Radboud University

VU VRIJE UNIVERSITEIT AMSTERDAM

Universiteit Leiden

UNIVERSITEIT VAN AMSTERDAM

HOLLAND RESEARCH SCHOOL OF MOLECULAR CHEMISTRY

ANNUAL REPORT 2020

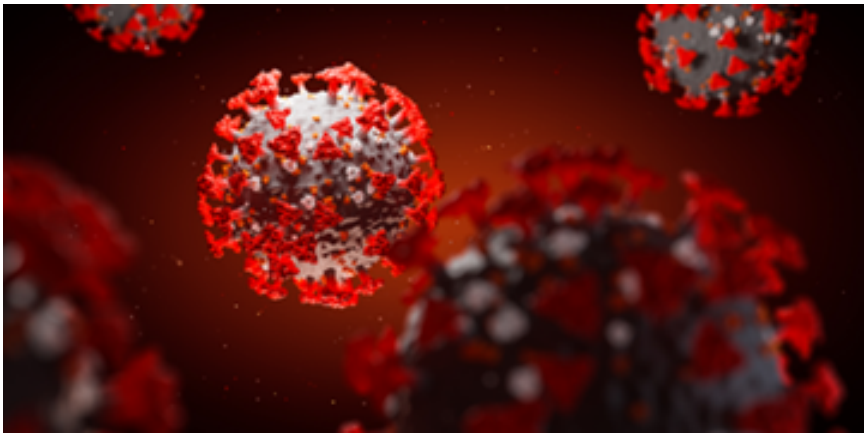


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1. General

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 2020. 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 2020

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, 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, Prof. dr. J.N.H. Reek, 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, 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	

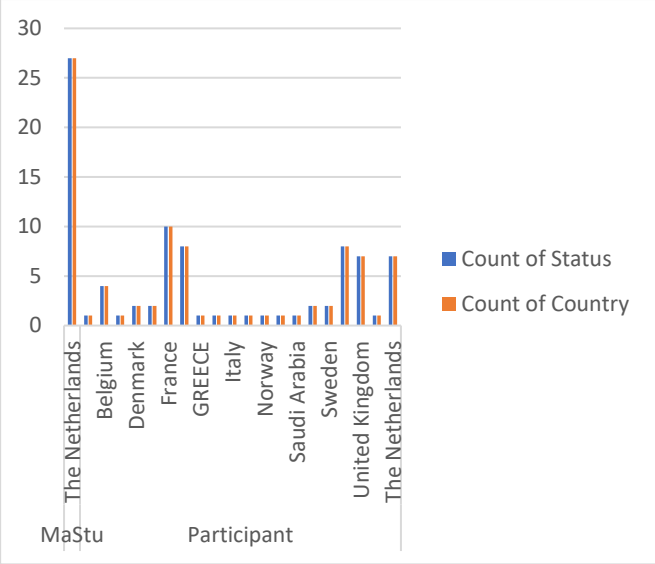
4. Research and Education

Molsim 2020 (January 6-17, 2020)
University of Amsterdam

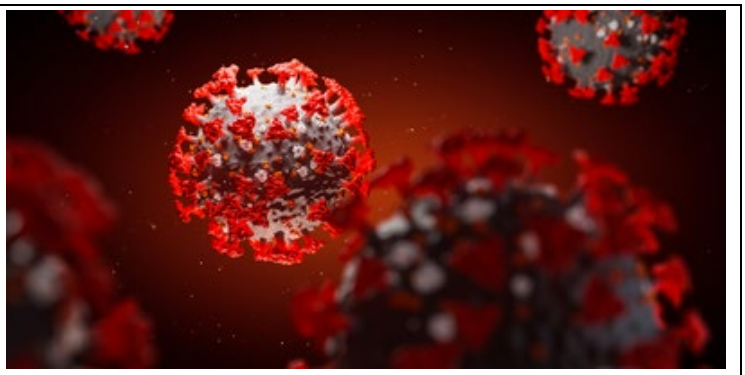
62 students from Saudi Arabia, and Europe
27 Students from Dutch Universities

Lectures by Prof. Daan Frenkel (Cambridge University), Prof. Berend Smit (EPFL), Prof. Dr. Thijs Vlugt (TU Delft), Dr. Sanne Abeln (Vrije Universiteit Amsterdam), Dr. Tristan Bereau, Prof. Peter Bolhuis, Prof. Evert Jan Meijer,
Workshops by Dr. Bernd Ensing, Dr. David Dubbeldam, Dr. Kevin Jablonka (EPFL), Dr. Mohammad Moosavi (EPFL)

Guest Lecturer: Prof. Nicola Marzari (EPFL, Lausanne)



And then there was COVID.....
Early in 2020 (February 27 officially) SARS-CoV-2 was discovered in the Netherlands and this led to a severe pandemic, not only in the Netherlands but across the world. This disrupted most of our activites as access to university buildings was restricted and travel and more was prohibited. Regular courses were given on-line but for the HRSMC activities the Board decided to defer further schools and courses, also our Annual Symposium was cancelled.



