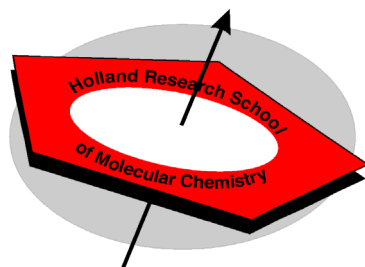


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**Holland Research School of Molecular Chemistry**



**Annual Report  
2010**

**LEIDEN UNIVERSITY  
UNIVERSITY OF AMSTERDAM  
VU UNIVERSITY**

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# Holland Research School of Molecular Chemistry

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**Colophon**

Lay-out: H.E. Zwaan – van der Plas / R. Weijer

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March 2011

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# 1. General

## 1.1 Preface

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 2010. The research school was founded in 1994 and has been twice re-accredited by the Royal Netherlands Academy of Arts and Sciences (KNAW). The HRSMC is now in the third period 2005-2012 (Formally, the third period is from 2005-2011. However, in 2009 the HRSMC received a one year extension from the KNAW because of the Research Quality Assessment 2001-2009 that would take place in 2010 at the institutes). The HRSMC comprises research groups of the following institutes and universities:

- the van 't Hoff Institute of Molecular Chemistry (HIMS) of the University of Amsterdam (UvA)
- the Institute for Electrons and Molecular Structure (EMS) of the VU University (VU)
- the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Leiden University (UL)

The research takes place in the heart of chemistry and focuses on the physical, chemical and biological properties of small to moderately sized molecules in relation to their electronic and spatial structures.

The HRSMC creates the conditions for a fruitful collaboration between the research groups, exerts itself to improve their infrastructure, and offers an extensive training programme for the PhD students in inorganic, organic, physical and theoretical chemistry. The participating universities provide the financial support by which the school can accomplish these tasks, including the invitation of foreign lecturers for the interuniversity courses and summer schools, and the organisation of the annual symposium.

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, clusters in the three HRSMC research themes: (1) Synthesis, Characterisation, Reactivity and Properties of Molecules, (2) Photochemistry and (Laser) Spectroscopy, and (3) Theoretical Chemistry.

## 1.2 Organisation and Mission

The HRSMC is a graduate research school in which research groups from the two Universities in Amsterdam and Leiden University participate. In accordance with the resolutions of the Government concerning the Graduate Research Schools, the HRSMC aims to set up and maintain a high-level training programme for its PhD students. In addition to the research training, the HRSMC offers a selection of courses to the students, which are collected in chapter 3.1 and on the HRSMC website ([www.hrsmc.nl](http://www.hrsmc.nl)). Some of these courses are given by staff members from all three universities, others by guest lecturers from abroad. Furthermore, summer schools are regularly organised on the main research themes of the HRSMC. A certificate is presented to those PhD students, who have fulfilled their education programme (18 ECTS, see Annex 4.5).

In order to promote the co-operation and exchanges of expertise and ideas, the members are informed about the activities and facilities of the research groups via reports, symposia, the news page of the HRSMC website and the HRSMC newsletter (three or four times a year).

The University of Amsterdam legally represents the HRSMC. The management consists of a board of three members and a scientific director (Prof. dr. W.J. Buma). In 2010, the HRSMC board consisted of Prof. dr. F.M. Bickelhaupt (VU), chairman, Prof. dr. M. Koper (UL) and Prof. dr. C.J. Elsevier (UvA).

The scientific director is assisted by an executive secretary (Mrs. Drs. H.E. Zwaan – van der Plas) and an administrative officer (Mrs. I. Weijer). In addition, an external advisory committee, the PhD platform and internal committees for education and research advise the board (see Annex 4.1). The organisation of the HRSMC is schematically depicted in Fig. 1.1, Annex 4.1. gives the composition of the committees and the PhD platform.

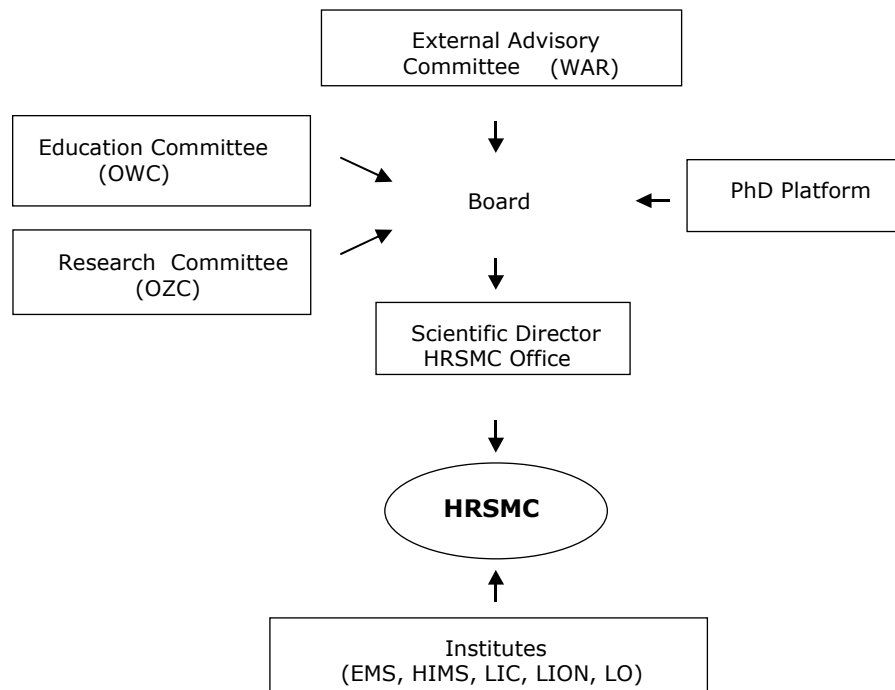


Figure 1.1 Schematic organisation of the HRSMC

On December 31, 2010 about 245 persons were employed within the HRSMC (several are not full-time involved in research, for details see Annex 4.3).

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### 1.3 General Activities and Headlines of 2010

In 2010, the HRSMC has put much effort in providing the PhD students with outstanding courses and maintaining the co-operations with other research groups and institutions.

The following major events took place in 2010:

- The annual HRMSC Symposium was held at the Leiden University on November 25. Following the advice of the Education Committee and the PhD platform, the format of the symposium has been changed to stimulate even more the interactions between the various research groups (e.g. more PhD lectures, less posters per session and a public prize for the best poster in each HRSMC Research Theme).

Besides the guest lectures of Prof. dr. R. van Santen (TUE) and Dr. Dominik Megger (WWU Münster), there were lectures of three PhD students and four lectures by senior scientists. Furthermore, the Dick Stufkens prize was awarded to Dr. N. Elders (Akzo Nobel), who also gave a lecture. In 2008 this annual prize has been established by the board of the HRSMC for the most outstanding PhD thesis within the HRSMC. The prize, consisting of (i) a certificate and (ii) 1,000 Euro in cash, is named after the scientific director of the HRSMC from 1997 to 2001.

The symposium, which was attended by ca. 140 scientists, also included poster sessions with 46 posters, mainly presented by PhD students. Further details regarding this symposium can be found in Chapter 3.2.

- The HRSMC educational activities of 2010 consisted of:
  - the two weeks Course 'Molecular Simulation', organised under the auspices of CECAM (January 4-15, 2010, UvA)
  - the Course Photophysics, Photochemistry & Photobiology, (May 31 - June 11 2010, UvA/VU)
  - the Autumn School 'Advanced Metal-Organic Chemistry', (September 26 - 29, hotel Zonheuvel, Doorn)

In addition to these Schools and Courses, the research groups of Prof. dr. H. Hiemstra (UvA), Prof. dr. R.V.A. Orru (VU) and Prof. dr. H.S. Overkleeft/Prof. dr. G. van der Marel organized two 'Synthetic Chemistry problem solving sessions'.

In 2010, a new activity was organized together on May 25 with the KNCV (Royal Dutch Chemistry Association): the KNCV/HRSMC Career Advice Event for PhD students and postdocs.

An overview of all HRSMC inter-university Courses and Summer Schools can be found in Chapter 3.1. In this chapter, more information can be found as well on the educational activities of 2010 described above.

#### Research highlights

The following HRSMC staff members received the following prestigious grants and awards:

- Dr. N. Elders (VU) received the HRSMC annual Dick Stufkens Prize for the most outstanding PhD thesis within HRSMC.
- Prof. dr. Evert Jan Baerends (VU) received the Schrödinger Medal 2010, a medal awarded by the World Association of Theoretical and Computational Chemists (WATOC).

- 
- As of November, Prof. dr. K. Lammertsma is a Board member of NWO/CW.
  - Prof. dr. R.V.A. Orru (VU) and Prof. dr. J.N. Reek (UvA) received each a prestigious NWO TOP Grant.
  - Dr. F. Ariese, Prof. dr. C. Gooijer and Dr. G van der Zwan (VU) received a grant of 270k€ within the NWO-Middelgroot programme 2009-2010 (Laser Centre VU – Biomolecular Analysis & Spectroscopy).
  - Dr. E. Ruijter (VU) received a ZonMW grant for research into potential new targets for future antibiotics.
  - The NWO Astrochemistry programme included several HRSMC members (Prof. dr. F.M. Bickelhaupt (VU), Prof. dr. W.J. Buma (UvA), Prof. dr. H. Linnartz (UL), Prof. dr. E.F. van Dischoeck and Prof. dr J. Oomens (UvA).
  - Dr. F. Ariese (VU), in collaboration with VU-Petrology, received a PhD grant from NWO/ Netherlands Space Office.
  - Laser Centre VU was expanded with laser-oriented groups from UvA (Buma, Brouwer), VUMC and AMC and is now called the Institute for Lasers, Life and Biophotonics Amsterdam (LaserLaB). New research initiatives are supported with 800 k€ matching from VU CvB.
  - A FOM TBSC Grant was awarded to Prof. dr. J.N.H. Reek (UvA), Prof. dr. A.M. Brouwer (UvA).
  - Election of Prof. dr. M. Orrit (UL) at Academia Europaea
  - Invitation to deliver the Harkins Lecture at the University of Chicago (M. Orrit, November 2010)

#### VENI, VIDI, VICI grants:

In February, Prof. dr. H.V.J. Linnartz (UL, Laboratory Astrophysics and Astrochemistry) received a VICI grant with his proposal 'Unlocking the chemistry of the heavens'.

In November, Dr. D. Dubbeldam (UvA, Computational Chemistry) received a VIDI grant.

In November, Dr. V.P. Nicu (VU, Theoretical Chemistry) and Dr. P. Rodriguez (UL, Catalysis and Surface Chemistry) received a VENI grant.

Publications from all HRSMC research groups published in 2010, can be found in Annex 4.4. Many of these publications appeared in high-impact journals, such as for example:

- J. Wassenaar, E. Jansen, W.-J. van Zeist, F. M. Bickelhaupt, M. A. Siegler, A. L. Spek, J. N. H. Reek; Survival of the Weakest: Catalyst Selection based on Intermediate Stability measured by Mass Spectrometry. *Nature Chemistry* **2010**, 2, 417-421. (Nature Chemistry publication as result of HRSMC and NRSC-C collaboration of the groups of Prof. dr. J.N. Reek and Prof. dr. F.M. Bickelhaupt)
- Witte, M. D.; Kallemeijn, W. W.; Aten, J.; Li, K. Y.; Strijland, A.; Donker-Koopman, W. E.; van den Nieuwendijk, A.; Bleijlevens, B.; Kramer, G.; Florea, B. I.; Hooibrink, B.; Hollak, C. E. M.; Ottenhoff, R.; Boot, R. G.; van der Marel, G. A.; Overkleeft, H. S.; Aerts, J., Ultrasensitive in situ visualization of active glucocerebrosidase molecules. *Nature Chemical Biology* **2010**, 6, (12), 907-913
- Meeuwissen, J.; Reek, J. N. H., Supramolecular catalysis beyond enzyme mimics. *Nature Chemistry* **2010**, 2, (8), 615-621.

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- De Boer, W.; Timmerman, D.; Dohnalova, K.; Yassievich, I. N.; Zhang, H.; Buma, W. J.; Gregorkiewicz, T., Red spectral shift and enhanced quantum efficiency in phonon-free photoluminescence from silicon nanocrystals. *Nature Nanotechnology* **2010**, 5, (12), 878-884.
  - De Boer, W., Timmerman, D., Dohnalova, K., Yassievich, I., Zhang, H. Buma, W.J., Gregorkiewicz, T., Red spectral shift and enhanced quantum efficiency of no-phonon emission from silicon nanocrystals, *Nature Nanotechnology* **2010**, 5, (12), 827-828.
  - Orrit, M., Single-photon sources: Frequency jitter of a nano-emitter. *Nature Photonics* **2010**, 4, (10), 667-668.
  - Angamuthu, R.; Byers, P.; Lutz, M.; Spek, A. L.; Bouwman, E., Electrocatalytic CO<sub>2</sub> Conversion to Oxalate by a Copper Complex. *Science* **2010**, 327, (5963), 313-315.
  - Panman, M. R.; Bodis, P.; Shaw, D. J.; Bakker, B. H.; Newton, A. C.; Kay, E. R.; Brouwer, A. M.; Buma, W. J.; Leigh, D. A.; Woutersen, S., Operation Mechanism of a Molecular Machine Revealed Using Time-Resolved Vibrational Spectroscopy. *Science* **2010**, 328, (5983), 1255-1258.
  - Gaiduk, A.; Yorulmaz, M.; Ruijgrok, P. V.; Orrit, M., Room-Temperature Detection of a Single Molecule's Absorption by Photothermal Contrast. *Science* **2010**, 330, (6002), 353-356.

