (University, Institute) and Staff members**

1	Homogeneous, Supramolecular and Bio-Inspired Catalysis (UvA, HIMS) Prof. dr. B. de Bruin, Prof. dr. J.N.H. Reek, Prof. dr. C.J. Elsevier, Dr. A.W. Ehlers, Dr. T.J. Mooibroek, Dr. Ir. J.I. van der Vlugt (guest appointment), Dr. S. Pullen
	Functional Materials (UvA, HIMS) Dr. S. Grecea
	Heterogeneous Catalysis and Sustainable Chemistry (UvA, HIMS) Prof. dr. G. Rothenberg, Dr. N. Yan, Dr. A. Garcia
	Catalysis Engineering (UvA, HIMS) Dr. N.R. Shiju
	Synthetic Organic Chemistry (UvA, HIMS) Prof. dr. J.H. van Maarseveen, Prof. dr. P. Timmerman, Dr. M.Á. Fernández-Ibáñez, Dr. S. Ingemann, Dr. J.C. Sootweg
	Biocatalysis (UvA, HIMS) Prof. dr. F. Mutti
	Flow Chemistry (UvA/HIMS) Prof. dr. T. Noël
	Biomimetic and Biomolecular Chemistry (VU, AIMMS) Prof. dr. T.Grossmann, Dr. S. Hennig, Dr. I. Drienovská
	Synthetic Organic Chemistry & Catalysis (VU, AIMMS) Prof. dr. E. Ruijter, Prof. dr. ir. R.V.A. Orru (guest appointment)
	Supramolecular and Biomaterials Chemistry (UL, LIC) Dr. S.J. Wezenberg
	Metals in Catalysis, Biomimetics & Inorganic Materials (UL, LIC) Prof. dr. E. Bouwman, Prof. dr. S. Bonnet, Dr. D.G.H. Hettterscheid
	Synthetic Organic Chemistry (RU/IMM) Prof. dr. F.P.T.J. Rutjes, Dr. T.J. Boltje, Dr. M.C. Feiters

2

Molecular Photonics (UvA, HIMS)

Prof. dr. A.M. Brouwer, Prof. dr. W.J. Buma, Prof. dr. S. Woutersen, Dr. ir. A. Petrigani-Taube, Dr. R. M. Williams, Dr. H. Zhang

Chemistry for Art Conservation (UvA, HIMS)

Prof. dr. K. Keune

Biophotonics and Medical Imaging (VU, LaserLaB)

Dr. F. Ariese

BioAnalytical Chemistry (VU, AIMMS)

Prof. dr. A.M. Rijs

PhotoConversion Materials (VU)

Prof. dr. E.L. von Hauff, Dr. C. Ramanan, Dr. A. Baldi

Biophysical Organic Chemistry (UL, LIC)

Prof. dr. H.J.M. de Groot, Dr. Alia, Dr. F. Buda, Dr. G.J.A. Sevink

Molecular Nano-Optics and Spins (UL, LION)

Prof. dr. E.J.J. Groenen, Prof. dr. M. Orrit, Dr. P. Gast, Dr. M. I. Huber

Laboratory Astrophysics and Astrochemistry (UL, LION)

Prof. dr. H. Linnartz

Surface Chemistry and Catalysis (UL, LIC)

Prof. dr. M. Koper, Dr. W.T. Fu, Dr. I.M.N. Groot, Dr. D.G.H. Hetterscheid, Dr. L.B.F. Juurlink, Dr. R.V. Mom

Bioelectrochemistry and Biocatalysis (UL, LIC)

Prof. dr. L.J.C. Jeuken

FELIX Laboratory (RU)

Prof. dr. J. Oomens, Dr. J.M. Bakker, Dr. S. Brünken, Prof. dr. W.J. Buma (extraordinary professor)

3

Computational Chemistry (UvA, HIMS)

Prof. dr. P.G. Bolhuis, Prof. dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede

Theoretical Chemistry (VU, EMS)

