HOLLAND RESEARCH SCHOOL
OF MOLECULAR CHEMISTRY

ANNUAL REPORT

2022

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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 2022. 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 2022

Theme	**Group (University, I**nstitute**) 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. Slootweg
	Biocatalysis (UvA, HIMS) Prof. dr. F. Mutti
	Flow Chemistry (UvA/HIMS) Prof. dr. T. Noël
	Industrial Sustainable Chemistry (UvA/HIMS) Prof. dr. G.J.M. Gruter
	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, Dr. T. Hansen 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. Hetterscheid

	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. Petrignani-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
	Cellular Metabolism (VU/AIMMS) Dr. S. Moco
	BioAnalytical Chemistry (VU, AIMMS) Prof. dr. A.M. Rijs, Dr. M. Bärenfänger
	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, Dr. I.M. Ilie
	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.A. Hamlin, Dr. P. Vermeeren, Dr. A. Förster
	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 2022

January 10-21, 2022, online

HRSMC Course 'Targeted Synthesis Challenges'

January 26, 2022, UvA

A total of 12 participants attended this very well evaluated course, of which six HRSMC members (VU: 3, UvA: 3) and 6 M.Sc. students (VU: 3, UvA: 3).

Organizers: Jan van Maarseveen (UvA), Eelco Ruijter (VU), Ineke Weijer (HRSMC), Laura Bastiaans (HRSMC), Rachel Scheffelaar (HRSMC)

HRSMC Course 'Physical Methods in Inorganic Chemistry'

May 12 – 20, 2022, UvA Roeterseiland and Sciencepark/UL/VU

A total of 28 PhD students attended this course of which 19 HRSMC members (UvA: 9 , UL: 12, TUD: 5, UU: 1, WUR: 1)

The invited speakers were Jörg Meyer (UL), Rik Mom (UL), Dennis Hetterscheid (UL), Marc Koper (UL), Ludo Juurlink (UL), Sylvestre Bonnet (UL), Freek Ariese (VU), Matthias Bickelhaupt (VU), Huub Kooijman, Fred Brouwer (UvA), Stefania Grecea (UvA), Bas de Bruin (UvA), Andreas Ehlers (UvA)

Organizers: Lies Bouwman (UL), Sylvestre Bonnet (UL), Bas de Bruin (UvA), Laura Bastiaans (UvA, HRSMC), Rachel Scheffelaar (UvA, HRSMC)

HRSMC Course Molecular Modeling

April 5-29, 2022, VU Amsterdam

A total of 9 participants attended this course of which 7 HRSMC members and 2 M.Sc. students (UvA: 2, VU: 4, UL: 1, RU: 1, TUE: 1).

Lectures were held by F. M. Bickelhaupt, C. Fonseca Guerra, and Trevor A. Hamlin

HRSMC/EPA Advanced Summer School on Photochemistry

14-17 July 2022, Noordwijk, The Netherlands

A total of 53 participants attended this school of which 25 HRSMC members (UvA: 10, UL: 11, VU: 4, RUG: 1, UU: 3, TUD: 1 other: 23).

Lectures were held by Timothy Noël (University of Amsterdam); Roberta Croce (Vrije Universiteit Amsterdam); Roel van de Krol (Helmholtz-Zentrum Berlin); Roberto Etchenique (Universidad de Buenos Aires); Ilaria Ciofini ((PSL University Chimie ParisTech).
Organizers: Sylvestre Bonnet, Chair (UL); Fred Brouwer (UvA); Charusheela Ramanan (VU); Rachel Scheffelaar (HRSMC); Laura Bastiaans-Tomé (HRSMC); Brahim Bouichfar (HRSMC); Saskia Spruyt (UvA); Renate Hippert (UvA)

HRSMC/NIOK Summer School 'Advances Metal-Organic Chemistry and Catalysis'

30 September – 3 October 2022, Noordwijk, The Netherlands

A total of 34 participants attended this school of which 27 HRSMC/NIOK members and 1 Class of Excellence student (UvA: 9, UL: 5, RU: 3, RUG: 3, UU: 9, WUR: 1, other: 7)

Lectures were held by Matthias Driess (Technische Universität Berlin); Inke Siewert (Georg-August-Universität Göttingen); Carole Duboc (Université Grenoble Alpes); Maurice van Gastel (Max-Planck-Institut für Kohlenforschung); Oliver Wenger (University of Basel).