5. The Dick Stufkens Prize 2020
Dr. Mark Koenis (University of Amsterdam)

The Dick Stufkens Prize 2020 for the best PhD thesis of the Holland Research School of Molecular Chemistry has been awarded to Dr Mark Koenis. Koenis graduated 21 February with the distinction cum laude on his thesis 'Advanced Spectra Analysis to Determine Complex Structure and Chirality'. He describes the application of vibrational circular dichroism (VCD) as a powerful method for the analysis of molecular properties. With his research he has significantly improved the applicability of VCD.



Dr Mark Koenis obtained his PhD on 21 February 2020 with the distinction cum laude, for his thesis 'Advanced spectra analysis to determine complex structure and chirality'. Supervisors were Prof. Wybren Jan Buma (UvA) and Prof. Lucas Visscher (VU). Koenis is currently continuing his research as a postdoctoral researcher with the research group Molecular Photonics at the Van 't Hoff Institute for Molecular Sciences (University of Amsterdam).

The work of Mark Koenis represents an important step in rendering VCD an easily applicable tool for structure determination of so-called 'chiral' molecules. These are molecules that in their spatial structure can have two forms, which are each other's mirror image. Although the chemical properties of these two variants are almost identical, their biological activity can differ enormously. This is of great importance in the development of medicines. It even happens that one variant is an effective medicine, while the other variant is a poison. Chemists therefore want to be able to determine exactly which chiral variant results from a certain synthesis pathway.

The VCD method can distinguish chiral molecular variants using circularly polarized infrared light. But in practice, this is rather difficult. Under normal circumstances, molecules are always in motion; they wobble, they rotate, and molecule parts can rotate relative to each other. The latter is a problem for VCD analysis. Every shape of the molecule produces a different VCD spectrum, which renders the analysis very difficult. At the end of the previous century, researchers found a way out by comparing VCD measurements with predictions resulting from quantum chemical computer models. This makes it much easier to determine what chiral variant results from a particular synthesis technique. Alas, this method can only be used with relatively simple molecules. And many active ingredients of drugs consist of rather complex molecules.

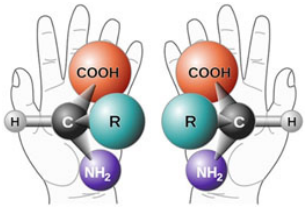
Algorithm

As a result of the research done by Mark Koenis VCD can now also be routinely applied to complex internally rotating molecules. In his greatly improved approach a genetic algorithm plays an important role. He designed an adaptive system, based on evolutionary principles, that is capable of chiral determination even with complex molecules. But the thesis describes many more striking applications of VCD, combining experimental and calculated VCD spectra. This concerns, for instance, the study of self-assembly of supramolecular polymers, the use of VCD as analytical tool to determine the level of diastereomers, and the use of VCD as a tool for the study of mechanically interlocking molecules (rotaxanes). The work is not limited to VCD. Other spectroscopic techniques have been employed by Koenis in further studies.

The jury of the Dick Stufkens prize was impressed by the quality and the breadth of Koenis' research. That he has greatly advanced the field of VCD applications to structure determination of chiral molecules was another reason for awarding him the prize. In addition, the jury report mentions the way Koenis presents his work in a convincing and engaging manner, which had already earned him well-deserved praise from referees. Because of the excellent quality of other candidates (all received the distinction cum laude) it was a difficult decision, but in the end the jurors unanimously awarded Mark Koenis the Dick Stufkens prize.

The research of Mark Koenis was funded by means of a Technology Area grant of the Dutch Research Foundation NWO to his promotors Wybren Jan Buma (UvA) and Lucas Visscher (VU) and co-promotor Paul Nicu (VU, at the time). It was supported by the companies BioTools (VCD spectrometers) and Software for Chemistry & Materials (SCM, quantum chemistry software with VCD functionality).