Prof. dr. F.M. Bickelhaupt, Prof. dr. L. Visscher, Prof. dr. C. Fonseca Guerra, Prof. dr. P. Gori Giorgi, Dr. O. Gritsenko, Dr. K. J. H. Giesbertz, Dr. T. Hamlin

Biomolecular Simulation and Modeling (VU, EMS)

Dr. D.P. Geerke

Theoretical Chemistry (UL, LIC Energy & Sustainability)

Prof. dr. G. J. Kroes, Dr. J. Meyer, Dr. M.F. Somers, Dr. A.L.M. Lamberts, Prof. C. Fonseca Guerra (extraordinary professor)

Theory in Surface science and electrochemistry (UL, LIC)

Dr. Katharina Doblhoff-Dier

Theoretical Chemistry (RU)

Prof. dr. ir. G.C. Groenenboom, Prof. dr. H.M. Cuppen, Prof. dr. F.M. Bickelhaupt (extraordinary professor)

Research and Education

HRSMC Course 'Understanding Molecular Simulation', Molsim 2021

4-15 January 2021, online

A total of 84 participants attended this course, of which 24 UvA MSc students (3 HRSMC Class of Excellence students), 13 Dutch PhD students (2 HRSMC members) and 47 participants from foreign universities.

Lectures were held by Daan Frenkel (University of Cambridge), Berend Smit (EPFL), Thijs Vlugt (Delft University of Technology), Seyed Mohamad Moosavi (EPFL), Kevin Jablonka (EPFL), Peter Bolhuis (University of Amsterdam), Evert Jan Meijer (University of Amsterdam), Bernd Ensing (University of Amsterdam), David Dubbeldam (University of Amsterdam) and Jocelyne Vreede (University of Amsterdam)

Organizers: Evert Jan Meijer (University of Amsterdam), Berend Smit (EPFL), Daan Frenkel (University of Cambridge), Ensing Bernd (University of Amsterdam), David Dubbeldam (University of Amsterdam), Jocelyne Vreede (University of Amsterdam), Ineke Weijer (University of Amsterdam) and Laura Bastiaans-Tomé (University of Amsterdam).

Dutch Photochemistry Days

10 and 17 May 2021, online

In total, 74 participants attended on the 10th of May, and 55 on the 17th of May.

Organizers: Sylvestre Bonnet (chair), Fred Brouwer, Elizabeth von Hauff, Laura Bastiaans-Tomé, Rachel Scheffelaar

High Impact Writing Course

June 2021, online

This very well reviewed course was given by Prof. dr. Ulrike Müller and Dr. Otto Berg (California State University Fresno). 25 PhD students/Postdocs attended, of which 13 came from the UL, 6 from the VU and 6 from the UvA.

HRSMC Organic Synthesis Summer School

5-8 July 2021, Deurne, The Netherlands

A total of 61 participants attended the Summer School (HRSMC Class of Excellence Students: 4, Industry: 9, VU: 5, UvA: 9; UL: 6; RU: 7; Maastricht University: 4; RUG: 8; Eindhoven University of Technology: 1; UU: 5; Wageningen University: 3).

Lectures were held by Francesca Paradisi (University of Bern, Switzerland); Géraldine Masson (Institut de Chimie des Substances Naturelles, France); Timothy Noël (University of

Amsterdam, The Netherlands); Daniele Leonori (University of Manchester, UK); Tom Wennekes (Utrecht University, The Netherlands); Jan van Maarseveen (University of Amsterdam, The Netherlands); Phil Baran (Scripps Research Institute, California USA, Evening Lecture Zoom); Anita Wegert (Symeres, The Netherlands, evening lecture).

HRSMC Course Photophysics, Photochemistry and Photobiology

28 October – 12 November 2021, Amsterdam

20 participants attended this course. 19 participants were PhD students, of which 16 HRSMC members (VU: 9, UvA: 2, UL: 4, RU: 2, UT: 2), and 1 was a HRSMC Class of Excellence Student.