#### Personnel mutations

At the Institute for Electrons and Molecular Structure (EMS) of the Vrije Universiteit (VU):

- No changes

At the van 't Hoff Institute of Molecular Chemistry (HIMS) of the Universiteit van Amsterdam (UvA):

- Prof. dr. A. Kleijn has been appointed as successor of Dr. R. Zsom as director of the van 't Hoff Institute of Molecular Chemistry

At the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Universiteit Leiden (UL):

- As of April 1, Prof. dr. E. Bouwman has been appointed as professor 'Inorganic Chemistry'. With her appointment, she succeeded Prof. dr. J. Reedijk as a group leader of the group 'Coordination and Bio-inorganic Chemistry'. The name of the group changed into 'Metals in Catalysis, Biomimetics & Inorganic Materials'.

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## 1.4 Joint Activities

The main mission of the HRSMC is the training and education of PhD students. Although the main part of the training is individual and specialised, the school offers the PhD students also a broad programme of courses and summer schools, which are given by a team of staff members from all three participating institutes and by guest lecturers from other universities and countries. In addition, the board of the school seeks to promote the research co-operation between groups of the HRSMC. These collaborations resulted in about 11 joint publications in 2010 while several joint applications at CW-NWO were awarded. Apart from this, many groups share their expertise and equipment (see annex 4.6).

### International Research Training Group (IRTG)

The board has also extended its activities outside the school; a fruitful collaboration has been established between the HRSMC and the Westfälische Wilhelms Universität Münster and is expressed in the International Research Training Group (IRTG) "Generation of Supramolecular Functional Cavities - Container Molecules, Macrocycles and Related Compounds". This IRTG promotes and supports the exchange of guest lecturers and PhD students, and the organisation of joint courses and summer schools. This program has been approved by DFG in 2006. At the Dutch side, the application was submitted in 2006, containing a request for the funding of PhD students. NWO approved the application in February 2007. However, without funding of PhD students as this is not in line with the guidelines of the Dutch program.

The IRTG program will continue until 2011. HRSMC staff members Prof. dr. F.M. Bickelhaupt, Prof. dr. C.J. Elsevier, Prof. dr. K. Lammertsma, Prof. dr. R.V.A. Orru, Prof. dr. J. Reedijk and Prof. dr. G. Rothenberg have established this cooperation with their partners from the Westfälische Wilhelms-Universität in Münster (see also chapter 2.4).

The IRTG finds a precedent in an earlier collaboration between the HRSMC and the Westfälische Wilhelms Universität Münster. In 2000, NWO and the DFG have recognised the International Graduate College 'Template Directed Chemical Synthesis', a cooperation between five research groups from the Holland Research School of Molecular Chemistry and eleven research groups from the University of Münster, for the period 2001-2004. Re-accreditation for the period 2004-2005 was obtained.

### National Research School Combination 'Catalysis' (NRSC-Catalysis)

Last but not least, the HRSMC takes part with several groups in the National Research School Combination Catalysis Controlled by Chemical Design (NRSC-Catalysis), which was founded and accredited in 1998. The participating groups (Baerends, Bickelhaupt, Elsevier, Hiemstra, Koper, Lammertsma, Orru, Bouwman/Reedijk, Reek and Wever) received appreciable additional funding for the period 2009-2013.

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## 2. Research

The research topics of the HRSMC are collected in the three research themes 'Synthesis, Characterisation, Reactivity and Properties of Molecules' (Theme 1), 'Photochemistry and (Laser) Spectroscopy' (Theme 2), and 'Theoretical Chemistry' (Theme 3). Of course the co-operations are not restricted to research groups of a single theme.

In Table 2.1 the names of the group leaders involved in the HRSMC in 2010 and their research themes are collected. The names of all staff members, graduate students, postdocs and technical staff are listed in Annex 4.3.

*Table 2.1 HRSMC group leaders and their research themes in 2010*

Theme	Group leader(s)	Institute	Workgroup
1	Bouwman <sup>1,2</sup>	LIC	Metals in Catalysis, Biomimetics & Inorganic Materials <sup>3</sup>
	Elsevier <sup>1,2</sup>	HIMS	Co-ordination and Organometallic Chemistry
	Hiemstra <sup>1,2</sup> / Timmerman	HIMS	Synthetic Organic Chemistry
	Lammertsma <sup>2</sup>	EMS	Organic and Organometallic Chemistry
	Orru <sup>2</sup>	EMS	Synthetic and Bio-organic Chemistry
	Overkleef/vd Marel	LIC	Bio-organic Synthesis
	Reek <sup>1,2</sup> /Hartl	HIMS	Supramolecular Catalysis
	Wever <sup>1,2</sup>	HIMS	Biocatalysts and Bio-organic Chemistry
2	Buma/Brouwer	HIMS	Molecular Photonics
	Gooijer	EMS	Biomolecular Analysis and Spectroscopy
	Groenen/Orrit/Völker	LION	Molecular Nano-Optics and Spins
	de Groot	LIC	Biophysical Organic Chemistry
	Janssen	EMS	Physical Chemistry
	Koper <sup>1,2</sup>	LIC	Surface Chemistry and Catalysis
	Linnartz	LO	Laboratory Astrophysics and Astrochemistry
3	Baerends <sup>2</sup> /Bickelhaupt <sup>1,2</sup> / Visscher	EMS	Theoretical Chemistry
	Bolhuis/Meijer	HIMS	Computational Chemistry & Physics
	Neugebauer	LIC	Theoretical Chemistry

<sup>1</sup>also NIOK; <sup>2</sup>also NRSC-Catalysis; <sup>3</sup>until 2009 this was the group 'Coordination and Bio-inorganic Chemistry', under leadership of Prof. dr. J. Reedijk, who retired in 2009.

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## 2.1 Theme 1 - Synthesis, Characterisation, Reactivity and Properties of Molecules

### Aims, activities and achievements

The design and synthesis of compounds with novel structures are among the most essential activities in molecular chemistry research. The incentives to prepare such new molecules are, apart from curiosity, their anticipated physical, chemical or biological properties. Strategic aspects of the HRSMC synthetic research are the development of new (bio)catalytic reactions and the investigation of their mechanisms, the synthesis of magnetic and conducting materials, and the development of methodologies for the synthesis of bioactive compounds. A great variety of techniques is used for the synthesis of the compounds as well as for the elucidation of their molecular structure and physical-chemical and biological properties. From the three universities eight different groups are active in this area.

The **Bouwman** (former Reedijk) group is involved in the synthesis and study of the properties of transition-metal coordination compounds and their potential applications as material or precursor for the development of new magnetic and luminescent materials, homogeneous catalysts, molecular machines, and models for the active sites in metalloproteins. The group participates in NIOK, NRSC-Catalysis and IRTG.

The research activities of the **Elsevier** group are in the field of molecular inorganic and organometallic chemistry and concern the mechanisms of selective metal-catalysed reactions. The main aim is to synthesise new metal compounds that show novel (catalytic) properties of bond formation and breaking. Furthermore, efforts are made to address immobilization and compartmentalization of molecular inorganic compounds that are used as (pre) catalysts, in order to promote recycling of the ligand and/or such a catalyst. The group participates in the International Research Training Group (IRTG) and in two other research schools: the National Research School Combination Catalysis Controlled by Chemical Design (NRSC-Catalysis) and in the Netherlands Institute for Catalysis Research (NIOK).

The **Hiemstra** group develops new synthetic methodologies, in particular directed to the total synthesis of novel, and structurally challenging bioactive natural products. Key areas of the group 's research are asymmetric organocatalysis with novel chiral Brønsted acids and bases, and the synthesis of cyclic tetra- and pentapeptides via novel cyclisation strategies. The group participates in the NRSC-Catalysis and NIOK.

**Lammertsma** and his group synthesize and study novel classes of organophosphorous compounds in the context of sustainability, using metal-template directed methods akin to the carbene complexes, such as the electrophilic Fischer (e.g.,  $\text{Ph-P=W(CO)}_5$ ) and nucleophilic Schrock-type complexes. The synthetic designs are supported by DFT calculations to anticipate the impact of substituents, transition metals and ligands. The group participates in the NRSC-Catalysis and IRTG.

The central theme in **Orru** group is the development of new synthetic methodology for the efficient and selective generation of (libraries of) biologically relevant molecules. Key topics are improvement of atom and process efficiency in organic synthesis, the development of novel tandem and multicomponent reactions for diversity and/or biology

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oriented synthesis, and application of advanced (bio)catalysis in synthesis. The group participates in the NRSC-Catalysis and IRTG.

The **Overkleeft/vd Marel** group develops methodologies for the synthesis of biologically active molecules such as nucleic acids, peptides and carbohydrates. These compounds form the basis of medicinal chemistry and chemical biology studies, which are performed both in house and in collaboration with academic partners from the Dutch University Medical Centres, the Netherlands Cancer Institute and international parties.

The catalysis group of **Reek** develops new catalysts for known and new important conversions. Important issues comprise of the atom-efficiency, the chemo-, regio-, and stereo-selectivity, and the activity and stability of the catalyst. In addition, new solutions to the problem of homogeneous catalyst separation and recycling are investigated. The group also participates in NRSC-Catalysis and NIOK.

The group **Wever** focuses on the use and development of biocatalysts in synthetic organic chemistry as a "green" alternative for existing chemical procedures. The group developed a novel procedure using a cascade of enzymes in one pot and starting from simple carbon compounds it was possible to synthesize a variety of complex and chiral carbohydrates. Furthermore, the group has research activities focused on protein engineering of vanadium haloperoxidases. The group also participates in NRSC-Catalysis and NIOK.

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## Metals in Catalysis, Biomimetics & Inorganic Materials

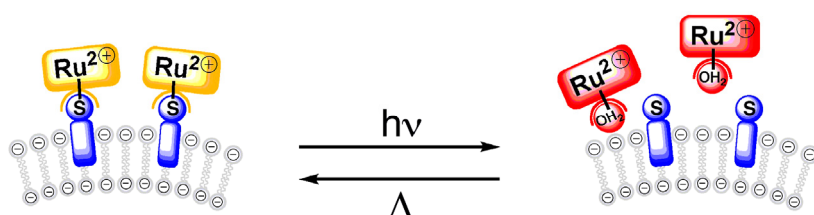
*Prof. dr. E. Bouwman, Prof. dr. J. Reedijk, Dr. S. Bonnet, Dr. W.T. Fu (UL)*

### Research topics

- Biomimetic and bioinorganic chemistry
- Molecular and solid-state materials
- Homogeneous catalysis (reported within NIOK)
- (Photo)coordination chemistry at lipid bilayers

### Summary of research activities

In a project aimed at the development of coordination complexes as potential phosphor materials for LED-based solid-state lighting new ligand systems have been screened. Ligands with the acetylacetonate structural motif are known to efficiently sensitize Eu(III) and have long been the subject of intensive research. Using these molecules as a starting point, some new ligands have been synthesized. While acetylacetonate usually forms stable complexes with the lanthanides, the  $\beta$ -enaminoketone and  $\beta$ -diketimine ligands do not seem to be capable of doing so since no Ln complexes could be isolated. Synthesis of some N-acylamide ligands was successful, but also in this case complex synthesis turned out to be troublesome due to the instability of the ligands. A series of Eu(III) and Tb(III) complexes using furan-2,5-dicarboxylate as a ligand has been synthesized, yielding white, microcrystalline materials that are moderately luminescent under UV excitation.



Light, this time in the visible region, is also used to trigger molecular motion at lipid bilayers. By synthesizing thioether-cholesterol conjugates

that bind to ruthenium through their sulfur atom and intercalate into bilayers through their apolar tail, we were able to prepare ruthenium-decorated unilamellar vesicles. Upon visible light irradiation, the ruthenium-sulfur bond is selectively broken, releasing the ruthenium complex. Depending on the charge of the lipids, the complex either diffuses in solution, or stays close to the membrane and can be re-bound by thermal treatment (S. Bonnet, B. Limburg, J. Meeldijk, R. J. M. Klein Gebbink, and J. A. Killian, *J. Am. Chem. Soc.* **2011**, *133*, 252-261). We aim at using this kind of systems to achieve unidirectional motion of molecules at biomimetic membranes.