Organizers: Bas de Bruin (University of Amsterdam), chairman; Sylvestre Bonnet (Leiden University); Andreas Ehlers (University of Amsterdam); Marc-Etienne Moret (Utrecht University); Dennis Hetterscheid (Leiden University); Edwin Otten (University of Groningen); Sonja Pullen (University of Amsterdam); Jana Roithova (Radboud University Nijmegen); Rachel Scheffelaar (HRSMC); Laura Bastiaans-Tomé (HRSMC/UvA); Brahim Bouichfar (HRSMC/UvA); Saskia Spruyt (HRSMC/UvA)

HRSMC Symposium

11 November 2022, O|2 Labbuilding, VU Amsterdam

A total of 179 people attended the symposium.

Guest lecturer:

- Prof. Fernando P. Cossio (Universidad del País Vasco, Spain)

HRSMC staff lecturers:

- Prof. dr. S.A. (Sylvestre) Bonnet (Leiden University) – Theme 1
- Dr. C. (Charusheela) Ramanan (VU Amsterdam) – Theme 2
- Dr. D. (David) Dubbeldam (University of Amsterdam) – Theme 3

PhD lecturers:

- Vivi Sukowski (University of Amsterdam)
- Eva Meeus (University of Amsterdam)
- Elahe (Eli) Motaee (Leiden University)
- Nipon Deka (Leiden University)
- Dani Rodrigues Silva (VU Amsterdam)

The Dick Stufkens Prize 2022

The Dick Stufkens Prize 2022 for best PhD thesis of the Holland Research School of Molecular Chemistry (HRSMC) has been awarded to Dr Tessel Bouwens for her thesis 'Pseudorotaxane Strategies for Guiding Self-Assembly and the Application of Molecular Machinery in Photoelectrochemical Devices'. Bouwens, who is now a postdoctoral fellow at the University of Cambridge, obtained her doctorate with the qualification 'cum laude' from the University of Amsterdam on 15 September 2021.

In her thesis, Bouwens describes studies towards the understanding of self-assembly through non-covalent bond formation and the application of such supramolecular interactions to enhance the efficiency of electron transfer in photoelectrochemical cells. Selecting the winner from eight excellent candidates, the jury for the Dick Stufkens prize 2022 unanimously decided for Tessel Bouwens. The jury was impressed by the quality of her research and the width of her scientific approach. Her experimental production is considered remarkable, particularly in view of the limitations imposed by the corona measures. Her easy to read thesis testifies to an enterprising researcher, who operates independently already early in her career.

Pursuing her own research idea

Bouwens' PhD research originated from her participation in the Excellence Program of the Holland Research School of Molecular Chemistry. At the time, this offered its students the opportunity to propose their own PhD research. Bouwens was among the few top students that saw their proposal awarded with a PhD fellowship. At its heart was the idea to enhance the efficiency of photo-electrochemical devices such as dye-sensitized solar cells by physically separating the charges and thus reducing electron-hole recombination. To achieve such physical separation, she proposed to use pseudorotaxane molecules that consist of a redox-active macrocyclic ring that can bind in a reversible, non-covalent fashion with a molecular thread. Connected to a molecular dye, these molecules could act as 'photoredox shuttles', carrying away the electrons generated by the dye and thus preventing recombination.

Demonstrating the viability of her idea turned out far from trivial. Her thesis shows how Bouwens successfully passed the many hurdles in an experimental 'tour-de-force'. She synthesized the building blocks of the photoredox shuttles and characterized these by spectroscopic and electrochemical techniques. She then implemented the supramolecular constructs into a solar cell, which required practical skills in materials science. This solar cell confirmed the concept, but its performance was limited. Inspired by natural photosynthesis, Bouwens continued to redesign the molecular components based upon her understanding of the supramolecular interactions, systematically further suppressing charge recombination and enhancing performance.