Chirality



Chiral molecules exist in two forms (stereoisomers), which are related by mirror symmetry (the name stems from the Greek for hand, referring to the mirror symmetry between left and right hand). Since all chemical properties of the two stereoisomers, called enantiomers, are identical, it is hard to establish which one is present (i.e. determine the absolute configuration). Nevertheless, biological action of the two enantiomers may be very different. Where one is a beneficial drug, the other one can be very harmful. This was dramatically demonstrated in the softenon disaster. Being able to distinguish between enantiomers is therefore extremely important in the pharmaceutical industry.

A very promising technique is vibrational circular dichroïsm (VCD): the absorption of right and left circularly polarized infrared radiation (for vibrational transitions) is different in a chiral molecule, and the differences are exactly opposite in the two enantiomers. This gives different spectra for the two enantiomers. Comparison to quantum chemical VCD calculations is then needed to determine which experimental spectrum belongs to which enantiomer.

When the enantiomers are rigid this works splendidly. But most molecules of interest are not at all rigid, but have many conformers, generated by rotations around single bonds, that are accessible at room temperature. All these conformers will give different VCD spectra. This is a major obstacle in the application of the VCD technique to the determination of absolute configurations.

6. HRSMC Class of Excellence and Pitch Prize

In September 2020 seven (7) students started the HRSMC Class of Excellence. Four students obtained their certificate this year after successfully graduating from the programme.

Melania Kozdra has won the HRSMC Class of Excellence Pitch Prize 2020



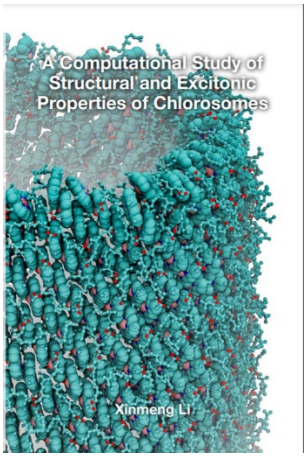
On June 23, five students of the HRSMC Class of Excellence have defended their research proposal for a jury of HRSMC staff members and two members of the external advisory committee of the HRSMC. The research proposal is an obligatory part of the HRSMC Class of Excellence, a programme for excellent chemistry master students. Although the jury explicitly remarked that all students had done an excellent job, they voted Melania Kozdra as the winner of the pitch contest. The jury was very much impressed by her pitch and the subsequent discussion with the jury members, and therefore decided to award her with the HRSMC Class of Excellence Pitch Prize. The prize consists of €1500,- (for a contribution) to attend a conference or course/training. This conference or course/training needs to take place within one year after graduation and needs to be approved by the HRSMC.

7. PhD Theses

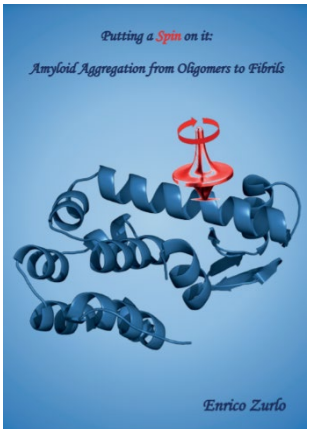
Listed here are PhD theses with HRSMC group leaders as supervisor and/or co-supervisor.
In 2020 8 HRSMC PhD Certficates have been rewarded

Leiden University

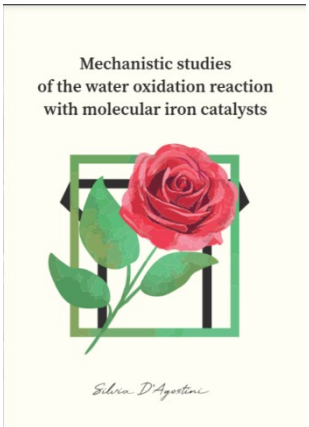
May 6, 2020
A computational study of structural and excitonic properties of chlorosomes
Author: X. (Xinmeng) Li
Supervisor: H.J.M. de Groot, H.J.M. de
Co-supervisor: G.J. Agur Sevink
Group: Biophysical Organic Chemistry
Link: Read or download this thesis



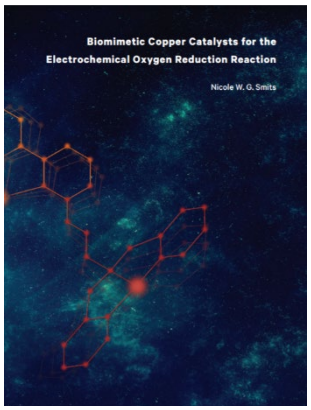
July 9, 2020
Putting a spin on it: amyloid aggregation from oligomers to fibrils
Author: E. (Enrico) Zurlo
Supervisors: Huber, M.I.; Eliel, E.R.
Group: Molecular Nano-Optics and Spins
Link: Read or download this thesis