Following our discovery of the strongly cooperative spin-crossover mononuclear compounds  $[\text{Fe}(\text{bapbpy})(\text{NCS})_2]$  (see reports of 2008 and 2009), we have been focusing on studying how introducing organic substituents on the tetrapyrridyl bapbpy ligand modifies the spin-transition properties of its iron(II) complex. Notably, we discovered that solid materials made of isomers of the same molecule show completely different spin-crossover properties. Meanwhile, in a collaboration with the CNRS in Toulouse we have studied by Raman mapping and optical microscopy the two independent spin transitions of  $[\text{Fe}(\text{bapbpy})(\text{NCS})_2]$  (S. Bedoui, G. Molnár, S. Bonnet, C. Quintero, H. J. Shepherd, W. Nicolazzi, L. Salmon, A. Bousseksou, *Chem. Phys. Lett.* **2010**, *499*, 94-

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99). These studies prove that both spin transitions follow completely different mechanisms. Together with collaborators from Lyon we also published a theoretical study on that topic.

### **Key publications 2007-2010**

- ♦ R. Angamuthu, P. Byers, M. Lutz, A.L. Spek and E. Bouwman; Electrocatalytic CO<sub>2</sub> Conversion to Oxalate by a Copper Complex; *Science*, **2010**, 327, 313-315.
- ♦ M.T.M. Koper and E. Bouwman; Electrochemical Hydrogen Production: Bridging Homogeneous and Heterogeneous Catalysis; *Angew. Chem. Int. Ed.*, **2010**, 49, 3723-3725.
- ♦ M. Kepenekian, J. Sanchez-Costa, B. Le Guennic, P. Maldivi, S. Bonnet, J. Reedijk, P. Gamez, V. Robert; Reliability and Storage Capacity: a Compromise Illustrated in the Two-step Spin-Crossover System [Fe(bapbpy)(NCS)<sub>2</sub>]; *Inorg. Chem.* **2010**, 49, 11057-11061.

### **Future developments**

In the topic of biomimetics we plan to continue the research towards the catalytic conversion of CO<sub>2</sub>. By varying the steric and electronic properties of the ligands, attempts will be undertaken to tune the structural and redox properties of the copper complexes. Future studies will also be directed to the synthesis of novel ligand systems that allow for anchoring of the copper catalyst on an electrode surface.

With the appointment of Dr. Bonnet, two projects are added to the bioinorganic topic: one aimed at controlling the motion of molecules with light (Veni grant), and one aimed at the light-activation of ruthenium-based anticancer drugs. For the first project a new PhD student started in November 2009 (Azadeh Bahreman). We also continue research in spin-transitions materials, for which a new PhD student started in May 2010 (Sipeng Zheng). The influence of modifications of the bapbpy ligands on the spin crossover of its iron complexes will be continued, as well as the study of spin crossover at gold surfaces.

In the project aimed at the development of coordination complexes as potential phosphor materials for LED-based solid-state lighting new ligand systems will be developed specifically for Tb and Eu. 1,3,5-Triazapentadienes (a group of ligands that resemble the β-diketone ligands) offer ample possibilities for substitution, which allows for tuning the ligand to the acceptor levels on the lanthanide. Complexes of Eu and Tb with these ligands will be synthesized in collaboration with the Universität Münster.

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# Co-ordination and Organometallic Chemistry

*Prof. dr. C.J. Elsevier (UvA)*

## **Research topics**

Organometallic and coordination chemistry

Catalytic bond-formation and -breaking

High-pressure NMR and transition metal NMR spectroscopy

N-heterocyclic carbenes as ligands

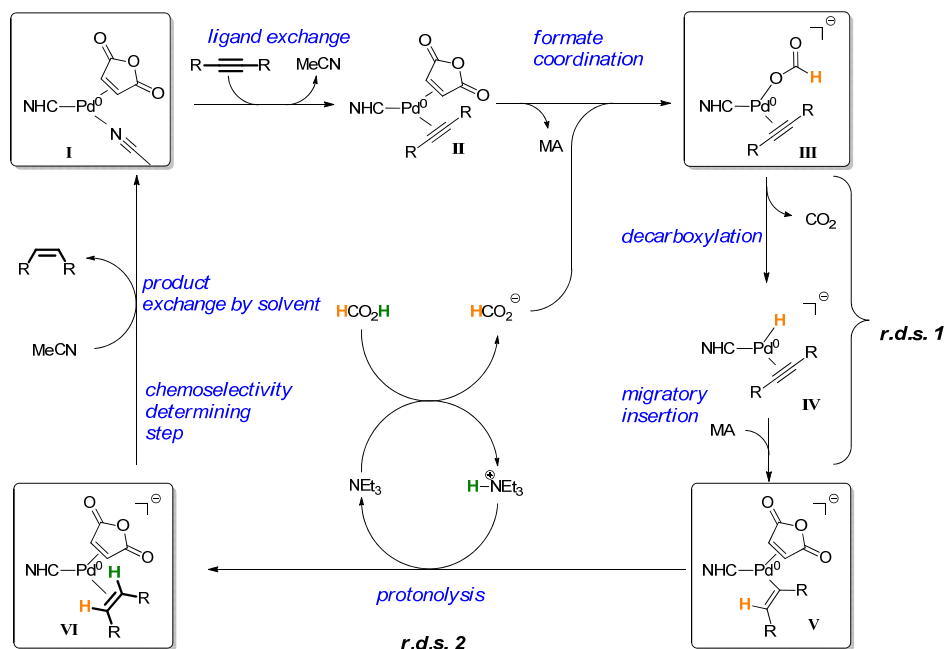
## **Summary of research activities**

The group Molecular Inorganic Chemistry at the University of Amsterdam is involved in fundamental research in Coordination and Organometallic Chemistry, notably the synthesis, characterization and application of organometallic compounds and homogeneous catalysts. We try to approach catalysis in a rational way by studying single steps and constitute new catalytic cycles from these building blocks. We also engage in finding alternatives to existing reactions, for instance hydrogenations, by knowledge-driven choice and engineering of the metal-ligand combinations. The counterpart lies in careful analysis of the mechanism of homogeneous catalytic, metal-mediated reactions and to discover new solutions and improvement of processes, based on understanding of its details. Organometallic chemistry, which resides at the basis of all catalytic processes, is the main topic of the activities in the group. The reactions concerned are mainly bond-forming and bond-breaking reactions between carbon and the other elements, with emphasis on carbon, hydrogen, and late transition metals. Processes studied are, e.g., hydrogenation, hydrosilylation, C-C coupling reactions. Several of these have been studied under pressure and in neoteric solvents, e.g. supercritical fluids. Spectroscopic studies of reactions under pressure are carried out to evaluate the reaction and intermediates under conditions similar to those in the catalytic reactions studied. The research of the group has in the past partly aimed at the design and implementation of self-organizing amphiphilic metal-organic molecules, especially a novel class of metallo-amphiphiles that are characterized by the intrinsic presence of a metallic group as part of the amphiphile, that acts as the polar headgroup. These systems are particularly amenable to the formation of micelles and inverted micelles, or vesicles, with the aim to enhance catalysis and bond activation taking place at the interface of polar and apolar media (such as water/alkane).

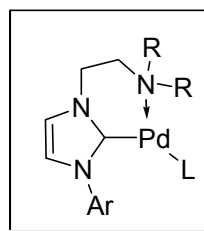
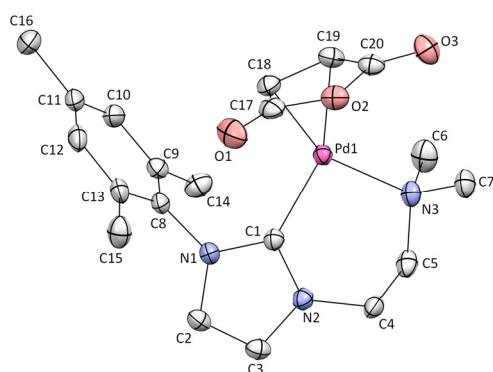
The design and implementation of N-heterocyclic carbene (NHC) ligands as well as rigid bidentate N-ligands in late transition metal compounds aimed at catalytic carbon-element bond forming reactions continues to be an important research topic in the group.

This year, the studies concerning the mechanism of palladium(NHC)-catalyzed *transfer* hydrogen-ation of alkynes has been completed and published (*J. Am. Chem. Soc.* **2010**, *132*, 16900-16910). This methodology for the catalytic synthesis of *Z*-alkenes from alkynes *without* reduction to alkanes attracts a lot of interest. Our research provided insight in details of the mechanism due to careful kinetic measurements including deuterium isotope effects of all isotopomers of formic acid that is used as the hydrogen donor. In addition, *in situ* NMR measurements provided insight in the structure of

accumulating intermediates. Altogether we were able to provide a convincing mechanism of this new reaction (Scheme below), proceeding by ligand exchange between **VI**, **I** and **II**, that critically depends on the coordinative properties of the solvent with respect to the substrate (stronger) and product (weaker). This feature ensures complete reduction of the alkynes to the alkenes, preventing further reduction from occurring.



Next, formate coordination (**III**) and CO<sub>2</sub> extrusion to give the active palladiumhydride **IV** occurs, which is followed by rate determining insertion of the alkyne in a palladium hydride to give Pd-alkenyl complex **V**. The second rate determining step concerns the protonolysis of the alkenyl intermediate providing the *cis*-alkene coordinated to palladium.



Currently, one of the focal points of our research concerns the design and application of late transition metal complexes with heterotopic carbene and N-ligands for coordination chemistry and applications in homogeneous catalysis. This year we have synthesized a number of heterobidentate NHC ligands containing a secondary nitrogen-donor. Combining a strong donor with a more weakly coordinating donor, we intend to gain access to a class of catalysts which benefits from the hemilabile behaviour of the weaker donor N-ligand. Additionally, the basicity of the secondary nitrogen-donor is easily varied to obtain the desired functionality. Various electron-rich palladium complexes bearing an NHC-ligand functionalized with N-donors such as a pyridyl, pyrimidyl, and pyrazolyl donors have been studied. Varying their

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basicity, hence coordinative properties, leads to specific behaviour in e.g hydrogenation reactions. Several papers have appeared and will appear on this subject.

Part of this project has been carried out in collaboration with Taiwanese colleagues (in a project financed by NWO and NSC): this led to the synthesis of iridium-NHC complexes for catalytic indole synthesis and reductive amination (C-N bond formation), and palladium-NHC complexes for C-S bond formation. The palladium(NHC) systems with various tethers are unprecedented hydrogenation catalysts, since they catalyze *transfer* hydrogenation of alkynes to give *cis*-alkenes selectively. Usually transfer hydrogenation is restricted to ketones and imines. This collaboration has given rise to 13 papers, 6 of which appeared in 2010.

Furthermore, we have started a project on immobilization of NHC-transition metal complexes for catalysis, with the aim of recycling, on which we will report next year.

### Key publications 2007-2010

- P. Hauwert, G. Maestri, J.W. Sprengers, M. Catellani, C.J. Elsevier; Transfer Semihydrogenation of Alkynes Catalyzed by a Zero-Valent Palladium N-Heterocyclic Carbene Complex. *Angew. Chem. Int. Ed.* 47 **2008** 3223-3226.
- S. Warsink, S.Y. de Boer, L.M. Jongens, C.-F. Fu, S.-T. Liu, J.-T. Chen, M. Lutz, A.L. Spek, C.J. Elsevier. Synthesis and characterization of Pd(II)-methyl complexes with N-heterocyclic carbene-amine ligands: resistance to reductive elimination. *Dalton Transactions* 35 **2009** 7080-7086.
- P. Hauwert, R. Boerleider, S. Warsink, J.J. Weigand, C.J. Elsevier. Mechanism of Pd(NHC)-catalyzed transfer hydrogenation of alkynes. *J. Am. Chem. Soc.* 132 **2010** 16900-16910.

### Future developments

The research for the immediate future will generally be aimed at design and synthesis of molecular inorganic and organometallic compounds for stoichiometric and homogeneous catalytic reactions. These will particularly be aimed at the addition and insertion of small molecules to unsaturated compounds, such as in hydrogenation and carbonylation reactions. In this respect, the important recent discovery that late-transition metal *N*-heterocyclic carbene compounds, notably palladium(NHC) compounds, appear to be stable and exceptionally selective catalysts for selective hydrogenation reactions, either using molecular hydrogen or hydrogen transfer agents, will receive ample attention. Especially the mechanism and implications of transfer-hydrogenations using palladium(NHC) complexes will be pursued. We will attempt to find suitable first-row transition elements to replace palladium in a number of cases. Furthermore, the design of man-made ligands will continue to be important, especially in relation to carbon-element bond forming reactions, carbonylations and related reactions.

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We will also make efforts on immobilization and compartmentalization of molecular inorganic (pre) catalysts, in order to promote recycling of the ligand and catalyst. Furthermore, the behaviour and reactivity of systems involving metallosurfactants and metals ligated by amphiphilic ligands will continue to receive some attention.

Transition metal NMR spectroscopy and NMR of other 'less commonly measured' nuclei continues to be of interest to complement our studies, especiall those involving N-ligands and metals such as rhodium and ruthenium.