International recognition

Bouwens' concept of integrating molecular machinery to enhance the efficiency of solar cells received international recognition. Her idea and first results were published already at an early stage as a communication paper in the renowned journal Faraday Discussions. Oral contributions followed at

multiple national and international conferences. While pursuing her initial idea in a practical sense, she also explored the role of supramolecular bond formation in the control of self-assembly on a more fundamental level. This is presented in the first part of her thesis, where Bouwens shows in various, original ways how the interaction of the thread and the ring can guide self-assembly. She incorporated this in two strategies based upon pseudorotaxane formation. In the first one the macrocyclic ring kinetically guides the self-assembly of so-called Fujita-type nanospheres where pseudorotaxane formation functions as catalyst. In the second strategy, ring binding influences the distribution of such nanospheres to guide the outcome of multi-ligand architectures and thereby the level of organisation obtained upon self-assembly.

HRSMC Class of Excellence

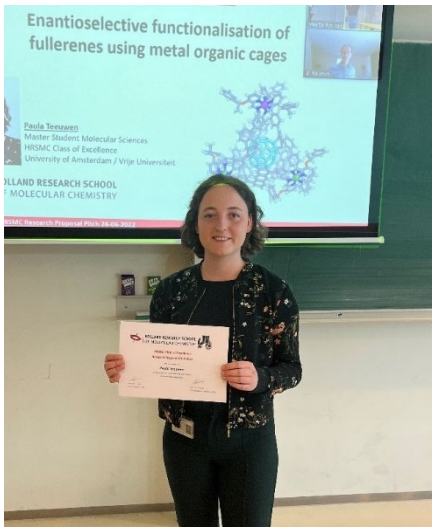
In September 2022 six (6) students started the HRSMC Class of Excellence. Three (3) students obtained their certificate this year after successfully graduating from the programme.

Class of Excellence Pitch Prize 2022

On June 28, two 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 both students gave an excellent pitch, they voted **Paula Teeuwen** as the winner of the pitch contest 2022. The jury was very much impressed by her pitch. It was indicated that she had also answered the questions of the jury members in great detail. They therefore decided to award her with the HRSMC Class of Excellence Pitch Prize.

The prize consists of a certificate and € 1500,- (for a contribution) to attend a conference or course/training or € 450,- free to spend.

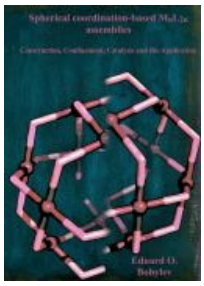


PhD Theses

Listed here are PhD theses with HRSMC group leaders as supervisor and/or co-supervisor. In 2022 9 HRSMC PhD certificates have been rewarded.

University of Amsterdam

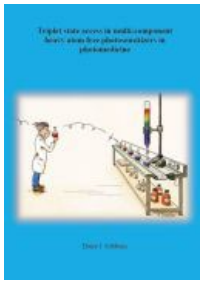
1/27/2022



Spherical coordination-based MnL2n assemblies: Construction, confinement, catalysis and bio application
Author: E.O. (Oleksandrovič) Bobylev
Supervisor: J.N. H. Reek, B. de Bruin
Co-supervisor: -
Group: Homogeneous and Supramolecular Catalysis

Link: Read or download this thesis

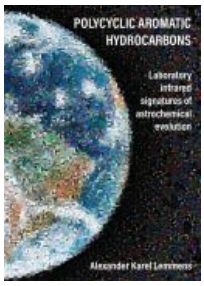
1/28/2022



Triplet state access in multi-component heavy atom free photosensitizers in photomedicine
Author: D. (Dáire) J. Gibbons
Supervisor: A.M. Brouwer, S. Leroy-Lhez
Co-supervisor: R.M. Williams, N. Villandier
Group: Spectroscopy and Photonic Materials

