Radboud University

VU VRIJE UNIVERSITEIT AMSTERDAM

Universiteit Leiden

UNIVERSITEIT VAN AMSTERDAM

25 YEARS ANNIVERSARY HRSMC

ANNUAL REPORT 2019



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1. 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 2019. 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 fourth period 2012-2018. The HRSMC is a collaboration between top research groups of four Dutch Universities: the University of Amsterdam (UvA), the VU University 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 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, Symposia and other activities like career advice events) 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 Programme, which has been established in 2015.

Prof. dr. Wybren Jan Buma
Scientific Director of the HRSMC

2. The research program

The research program of the HRSMC is embedded in top research groups of the VU University 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.

3. Overview of the Research Groups in 2019

Theme 1 Synthesis, Characterisation, Reactivity and Properties of Molecules	
Group /staff members	**University/Group**
Biocatalysis Dr. F. Mutti	UvA/HIMS
Biomimetic Synthesis and Biomolecular Chemistry Prof. dr. T.N. Grossmann, Dr. Ivana Drienovská, Dr. Sven Hennig	VU/AIMMS
Heterogeneous Catalysis and Sustainable Chemistry Prof. dr. G. Rothenberg[1], Dr. N. Yan	UvA/HIMS
Functional Materials Dr. S. Grecea	UvA/HIMS
Catalysis Engineering Dr. N.R. Shiju	UvA/HIMS
Homogeneous, Supramolecular and Bio-Inspired Catalysis Prof. dr. B. de Bruin[1], Prof. dr. J.N.H. Reek[1], Dr. A.W. Ehlers, Prof. dr. C.J. Elsevier, Dr. T.J. Mooibroek, Dr. Ir. J.I. van der Vlugt	UvA/HIMS
Metals in Catalysis, Biomimetics & Inorganic Materials Prof. dr. E. Bouwman[1] , Prof. dr. S. Bonnet, Dr. D. Hetterscheid	UL/LIC
Synthetic and Bio-organic Chemistry Prof. dr. ir. R.V.A. Orru, Dr. E. Ruijter	VU/AIMMS
Synthetic Organic Chemistry Prof. dr. H. Hiemstra1, Prof. dr. J.H. van Maarseveen, Prof. dr. P. Timmerman, Dr. M.Á. Fernández-Ibáñez, Dr. S. Ingemann, Dr. J.C. Slootweg	UvA/HIMS
Synthetic Organic Chemistry Prof. dr. F.P.J.T. Rutjes, Dr. T.J. Boltje, Dr. M.C. Feiters	RU/SOC

Theme2 Synthesis, Characterisation, Reactivity and Properties of Molecules	
Group /staff members	**University/Group**
Biomolecular Spectroscopy Dr. F. Ariese	(VU/LaserLaB)
Biophysical Organic Chemistry Prof. dr. H.J.M. de Groot, Dr. Alia, Dr. F. Buda, Dr. G.J.A. Sevink	(UL/LIC)
Hybrid Solar Energy Conversion Dr. Elizabeth von Hauff	VU/AIMMS
Laboratory Astrophysics and Astrochemistry Prof. dr. H. Linnartz	(UL/LION)
Molecular Nano-Optics and Spins Prof. dr. E.J.J. Groenen, Prof. dr. M. Orrit, Dr. P. Gast, Dr. M. I. Huber	(UL/LION)
Molecular Photonics Prof. dr. A.M. Brouwer, Prof. dr. W.J. Buma, Prof. dr. S. Woutersen, Dr. ir. A. Petrignani-Taube, Dr. R. M. Williams, Dr. H. Zhang Guest Appointment: Dr. S. Castellanos Ortega (ARCNL)	(UvA/HIMS)
Molecular Structure and Dynamics - FELIX / Molecular and Biophysics Prof. dr. J. Oomens, Dr. J.M. Bakker, Dr. A.M. Rijs	(RU/IMM)

Surface Chemistry and Catalysis Prof. dr. M. Koper1, Dr. W.T. Fu, Dr. I.M.N. Groot, Dr. D. Hetterscheid, Dr. L.B.F. Juurlink	(UL/LIC)
Biomolecular Simulation and Modeling Dr. D.P. Geerke	(VU/AIMMS)

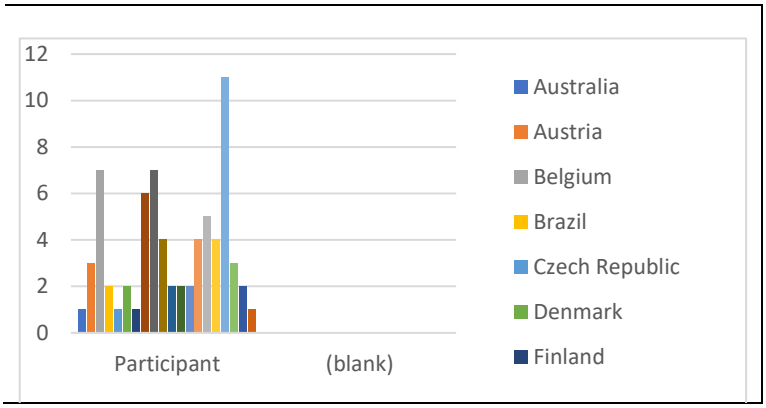
Theme 3 Theoretical Chemistry	
Computational Chemistry Prof. dr. P.G. Bolhuis, Prof. dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede	(UvA/HIMS)
Theoretical Chemistry *Prof. Dr. F. Matthias Bickelhaupt, Prof. Dr. Lucas Visscher, Prof. Dr. Célia Fonseca Guerra,* Dr. P. Gori Giorgi, Dr. O. Gritsenko *Dr. Klaas J. H. Giesbertz,* Dr. Trevor A. Hamlin	(VU/EMS)
Theoretical Chemistry Prof. dr. G.J. Kroes, Dr. J. Meyer, Prof. dr. C. Fonseca Guerra (Extraordinary Professor)	(UL/LIC)
Theoretical Chemistry Prof. dr. ir. G.C. Groenenboom, Dr. H.M. Cuppen, Prof. dr. F.M. Bickelhaupt (Extraordinary Professor)	(RU/IMM)
Theory in Surface Chemistry and Catalysis Dr. Katharina Doblhoff-Dier	