# Synthetic Organic Chemistry

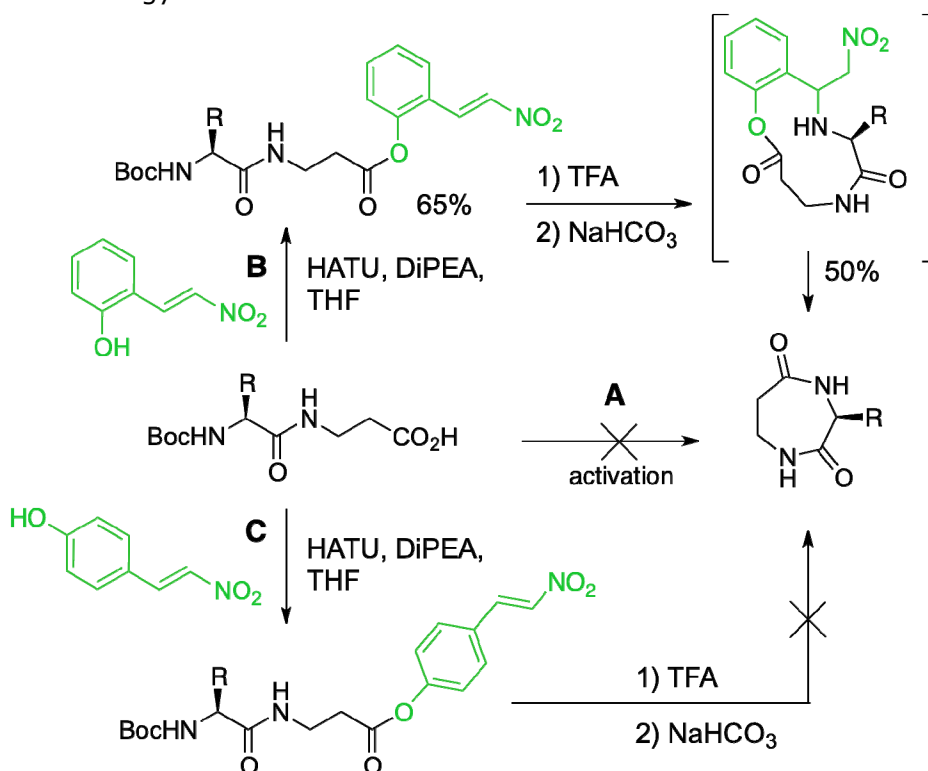
Prof. dr. H. Hiemstra, Prof. dr. P. Timmerman, Dr. J.H. van Maarseveen, Dr. S. Ingemann (UvA)

## Research topics

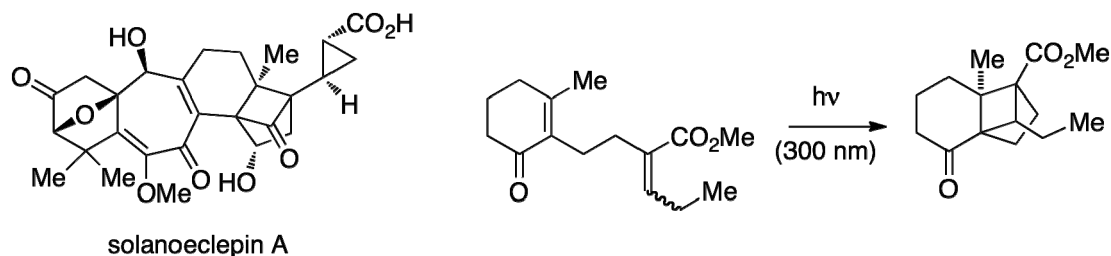
- Synthetic methodology development
- Target-oriented synthesis
- Organocatalysis
- Chemical biology

## Summary of research activities

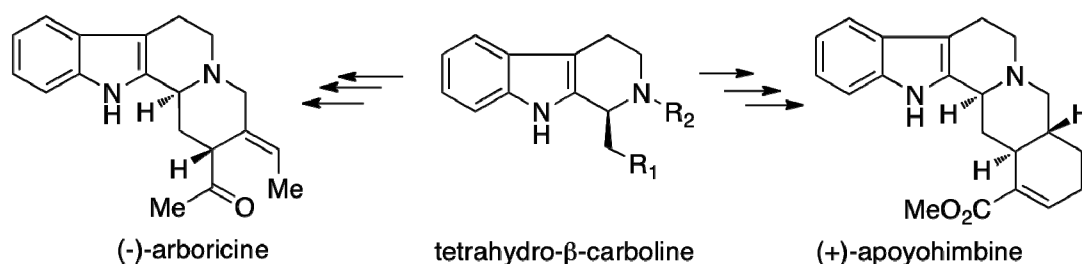
*Synthetic methodology development:* As is shown below, dipeptides containing one  $\beta$ -amino acid do not easily cyclize to 7-membered lactams (route A). Therefore, they are ideally suited for the development of methods to synthesize by ring-closure naturally occurring and biologically relevant strained lactams. It was found that esterification of N-terminal protected  $\beta$ -peptides with commercially available *o*-hydroxy- $\beta$ -nitrostyrene, followed by liberation of the N-terminus is followed by facile 7-membered lactam formation (route B). Carrying out the same reaction sequence for *p*-hydroxy- $\beta$ -nitrostyrene predominantly yields the unwanted cyclic dimer, as is found by lactamization attempts of the same  $\beta$ -peptides (route C). This result suggests in the case of *o*-hydroxy- $\beta$ -nitrostyrene the intermediacy of an 11-membered macrocyclic intermediate, formed via an intramolecular aza-Michael reaction, which collapses to the 7-membered lactam via a ring-contractive O $\rightarrow$ N acyl-transfer reaction, followed by a retro-aza-Michael reaction liberating the lactam. This method is now further developed for the ring-closure of naturally occurring small cyclic peptides that cannot be addressed using the current synthetic methodology.



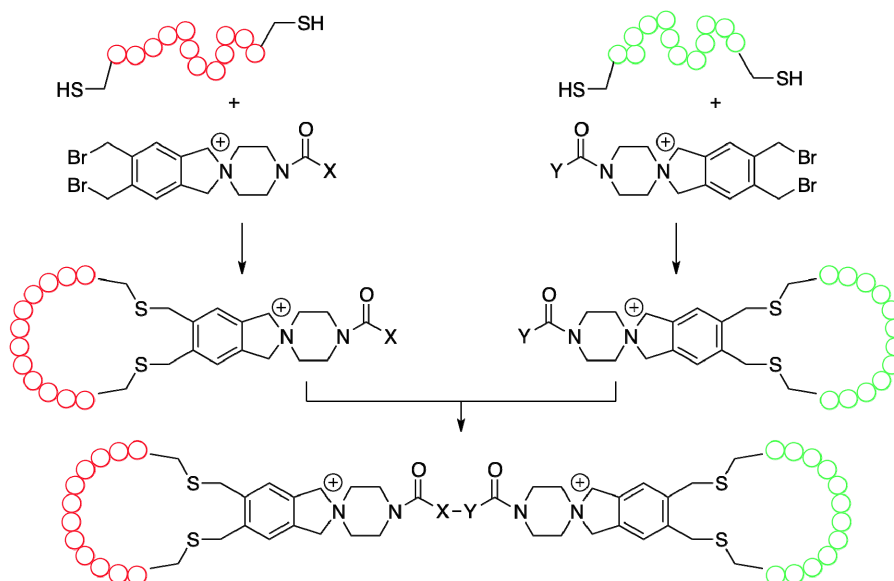
*Target-oriented synthesis:* Our research towards the total synthesis of the terpenoid hatching agent solanoeclepin A should eventually lead to simple active analogues in order to combat potato cyst nematodes as parasites in potato production. In 2010 our insight into the [2+2]-photocycloaddition towards the tricyclic core of the natural product was considerably enhanced by the successful construction of the tricyclic ester from the cyclohexenone precursor in the correct regiochemical (crossed) sense.



*Organocatalysis:* Chiral biarylphosphoric acids were used to catalyse Pictet-Spengler reactions in order to prepare tetrahydro- $\beta$ -carbolines in high ee's. These *N*-heterocycles are suitable substrates for the asymmetric synthesis of indole alkaloids through cyclization reactions between the C1 and N2 substituents, either via transition metal catalysis or Diels-Alder chemistry. In these ways the first total syntheses of (-)-arboricine and (+)-apoyohimbine were achieved.



*Chemical biology:* The CLIPS technology developed at Pepscan Therapeutics, Lelystad, by Timmerman and coworkers was further expanded by the introduction of additional reactive tags to the scaffolds to allow the covalent connection of different CLIPS-constrained peptides thus mimicking discontinuous protein epitopes. In addition, these tags were attached via an ammonium moiety to improve the water solubility. Covalent ligation of these highly functionalized *unprotected* CLIPS-peptides may be conducted by click-type transformations such as the CuAAC-reaction, oxime-formation or the thiol-ene reaction.



### Key publications 2007-2010

- Enantioselective copper-catalyzed propargylic amination, R.J. Detz, M.M.E. Delville, H. Hiemstra, J.H. van Maarseveen, *Angew. Chem. Int. Ed.* **47**, 3777-3780 (2008).
- Backbone amide linker strategy for the synthesis of 1,4-triazole-containing cyclic tetra- and pentapeptides, J. Springer, K.R. de Cuba, S. V. Calvet-Vitale, J.A.J. Geenevasen, P.H.H. Hermkens, H. Hiemstra, J.H. van Maarseveen, *Eur. J. Org. Chem.* 2592-2600 (2008).
- Organocatalytic enantioselective total synthesis of (-)-arboricine, M.J. Wanner, R.N.A. Boots, B. Eradus, R. de Gelder, J.H. van Maarseveen, H. Hiemstra, *Org. Lett.* **11**, 2579-2581 (2009).
- Selective enrichment of azide-containing peptides from complex mixtures, M.A. Nessen, G. Kramer, J.W. Back, J.M. Baskin, L.E.J. Smeenk, L.J. de Koning, J.H. van Maarseveen, L. de Jong, C.R. Bertozzi, H. Hiemstra, C.G. De Koster, *J. Proteome Res.* **8**, 3702-3711 (2009).
- Expedient pyrrolizidine synthesis by propargylsilane addition to *N*-acyliminium ions followed by gold-catalyzed  $\alpha$ -allenyl amides cyclization, A.C. Breman, J. Dijkink, J.H. van Maarseveen, S.S. Kinderman, H. Hiemstra, *J. Org. Chem.* **74**, 6327-6330 (2009).

### Future developments

The principles of our lactamization auxiliaries that use a ring-contractive O $\rightarrow$ N acyl transfer reaction as the key step have been validated for the synthesis of 7-membered strained bislactams. In the following year these auxiliaries will be used to ring-close natural small cyclic peptides that cannot be prepared using the current methodologies. Also, derivatives of the auxiliaries will be developed that can be used in catalytic amounts.

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Our research toward the total synthesis of solanoeclepin A, the hatching agent of potato cyst nematodes will be further concentrated on the smooth construction of eastern substructure in such a manner that the total synthesis can eventually be completed.

In organocatalytic research efforts are now directed at structural modification of cinchona alkaloids in the quinuclidine portion, in order to assess the relevance of skeletal subtleties for catalytic and biological activity. Chiral Bronstedt acid organocatalysis will remain an important tool to effect iminium ion cyclizations with high enantioselectivity.

So far, covalent ligation of the two different CLIPS peptides using the water-soluble scaffolds was successfully conducted by oxime formation. In addition, the thiol-ene reaction and the strain-promoted azide-alkyne cycloaddition will be optimized for our ligation purposes. Using the Pepscan technology libraries of discontinuous protein epitope mimics based on the new water-soluble/ligatable CLIPS-scaffolds will be made and screened for their ability to trigger the immune system to raise antibodies against them. Eventual hits will be resynthesized on larger scales to allow wider pharmacochemical and biological studies

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# Organic Chemistry

*Prof. dr. K. Lammertsma, Dr. A.W. Ehlers, Dr. J.C. Slootweg (VU)*

## Research topics

- Syntheses and applications of organophosphorus and organometallic reagents and compounds.
- Recycling current organophosphorus waste products.
- Catalytic reactions that eliminate organophosphorus waste.
- Transition metal complexes with low valent phosphorus ligands.
- Sustainable building blocks, polydentate ligands, and catalysts.
- Computational studies on metalloenzymes.