Link: Read or download this thesis

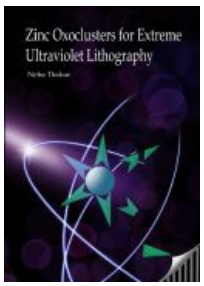
3/10/2022



Polycyclic aromatic hydrocarbons: Laboratory infrared signatures of astrochemical evolution
Author: A. (Sander) K. Lemmens
Supervisor: W.J. Buma, A.M. Rijs
Co-supervisor: -
Group: Molecular Spectroscopy

Link: Read or download this thesis

3/28/2022



Zinc oxoclusters for extreme ultraviolet lithography
Author: N. (Neha) Thakur
Supervisor: A.M. Brouwer
Co-supervisor: S. Castellanos Ortega
Group: Spectroscopy and Photonic Materials

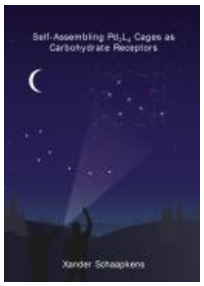
Link: Read or download this thesis

4/20/2022

Redox mediation in dye-sensitized photoelectrochemical cells: Coupling solar-driven oxidative catalysis to fuel generation
Author: D. (Didjay) F. Bruggeman
Supervisor: J.N.H. Reek
Co-supervisor: S. Mathew, R.J. Detz
Group: Homogeneous and Supramolecular Catalysis

Link: Read or download this thesis

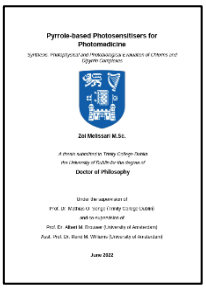
5/12/2022



Self-assembling Pd2L4 cages as carbohydrate receptors
Author: X. (Xander) Schaapkens
Supervisor: J.N.H. Reek
Co-supervisor: T.J. Mooibroek
Group: Homogeneous and Supramolecular Catalysis

Link: Read or download this thesis

5/30/2022



Pyrrole-based photosensitisers for photomedicine
Author: Z. (Zoi) Melissari
Supervisor: A.M. Brouwer, M.O. Senge
Co-supervisor: R.M. Williams
Group: Spectroscopy and Photonic Materials

Link: Read or download this thesis

6/30/2022

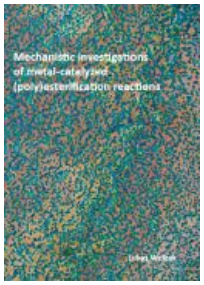
Stepping stones in CO2 utilization: Towards process development of oxalic and glycolic acid monomers
Author: E. (Eric) O. Schuler
Supervisor: G.J.M. Gruter
Co-supervisor: N.R. Shiju
Group: Sustainable Chemistry Industrial

Link: Read or download this thesis

7/5/2022

Mechanistic investigations of metal-catalyzed (poly)esterification reactions
Author: L. (Lukas) A. Wolzak
Supervisor: M. Tromp, J.N.H. Reek
Co-supervisor: T.J. Korstanje
Group: Catalyst Characterisation

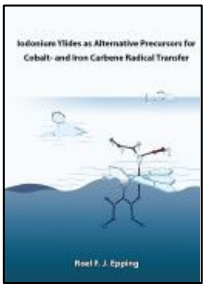
Link: Read or download this thesis



9/12/2022

Iodonium ylides as alternative precursors for cobalt- and iron carbene radical transfer
Author: R. (Roel) F.J. Epping
Supervisor: B. de Bruin
Co-supervisor: J.N.H. Reek
Group: Homogeneous and Supramolecular Catalysis

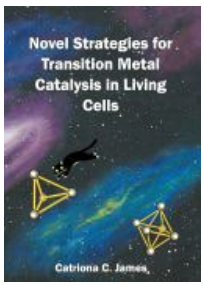
Link: Read or download this thesis



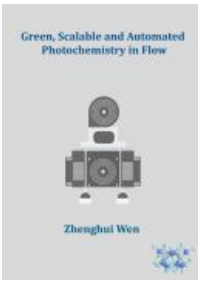
10/11/2022

Novel strategies for transition metal catalysis in living cells
Author: C. (Catriona) C. James
Supervisor: J.N. H. Reek, B. de Bruin
Co-supervisor: -
Group: Homogeneous and Supramolecular Catalysis