Lectures were held by Prof. dr. Fred Brouwer (UvA), Prof. dr. Maurice Aalders (UvA/AMC), Dr. Francesco Buda (UL), Dr. René Williams (UvA), Dr. Ivo van Stokkum (VU), Dr. Charusheela Ramanan (VU), Dr. Freek Ariese (VU).

Organizers: Dr. René Williams (UvA), Ineke Weijer (UvA, HRSMC), Laura Bastiaans (UvA, HRSMC), Rachel Scheffelaar (UvA, HRSMC)

The Dick Stufkens Prize 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, who is now a postdoctoral fellow at the University of Hong Kong, obtained his doctorate with the qualification 'cum laude' from the University of Amsterdam at the end of 2020.



In his thesis, Van Leest describes his studies on cobalt catalysts to achieve selective C–N and S–N bond formation via radical-type nitrene transfer. He provides a profound understanding of the underlying mechanisms of these catalysed conversions that are of relevance to the synthesis of medicines and other bio-active molecules.

Selecting the winner from a selection of excellent candidates, the jury for the Dick Stufkens prize 2021 unanimously decided for Klaas van Leest. They were impressed by the quality of his research and applaud his enormous productivity. Not only has Van Leest advanced the catalysis type that was the main subject of his study, he also contributed to studies on a variety of metal catalysts for a range of catalytic processes. While he reported on his PhD research in 9 papers, a further number of 22 other high-quality papers hold his name, and his publications have already been cited over 500 times. According to the jury, Van Leest thus displays an unusual combination of very high productivity with very high-quality, interesting catalysis research, achieved by fostering numerous collaborations within the HRSMC and outside the Netherlands.

Novel approach to improve atom efficiencies

The formation of carbon-nitrogen and heteroatom-nitrogen bonds often is a key step in the synthesis of medicines and other bio-active molecules. The general strategy for these conversions involves functional groups exchange, preorganisation and/or deprotecting steps, all resulting in a reduction of the atom efficiency. Employing catalytic conversions to form C–N and S–N bonds could substantially improve this. However, such an approach poses major challenges, especially for chemists searching to employ abundant first-row transition metal ions instead of precious second- or third row metals. The latter often operate via two-electrons reactions, whilst the first-row metal complexes often exhibit one-electron (radical) reactivity. The particularly challenging tasks for chemists are to control the often nonselective radical processes in the desired transformation; to employ nontrivial

Highly efficient nitrene radical transfer reactions under mild conditions

Klaas van Leest has managed to overcome all these challenges in a beautiful manner. He employed a redox-active ligand bound to cobalt that can act as an electron reservoir allowing radical nitrene transfer reactions to occur. To succeed in this novel approach, he developed an understanding of the role of the redox-active ligand on the spin-state of the cobalt complex. He also had to develop new reactions for N-group transfer to sp^3 hybridized C–H bonds, and for the selective formation of reactive nitrene radicals on cobalt by using a redox active ligand. His efforts resulted in highly efficient nitrene radical reactions using such a cobalt complex, performed under mild conditions, in air, in the presence of moisture.

The jury was particularly impressed by Van Leest's investigations on cobalt complexes containing the macrocyclic TAML ligand, where he used a variety of techniques to elucidate the nature of the radical nitrene reactions. Noteworthy further is that the theoretical calculations were not only based on standard DFT calculations, but also highly advanced multireference NEVPT2-CASSCF calculations were used. The Co-TAML catalyst is extremely fast and shows a high turnover number. Since the TAML ligand has already been upscaled for catalytic oxidation reactions (as an iron complex), there might be a potential to apply the Co-TAML complex for nitrene conversions on an industrial scale.

HRSMC Class of Excellence

In September 2021 five (5) students started the HRSMC Class of Excellence. Six (6) students obtained their certificate this year after successfully graduating from the programme.

Class of Excellence Pitch Prize 2021

On June 28, 2021 four students of the HRSMC Class of Excellence have defended their research proposal for a jury of HRSMC staff members and one member of the external advisory committee of the HRSMC. The research proposal is an obligatory part of the HRSMC Class of Excellence, a programme for excellent chemistry master students.