## Summary of research activities

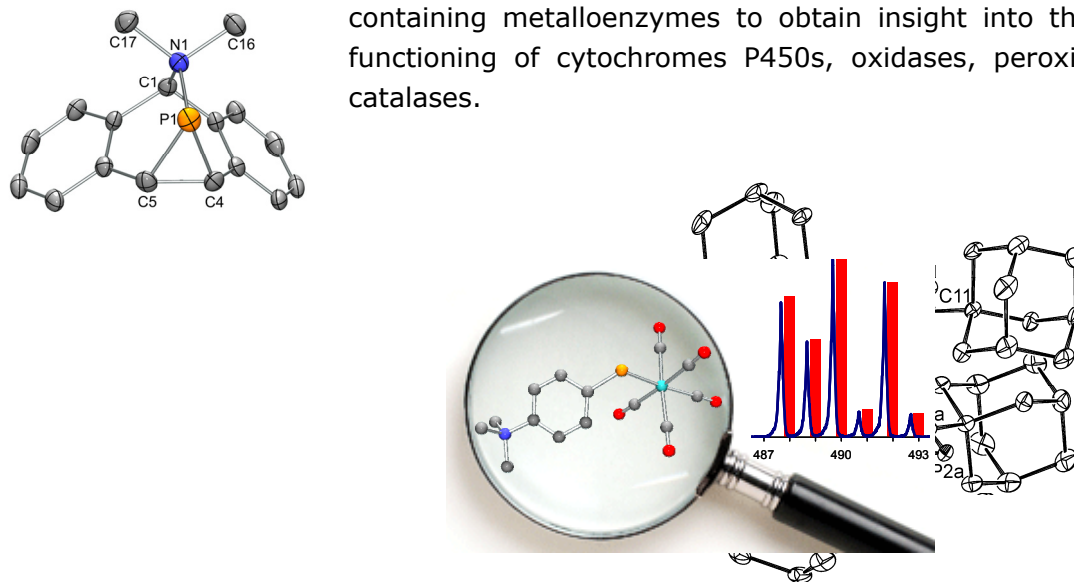
Our organophosphorus research explores new vistas with focus on the sustainability of phosphorus, an essential element in the life cycle, that will become scarce within this century at the current rate of consumption of the world's reserves. By combining synthetic methodologies with high-level theoretical modeling new reagents, tailor-made building blocks, novel compounds classes, catalysts, ligands, and (opto-electronic and polymeric) materials are designed in atom- and step-efficient manners for synthetic and catalytic applications. By exploring the relationship between phosphorus and carbon, the electronic influence on transition metals, and the valency of phosphorus, new venues are probed for the sustainable and versatile use of organophosphorus compounds.

Specifically, as a leader in organophosphorus chemistry my group mapped, since the discovery of the transient phosphinidene complex  $R-P=W(CO)_5$ , the scope of this electrophilic carbene-like complex, synthesized an abundance of unique products (ylids, polycyclic rings (condensed, catenated), (poly)spiranes, baskets, cages, 'frozen' transition structures, etc.), and new precursors. We showed the similarity with hydrocarbon chemistry through pericyclic rearrangements and additions with a molecular bevel gear as highlight. We rekindled the interest in nucleophilic phosphinidene complexes, synthesized new transition metal complexes (Co, Ru, Rh, Os, Ir), demonstrated their reactivities, and illustrated their potential as catalysts, such as for generating phosphalkenes. We showed the reagents to relate to the isoelectronic Fischer- and Schrock-type carbene complexes.

We developed new macrocycles (P/C/Al) from, conjugated rings and frames, multi-purpose fluorescent P-based polyarenes, P/C-polymers, and are preparing self-healing polymeric phospho-scorpionate catalysts. We showed phosphalkynes ( $P\equiv CR$ ) to react with phosphinidene complexes to P/C-frames and to condense with Fe- and Co-metallates to sandwiches of which the electronic states can be varied. We showed the incorporation of popular isocyanides into the P-based complexes, developed nitrilium salts as perfect building blocks for dynamic P/N-ligands suitable for coordination to many transition metals including gold, are generating several new classes of P/Al- and P/B-based Frustrated Lewis Pairs, and have developed clean reduction protocols for

phosphine oxides.

In our laboratories we also design stable non-chelating all-carbon chiral silicates and investigate the principles for the stereomutation of pentacoordinate systems. We further conduct research on artizymes and perform high-level theoretical studies on heme-containing metalloenzymes to obtain insight into the catalytic functioning of cytochromes P450s, oxidases, peroxidases and catalases.



**Figure.** Left: X-ray crystal structure of a BABAR-Phos; Middle: X-ray crystal structure of  $[\text{Co}(\eta^4\text{-P}_2\text{C}_2\text{Ad}_2)_2]^-$  complex; Right: Graphical display and MS spectrum of  $[\text{Me}_3\text{NC}_6\text{H}_4\text{-P}=\text{W}(\text{CO})_5]^+$

### Key publications 2007-2010

- H. Aktas, J.C. Slootweg, and K. Lammertsma, Nucleophilic phosphinidene complexes – access and applicability; *Angew. Chem. Int. Ed.* 49 **2010** 2102 – 2113; *Angew. Chem. Int. Ed.* 122 **2010** 2148 – 2159. (inside cover)
- E.P.A. Couzijn, J.C. Slootweg, A.W. Ehlers, and K. Lammertsma, Stereomutation of Pentavalent Compounds. Validating the Berry Pseudorotation, Redressing the Ugi's Turnstile Rotation, and Revealing the Two- and Three-Gated Turnstiles; *J. Am. Chem. Soc.* 132 **2010** 18127 – 18140.
- H. Jansen, M.C. Samuels, E.P.A Couzijn, J.C. Slootweg, A.W. Ehlers, P. Chen, and K. Lammertsma, A carbene-like phosphinidene complex caught in the act; *Chem. Eur. J.* 16, **2010** 1454 – 1458. (front cover)
- R. Wolf, J.C. Slootweg, A.W. Ehlers, F. Hartl, B. de Bruin, M. Lutz, A.L. Spek, and K. Lammertsma; A phosphorus analogue of bis( $\eta^4$ -cyclobutadiene)iron(0); *Angew. Chem. Int. Ed.* 48 **2009** 3104 – 3107; *Angew. Chem. Int. Ed.* 121 **2009** 3150 – 3153. (front cover)
- S. Burck, S.G.A. van Assema, B. Lastdrager, J.C. Slootweg, A.W. Ehlers, J.M. Otero, B. Dacunha-Marinho, A.L. Llamas-Saiz, M. Overhand, M.J. van Raaij, and K. Lammertsma, Bis-phosphine-functionalized cyclic decapeptides based on the natural

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product gramicidin S: a potential scaffold for transition-metal coordination; *Chem. Eur. J.* 15 **2009** 8134 – 8145. (frontispiece)

- A.R. Groenhof, A.W. Ehlers, and K. Lammertsma, Proton assisted oxygen-oxygen bond splitting mechanism in cytochrome P450; *J. Am. Chem. Soc.* 129 **2007** 6204 – 6209.

### **Future developments**

Our research is directed to use our expertise in organophosphorus chemistry blended with a physical-organic approach to advance sustainability in phosphorus. The issue is of eminent importance as phosphate ore, the source of all phosphorus products, may be depleted within one century. As phosphorus is an essential element in the life cycle, it is important that the chemical sector implements sustainability in phosphorus. This is still not the case. Our research will focus on all aspects of closing the cycles for use and re-use of phosphorus products, eliminating waste, while advancing the beneficial feature of novel compounds, ligands, catalysts, and materials.

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# Synthetic & Bio-Organic Chemistry

*Prof. dr. ir. R.V.A. Orru, Dr. F.J.J. de Kanter, Dr. E. Ruijter (VU)*

## Research topics

- Natural product chemistry
- Diversity oriented synthesis
- Biology oriented synthesis
- Multi-component reactions
- Biocatalysis

## Summary of research activities

Since entering the field (see *Synthesis* 2003, 1471, cited almost 400 times) the Synthetic & Bioorganic Chemistry (SBC) Chair has developed important novel entries in the emerging, highly competitive area of multicomponent reactions (MCRs) and strategies for Diversity Oriented Synthesis. The approach, using simple starting materials to generate highly diverse libraries of functionalized small molecules in a single step, is not only very efficient, versatile, and environmentally friendly, but importantly provides rapid access to key compounds for fine chemicals with high added value, like small molecular probes for chemical biology research, building blocks for medicines or ligands for catalysis.

Both mechanistic aspects, stereochemistry using biocatalysis, optimization towards robust procedures and synthetic utility are studied in-depth and our chemistry proved already successful for the synthesis of potentially biologically active molecules (antitumor, antibiotics, hepatitis C) as well as ligands relevant to catalysis (N-heterocyclic carbene complexes, organocatalysts). A highlight of our research is a spectacular and unprecedented eight-component reaction, reported as Hot Paper in *Angewandte Chemie* (Int. Ed. 2009, 48, 5856-5859) and highlighted in *Nature*. As a result, we receive growing recognition as exemplified by an invitation from *Nature Chemical Biology* for a perspective on the impact of MCRs for DOS-based library design in chemical biology research.

As a result, the SBC-group is now one of the leading players in the field of multicomponent and Diversity Oriented Synthesis-related chemistry. For example, Orru chaired the 3rd International Conference on MCRs and Related Chemistry in July 2006 in Amsterdam ([www.mcr2006.nl](http://www.mcr2006.nl)) and was a main speaker at the follow-up conference in May 2009 in Yekaterinburg, Russia. Further, Orru was a guest editor of a special issue of the Wiley journal *QSAR & Combinatorial Sciences* (2006, vol. 25, issues 5-6) on MCR chemistry and currently, together with Dr. Ruijter, is the editor of two special volumes of the Springer series *Topics in Heterocyclic Chemistry on MCRs in heterocyclic chemistry*.

## Key publications 2007-2010

- B. Groenendaal, E. Ruijter, R.V.A. Orru; 1-Azadienes in cycloaddition and multicomponent reactions towards N-heterocycles, *Chem. Commun.* 5474 **2008**

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- N. Elders, D. van der Born, L.J.D. Hendrickx, B.J.J. Timmer, A. Krause, E. Janssen, F.J.J. de Kanter, E. Ruijter, R.V.A. Orru; The Efficient One-Pot Reaction of up to Eight Components by the Union of Multicomponent Reactions, *Ang. Chem.Int. Ed.* 48 (32) **2009** 5856-5859
  - Znabet, E. Ruijter, F.J.J. de Kanter, V. Kohler, M. Helliwell, N.J. Turner, R.V.A. Orru; Highly Stereoselective Synthesis of Substituted Prolyl Peptides Using a Combination of Biocatalytic Desymmetrization and Multicomponent Reactions, *Ang. Chem.Int. Ed.* 49 (31) **2010** 5289-5292

### **Future developments**

The research of the Synthetic & Bio-organic Chemistry (SBC) chair will continue to focus on domino (or tandem) processes in context of the topics mentioned above. Smart design of our synthetic strategies based on the concepts of Diversity Oriented Synthesis (DOS) and Biology Oriented Synthesis (BIOS) take advantage of the potential of MCRs allowing molecular complexity and diversity to be created by facile formation of several covalent bonds in one-pot transformations. At the same time our reactions proceed with high atom economy and low E factors thus minimizing the number of functional group manipulations towards a given complex molecular target and avoiding the use of protective groups.

The SBC group will further expand the synthetic tool-box with highly efficient novel tandem- and multicomponent reactions covering the chemical space effectively and providing small molecules and ligands for chemical biology and medicinal chemistry research as well as for catalysis.

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## Bio-organic Synthesis

*Prof. dr. H.S. Overkleeft, Prof. dr. G.A. van der Marel,  
Prof. dr. J. Lugtenburg, Dr. ing. M. Overhand, Dr. G. Lodder,  
Dr. D. Filippov, Dr. J.D.C. Codée, Dr. R.J.B.H.N. van den Berg (UL)*

### Research topics

The central theme of the BIOSYN research group comprises the development of synthetic methodologies towards the assembly of naturally occurring molecules as well as analogs thereof. Both solution - and solid phase approaches are pursued. The developed methodologies are implemented in the design and synthesis of molecular probes such as enzyme inhibitors and proteomic tags. The synthetically prepared molecules are applied as tools in biochemical and biophysical studies to elucidate and interfere in biological processes.

### Summary of research activities

Medicinal Chemistry: Development of cell permeable selective inhibitors for each of the proteasome active sites, beta1, beta2 and beta5. Development of selective inhibitors of the three enzymes involved in glucosylceramide metabolism, GBA1, GBA2 and GCS

Chemical Biology: The first activity-based probes with which endogenous glycosidase levels in cell extracts and living cells can be monitored were developed.

Synthetic methodology: new ways to create pyrophosphates in complex biomolecules (Leloir donor saccharides, ADP-ribosylated proteins) were developed. Detailed insight in the glycosylating properties of inactive donor glycosides was obtained and applied in the construction of bacterial source oligosaccharides.

Peptide structural chemistry: A link relating hydrophobicity, haemolytic activity and bactericidal activity of structurally well-defined cyclic peptides related to the natural antibiotic gramicidin S has been established.

### Key publications 2007-2010

- M. Walvoort, G. Lodder, J. Mazurek, H. Overkleeft, J. D. C. Codée and G. van der Marel, Equatorial anomeric triflates from mannuronic acid esters, *J. Am. Chem. Soc.* **2009**, *131*, 12080.
- G. J. van der Heden van Noort, M. G. van der Horst, H. S. Overkleeft, G. A. van der Marel and D. V. Filippov, Synthesis of mono-ADP-ribosylated oligopeptides using ribosylated amino acid building blocks, *J. Am. Chem. Soc.* **2010**, *132*, 5236.
- P. P. Geurink, B. I. Florea, N. Li, M. D. Witte, J. Verasdonck, C.-L. Kuo, G. A. van der Marel and H. S. Overkleeft, A cleavable linker based on the levulinoyl ester for activity-based protein profiling, *Angew. Chem. Int. Ed.* **2010**, *49*, 6802.
- V. V. Kapoerchan, A. D. Knijnenburg, M. Niamat, E. Spalburg, A. J. de Neeling, P. H. Nibbering, R. H. Mars-Groenendijk, D. Noort, J. M. Otero, A. L. Llamas-Saiz, M. J. van Raaij, G. A. van der Marel, H. S. Overkleeft and M. Overhand, An adamantyl amino acid containing gramicidin S analogue with broad spectrum

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antibacterial activity and reduced hemolytic activity, *Chem. Eur. J.* **2010**, *40*, 12174.