September 17, 2020
Mechanistic studies of the water oxidation reaction with molecular iron catalysts
Author: S. (Sylvia) D'Agostini
Supervisors: E. Bouwman
Co-supervisor: D.G.H. Hetterscheid
Group: Metals in Catalysis, Biomimetics & Inorganic Materials
Link: Read or download this thesis

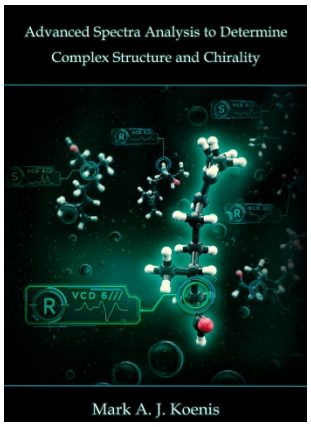


November 26, 2020
Biomimetic copper catalysts for the electrochemical oxygen reduction reaction
Author: N. (Nicole) W.G. Smits
Supervisors: E. Bouwman
Co-supervisor: D.G.H. Hetterscheid
Group: Metals in Catalysis, Biomimetics & Inorganic Materials
Link: Read or download this thesis

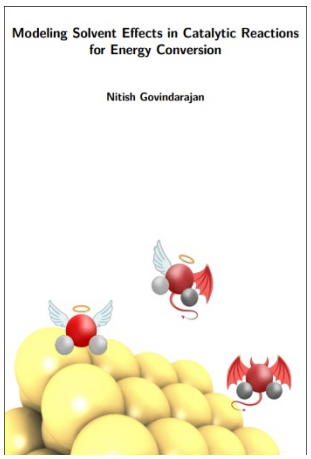


University of Amsterdam

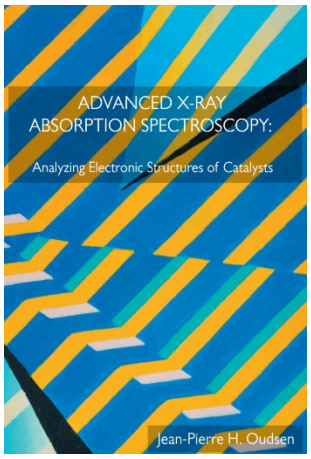
21 February 2020
Advanced spectra analysis to determine complex structure and chirality
Author: M. (Mark) A.J. Koenis
Supervisors: W.J. Buma, L. Visscher
Co-supervisor: V.P. Nicu
Group: Molecular Photonics
Link: Read or download this thesis



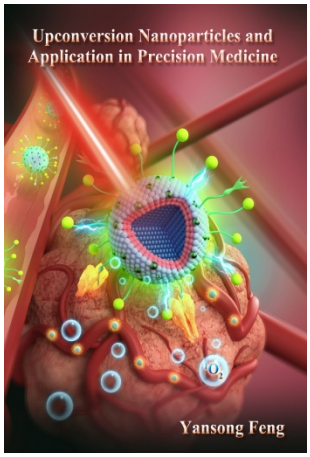
14 April 2020
Modeling solvent effects in catalytic reactions for energy conversion
Author: N. (Nitish) Govindarajan
Supervisor: E.J. Meijer
Co-supervisor: P.G. Bolhuis
Group: Computational Chemistry
Link: Read or download this thesis



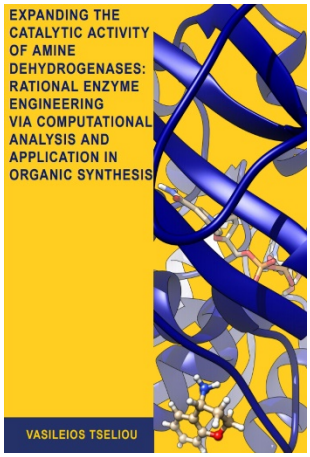
15 April 2020
Advanced x-ray absorption spectroscopy
Analyzing electronic structures of catalysts
Author: J.P. (Jean-Pierre) H. Oudsen
Supervisors: M. Tromp, J.N.H. Reek
Co-supervisor: T.J. Korstanje
Link: Read or download this thesis