Although the jury explicitly remarked that all students gave an excellent pitch, they voted **Demi Snabilié** as the winner of the pitch contest 2021. The jury was very much impressed by her pitch and with the answers she gave to the jury's questions. They therefore decided to award her with the HRSMC Class of Excellence Pitch Prize.

The prize consists of a certificate and € 450,- free to spend.



PhD Theses

Listed here are PhD theses with HRSMC group leaders as supervisor and/or co-supervisor. In 2021 13 HRSMC PhD Certificates have been rewarded.

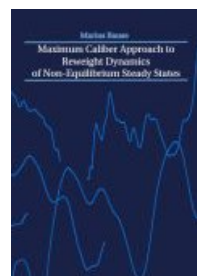
University of Amsterdam

1/26/2021

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 Science Lab (IVI, FNWI)

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



2/9/2021

Peptide cyclization strategies in confined spaces

Author: A. (Arnout) P.T. Hartendorp
Supervisor: J.N. H. Reek, J.H. van Maarseveen
Co-supervisor: -
Group: Homogeneous and Supramolecular Catalysis

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

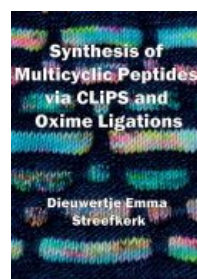


2/16/2021

Synthesis of multicyclic peptides via CLIPS and oxime ligations

Author: D. (Dieuwertje) E. Streefkerk
Supervisor: J.H. van Maarseveen, P. Timmerman
Co-supervisor: -
Group: Synthetic Organic Chemistry

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

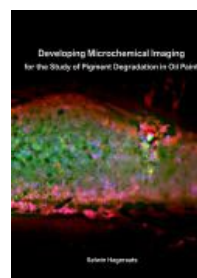


3/3/2021

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

Author: S. (Selwin) Hageraats
Supervisor: K. Keune
Co-supervisor: M. Thoury
Group: Catalyst Characterisation

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



3/9/2021

Transition path sampling of clathrate hydrate formation

Author: A. (Arjun) Wadhawan
Supervisor: P.G. Bolhuis
Co-supervisor: N. Shahidzadeh
Group: Simulation of Biomolecular Systems

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



3/11/2021

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](#)

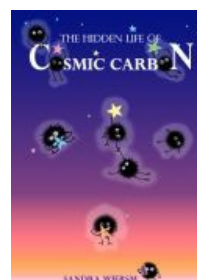


3/17/2021

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

Author: S. (Sandra) D. Wiersma
Supervisor: W.J. Buma
Co-supervisor: A. Petrignani
Group: Molecular Spectroscopy

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

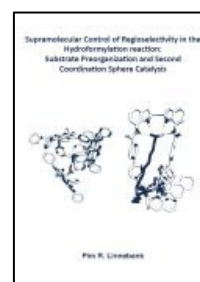


3/31/2021

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 and Supramolecular Catalysis

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



4/7/2021

Sustainable selective oxidations in confined spaces

Author: I. (Ilse) M. Denekamp
Supervisor: G. Rothenberg, D.
Dubbeldam
Co-supervisor: -
Group: HCSC+

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

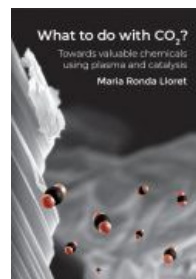


4/9/2021

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

Author: M. (Maria) Ronda Lloret
Supervisor: N.R. Shiju, G.
Rothenberg
Co-supervisor: -
Group: HCSC+

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



4/12/2021

Understanding confinement effects and nano structuring in heterogeneous catalysis

Author: T. (Thierry) K. Slot
Supervisor: G. Rothenberg, N.R.
Shiju
Co-supervisor: -
Group: HCSC+

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



4/26/2021

Structural characterisation studies during synthesis of industrial mixed metal oxide catalysts

Author: M. (Michelle) Hammerton
Supervisor: M. Tromp, K. Köhler
Co-supervisor: G. Mestl
Group: Catalyst Characterisation

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



6/3/2021

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: Spectroscopy and Photonic Materials

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



9/15/2021

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 and Supramolecular Catalysis

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



9/22/2021

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: Molecular Simulations

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



10/8/2021

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

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

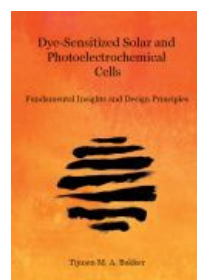
Supervisor: J.N. H. Reek

Co-supervisor: S. Mathew, R.J.