Link: Read or download this thesis



10/19/2022



Green, scalable and automated photochemistry in flow
Author: Z. (Zhenghui) Wen
Supervisor: T. Noël
Co-supervisor: B. de Bruin
Group: HCSC+

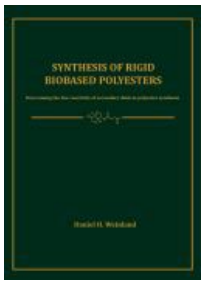
Link: Read or download this thesis

10/20/2022

Stepping stones in CO2 utilization: Synthesis and evaluation of oxalic- and glycolic acid (co)polyesters
Author: M. (Maria) A. Murcia Valderrama
Supervisor: G.J.M. Gruter
Co-supervisor: R.J. van Putten
Group: Industrial Sustainable Chemistry

Link: Read or download this thesis

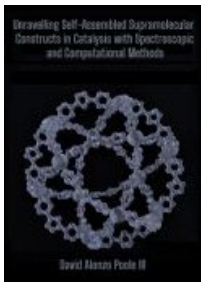
10/27/2022



Synthesis of rigid biobased polyesters: Overcoming the low reactivity of secondary diols in polyester synthesis
Author: D. (Daniel) H. Weinland
Supervisor: G.J.M. Gruter
Co-supervisor: R.J. van Putten
Group: Sustainable Chemistry Industrial

Link: Read or download this thesis

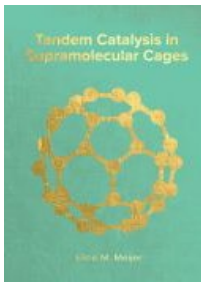
11/8/2022



Unravelling self-assembled supramolecular constructs in catalysis with spectroscopic and computational methods
Author: D. (David) A. Poole III
Supervisor: J.N. H. Reek
Co-supervisor: S. Mathew
Group: Homogeneous and Supramolecular Catalysis

Link: Read or download this thesis

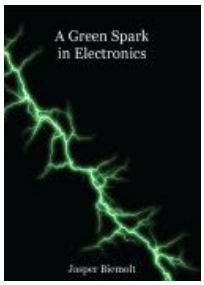
11/16/2022



Tandem catalysis in supramolecular cages
Author: E. (Eline) M. Meijer
Supervisor: J.N. H. Reek, B. de Bruin
Co-supervisor: -
Group: Homogeneous and Supramolecular Catalysis

Link: Read or download this thesis

12/1/2022



A green spark in electronics: Electrochemical innovations for a sustainable printed circuit board industry
Author: J. (Jasper) Biemolt
Supervisor: G. Rothenberg
Co-supervisor: N. Yan
Group: HCSC+

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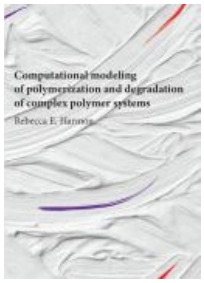
12/1/2022



Computational modeling of polymerization and degradation of complex polymer systems
Author: R. (Becca) E. Harmon
Supervisor: P.D. Iedema, L.J. Broadbelt
Co-supervisor: -
Group: CC overig

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12/2/2022

Environmental biodegradability of hydrolysable polyesters from renewable resources
Author: Y. (Yue) Wang
Supervisor: G.J.M. Gruter
Co-supervisor: R.J. van Putten, A. Tietema
Group: Sustainable Chemistry Industrial

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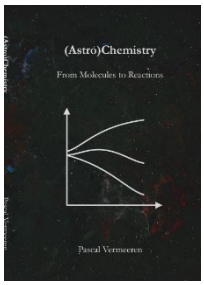
VU Amsterdam

2/15/2022



(Astro)Chemistry: From Molecules to Reactions
Author: P. (Pascal) Vermeeren
Supervisor: M. Bickelhaupt
Co-supervisor: T.A. Hamlin
Group: TC