4. Research and Education

Molsim 2019 (January 6-17, 2019)

70 students from Australia, Brazil and Europe18 master students from University of Amsterdam
Lectures by Prof. Daan Frenkel, Prof. Berend Smit, Prof. Dr. Thijs Vlugt, Dr. Sanne Abeln, Leopold Talirz, Sasha Yakutovich, Danielle Ongari Dianne Ortega From UvA:
Prof. Peter Bolhuis, Prof. Evert Jan Meijer, Dr. Bernd Ensing, Dr. David Dubbeldam

Guest Lecturer: Ignacio Pagonabarraga (University of Barcelona)



PhMIC2019 (January 21 - February 1, 2019)
Leiden University

A total of 31 students,
9 Masterstudents
10 PhD students Leiden University
6 PhD students from University of Amsterdam
2 PhD students from VU University
4 Excellence Master Students (1 from Leiden, 3 from UvA)

Sustainability workshop: Towards a circular Economy (April 4, 2019)

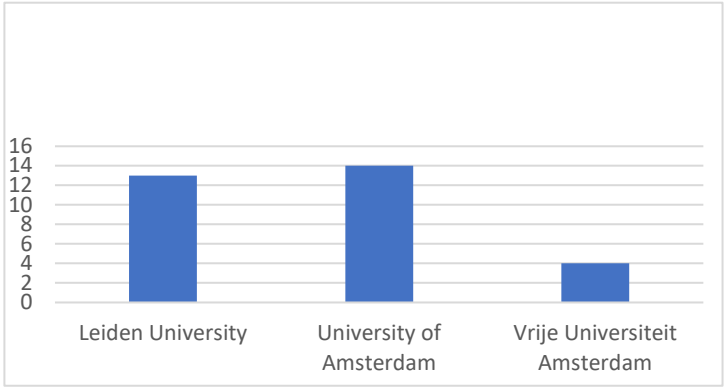
Universiteit van Amsterdam, in co-operation with HIMS-

69 Participants

The workshop, organized in the context of the UvA's Research Priority Area Sustainable Chemistry, is intended for PhD students, postdocs, staff members and other insterested parties.



Tessel Bouwens (University of Amsterdam) and David Klein (Leiden University), who were the last students to get a NWO Graduate PhD-position offered, organised this NWO Graduate Programme.



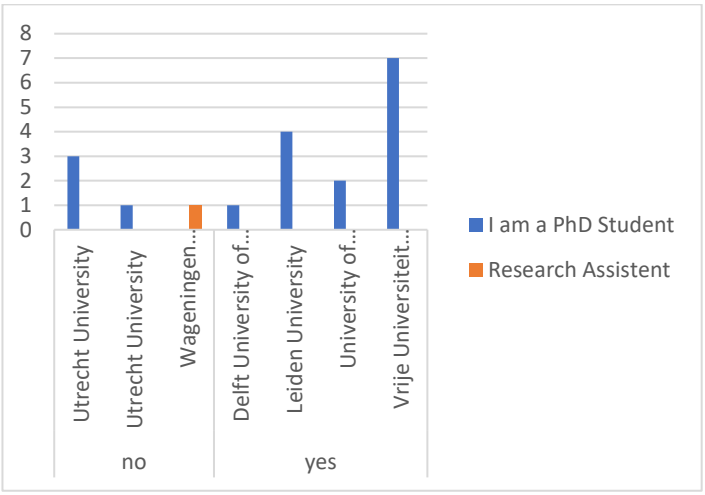
Lectures by Marjan Minnesma (Urgenda), Krijn de Jong (Utrecht University), Gert-Jan Gruter (Avantium/UvA), Shiju Raveendran (UvA) & Niek Persoon (Amsterdam Green Campus)

HRSMC-KNCV Career Event (April 11, 2019)
University of Amsterdam

About 60 Interested students visited the evening, organised by the KNCV in cooperation with HRSMC to help PhD students boost their future career.