- M. D. Witte, W. W. Kallemeijn, J. Aten, K.-Y. Li, A. Strijland, W. E. Donker-Koopman, B. Blijlevens, G. Kramer, A. M. C. H. van den Nieuwendijk, B. I. Florea, B. Hooibrink, C. E. M. Hollak, R. Ottenhoff, R. G. Boot, G. A. van der Marel, H. S. Overkleeft and J. M. F. G. Aerts, Ultrasensitive *in situ* visualization of active glucocerebrosidase molecules, *Nat. Chem. Biol.* **2010**, *6*, 907.

### **Future developments**

Medicinal chemistry: the creation of dedicated libraries aimed at glycosidases and glycosyl transferases in relation to lysosomal storage disorders, and at kinases in relation to cancer, is envisaged.

Chemical biology: activity-based probes for glycosidases other than GBA1, as well as kinases and yet uncharted enzymes is envisaged.

Synthetic methodology: we envisage application of or phosphorylation and glycosylation expertise in the construction of complex bioconjugates with the aim to modulate immunological events in relation to vaccine development.

Peptide structural chemistry: we intend to both extend our work in the direction of non-haemolytic gramicidin S analogues and in the direction of materials design.

# Supramolecular Catalysis and Spectro-electrochemistry

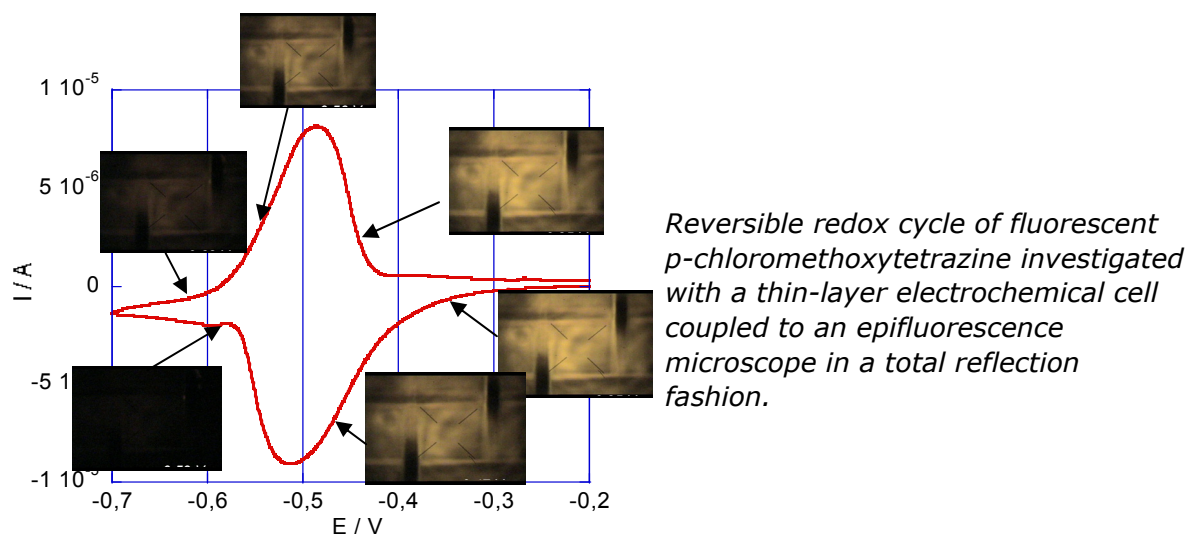
Prof. dr. J.N.H. Reek, Prof. dr. F. Hartl, Dr. B. de Bruin, Dr. J. I. van der Vlugt (UvA)

## Research topics

- ♦ Development of spectro-electrochemical techniques and their application in homogeneous and heterogeneous catalysis, photocatalysis, redox catalysis and biocatalysis.
- ♦ Energy and electron transfer in (supra)molecular dyad and triad systems driven and controlled by light absorption and/or a redox reaction.
- ♦ Photo- and electrocatalytic activation of carbon dioxide and generation of molecular hydrogen.
- ♦ Development of new approaches in transition metal catalysis and catalyst recovery, including supramolecular approach, ligand design, noninnocent ligands and metal complexes in unusual oxidation states.
- ♦ Combinatorial catalysis and kinetic analysis using robotics and HTE.
- ♦ Development of new reactions using rational approaches based on spectroscopic analysis, kinetics and dft calculations.

## Summary of research activities

We have reported first applications of thin-layer spectroelectrochemistry in combination with vibrational circular dichroism (in collaboration with the Buma group) and epifluorescence microscopy (in collaboration with ENS Cachan, France). The latter technique is a very useful and efficient tool for investigating properties of surface confined species, also in catalysis.



Photocatalytic formation of molecular hydrogen was further investigated with promising [Fe<sub>2</sub>S<sub>2</sub>]-linker-metal porphyrin triads featuring phosphoramidite bridges. The systems show improved photostability, performance and versatility compared with assemblies containing pyridylphosphine linkers.

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Diverse projects targeting electro- and photocatalytic reduction of carbon dioxide have been in progress. Most remarkable is the discovery of photocatalytic activity of low-valent manganese complexes with non-aromatic  $\alpha$ -diimine ligands, which does not require addition of sacrificial electron donors.

### Key publications 2007-2010

- R. T. F. Jukes, V. Adamo, P. Belsler, F. Hartl\* and L. De Cola; Photophysical and Photochemical Properties of Novel Fulgimide Derivatives with Attached 2,2'-Bipyridine (bpy) and  $M(\text{bpy})_3^{2+}$  ( $M = \text{Ru}$  and  $\text{Os}$ ) Moieties. *Dalton Trans.* **2009**, 3993-4002. Special Theme Issue - Supramolecular Photochemistry.
- F. Hartl, A. K. Renfrew, F. Lafalet, T. Mahabiersing, M. J. Calhorda, S. Chardon-Noblat, M. Haukka and A. Deronzier; Soluble Redox-Active Polymetallic Chains  $[\{\text{Ru}^0(\text{CO})(\text{L})(\text{bpy})\}^m]_n$  (bpy = 2,2'-bipyridine L = PrCN, Cl-;  $m = 0, -1$ ): Electrosynthesis and Characterization. *Inorg. Chem.* **2009**, 48, 8233-8244.
- A.M. Kluwer, R. Kapre, F. Hartl, M. Lutz, A.L. Spek, A.M. Brouwer, P.W.N.M van Leeuwen and J.N.H. Reek; Self-assembled Biomimetic  $[2\text{Fe}_2\text{S}]$ -Hydrogenase Based Photocatalyst for Molecular Hydrogen Evolution. *PNAS* **2009**, 106, 10460-10465.
- F.W. Patureau, M. Kuil, A.J. Sandee, J.N.H. Reek, "METAMORPhos: Adaptive supramolecular ligands and their mechanistic consequences for asymmetric hydrogenation" *Angew. Chem. Int. Ed.* **2008**, 47, 3180.
- E. Jellema, P.H.M. Budzelaar, J.N.H. Reek, B. de Bruin, "Rh-mediated polymerization of carbenes: Mechanism and stereoregulation" *J. Am. Chem. Soc.* **2007**, 129, 11631-11641.
- X.-B. Jiang, L. Lefort, P. E. Goudriaan, A. H. M. de Vries, P. W. N. M. van Leeuwen, J. G. de Vries, and J. N. H. Reek, "Robotic screening of a supramolecular catalyst library in the search for selective catalysts for the asymmetric hydrogenation of a difficult enamide substrate" *Angew. Chem. Int. Ed.* **2006**, 45, 1223.

### Future developments

The NWO ECHO project *Light-Driven Dihydrogen Production in  $[2\text{Fe}_2\text{S}]$ -Metalloporphyrin Supra-molecular Assemblies* will be continued in Amsterdam until 2012. The main targets for the coming period are full understanding of the mechanism of the photoinduced electron transfer to the catalyst site, improved photostability of the assemblies, introduction of new light harvesting metalloporphyrins and anchoring bases, and methodology for accurate quantitative determination of photogenerated molecular hydrogen.

The existing and novel spectro-electrochemical techniques and instruments, developed also for applications in photo-, electro- and heterogeneous catalysis, will be introduced to world markets jointly with Specac Ltd. (Orpington, UK).

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## Biocatalysts and Bio-organic Chemistry

*Prof. dr. R. Wever, Dr. M.A. Van der Horst, A.F. Hartog, MSc. L. Babich (UvA)*

### Research topics

- ♦ Vanadium haloperoxidases
- ♦ Acid phosphatases, phosphorylation reactions and directed evolution
- ♦ Enzyme cascade reactions and production of chiral non natural carbohydrates

### Summary of research activities

A four enzyme one-pot cascade reaction was developed by which it was possible to synthesize a wide variety of non-natural carbohydrates starting from glycerol and a variety of aldehydes, using pyrophosphate as an energy rich phosphorylating agent to drive the reaction to completion. This was carried out in collaboration with the group of prof. Rutjes (RUN). Directed evolution was used to modify the enzymes (acid phosphatase, aldolases) involved. Immobilized enzymes in a flow reactor are NOW used to produce phosphorylated compounds and carbohydrates at a gram scale.

The antimicrobial and antiviral effect of the vanadium chloroperoxidase and a mutant obtained by directed evolution was also investigated. It is concluded that this enzyme and its reaction products form a potent antimicrobial system and that the enzyme could have potential as mouth rinse.

### Key publications 2007-2010

- T. Van Herk, A.F. Hartog, L. Babich, H.E. Schoemaker, R. Wever; Improvement of an acid phosphatase –DHAP dependent aldolase cascade reaction by directed evolution. *ChemBioChem*. **10** (2009) 2230 – 2235.
- R Renirie, J. M. Charnock, C.D. Garner, R. Wever; Vanadium K-edge XAS studies on the native and peroxo-forms of vanadium chloroperoxidase from *Curvularia inaequalis*. *J Inorg Biochem* **104** (2010) 657-664.

### Future developments

We will further explore a novel approach to combine the catalytic activity of up to 3 enzymes in a single fusion enzyme product that catalyses consecutive reactions in a pathway that offers the possibility of an efficient and selective way of product formation. The physical association of enzymes may bring the active sites in close proximity resulting in channelling of the product from the first enzyme to the active site of the second enzyme rather than random diffusion to the active site. The substrate channelling in which the product is directly transferred from the first to the second enzyme without exposure to bulk solution would offer maximal transfer efficiency and may protect instable intermediates from the solvent. We will also try to immobilize the 4 enzymes used in our cascade and use them in flow reactor to further optimize product formation. The cooperation with prof. Crielaard (ACTA) on the use of the vanadium chloroperoxidase in preventing biofilm formation in the oral cavity will be continued.

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## 2.2 Theme 2 - Photochemistry and (Laser) Spectroscopy

The interaction between light and molecular matter is central in a large number of fundamental and applied research areas in molecular chemistry and physics. In HRSMC it is employed to probe and utilize fundamental processes such as reaction mechanisms and dynamics, catalytic events, energy and electron transfer, conformational dynamics, and dynamic life processes. Concurrently, advanced spectroscopic techniques are used to elucidate inter- and circumstellar chemistry, and for analytical applications. Many of the groups working in this area are renowned for their development and application of new spectroscopic techniques. Various groups in the Netherlands conduct scientific research in spectroscopy, but photo-chemical and photo-physical research of inorganic and organic compounds in gas and condensed phases is increasingly confined to groups within HRSMC.

The group of **Buma/Brouwer** aims to extend the fundamental knowledge of excited states. The spectroscopic tools and the scientific competences that are required to do this enable the team to enter into numerous projects in which light-matter interaction is essential. This leads to the application of a photonic approach to the broader scientific and technological fields of molecular biology, polymer science, nanoscience, catalysis, solar energy conversion and medical imaging and phototherapies.

In the group of **Gooijer** in the area of Applied Spectroscopy (Biomolecular Spectroscopy) laser spectroscopic methods such as Raman Spectroscopy (RS) and time-resolved luminescence spectroscopy in a variety of modes are involved and/or developed for bioanalytical and biophysical purposes. Emphasis is on the structure and dynamics of ligand protein interactions.

In the Molecular Nano-Optics and Spins group, the subgroup of **Orrit** is interested in the optical detection and study of single fluorescent molecules and of single gold nanoparticles. The projects have contacts with biophysics, physical chemistry, soft matter physics and solid state physics. The subgroup of **Groenen** uses electron spin resonance spectroscopy to study the structure and dynamics of (bio)molecules. An important part of the activity is devoted to spin-labeled proteins and metalloenzymes. The subgroup of **Völker** studies the optical properties and the dynamics of fluorescent proteins by spectroscopic techniques, in particular spectral hole-burning at low temperatures.