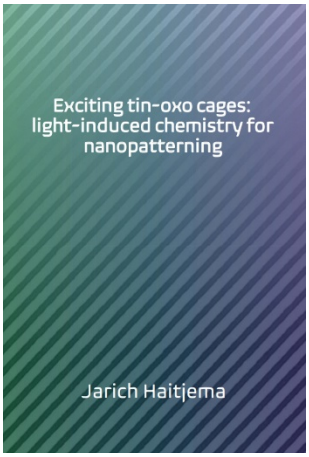
22 April 2020
Upconversion nanoparticles and application in precision medicine
Author: Y. (Yansong) Feng
Supervisor: H. Zhang
Co-supervisor: W.J. Buma
Group: Molecular Photonics
Link: Read or download this thesis



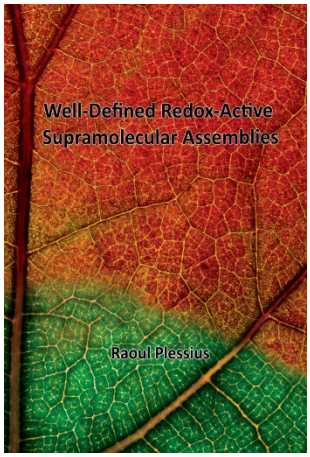
12 May 2020
Expanding the catalytic activity of amine dehydrogenases
Author: V. (Vasileios) Tseliou
Supervisors: F. Mutti, J.H. van Maarseveen
Group: Biocatalysis
Link: Read or download this thesis



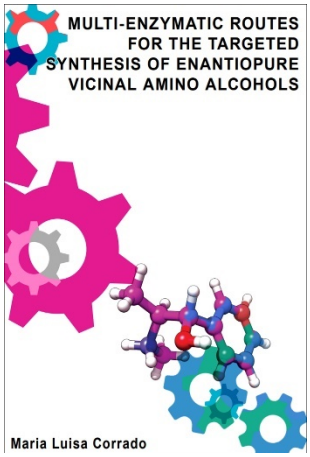
3 June 2020
Exciting tin-oxo cages
Light-induced chemistry for nanopatterning
Author: J. (Jarich) Haitjema
Supervisor: A.M. Brouwer
Co-supervisor: S. Castellanos Ortega
Group: Molecular Photonics
Link: Read or download this thesis



16 June 2020
Well-defined redox-active supramolecular assemblies
Author: R. (Raoul) Plessius
Supervisor: J.I van der Vlugt, J.N.H. Reek
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis



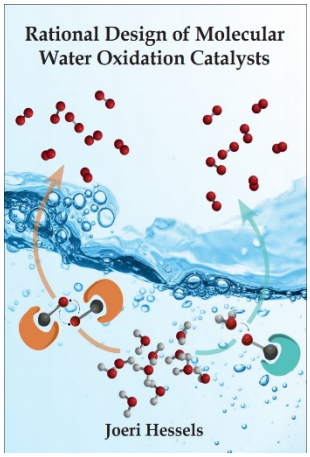
24 June 2020
Multi-enzymatic routes for the targeted synthesis of enantiopure vicinal amino alcohols
Author: M. (Maria) Luisa Corrado
Supervisors: F. Mutti, J.H. van Maarseveen
Group: Biocatalysis
Link: Read or download this thesis



29 June 2020

Rational design of molecular water oxidation catalysts

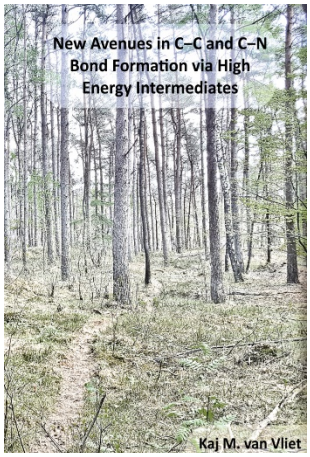
Author: J. (Joeri) Hessels
Supervisor: J.N.H. Reek
Co-supervisor: R.J. Detz
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis



03 July 2020

New avenues in C–C and C–N bond formation via high energy intermediates

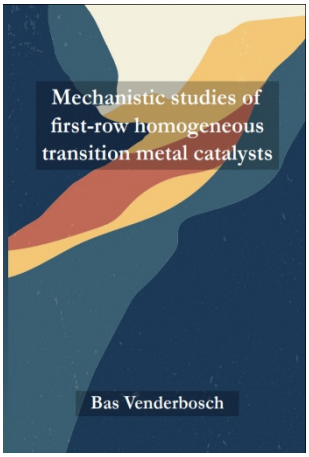
Author: K. (Kay) M. van Vliet
Supervisor: B. de Bruin
Co-supervisor: A.M. Brouwer
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
Link: Read or download this thesis