Molecular Modeling Course
Vrije Universiteit Amsterdam

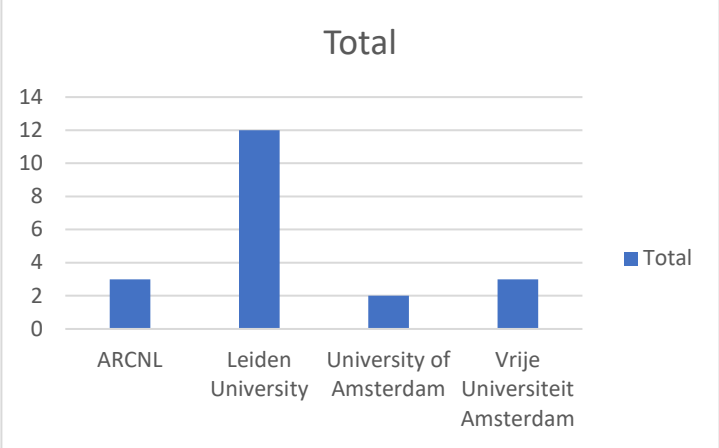
18 PhD Students, 1 Research Assistant from Delft University (1), Leiden University (4), University of Amsterdam (2), Utrecht University (4), Vrije Universiteit Amsterdam (7) and Wageningen University and Research (1)



High Impact Writing Course (June 11-14, 2019)
Leiden University

By Dr. Ulrike Muller
(California State University at Fresno

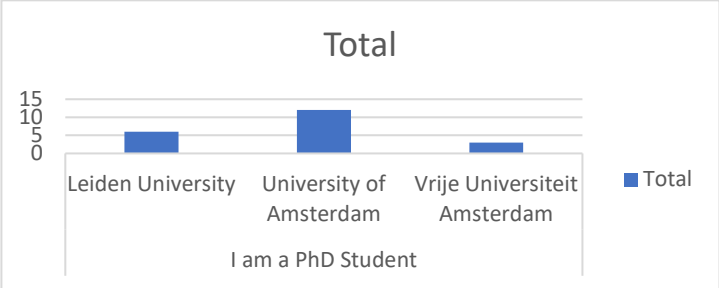
20 students
3 students from UvA/ARCNL
12 from Leiden University
2 students from University of Amsterdam
3 students from Vrije Universiteit Amsterdam



PPP2019 (October 18 – October 31, 2019)

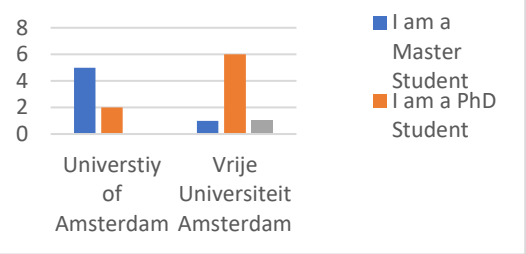
At University of Amsterdam and Vrije Universiteit Amsterdam

A total of 23 students
2 Excellence Master Students
21 PhD Students
(Leiden University 6, University of Amsterdam 12, VU University 3)



Targeted Synthesis Meeting 2019 (17 october 2019)

15 students:
6 Master Students
8 PhD students
1 Postdoctoral Student



Lustrum Symposium
November 14-15, 2019
at Royal Tropical Institute (KIT)

216 Participants

We had a special 2 day programme, with a grand opening by Prof.dr. Wybren Jan Buma (Scientific Director HRSMC) and Prof.dr. Hubertus Irth (Interim Dean Faculty of Science, Leiden University).
Also, Prof. dr. Jan Reedijk gave a presentation on the history of the HRSMC.
Special Invited Lecturers were:
Prof. Jens K. Nørskov (Technical University Denmark)
Prof.dr. Ben L. Feringa (University of Groningen)
Prof. Jeffrey R. Long (University of California at Berkeley)
Prof.dr. Michel A.G.J. Orrit (Leiden University)
Prof. Thomas Ebbesen (University of Strasbourg.
The first day was closed by
Prof.dr. Vinod Subramaniam (Rector Magnificus, Vrije Universiteit Amsterdam)

On Friday November 15 the programme continued with staff lectures by
dr. Tati Fernández Ibáñez (University of Amsterdam)
dr. Irene Groot (Leiden University)
dr. Daan Geerke (Vrije Universiteit Amsterdam)
and final closure by Closure Prof.dr. Peter van Tienderen (Dean Faculty of Science, University of Amsterdam)

The Dick Stufkens Prize 2019
Dr. Thom Hersbach
(Leiden University)



The Dick Stufkens Prize 2019 for the best PhD thesis of the Holland Research School of Molecular Chemistry (HRSMC) will be awarded to Dr Thom Hersbach. In his thesis, Hersbach presents a thorough analysis of cathodic corrosion. His comprehensive research, on which he graduated with the distinction cum laude, sheds light on the initial stages and the exact chemical nature of this relatively unknown and underestimated phenomenon.
Dr Thom Hersbach obtained his PhD from Leiden University on 19 December 2018. He is currently a postdoctoral fellow at the University of Texas at Austin.
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Thom Hersbach performed his PhD research with Marc Koper, Professor in Fundamental Surface Science at Leiden University. A phenomenon first observed by the great German chemist Fritz Haber at the end of the 19th century, cathodic corrosion was 'rediscovered' at the Koper research group in Leiden in 2011. It refers to the etching, restructuring and degradation of metallic electrode materials under highly reductive conditions, that is under very negative applied potentials. The PhD assignment of Thom Hersbach was to uncover what exactly happens at the onset of cathodic corrosion, and which chemistry is involved.

With his seminal work, Thom Hersbach has written a new chapter in the book of corrosion science, and it will probably feature as such in many future Corrosion Handbooks. He established that cathodic corrosion can be detrimental to many metals, notably to platinum. He discovered that the deterioration of this precious metal

starts at surprisingly low cathodic potentials, results in intriguing anistropic etching, and involves the formation of complex metal hydrides. He used this knowledge to improve platinum's catalytic activity for the conversion of oxygen to water, an important reaction in fuel cells present in hydrogen-powered vehicles.