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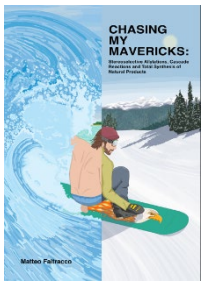
3/15/2022



Chasing my Mavericks: Stereoselective Allylations, Cascade Reactions and Total Synthesis of Natural Products
Author: M. (Matteo) Faltracco
Supervisor: E. Ruijter
Co-supervisor: R. Orru
Group: OC

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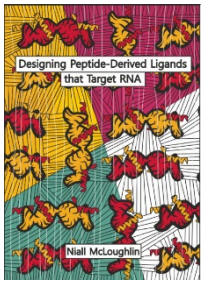
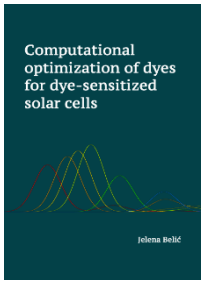
3/28/2022



Designing Peptide-Derived Ligands that Target RNA
Author: N. (Niall) M. McLoughlin
Supervisor: T. Grossmann
Co-supervisor: S. Hennig
Group: OC

Link: Read or download this thesis

11/23/2022



Computational optimization of dyes for dye-sensitized solar cells
Author: J. (Jelena) Belić
Supervisor: L. Visscher
Co-supervisor: F. Buda
Group: TC

Link: Read or download this thesis

12/9/2022

Many-Body Perturbation Theory with Slater Type Orbitals
Author: A. (Arno) T.L. Förster
Supervisor: L. Visscher
Co-supervisor: K. Giesbertz
Group: TC

Link: Read or download this thesis

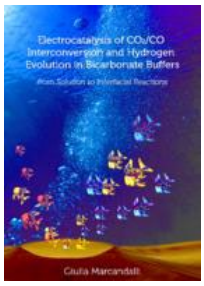
Leiden University

1/19/2022

Insights into the mechanism of electrocatalytic CO2 reduction and concomitant catalyst degradation pathways
Author: S.J. (Stefan) Raaijman
Supervisor: M.T.M. Koper
Co-supervisor: G. Mul
Group: Catalysis and Surface Chemistry

Link: Read or download this thesis

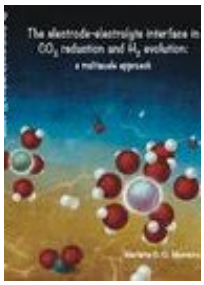
2/3/2022



Electrocatalysis of CO2/CO interconversion and hydrogen evolution in bicarbonate buffers: from solution to interfacial reactions
Author: G. (Giulia) Marcandalli
Supervisor: M.T.M. Koper
Co-supervisor: D.A. Vermaas
Group: Catalysis and Surface Chemistry

Link: Read or download this thesis

2/15/2022



The electrode-electrolyte interface in CO2 reduction and H2 evolution: a multiscale approach
Author: M. (Mariana) Cecilio de Oliveira Monteiro
Supervisor: M.T.M. Koper
Co-supervisor: López, N.
Group: Catalysis and Surface Chemistry

Link: Read or download this thesis

3/3/2022

Photoinduced processes in dye-sensitized photoanodes under the spotlight: a multiscale in silico investigation
Author: J.P. (Jan Paul)Menzel
Supervisor: H.J.M. de Groot
Co-supervisor: F. Buda
Group: Biophysical Organic Chemistry

Link: Read or download this thesis

4/20/2022

CO2 reduction on post-transition metals and their alloys: an industrial approach
Author: D. (Davide) Pavesi
Supervisor: M.T.M. Koper
Co-supervisor: K.J.P. Schouten, G.J.M. Gruter
Group: Catalysis and Surface Chemistry

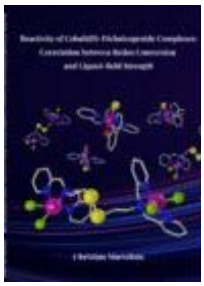
Link: Read or download this thesis

6/8/2022

Towards photocatalytic water splitting in homogeneous solutions using molecular metalloporphyrin photosensitizers and catalysts
Author: C. (Chengyu) Liu
Supervisor: E. Bouwman, S.A. Bonnet
Co-supervisor: -
Group: Metals in Catalysis, Biomimetics & Inorganic Materials