Detz

Group: Homogeneous and Supramolecular Catalysis

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



10/22/2021

Confinement effects in homogeneous catalysis using well-defined supramolecular architectures

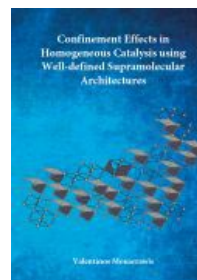
Author: V. (Valentinos) Mouarrawis

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

Co-supervisor: -

Group: Homogeneous and Supramolecular Catalysis

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



11/24/2021

Unraveling the mechanism of biomimetic hydrogen fuel production: A computational study

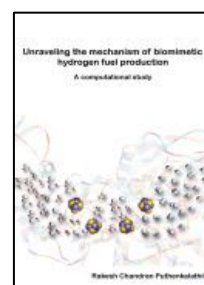
Author: R. (Rakesh) C. Puthenkalathil

Supervisor: B. Ensing, P.G. Bolhuis

Co-supervisor: -

Group: Simulation of Biomolecular Systems

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



11/26/2021

Radicals and London dispersion in frustrated Lewis pair chemistry

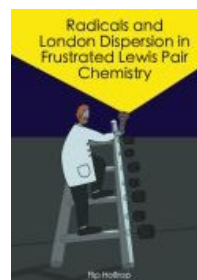
Author: F. (Flip) Holtrop

Supervisor: J.C. Slootweg

Co-supervisor: A.R. Jupp, J.H. van Maarseveen

Group: Synthetic Organic Chemistry

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



VU Amsterdam

3/11/2021

Calibration of next generation first-principle derived polarizable force fields

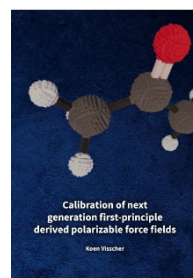
Author: K. (Koen) M. Visscher

Supervisor: N. Vermeulen

Co-supervisor: D. Geerke

Group: MedChem

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



6/25/2021

Advanced Computational Strategies in the Dirac-Kohn-Sham Framework: Optical Properties in the Strong Spin-Orbit Coupling Regime and Strong Fields

Author: M. (Matteo) De Santis

Supervisor: L. Visscher

Co-supervisor: F. Tarantelli, L.

Belpassi

Group: TC

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



9/13/2021

Transition Metal-Catalyzed Isocyanide Insertions: From Noble to Base Metal Catalysis

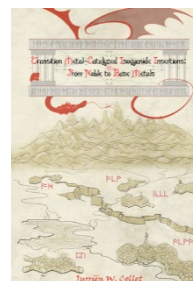
Author: J. (Jurriën) W. Collet

Supervisor: R. Orru

Co-supervisor: E. Ruijter

Group: OC

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



9/20/2021

A quantitative Kohn-Sham approach to elementary redox reactions in artificial, bio-inspired and biological catalysis

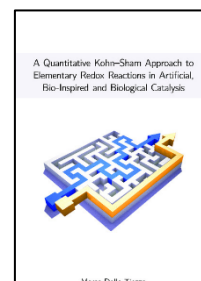
Author: M. (Marco) Dalla Tiezza

Supervisor: M. Bickelhaupt

Co-supervisor: L. Orian

Group: TC

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



11/2/2021

**Intermolecular Covalent Interactions:
A Quantitative Molecular Orbital Perspective**

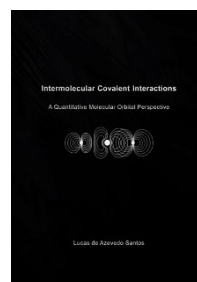
Author: L. (Lucas) de Azevedo Santos

Supervisor: M. Bickelhaupt, T. de
Castro Ramalho

Co-supervisor: T.A. Hamlin

Group: TC

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



11/22/2021

**Conformation and Bonding: Theoretical Studies on
Conformational Effects and Lewis Pair Stability**

Author: D. (Daniela) Rodrigues Silva

Supervisor: C. Fonseca Guerra, M.