Elusive metal anions

The more well-known and well-studied corrosion phenomenon is that of anodic corrosion. It involves the oxidation of metals: they lose electrons so that they can dissolve or convert to compounds like metal oxides (e.g., in the case of iron, rust). This can have catastrophic consequences to structures like bridges or oil pipelines. Fortunately, anodic corrosion can be prevented by "cathodic protection" which entails lowering a metal's potential to stabilize it in its un-oxidized state. The general assumption was that this protection held at any sufficiently negative potential. However, in 2011 the Leiden chemists established that at more negative potentials, beyond those of the cathodic protection, metals can again start to corrode. This has now been confirmed in detail by the research of Thom Hersbach. Furthermore, since cathodic corrosion would not involve the *loss*, but the *gain* of electrons, it was hypothesized that this electron gain would involve the creation of exotic yet very unstable metal anions. It is the highlight of Thom Hersbach's research that he has indeed been able to detect the formation of PtH_6^{2-} anions during the cathodic corrosion of platinum. This involved repeated sophisticated in-situ X-ray absorption experiments at the synchrotron at Stanford University (U.S.). The discovery considerably advanced the fundamental understanding of cathodic corrosion.

Independence and perseverance

The jury of the Stufkens prize 2019 rewards the thesis of Thom Hersbach for its surprising findings, its quality and its broad scope. It stands out as a milestone in the understanding of cathodic corrosion, as well as in its possible applications, such as in catalysis. The jury appreciates his high degree of independence as a researcher and the great perseverance he displayed during the X-ray measurements at the Stanford synchrotron, which required a redesign of the electrochemical cell and a second round of experiments. The jury also notes that for 2019 the number of applications for the Stufkens prize was very high, on a wide variety of subjects, and on average of high quality. Nonetheless, the jury was able to arrive at a unanimous nomination of the top three, after which Thom Hersbach was unanimously voted as the winner on the basis of his originality and productivity.

HRSMC Class of Excellence and Pitch Prize

In September 2019 six (6 students started the HRSMC Excellence Master Programme. Two students obtained their certificate this year after successfully graduating from the programme.
Celine Nieuwland started as PhD student in the **Theoretical Chemistry** Group of Prof.dr. Celia Fonseca Guerra and **Felix de Zwart** in the group **Homogeneous, Supramolecular and Bio-Inspired Catalysis** of Prof. dr. Joost Reek.

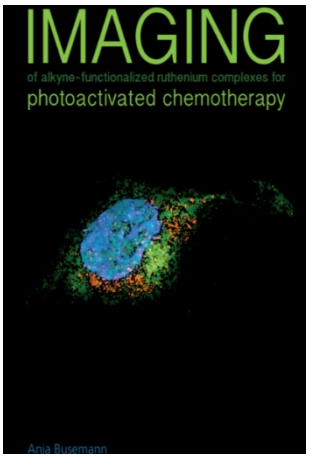


On September 30, **Eva Meeus** has defended her research proposal for a jury of HRSMC staff members and a member of the external advisory committee of the HRSMC. The research proposal is an obligatory part of the HRSMC Class of Excellence, a programme for excellent chemistry master students. The jury was very much impressed with her pitch and the subsequent discussion with the jury members, and therefore decided to award her with the HRSMC Excellence Programme Pitch Prize
The prize consists of a certificate and € 450,- in cash.

5. PhD Theses

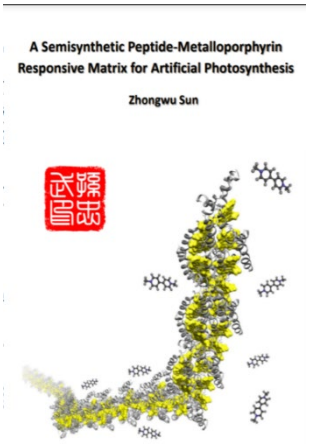
Listed here are PhD theses with HRSMC group leaders as supervisor and/or co-supervisor.
In 2019 15 HRSMC PhD Certficates have been rewarded.

Leiden University

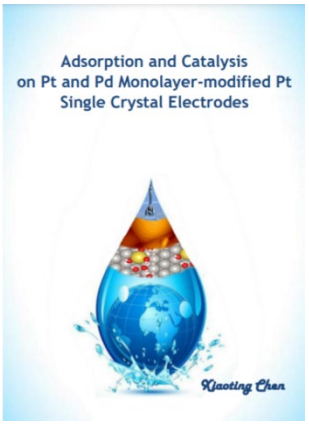


October 1, 2019

Author: A. (Anja) Busemann
Supervisors: S. Bonnet; E.Bouwman
Group: Metals in Catalysis, Biomimetics & Inorganic Material**s**
Link: Read or download this thesis



November 20, 2019
A semisynthetic peptide-metalloporphyrin responsive matrix for artificial photosynthesis
Author Z. (Zhongwu) Sun
Supervisor**:** H.J.M. de Groot
Group: Biophysical Organic Chemistry
Link: Read or download this thesis



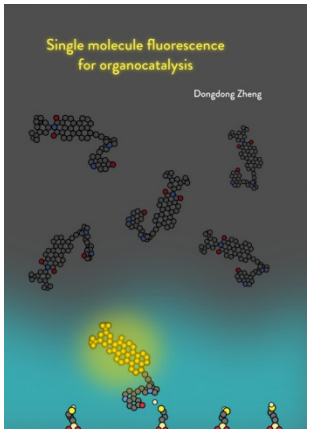
December 5, 2019
Adsorption and catalysis on Pt and Pd monolayer-modified Pt single crystal electrodes
Author: X. (Xiaoting) Chen
Supervisor: M.T.M. Koper
Co-supervisor: M.C. Figueiredo
Group: Surface Chemistry and Catalysis
Link: Read or download this thesis