The group of **De Groot** is highly recognised for its studies in high-resolution Magic Angle Spinning Solid State NMR studies. The research takes part in the European centre for ultra high field solid state NMR in Leiden and is mainly concerned with the electronic and spatial structure of membrane proteins involved in visual signal transduction and photosynthetic energy conversion.

The group of **Janssen** at LaserLaB Amsterdam performs laser-spectroscopic studies to advance the understanding and to develop the control of (nonadiabatic) dynamics in photochemical reactions. The group integrates and utilizes quantum-state selectors, (ultrafast) lasers, pulse shaping and position sensitive electron- and ion imaging detectors in photochemistry to study, manipulate, and control (nonadiabatic) effects in molecular photo-induced dynamics, with special interest in coherences from quantum interference.

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The **Koper** group studies chemical reactions on well-defined, mostly single crystalline, surfaces at the molecular level. The group combines state-of-the-art experimental setups to study surface catalytic reactions using a variety of spectroscopic techniques, both at the metal-uhv and metal-liquid interface, with computational techniques. Their aim is to unravel mechanistic and kinetic aspects of important catalytic reactions that feature in industrial processes, fuel reforming, fuel cells, the hydrogen economy, and environmental catalysis. The group is also part of NRSC-Catalysis and NIOK.

The group of **Linnartz** represents one of the very few places worldwide where physical and chemical laboratory research is fully dedicated to characterize inter- and circumstellar chemistry. The laboratory comprises several spectrometers to guide and interpret results from large scale astronomical facilities. In addition, the research covers the emerging field of solid state astrochemistry in which icy dust grains are exhibited to thermal and UV processing and bombarded by individual atoms to generate both simple and complex molecules under conditions as typical in space.

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## Molecular Photonics

*Prof. dr. W.J. Buma, Prof. dr. A.M. Brouwer, Prof. dr. J.W. Verhoeven, Dr. R. M. Williams, Dr. S. Woutersen, Dr. H. Zhang (UvA), Prof. dr. H.J. Bakker (AMOLF), Prof. dr. J. Oomens (FOM Rijnhuizen)*

### Research topics

- Dynamics of supramolecular and biomolecular systems
- Photoprocesses in nanostructures
- Photochemical processes

### Summary of research activities

Molecular nanotechnology:

We have shown how in the gas phase binding interactions between the thread and the macrocycle of a [2]rotaxane can be tuned in a quasi-continuous manner by adding hydrogen-bond-forming solvent molecules one at a time to an isolated [2]rotaxane molecule. In this way conformational changes have been induced that detach controllably the thread from the macrocycle (*Angew. Chem. Int. Ed.* **2010**, 49, 3896-3900).

Molecular machines in motion:

Using time-resolved vibrational spectroscopy, we have investigated the operation mechanism of a rotaxane-based molecular shuttle. The shuttling involves two steps: thermally driven escape from the initial station, followed by fast motion along the track ending either at the initial or final station. The fast motion approximates a biased random walk. Surprisingly, the direction of the overall motion is opposite that of the bias (*Science* **2010**, 328, 1255-1258). A modification of the molecular design led to a bistable molecular shuttle. The thermodynamics of this system could be studied with high precision, which revealed the importance of entropy and heat capacity differences between the two co-conformational states (*Chem. Commun.* **2010**, 46, 2061-2063).

Tunneling electrons through bends and around corners:

A simple theoretical model has been developed that describes orientation effects in electron transfer. In this model the twist and dihedral angles between electron donor (D) and acceptor (A) play a role in the distance dependence of charge transfer (CT), next to the conventional distance dependence of electron transfer that is not influenced by the angles between D and A. This can be applied to, for example, helical bridges, when twist and dihedral angles can modulate the rate. The new equation is dubbed: Karplus Relation for Charge Transfer Interaction. It can be used to describe orientation effects and non-linear plots of  $\ln(k_{cs})$  vs. distance (*Photochem. Photobiol. Sci.* **2010**, 9, 1018-1026). Furthermore, charge separation processes in two low-band gap oligomer/fullerene C<sub>60</sub> triads that are models for new organic solar cell materials were studied in collaboration with TU-Eindhoven (*Photochem. Photobiol. Sci.* **2010**, 9, 1055-1065; *J. Phys. Chem. B*, **2010**, 114, 14149-14156).

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#### Photoactive proteins:

A series of high-resolution laser spectroscopic studies have been performed on para-coumaric acid and derivatives, chromophores of the Photoactive Yellow Protein. These have led to the first characterization of their electronically excited-state manifold under isolated-molecule conditions (*J. Am. Chem. Soc.* **2010**, *132*, 6315-6317).

#### Ion spectroscopy:

A new method has been developed that allows for the observation of IR and UV/Vis spectra of cold and isolated molecular ions with unprecedented sensitivity. To this purpose ions are captured in nanodroplets of superfluid helium. The study opens up exciting new opportunities for the investigation of ionic that may range from biomolecular ions such as polypeptides and proteins to ionic clusters (*J. Am. Chem. Soc.* **2010**, *132*, 14086-14091).

#### Silicon nanocrystals:

In collaboration with the group of T. Gregorkiewicz (Van der Waals – Zeeman Institute, UvA), no-phonon optical transitions that are tunable into the visible range have been identified in silicon nanocrystals. The enhanced quantum efficiency of this emission compared to bulk silicon (three orders of magnitude for 2.5-nm-diameter nanocrystals) creates new opportunities in photonic, photovoltaic and optoelectronic applications of silicon nanocrystals (*Nature Nanotech.* **2010**, *5*, 878-884).

#### Designing nanoplatfoms for homogeneous assay and cancer detection and therapy:

Various nanostructures/complexes have been tailor-designed for the biological application. Au/SiO<sub>2</sub> core/shell nanoparticles have been designed to enhance significantly sensitivity of the homogeneous assay based on FRET from QDs to organic fluorophores in solution (*Chem. Comm.* **2010**, *46*, 6479-6481). Multi-targeting single fiber-optic biosensor based on evanescent wave and quantum dots was realized for the first time (*Biosensors and Bioelectronics* **2010**, *26*, 149-154).

#### Single molecular spies:

A new mechanism for single molecule fluorescence switching based on photoinduced electron transfer was exploited to detect spatial and temporal heterogeneities in thin polymer films. The electron transfer process requires a sufficiently large free volume to occur. As a result, fluorescence is switched off when heating the material from temperatures below the glass transition to a few degrees above it (*J. Am. Chem. Soc.* **2010**, *132*, 1240-1242).

#### Fluorescence microscopy assists catalyst development:

In a collaboration with the HIMS homogeneous catalysis group, two-photon fluorescence imaging pointed the way to a large improvement in the preparation of immobilized catalysts. A simple change in the experimental procedure avoided the formation of clusters of ligands in solution, prior to condensation on the substrate. The catalyst thus produced was very active and could be recycled effectively (*Angew. Chem. Int. Ed.* **2010**, *49*, 5480 –5484).

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### Key publications 2007-2010

- M. de Groot, R.W. Field, W.J. Buma; Intersystem crossing in acetylene: interference effects reveal a double doorway mechanism. *Proc. Natl. Acad. Sci. USA* **106** (2009) 2510-2514.
- A.M. Kluwer, R. Kapre, F. Hartl, M. Lutz, A.L. Spek, A.M. Brouwer, P.W.M.N. van Leeuwen, J.N.H. Reek; Self-assembled biomimetic [2Fe2S]-hydrogenase-based photocatalyst for molecular hydrogen evolution. *Proc. Natl. Acad. Sci. USA* **106** (2009) 10460-10465.
- F. Marras, A.M. Kluwer, J.R. Siekierzycka, A. Vozza, A.M. Brouwer J.N.H. Reek; Phosphorus ligand imaging with two-Photon fluorescence spectroscopy: towards rational catalyst immobilization. *Angew. Chem. Int. Ed.* **49** (2010), 5480–5484.
- M.R. Panman, P. Bodis, D.J. Shaw, B.H. Bakker, A.C. Newton, E.R. Kay, A.M. Brouwer, W.J. Buma, D.A. Leigh, S. Woutersen; Operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy. *Science* **328** (2010), 1255-1258.
- A.M. Rijs, N. Sändig, M.N. Blom, J. Oomens, J.S. Hannam, D.A. Leigh, F. Zerbetto, W.J. Buma; Controlled hydrogen-bond breaking in a rotaxane by discrete solvation. *Angew. Chem. Int. Ed.* **49** (2010), 3896-3900.
- W.D.A.M. de Boer, D. Timmerman, K. Dohnalova, I.N. Yassievich, H. Zhang, W.J. Buma, T. Gregorkiewicz; Red spectral shift and enhanced quantum efficiency in phonon-free photoluminescence from silicon nanocrystals. *Nature Nanotech.* **5** (2010), 878-884.

### Future developments

High-resolution laser spectroscopy of large molecular systems will continue to be one of the main lines of research. Topical areas of application are molecular nanotechnology and (photo-induced) biomolecular conformational dynamics. The emphasis of this research will shift towards the time-resolved study of dynamical phenomena. A novel area we aim to apply our knowledge on are inorganic nano-clusters of importance for (photo)catalytic applications. The strong collaborations with the Free Electron Laser facilities (currently FELIX at FOM Rijnhuizen, in the future also FLARE at RU) will be continued and expanded.

The application of Vibrational Circular Dichroism (VCD) to study molecular conformational properties and dynamics will be continued. Initial experiments on a new approach to use optical amplification of VCD spectra have provided positive results, and will be expanded. In view of the expertise we are currently building up in this field and the potential VCD has for applications in core research areas of the HRSMC, we expect that the interest expressed by other groups for further collaboration will increase.

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Fluorescent probes are finding more and more applications, in polymer science and in the studies together with the physics institute on colloidal matter. The combination of molecular probes and optical microscopy is still relatively under-developed in these fields.

Next to further theoretical development and practical application of the "Karplus relation for charge transfer interaction", focus will be directed at photo-induced processes in new materials for organic solar cells as well as the development and study of new photocatalytic systems. Our long-standing knowledge in the field of photoinduced electron transfer will be exploited in a new project together with the Homogeneous Catalysis group aiming at the catalytic oxidation of water.

The application of two-dimensional vibrational spectroscopy to molecular machines and biomolecular systems will be expanded to include time-resolved 2D-IR experiments in the nanosecond to millisecond range. As a first step in this direction we have recently performed time-resolved visible-pump/IR-probe experiments on the Photoactive Yellow Protein in the ns-ms range, and we are currently extending the optical setup to also allow for 2D-IR probing.

The upconversion nanoplatfom will be optimized for the diagnosis and therapy of cancer cells, as well as for bacteria. We are developing new approaches to improve the upconversion efficiency from the structural optimization as well as doping concentration improvement. The new concept of fiber detection is developed and will be validated for biomedical applications.

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## Biomolecular Spectroscopy

*Prof. dr. C. Gooijer, Dr. F. Ariese, Dr. G. v.d. Zwan (VU)*

### **Research topics**

- Application of spectroscopic methods to study the structure and dynamics of ligand-protein complexes
- Hyphenation of liquid separation techniques and (laser) spectroscopic identification methods
- High-resolution fluorescence spectroscopy under cryogenic conditions
- UV-resonance and pico-second time-gated Raman spectroscopy
- Spectro-electrochemistry of redox protein systems

### **Summary of research activities**

In the past five years methods were developed that combine electrochemistry and spectroscopy. In particular, we now have a small volume flow cell that fits under the Raman microscope, in which a small silver working electrode fits, together with the counter and reference electrode. The Krypton laser line at 413 nm is eminently suited to study hemes by resonance enhanced Raman methods, and the silver gives even better results due to the surface enhancement effect at those wavelengths for silver. It being a flow cell also allows us to get oxygen free conditions, and to study the effect of substrate binding in a time-resolved manner. So far we mainly concentrated on the monooxygenases P4502D6 and P450BM3, and the electron transport protein cytochrome c. Currently other redox proteins are studied as well.

Time-resolved and steady state fluorescence methods were mainly concentrated on the antihistamines (inverse agonists) mepyramine and tripeleennamine. These were found to have complicated photophysics, as a consequence of tautomerism, internal hydrogen bonding, and intramolecular energy and electron transfer. Although this leads to complicated spectroscopic dependence on pH, solvent properties, and excitation wavelength, it also makes these compounds suitable for binding studies. Detailed information about the molecular structure of these antihistamines in aqueous solution (under sufficiently low concentrations to avoid aggregate formation) could be obtained by UV resonance Raman spectroscopy. Use was made of selective excitation at 229 nm and 257 nm.

Time-resolved Raman with a picosecond Ti:sapphire system and fast gated ICCD detection was used to record Raman spectra from deeper layers through diffusely scattering media. This was then applied to depth profiling and contrast studies within polymer layers, as a test case for biomedical imaging.

Time-resolved phosphorescence was coupled to capillary electrophoresis and could be used for the enantiospecific detection of (+) and (-)-camphorquinone.