Puggina de Freitas

Co-supervisor: T.A. Hamlin

Group: TC

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



11/23/2021

**Identification, characterization and modulation of
protein-protein interactions using modified peptides**

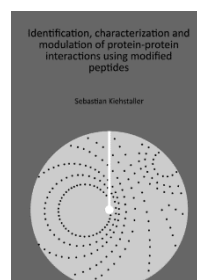
Author: S. (Sebastian) Kiehstaller

Supervisor: T. Grossmann

Co-supervisor: S. Hennig

Group: OC

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



11/30/2021

**Cyclic and Bicyclic Peptides that Target Protein-Protein
Interactions of Transcription Factors**

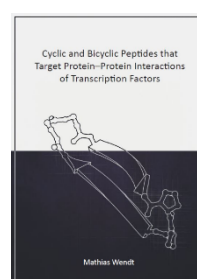
Author: M. (Mathias) Wendt

Supervisor: T. Grossmann

Co-supervisor: S. Hennig

Group: OC

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

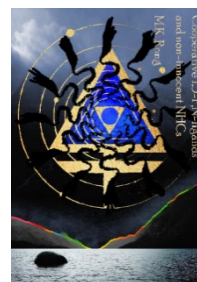


12/2/2021

Cooperative 1,3-P,N-ligands and non-innocent NHCs

Author: M. (Mark) K.Rong
Supervisor: K. Lammertsma
Co-supervisor: C. Slootweg, A.W.
Ehlers
Group: MedChem

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

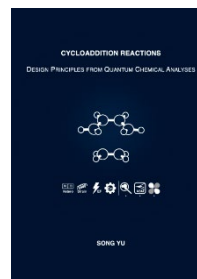


12/14/2021

Cycloaddition Reactions: Design Principles from Quantum Chemical Analyses

Author: S. (Song) Yu
Supervisor: M. Bickelhaupt
Co-supervisor: T.A. Hamlin
Group: TC

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



Leiden University

1/14/2021

**Molecular and Nano-engineering with iron, ruthenium and carbon:
Hybrid structures for sensing**

Author: E. (Erik) P. van Geest

Supervisor: S.A. Bonnet

Co-supervisor: G.F. Schneider

Group: Metals in Catalysis, Biomimetics & Inorganic Materials

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



2/24/2021

Accelerating the photocatalytic water splitting in catalyst-dye complexes

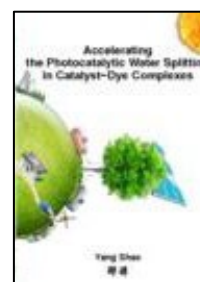
Author: Y. (Yang) Shao

Supervisor: H.J.M. de Groot

Co-supervisor: F. Buda

Group: Biophysical Organic Chemistry

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



3/10/2021

The role and analysis of molecular systems in electrocatalysis

Author: B. (Bas) van Dijk

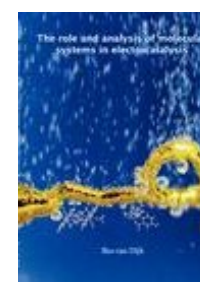
Supervisor: M.T.M. Koper, D.G.H.

Hetterscheid

Co-supervisor: -

Group: Catalysis and Surface Chemistry

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



3/11/2021

**Exploring structure dependencies of gas-surface interactions with
curved single crystals**

Author: S. (Sabine) V. Auras

Supervisor: M.T.M. Koper, L.B.F.