Link: Read or download this thesis

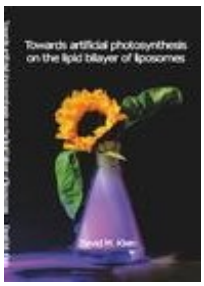
7/5/2022



Reactivity of cobalt(II)-dichalcogenide complexes: correlation between redox conversion and ligand-field strength
Author: C. (Christian) Marvelous
Supervisor: G.J. Kroes
Co-supervisor: C. Fonseca Guerra
Group: Theoretical Chemistry

Link: Read or download this thesis

9/15/2022



Towards artificial photosynthesis on the lipid bilayer of liposomes
Author: D. (David) M. Klein
Supervisor: A.M. Brouwer, S.A. Bonnet
Co-supervisor: -
Group: Metals in Catalysis, Biomimetics & Inorganic Materials

Link: Read or download this thesis

10/25/2022

Nuclear quantum effects in solid water: new insights from computational modeling
Author: S. (Soroush) Rasti
Supervisor: G.J. Kroes
Co-supervisor: J. Meyer
Group: Theoretical Chemistry

Link: Read or download this thesis

12/1/2022

Design of homogeneous water oxidation electrocatalysts
Author: D. (Daan) den Boer
Supervisor: E. Bouwman, D.G.H. Hetterscheid
Co-supervisor:
Group: Catalysis and Surface Chemistry

Link: Read or download this thesis

12/20/2022

Observing what cannot be observed: computational electrochemistry from carbon to hydrogen
Author: S. (Selwyn) R Hanselman
Supervisor: M.T.M. Koper
Co-supervisor: F. Calle Vallejo
Group: Catalysis and Surface Chemistry

Link: Read or download this thesis

Radboud University

4/11/2022

From peptide to aggregate: Advances in infrared action spectroscopy
Author: S. (Sjors) Bakels
Supervisor: J. Oomens, A.M. Rijs
Co-supervisor:
Group: Molecular Structure and Dynamics

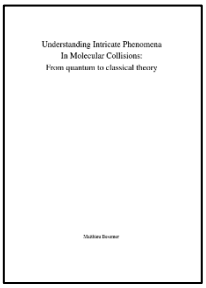
Link: Read or download this thesis

4/26/2022

Infrared spectroscopy of ionized fullerene derivatives: The astrophysical implications of breaking symmetries
Author: J. (Julianna) Palotás
Supervisor: J. Oomens
Co-supervisor: G. Berden
Group: Molecular Structure and Dynamics

Link: Read or download this thesis

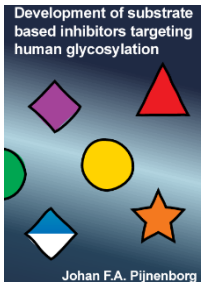
5/6/2022



Understanding Intricate Phenomena In Molecular Collisions: From quantum to classical theory
Author: M. (Matthieu) Besemer
Supervisor: S.Y.T. van de Meerakker, G.C. Groenenboom, A. van der Avoird
Co-supervisor: T. Karman
Group: Theoretical Chemistry

Link: Read or download this thesis

9/23/2022



Development of substrate based inhibitors targeting human glycosylation
Author: J. (Johannes) F.A. Pijnenborg
Supervisor: F.P.J.T. Rutjes
Co-supervisor: T.J. Boltje
Group: Synthetic Organic Chemistry

Link: Read or download this thesis

11/10/2022

Altering the Glycome Using Sialomimetics
Author: S. (Sam) J. Moons
Supervisor: F.P.J.T. Rutjes
Co-supervisor: T.J. Boltje
Group: Synthetic Organic Chemistry

Link: Read or download this thesis

12/16/2022

Epigenetics & Biomarkers. Exploring Modifications of Histone Tail Peptides & Novel biomarker discovery with Infrared Ion Spectroscopy
Author: J. (Jona) Merx
Supervisor: F.P.J.T. Rutjes
Co-supervisor: T.J. Boltje, J. Mecinovic
Group: Synthetic Organic Chemistry