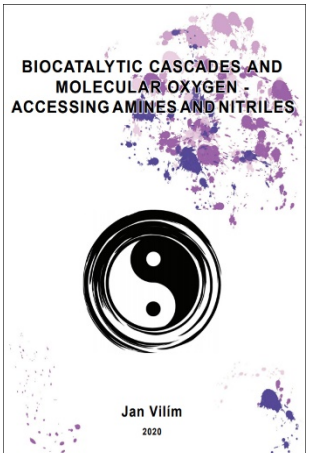
07 September 2020

Mechanistic studies of first-row homogeneous transition metal catalysts

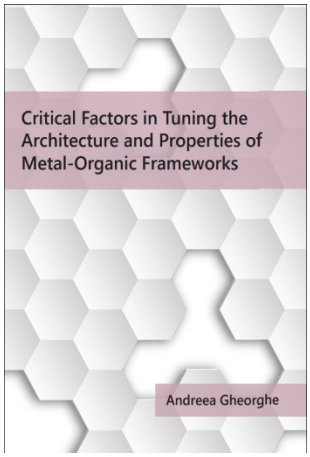
Author: B. (Bas) Venderbosch
Supervisors: M. Tromp, J.N.H. Reek
Co-supervisor: T.J. Korstanje
Link: Read or download this thesis



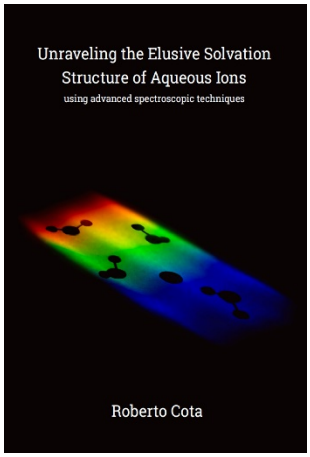
07 October 2020
Bio-catalytic cascades and molecular oxygen-accessing amines and nitriles
Author: J. (Jan) Vilím
Supervisors: F. Mutti, J.H. van Maarseveen
Co-supervisor: M.A. Fernández Ibáñez
Group: Biocatalysis
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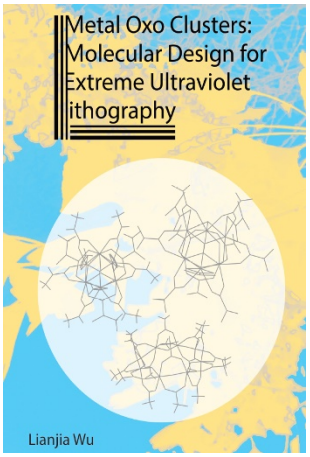
8 October 2020
Critical factors in tuning the architecture and properties of metal-organic frameworks
Author: A. (Andreea) Gheorghe
Supervisor: S. Grecea
Co-supervisor: G. Rothenberg
Group: Heterogeneous Catalysis and Sustainable Chemistry
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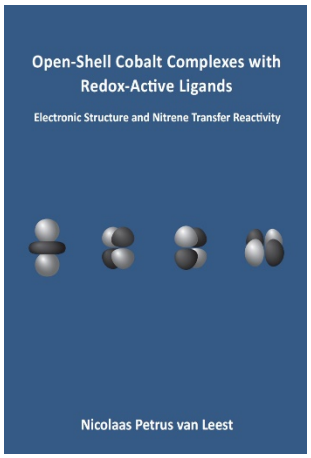
30 October 2020
Unraveling the elusive solvation structure of aqueous ions using advanced spectroscopic techniques
Author: R. (Roberto) O. Cota
Supervisors: S. Woutersen, H.J. Bakker
Group: Molecular Photonics
Link: Read or download this thesis



18 November 2020
Metal oxo clusters: molecular design for extreme ultraviolet lithography
Author: L. (Lianjia) Wu
Supervisors: A.M. Brouwer
Co-supervisor: S. Castellanos Ortega
Group: Molecular Photonics
Link: Read or download this thesis