Juurlink

Co-supervisor: -

Group: Catalysis and Surface Chemistry

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



3/17/2021

Electrochemical and surface studies of the effect of naphthalene-based additives on tin electrodeposition

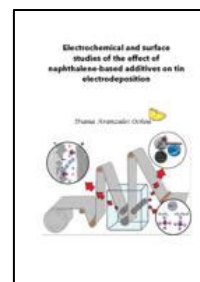
Author: D. (Diana) M. Aranzales Ochoa

Supervisor: M.T.M. Koper

Co-supervisor: J. Wijenberg

Group: Catalysis and Surface Chemistry

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



5/26/2021

The metallophilic interaction between cyclometalated complexes: photobiological applications

Author: X. (Xuequan) Zhou

Supervisor: E. Bouwman, S.A. Bonnet

Co-supervisor: -

Group: Metals in Catalysis, Biomimetics & Inorganic Materials

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



6/3/2021

Atomic insights into hydrodesulfurization

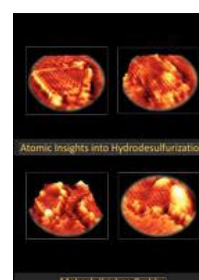
Author: M.K. (Mahesh Krishna) Prabhu

Supervisor: M.T.M. Koper

Co-supervisor: I.M.N. Groot

Group: Catalysis and Surface Chemistry

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



6/29/2021

Development of highly accurate density functionals for H2 dissociation on transition metals

Author: E.W.F. (Guido) Smeets

Supervisor: G.J. Kroes

Co-supervisor: M.F. Somers

Group: Theoretical Chemistry

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



9/16/2021

Microscopy and spectroscopy on model catalysts in gas environments

Author: S. (Sabine) Wenzel

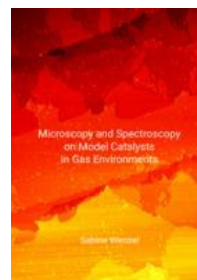
Supervisor: M.T.M. Koper, I.M.N.

Groot

Co-supervisor: L.B.F. Juurlink

Group: Catalysis and Surface Chemistry

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



9/23/2021

Accurate modeling of the dynamics of dissociative chemisorption on metal surfaces

Author: N. (Nick) Gerrits

Supervisor: G.J. Kroes

Co-supervisor: J. Meyer

Group: Theoretical Chemistry

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



10/12/2021

The electrochemical reduction of dioxygen and hydrogen peroxide by molecular copper catalysts

Author: M. (Michiel) Langerman

Supervisor: E. Bouwman, D.G.H.

Hetterscheid

Co-supervisor: -

Group: Catalysis and Surface Chemistry

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



Radboud University

5/20/2021

Exploring Glycosyl Cations

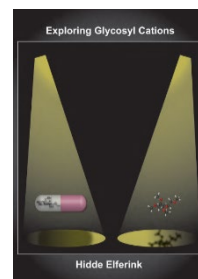
Author: H. (Hidde) Elferink

Supervisor: F.P.J.T. Rutjes

Co-supervisor: T.J. Boltje

Group: Synthetic Organic Chemistry

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



8/27/2021

The structure and reactivity of gas-phase copper clusters

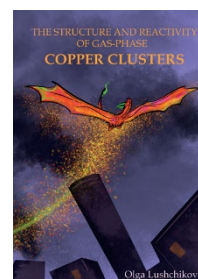
Author: O. (Olga) V. Lushchikova

Supervisor: A.I. Kirilyuk

Co-supervisor: J.M. Bakker

Group: Condensed Matter Physics

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



8/27/2021

Solid state deracemization: Viedma ripening versus temperature cycling

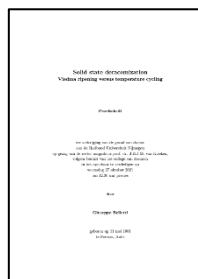
Author: G. (Giuseppe) Belletti

Supervisor: F.P.J.T. Rutjes, E. Vlieg

Co-supervisor: H. Meekes

Group: Synthetic Organic Chemistry

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



Fellowship Programme

13th call – April 2021



Dr. Thomas Mathew, Assistant Professor at the Department of Chemistry, St. John's College, Anchal, Kerala, India.