December 16, 2019
Steps in Gas Surface Reactions
Author: R. (Richard)van Lent
Supervisors: L.B.F. Juurlink; M.T.M. Koper
Co-Supervisor: M.A. Gleeson
Group: Surface Chemistry and Catalysis
Link: Read or download this thesis

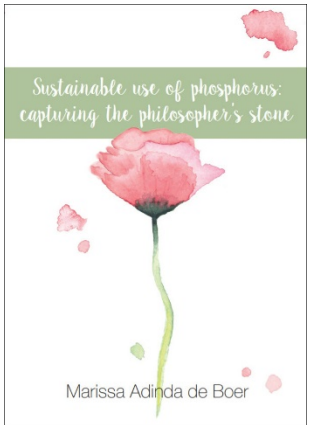


University of Amsterdam

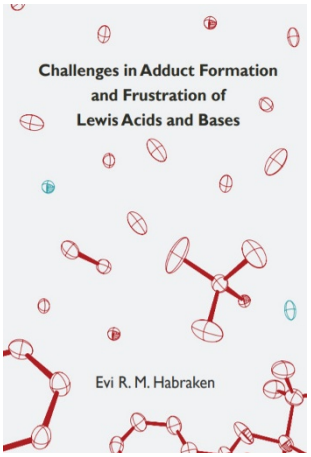
January 18, 2019
Single molecule fluorescence for organocatalysis
Author: D. (Dongdong) Zheng
Supervisor: A.M. Brouwer
Co-supervisor: R.M. Williams
Group: Molecular Photonics
Link: Read or download this thesis



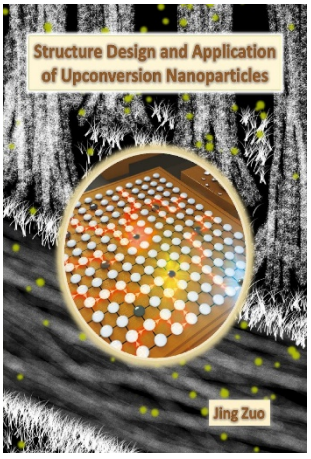
January 25, 2019
Sustainable use of phosphorus - Capturing the philosopher's stone
Author: M. (Marissa) A. de Boer
Supervisor: J.C. Slootweg
Co-supervisor: J.H. van Maarseveen
Group: Synthetic Organic Chemistry
Link: Read or download this thesis



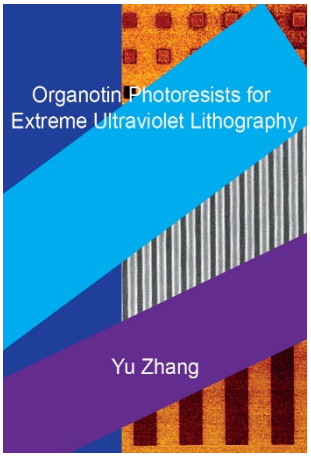
March 28, 2019
Challenges in adduct formation and frustration of Lewis acids and bases
Author: E. (Evi) R.M. Habraken
Supervisor: J.C. Slootweg
Co-supervisors: A.W. Ehlers, A.R. Jupp
Group: Synthetic Organic Chemistry
Link: Read or download this thesis



April 2, 2019
Structure design and applications of upconversion nanoparticles
Author: J. (Jing) Zuo
Supervisor: H. Zhang
Co-supervisor: W.J. Buma
Group: Molecular Photonics
Link: Read or download this thesis



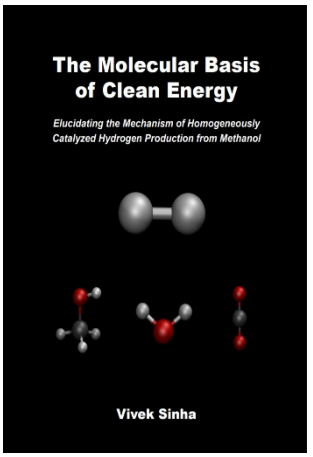
April 11, 2019
Organotin Photoresists for Extreme Ultraviolet Lithography
Author: Y. (Yu) Zhang
Supervisor: A.M. Brouwer
Co-supervisors: P.C.M. Planken, S. Castellanos Ortega
Group: Molecular Photonics
Link: Read or download this thesis



April 23, 2019

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

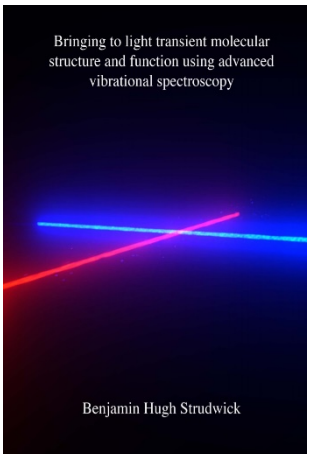
Author: V. (Vivek) Sinha
Supervisor: B. de Bruin
Co-supervisor: H. Grützmacher
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis



May 24, 2019

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

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



June 26, 2019

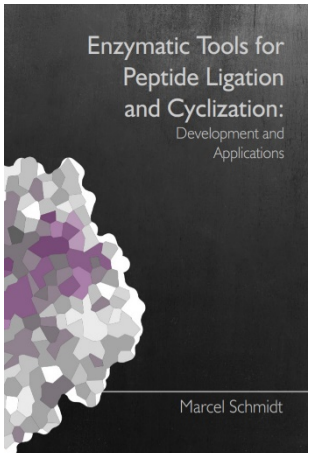
Author: D. (Dina) Petrova
Fluorescence nanoscopy
Applications in tribology
Supervisor: A.M. Brouwer
Co-supervisor: D. Bonn
Group: Molecular Photonics
Link: Read or download this thesis