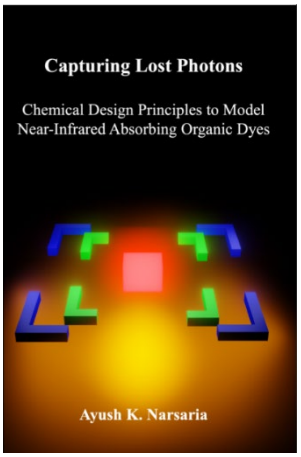


3 December 2020
Open-shell cobalt complexes with redox-active ligands
Electronic structure and nitrene transfer reactivity
Author: N. (Klaas) P. van Leest
Supervisor: B. de Bruin
Co-supervisor: J.I van der Vlugt
Group: Homogeneous, Supramolecular and Bio-Inspired Catalysis
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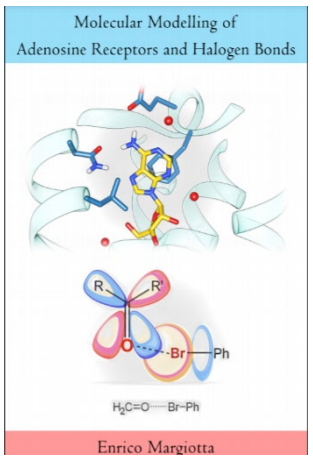
June 18, 2020
Capturing Lost Photons: Chemical Design Principles to Model Near-Infrared Absorbing Organic Dyes
Author: Ayush K. Narsaria
Supervisors: F.M. Bickelhaupt, K. Lammertsma, C. Fonseca Guerra
Co-supervisor: A.W. Ehlers
Group: Theoretical Chemistry
Link: Read or download the thesis



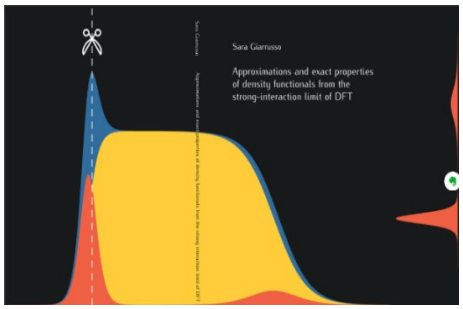
October 15, 2020
Author: Zakaria Boughlala
Cation affinities throughout the periodic table
Supervisors: F.M. Bickelhaupt,
Co-supervisor: C. Fonseca Guerra
Group: Theoretical Chemistry
Link: Read or download the thesis



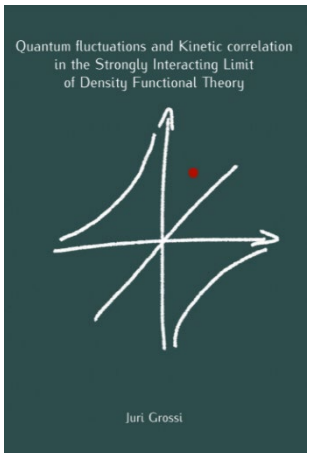
March 2, 2020
Molecular Modelling of Adenosine Receptors and Halogen Bonds
Author E. (Enrico) Margiotta
Supervisor: C. Fonseca Guerra
Group: Theoretical Chemistry
Link: Read or download this thesis



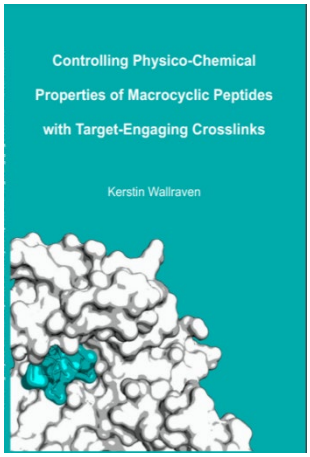
March 2, 2020
Approximations and exact properties of density functionals from the strong-interaction limit of DFT
Author: Sara Giarrusso
Supervisor: Gori Giorgi, P., Supervisor
Co-supervisor: K. Giesbertz
Group: Theoretical Chemistry
Link: Read or download the thesis



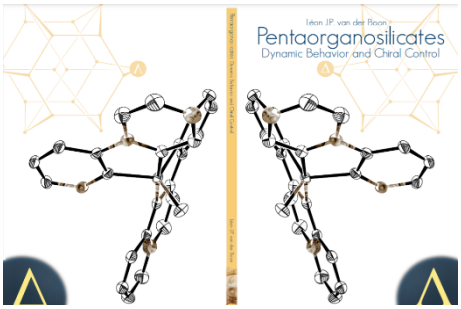
March 4, 2020
Quantum fluctuations and kinetic correlation in the strongly Interacting Limit of Density Functional Theory
Author: Juri Grossi
Supervisor: Gori Giorgi, P., Supervisor
Co-supervisor: K. Giesbertz
Group: Theoretical Chemistry
Link: Read or download the thesis



June 8, 2020
Macrocyclic Peptides with Target-Engaging Crosslinks
Supervisor: T. Grossmann,
Co-supervisorsor: S. Hennig
Group: Biomimetic Synthesis and Biomolecular Chemistry
Link: Read or download thesis