Link: Read or download this thesis

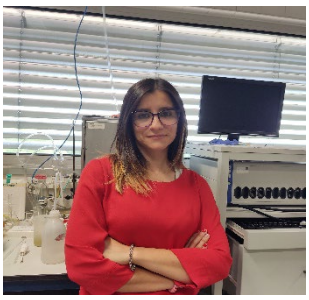
Fellowship Programme

15th call – April 2022

Dr. Sandra Marianne Lang, Akademischer Rat (Privatdozent, permanent position), Ulm University, Institute of Surface Chemistry and Catalysis, Germany.

Hosted by Prof. dr. Anouk Rijs (VU), Dr. Joost Bakker (RU), Dr. Hans Elemans (RU).

Stay: 5 months



Dr. Sara Realista, Junior researcher at the University of Lisbon, Faculty of Sciences, Biosystems and Integrative Sciences (BioISI) and Centro de Química Estrutural (CQE).

Hosted by Dr. Stefania Grecea (UvA) and Dr. Dennis G.H. Hetterscheid (UL).

Stay: 4 months

16th call – October 2022

No fellow grants this round.

PhD Mobility Programme

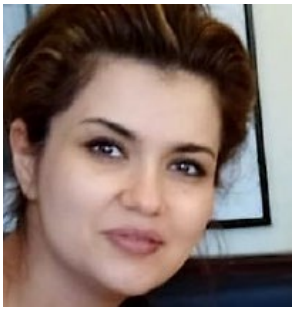
5th call – April 2022

Jan Sebastiaan Dominic Rodriguez from the group of Dr. Rik Mom and Prof.dr. Marc Koper (LEI) has visited Dr. Adam Squires (University of Bath, Department of Chemistry, UK).

Stay: 2 months

He Zhiyuan (Daniel) from the group of Prof. Jarl Ivar van der Vlugt and Prof. Bas de Bruin (UvA) had visited Prof. Michael Neidig at the University of Rochester, Department of Chemistry, USA.

Stay: 4 months



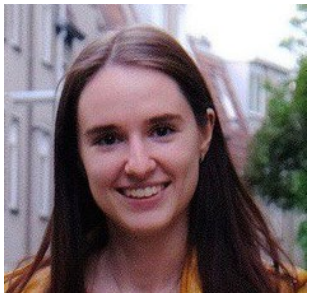
Selda Abyar from the group of Prof. Sylvestre Bonnet and Dr. Sylvia Le Dévédec (UL) has visited Prof. Giovanni Mann (King's college London, Vascular biology & inflammation)

Stay: 2 months

6th call – October 2022

Marlene Hoefnagel from the group of Dr. Dennis Hetterscheid (UL) and Dr. Stefania Grecea (UvA) has visited Prof. Sascha Ott (Uppsala University, Sweden).

Stay: 5 months



Iuliia Stroganova from the group of Prof. Dr. Anouk M. Rijs (VU) has visited Prof. Dr. Tuomas P.J. Knowles (University of Cambridge, UK)

Stay: 2 months

Financial Account 2022

Income			**Expenses**	
Contribution UvA 2022 - faculty[1]	150000		Donation HIMS Institute[1]	150.000
Contribution UvA 2022 - HIMS[1]	150000		Personnel Costs	78.871
Photochemistry School (fee and sponsoring)[2]	44425		Office and management costs incl. Annual report	1.200
AMOCC School (fee and sponsoring)[2]	35595		Fellowship Programme	34.000
			Dick Stufkens PhD prize	2.623
			Photochemistry School	50314
			AMOCC School	40.537
			HRSMC Symposium (moved from 2021)	24.470
			HRSMC Symposium	11.024
			HRSMC Class of Excellence	1.307
			Courses	1.306
			Social Activity PhD Students	2.474
			Other	105
	€ 380.020			**€ 398.231**
Income minus Expenses	€ -18.211			

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 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.