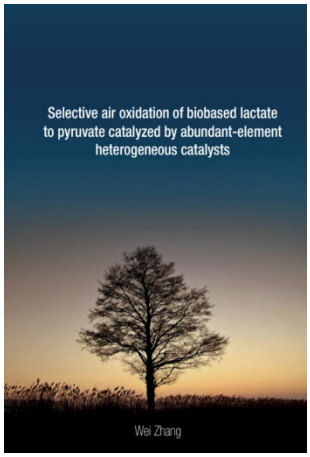
July 3, 2019
Author: A. (Anne) C.H. Jans
Exploring Gold-Catalyzed Reactions in Self-Assembled Hexameric Resorcin [4] arene Cages
Supervisor: J.N.H. Reek
Co-supervisor: J.I. van der Vlugt
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis



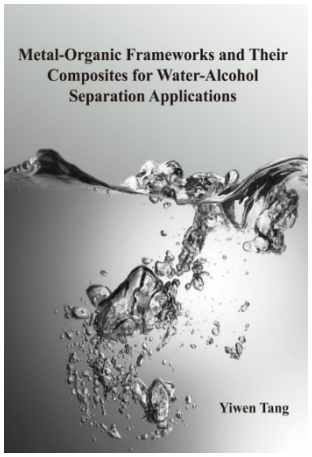
July 5, 2019
Author: M. (Marcel) Schmidt
Enzymatic Tools for Peptide Ligation and Cyclization
Development and Applications
Supervisors: J.H. van Maarseveen, T.N. Grossmann.
Co-supervisor: F. Mutti.
Group: Synthetic Organic Chemistry
Link: Read or download this thesis



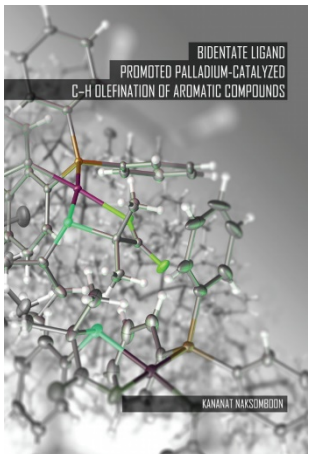
September 6, 2019
Author: W. (Wei) Zhang
Selective Air Oxidation of Biobased Lactate to Pyruvate Catalyzed by Abundant-Element Heterogeneous Catalysts
Supervisors: G. Rothenberg, N.R. Shiju.
Group: Heterogeneous Catalysis and Sustainable Chemistry
Link: Read or download this thesis



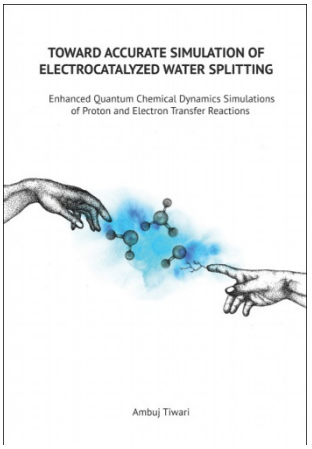
September 18, 2019
Author: Y. (Yiwen) Tang
Metal-organic frameworks and their composites for water-alcohol separation applications
Supervisors: S. Grecea, G. Rothenberg.
Group: Heterogeneous Catalysis and Sustainable Chemistry
Link: Read or download this thesis



October 10, 2019
Author: K. (Kananat) Naksomboon
Bidentate ligand promoted palladium-catalyzed C–H olefination of aromatic compounds
Supervisor: M.A. Fernández Ibáñez
Co-supervisor: J.H. van Maarseveen
Group: Synthetic Organic Chemistry
Link: Read or download this thesis



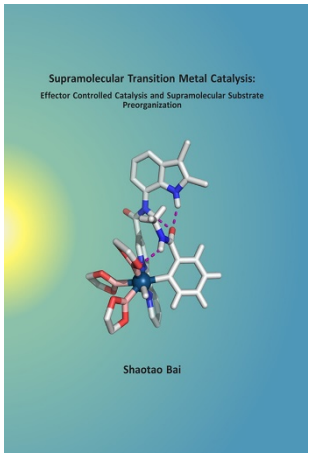
December 3, 2019
Toward accurate simulation of electrocatalyzed water splitting
Enhanced quantum chemical dynamics simulations of proton and electron transfer reactions
Author: A. (Ambuj) Tiwari
Supervisors: B. Ensing, P.G. Bolhuis
Group: Computational Chemistry
Link: Read or download this thesis



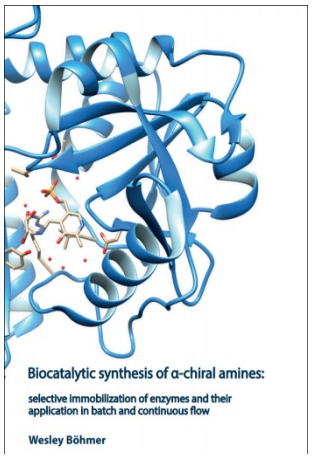
December 10, 2019
Author: L. (Lukas) J. Jongkind
Ligand based encapsulation strategies in homogeneous catalysis
Supervisor: J.N.H. Reek
Co-supervisor: J.I. van der Vlugt
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis