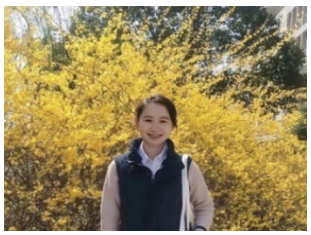


June 10, 2020
Pentaorganosilicates: Dynamic behavior and chiral control
L.J.P. van der Boon
Supervisors: K. Lammertsma, A.W. Ehlers
Ehlers, A.W.,
Co-supervisor: C. Slootweg
Group:
Link: Read or download the thesis



8. Fellowships
11th call May 2020

Dr. Yuan Gao (*School of Chemistry Engineering and Technology, China University of Mining and Technology***)**
Title of the Project: **Selective detection and removal of heavy metal ions using porousmaterials**
Hosted by Dr. Stefania Grecea and Dr. Hong Zhang (University of Amsterdam)



12th Call, October 2020

Dr. Zahra Yamshidi (*Sharif University of Technology, Tehran, Iran)*
Title of the Project: **Enhanced Vibrational Circular Dichroism Using Plasmonic Resonance**
Hosted by: Prof. dr. Lucas Visscher (Vrije Universiteit Amsterdam) and Prof. dr. Wybren Jan Buma (University of Amsterdam)
2 Visits: Total 3 months

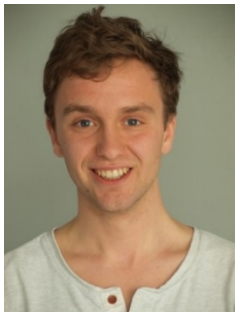


9. PhD Mobility Programme
1st round, May 2020

Pascal Vermeeren, from the group of Prof. Dr. F. Matthias Bickelhaupt and Dr. Trevor A. Hamlin (VU Amsterdam) will visit Prof. Henry F. Schaefer III and Prof. Steven E. Wheeler, University of Georgia
Title of the Project: **Rational Design of Metallylene Catalysts for Hydrogenation Reactions**



Alexander (Sander) Lemmens, from the Groups of Prof. Dr. Wybren Jan Buma (UvA)) and Dr. Anouk M. Rijs (Radboud University) will visit Prof. dr. Mattanjah de Vries, at University of California, Santa Barbara, CA Awarded by Stichting John van Geuns
Title of the Project: **Photophysics of PAHs: From ns to ps laser pulses**



Tessel Bouwens, from the group of Prof. Dr. Joost N.H. Reek (UvA) will visit Dr. Elizabeth A. Gibson (Newcastle University, School of Chemistry)
Awarded by Stichting John van Geuns
Title of the Project:**Unraveling the kinetics of the ring launching solar cell**



Dario Calvani, from the group of dr. F. Buda, Leiden University, going to Pennsylvania State University – Department of Mechanical Engineering Prof. Dr. Adri C.T. van Duin
Title of the Project**: Novel ReaxFF model for Water Oxidation Catalysts**



Zohre Eskandari Alughare from the group of Professor Dr. Michel Orrit, Leiden University will visit Prof. Dr. Don C. Lamb, Ludwig-Maximilians-Universität München
Title of the Project: **Kinetics of CO rebinding to single Myoglobin molecules using Förster Resonance Energy Transfer (FRET) at cryogenic temperatures**



Olga Lushchikova, From the group of Dr. Joost M. Bakker (Radboud University) will visit Prof. Dr. Paul Scheier (University of Innsbruck)
Title of the Project: **Spectral characterization of complexes with C60+ via He tagging**



2nd round October 2020

Celine Nieuwland from the group of Prof. F. Matthias Bickelhaupt, Prof. Dr. Célia Fonseca Guerra and Dr. Trevor A. Hamlin (VU Amsterdam) will visit the group of Prof. Dr. Marcel Swart at the University of Girona.

Celine Nieuwland
Title of the Project: **Understanding DNA replication using multi-scale modelling**



10. Financial Account 2020

Income			**Expenses**	
Contribution UvA 2020 - faculty[1]	150.000		Donation HIMS Institute[1]	150.000
Contribution UvA 2020 - HIMS[1]	150.000		Personnel Costs	83.286
Fellowship Programme John van Geuns (sponsoring)[2]	10.000		Office and management costs incl. Annual report	465
Correction Fellowship 2017	8.969		Fellowship Programme	35.250
Other	92		Dick Stufkens PhD prize	2.106
			HRSMC Class of Excellence	1.973
			Other	472
	€ 319.061			**€ 273.553**
Income minus Expenses[3]	€ 45.508			

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) In 2020 the balance had a positive outcome (+ € 45,508). This is caused by the COVID-19 pandemic, due to which almost all events and meetings had to be cancelled.