Hosted by Dr. Shiju Raveendran and Dr.ir. Bernd Ensing (University of Amsterdam).

Stay: 3 months

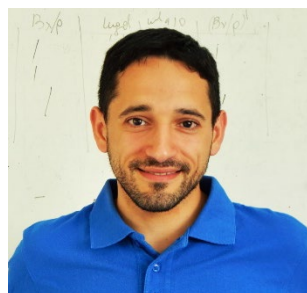
14th call – October 2021



Prof. Dr. Miquel Solà, Full Professor, Institute of Computational Chemistry and Catalysis, University of Girona (UdG), Spain.

Hosted by Prof. dr. F. Matthias Bickelhaupt and Dr. Trevor A. Hamlin (VU).

Stay: 1 month



Dr. Andre Nicolai Petelski, Research assistant (CONICET) and Assistant Professor (UTN – FRRe), National Scientific and Technical Research Council (CONICET) – Argentina, National Technological University – Regional Faculty of Resistencia (UTN –FRRe).

Hosted by Prof. dr. Célia Fonseca Guerra (VU).

Stay: 5 months

PhD Mobility Programme

3th call – April 2021



Nipon Deka from the group of Dr. Rik V. Mom and Prof. dr. Marc T.M. Koper (UL) has visited Dr. Axel Knop-Gericke (Fritz-Haber-Institute of the Max Planck Society, Berlin, Germany) and Dr. Ing. Ralph Krahnert (Technische Universität Berlin).

Stay: 3 months



Derk P. Kooi from the group of Prof. dr. Paola Gori Giorgi and Dr. Klaas J.H. Giesbertz (VU) planned to visit Prof. Paul W. Ayers (McMaster University, Hamilton, ON, Canada) for a duration of one month. Due to COVID-19 this visit has to be cancelled.

4th call – October 2021



Eva Meeus from the group of Prof. dr. J. Joost N. H. Reek and Prof. dr. B. Bas de Bruin (UvA) has visited Prof. dr. T. (Thomas) R. Ward (University of Basel, Philosophisch-Naturwissenschaftliche Fakultät, Departement Chemie).

Stay: 3 months

Financial Account 2021

Income		Expenses	
Contribution UvA 2021 - faculty ¹	150000	Donation HIMS Institute ¹	150.000
Contribution UvA 2021 - HIMS ¹	150000	Personnel Costs	84.194
Correction Fellowship 2018	8982	Office and management costs incl. Annual report	1.099
Writing Course (Ulrike Muller, sponsoring and fees)	1290	Fellowship Programme	29.000
Synthesis School (fee and sponsoring) ²	70651	Dick Stufkens PhD prize	2.426
		Synthesis School	55376
		Writing Course (Ulrike Muller)	4.257
		HRS MC Class of Excellence	3.850
		Courses (PPP)	1.689
		Other	120
	€ 380.923		€ 332.012
Income minus Expenses ³	€ 48.910		

1. As of 2014, a new agreement between the VSNU (Association of universities in the Netherlands) and SODOLA (the Dutch network of accredited research schools in all fields of academic research) has become applicable for the funding of Research Schools. Based on this agreement, as of 2015, the HRS MC should get funding of 300 KEuro. Instead of 50 KEuro from the faculty and 5 KEuro from the HIMS Institute, the contribution of the faculty is raised to 150 KEuro and 150 KEuro for the HIMS Institute. As this increase for the HIMS Institute would strongly affect HRS MC affiliated research groups from the UvA/HIMS Institute, the HRS MC Board decided to donate 150 KEuro to the HIMS Institute.
2. The HRS MC is grateful to the John van Geuns foundation for its financial support for the HRS MC Synthesis School
3. In 2021 the balance had a positive outcome (+ € 48,910). This is caused by the COVID-19 pandemic, due to which some meetings and events were moved to 2022.