December 16, 2019
Supramolecular Transition Metal Catalysis Effector controlled catalysis and supramolecular substrate preorganization
Author: S. (Shaotao) Bai
Supervisor: J.N.H. Reek
Co-supervisor: A.M. Kluwer
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis

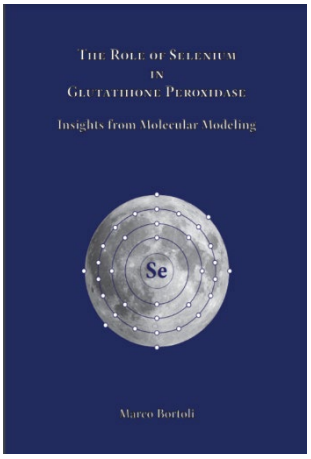


December 19, 2019
Biocatalytic synthesis of α-chiral amines Selective immobilization of enzymes and their application in batch and continuous flow
Author: W. (Wesley) Böhmer
Supervisors: F. Mutti, J.H. van Maarseveen
Group: Biocatalysis
Link: Read or download this thesis

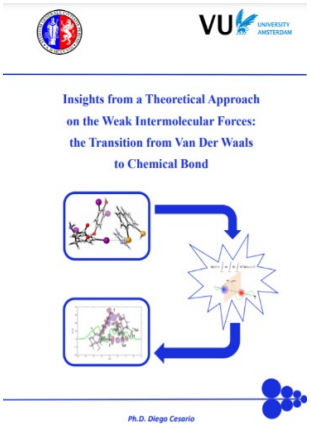


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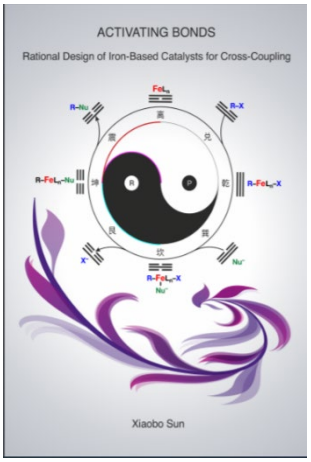
April 17, 2019
The Role of Selenium in Glutathione Peroxidase: Insights from Molecular Modeling
Author: M. (Marco) Bartoli
Supervisor: F.M. Bickelhaupt
Group: Theoretical Chemistry
Link: Read or download this thesis



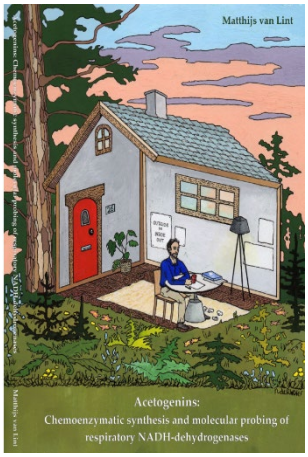
May 7, 2019
Insights from a Theoretical Approach on the Weak Intermolecular Forces: the Transition from Van Der Waals to Chemical Bond
Author: Diego Cesaria
Supervisors: F.M. Bickelhaupt
Co-supervisor: C. Fonseca Guerra
Group: Theoretical Chemistry
Link: Read or download this thesis



June 16, 2019
Activating Bonds
Author: Xiabo Sun
Supervisors: F.M. Bickelhaupt;
C. Fonseca Guerra
Co-supervisor: T.A. Hamlin
Group: Theoretical Chemistry
Link: Read or download this thesis



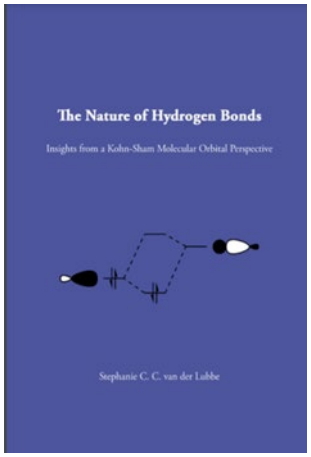
September 12, 2019
Acetogenins: Chemoenzymatic synthesis and molecular probing of respiratory NADH-dehydrogenases
Author: Matthijs van Lint
Supervisors:R.V.A. Orru;
H.V. Westerhoff
Co-supervisors: E. Ruijter;
R.van Spanning
Group: Synthetic and Bio-organic Chemistry
Link: Read or download this thesis



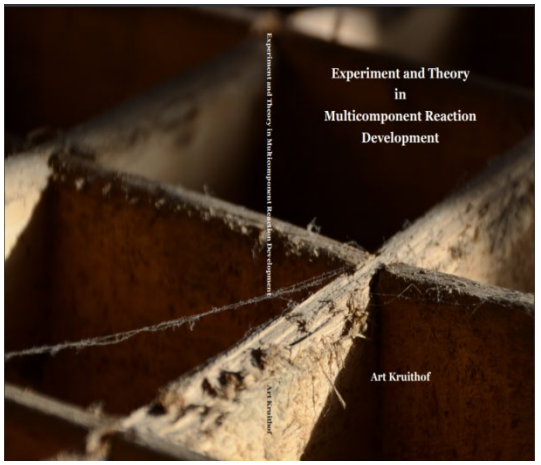
October 7, 2019
G-Quadruplexes: A Systematic Investigation on the Interaction of Cations with the Internal Channel Site
Author: Francesco Zaccaria
Supervisors: C. Fonseca Guerra;
F.M. Bickelhaupt
Group: Theoretical Chemistry
Link: Read or download this thesis



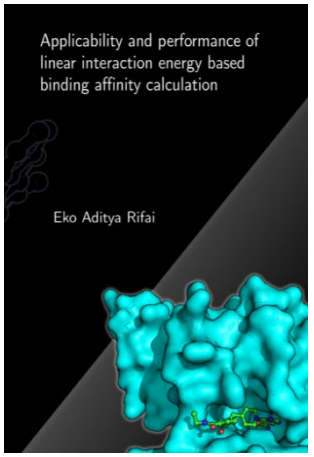
October 16, 2019
The Nature of Hydrogen Bonds: Insights from a Kohn-Sham Molecular Orbital Perspective
Author: Stephanie van der Lubbe
Supervisors: C**.** Fonseca Guerra; F.M. Bickelhaupt
Group: Theoretical Chemistry
Link: Read or download this thesis



November 26, 2019
Experiment and Theory in Multicomponent Reaction Development
Supervisor: R.V.A. Orru
Co-supervisor: E. Ruijter
Group: Synthetic and Bio-organic Chemistry
Link: Read or download this thesis



December 12, 2019
Applicability and performance of linear interaction energy based binding affinity calculation
Autho E. (Eko) A. Rifai
Supervisor: N.P.E. Vermeulen
Co-supervisor: D. Geerken
Group: Biomolecular Simulation and Modeling
Link: Read or download this thesis



PhD Fellowships

9th call April 2019

In Alphabetical order:

Dr. Nikita Durandin (*Tampere University, Finland)*;
Title of the Project: R**ed-light-triggered content release from liposomes via co-localized triplet-triplet annihilation upconversion**
Hosted by Prof. Sylvestre Bonnet (Leiden University) and Prof. Fred Brouwer (University of Amsterdam)
2 Visits, 3 months in total



Dr. J. Oscar C. Jimenez-Halla *(Universidad de Guanajuato, Mexico*)
Title of the Project: **Theoretical Study of the Oxidative Addition of Heteroatom Trihalides to a Pt(0) Complex Using Activation Strain Analyses**
Hosted by: Prof. Dr. F. Matthias Bickelhaupt (Vrije Universiteit Amsterdam).
A visit of *5 weeks* ???



Dr. David Swenson (*Postdoc, École Normal Supérieure de Lyon*)
Title of the Project: **Developing a framework to understand switching between different transitions**
Hosted by Prof. dr. P. Bolhuis and Dr. J. Vreede (University of Amsterdam)
2 Visits : total of 2 months



10th Call October 2019

In Alphabetical order:

Prof. dr. Vitaly Gitis, Associate (*Professor Ben Gurion University of the Negev (BGU), Israel)*
Title of the Project: **Zeolites by design: Towards a fundamental understanding of zeolite formation**
Hosted by Gadi Rothenberg, David Dubbeldam, Evert Jan Meijer (UvA)
Visit: Total of 3 months



Dr. Otto T. Berg *(California State University at Fresno, U.S.A.)*
Title of the Project: **Assigning IR modes for CO(2) and reaction products on Cu particles and surfaces**
Hosted by: Ludo Juurlink (UL). Joost Bakker (RU/FELIX). Jörg Meyer (UL)
Visit: 1,5 month



Dr. Eva Pluhařová
(J*. Heyrovský Institute of Physical Chemistry, Czech Republic*)
Title of the Project: **Catalysts for efficient capture and reduction of CO_2**
Hosted by Prof. Evert Jan Meijer (University of Amsterdam) and Prof. Jana Roithová (Radboud University)
3 Visits, Total of 7 weeks



Dr. André Severo Pereira Gomes (C*NRS University of Lille*)
Title of the project: **Relativistic coupled cluster theory in real-time**
Host: by Prof. dr. L.Visscher (VU)
2 Visits : total of 1.5 months



dr. William C. Swope (*IBM Almaden Research Center (San Jose, CA, USA*)
Title of the Project: **Including anisotropic electronic polarization into a polarizable force field derived from first principles**
Host: Daan Geerke (VU)
Visit: 2 weeks



Financial Account 2019

Income			**Expenses**	
Contribution UvA 2019 - faculty[1]	150.000		Donation HIMS Institute[1]	150.000
Contribution UvA 2019 - HIMS[1]	150.000		Personnel Costs	88.272
Lustrum Symposium (sponsoring)[2]	24.500		Office and management costs incl. Annual report	5.427
Writing Course (Ulrike Muller, sponsoring and fees)	6.030		Lustrum Symposium	53.090
Career Event - Contribution KNCV/Checkmark	478		Fellowship Programme	33.125
Sustainability Workshop - Contribution HIMS	1.443		HRSMC Writing Course (Ulrike Muller)	8.005
Correction Winter School	395		Career event	651
Interest	13		Sustainability Workshop	2.886
			Other courses/activities	2.464
			Dick Stufkens PhD prize	2.742
			HRSMC Excellence Traject	1.170
			PhD event	2.959
			Corrections 2018	2.619
	€ 332.859			**€ 353.410**
Income minus Expenses[3]	€ -20.551			

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 HRSMC 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 HRSMC affiliated research groups from the UvA/HIMS Institute, the HRSMC Board decided to donate 150 kEuro to the HIMS Institute.
2) The HRSMC is grateful to **the John van Geuns foundation** for its financial support for the HRSMC Lustrum Symposium
3) A negative outcome was expected since the estimated budget was also negative (-€44.654,-). Ultimately, we spent € 24,102 less than budgeted.