Cavity ring-down spectroscopy (CRDS) in evanescent-wave mode was used to study protein binding phenomena on silica and on various surface coatings. It enabled the direct observation of protein-wall interactions – a main point of concern in capillary electrophoresis of proteins – and the investigation of the performance of various coating layers utilized to prevent protein adsorption.

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### Key publications 2007-2010

- A. Bonifacio, A.R. Groenhof, P.H.J. Keizers, C. de Graaf, J.N.M. Commandeur, N.P.E. Vermeulen, A.W. Ehlers, K. Lammertsma, C. Gooijer, G. van der Zwan; Altered spin equilibrium in the T309V mutant of cytochrome P450<sub>2D6</sub>: a spectroscopic and computational study. *J. Biol. Inorg. Chem.* **12** (2007) 645-654.
- F. Ariese, H. Meuzelaar, M.M. Kerssens, J.B. Buijs, C. Gooijer: Picosecond Raman spectroscopy with a fast intensified CCD camera for depth analysis of diffusely scattering media. *Analyst* **134** (2009) 1192-1197.
- I. Lammers, J. Buijs, G. van der Zwan, F. Ariese, C. Gooijer: Phosphorescence for sensitive enantioselective detection in chiral capillary electrophoresis. *Anal. Chem.* **81** (2009) 6226-6233.

### Future developments

Current research on heme proteins focusses on the immobilization of cytochrome P450<sub>BM3</sub> mutants on modified silver electrodes, in order to design a system where electron transfer can be accomplished from the electrode, while allowing simultaneous spectroscopic measurements. A triggering system where electron transfer is induced by a potential jump and Raman spectra can be measured as a function of time after the jump is under development. In addition to P450's other heme proteins (Cytochrome C<sub>4</sub>, IDO, TDO) will be the topic of investigation. Present attention is on mutants of P450<sub>BM3</sub> which has an active site resembling that of human P450-2D<sub>6</sub>.

Exploring experiments have shown that UV-Resonance Raman is an appropriate technique to obtain detailed structural information about protein-ligand interactions in the liquid aqueous-state at sufficiently low protein concentrations. Much effort will be devoted to the (further) development of an appropriate set-up. The method will be exploited for various protein-ligand combinations.

Furthermore UV-Resonance Raman will be coupled to flow systems, such as CE.

Enantiomer-specific detection of chiral molecules is a hot topic in lifesciences and pharmacochemistry, since the two enantiomers of a compound often have completely different biological properties. Strategies are being developed to detect and identify enantiomers based on differences in phosphorescence lifetime, in combination with capillary electrophoresis (CE) separation. Present attention is on sensitised phosphorescence, to improve detection limits. Furthermore detailed interactions of bioactive compound with the transport protein human serum albumin (HAS) are studied.

Time-resolved Raman using fast gated detection is being explored to reject fluorescence interference and for time-gated detection for depth profiling, contrast studies and applications to biomedical imaging.

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## Molecular Nano-Optics and Spins

*Prof. dr. E.J.J. Groenen, Prof. dr. M. Orrit, Prof. dr. S. Völker,  
Dr. P. Gast, Dr. M. I. Huber (UL)*

### Research topics

- Electronic and geometric structure determination and dynamics by multifrequency, cw and pulsed Electron Paramagnetic Resonance (EPR) and Electron Nuclear Double Resonance (ENDOR).
- Single-molecule fluorescence and absorption spectroscopy, microscopy of single metal nanoparticles, optical trapping and diffusion of single nanoparticles.
- Photophysics, conformational dynamics and relaxation processes of (bio)molecular systems probed by high-resolution, site-selective laser spectroscopy and optical hole-burning.

### Summary of research activities

In the past few years, the Orrit subgroup has focused on the interplay of light and heat for the detection and study of single objects. The energy absorbed by a nanoparticle and released as heat in the environment can be used to detect and study the absorbing object. Recently, the sensitivity of these absorption experiments reached the single-molecule limit. The heat released upon absorption can also be used to activate various motions of single molecules, for example conformational changes of FRET-labeled peptides. One of group's foci is the optical manipulation and study of gold nanoparticles. We have recently trapped single gold nanorods as small as 60 nm in length and 25 nm in diameter and studied their rotation and translation dynamics in the optical trap.

The Groenen subgroup has developed a new probe head for continuous wave EPR spectroscopy at the unusually high microwave frequency of 275 GHz. Thereby the sensitivity and signal stability has been enhanced to such an extent that high-spin Fe(III) active centres in low-concentration protein solutions could be studied. Another focus concerns the investigation into the mechanism of oxygen reduction in multicopper oxidases, where we recently identified an unexpected transient biradical intermediate. We have demonstrated that spin-label EPR is an excellent tool to study the conformation of disordered proteins in the free and membrane-bound state. We have even detected aggregates of such proteins, which shows the scope of the approach.

### Key publications 2007-2010

- Drescher, M., Rooijen, B.D. van, Veldhuis, G., Subramaniam, V., Huber, M.; A Stable Lipid-Induced Aggregate of  $\alpha$ -synuclein.  
*J. Am. Chem. Soc.* **132** (2010) 4080-4082
- Kulzer, F., Xia, T., Orrit, M.; Single molecules as optical nanoprobe for soft and complex matter.  
*Angew. Chem. Int. Ed.* **49** (2010) 854-866.
- Purchase, R., Völker, S.; Spectral hole burning: examples from photosynthesis.  
*Photosynth. Res.* **101** (2009) 245-266

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### **Future developments**

In the next few years, the Orrit subgroup expects to manipulate single gold nanoparticles in complex environments, to explore such local properties as mechanical responses (stiffness, viscosity) or refractive index, and to correlate them with local structures and processes. An exciting field of application will be the exploration of live cells with this technique. Another fascinating subject is the study of single-molecule dynamics by the temperature jump method. Within the next four years, we expect to apply this technique to complex protein dynamics on a single-molecule basis. Finally, low-temperature spectroscopy experiments will be exploited in quantum optical projects and for the study of plasmon enhancement in the vicinity of metallic nano-antennas.

The Groenen subgroup will exploit the potential of multifrequency EPR in combination with high-field electron-nuclear double resonance in the study of enzymatic processes. A new approach will be pioneered at 275 GHz to try and increase the time resolution of kinetic EPR experiments. In addition, methods will be developed further to study the dynamics and interactions of molecules and proteins, both in solutions and membrane related systems.

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# Biophysical Organic Chemistry

*Prof. dr. H.J.M. de Groot, Dr. F. Buda, Dr. J. Matysik (UL)*

## **Research topics**

Membrane Proteins and Solid State NMR

## **Summary of research activities**

The long term goal of our group is to reach understanding of structure, dynamics and functional mechanisms of membrane proteins and self-organized biological assemblies and to translate this knowledge into new concepts for nano-devices, medicine, and new materials of technical importance. Central fundamental research theme is the electronic and spatial structure of membrane proteins involved in photosynthetic energy conversion and visual signal transduction. The fundamental research in the field of rhodopsin and the photosynthetic energy transformation has a spin off towards applications and research in the field of g-protein coupled receptors and artificial photosynthesis.

MAS NMR for structure determination:

Protein nuclear magnetic resonance (NMR) secondary chemical shifts are widely used to predict the secondary structure, and in solid-state NMR, they are often the only unambiguous structural parameters available. However, the employed prediction methods are empirical in nature, relying on the assumption that secondary shifts are only affected by shielding effects of neighboring atoms. We analyzed the secondary shifts of a photosynthetic membrane protein with a high density of chromophores and very tight packing, the light harvesting 2 (LH2) complex of *Rhodospseudomonas acidophila*. A relation was found between secondary shift anomalies and protein-protein or pigment-protein tertiary and quaternary contacts. For several residues, including the bacteriochlorophyll-coordinating histidines (RH31 and  $\beta$ H30) and the phenylalanine RF41 that has strongly twisted Cb-Ca-C and Ca-C-N conformations in the LH2 crystal structure, the perturbing effects on the backbone chemical shifts were tested by density functional theory (DFT) calculations. We propose that higher-order interactions in the tightly packed complex can induce localized perturbations of the backbone conformation and electronic structure, related to functional pigment-protein or protein-protein interactions.

Chlorosomes are the largest and most efficient light-harvesting antennae found in nature, and they are constructed from hundreds of thousands of self-assembled bacteriochlorophyll (BChl) pigments. Because they form very large and compositionally heterogeneous organelles, they had been the only photosynthetic antenna system for which no detailed structural information was available. By combining SSNMR and cryoEM techniques complemented by DFT calculations, we have determined the structure of a member of the chlorosome class and compared with the wild type to resolve how the biological light-harvesting function of the chlorosome is established.

The cyanobacterial phytochrome Cph1 can be photoconverted between two thermally stable states, Pr and Pfr. The photochemically induced Pfr  $\rightarrow$  Pr back-reaction has been followed at low temperature by magic-angle spinning (MAS) NMR spectroscopy, allowing two intermediates, Lumi-F and Meta-F, to be trapped. Employing uniformly  $^{13}\text{C}$ - and

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<sup>15</sup>N-labeled open-chain tetrapyrrole chromophores, all four states - Pfr, Lumi-F, Meta-F, and Pr - have been structurally characterized. In the first step, the double bond photoisomerization forming Lumi-F occurs. The second step, the transformation to Meta-F, is driven by the release of the mechanical tension. This process leads to the break of the hydrogen bond of the ring D nitrogen to Asp-207 and triggers signaling. The third step is protonically driven allowing the hydrogen bonding interaction of the ring D nitrogen to be restored. Compared to the forward reaction, the order of events is changed, probably caused by the different properties of the hydrogen bonding partners of N24, leading to the directionality of the photocycle.

Quantum chemical modeling:

Molecular Modeling and quantum chemical calculations based on density functional theory (DFT) and Car-Parrinello Molecular Dynamics (CPMD) simulations are also performed in our group to translate spectroscopic information into models and to investigate functional mechanisms. These computational techniques are currently applied to study fundamental processes in models of Bacterial Reaction Centres, and to get insight in the mechanism of water oxidation catalysts.

### **Key publications 2007-2010**

- Ganapathy, S., Oostergetel, G.T., Wawrzyniak, P.K., Reus, M., Chew, A.G.M., Buda, F., Boekema, E.J., Bryant, D.A., Holzwarth, A.R., de Groot, H.J.M. , Alternating syn-anti bacteriochlorophylls form concentric helical nanotubes in chlorosomes, *Proc. Natl. Acad. Sci. USA*, (2009) vol. 106, no. 21, pp. 8525-8530.
- Pandit, A., Wawrzyniak, P.K., van Gammeren, A.J., Buda, F., Ganapathy, S., de Groot, H.J.M. , Nuclear Magnetic Resonance Secondary Shifts of a Light-Harvesting 2 Complex Reveal Local Backbone Perturbations Induced by Its Higher-Order Interactions, *Biochemistry*, (2010) vol. 49, no. 3, pp. 478-486.
- Rohmer, T., Lang, C., Bongards, C., Gupta, K., Neugebauer, J., Hughes, J., Gartner, W., Matysik, J. , Phytochrome as Molecular Machine: Revealing Chromophore Action during the Pfr -> Pr Photoconversion by Magic-Angle Spinning NMR Spectroscopy, *J. Am. Chem. Soc.*, (2010) vol. 132, no. 12, pp. 4431-4437.

### **Future developments**

Development of advanced ultra high field solid-state MAS NMR technology for structure and structure-function determination: NMR structure determination is both an important and a highly significant enabling technology for our energy conversion studies. We will continue our efforts to develop and apply methodology for structure determination with solid state NMR in high and ultra high magnetic fields.

Quantum chemical calculations: Theoretical modeling is an integral part of our research (i) to translate spectroscopic information directly into models for the spatial and electronic structure and (ii) to formulate detailed hypotheses regarding operational

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mechanisms. We will focus on the mechanisms of photosynthetic oxygen production in natural and artificial photosynthesis.

From natural photosynthesis to artificial photosynthesis: Self-organised antenna and reaction center complexes are currently becoming widely considered as a paradigm for solar cell research. We plan to use a combination of solid state NMR and state-of-the-art modeling tools to resolve the structural dynamics and chemistry of crucial catalytic reactions in photosynthesis. A minimal model for the multielectron water splitting catalytic cycle in photosystem II (PSII) can serve as a starting point for the design of photoanodes comprising multivalent metal clusters embedded in man-made smart matrices. We expect to give proof of principle that including hierarchical organizational principles from biology can lead to improved photovoltaics technology.

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# Physical Chemistry

*Prof. dr. M.H.M. Janssen (VU)*

## **Research topics**

Our mission is to advance the understanding and to develop the control of (nonadiabatic) dynamics in photochemical reactions. Our scientific objectives are:

- to integrate and utilize quantum-state selectors, (ultrafast) lasers, pulse shaping and position sensitive electron- and ion imaging detectors in photochemistry.
- to study, manipulate, and control (nonadiabatic) effects in molecular photo-induced dynamics, with special interest in coherences from quantum interference.
- to foster the theoretical understanding and the quantitative ab initio modeling of (nonadiabatic) photochemical dynamics by providing fully quantum resolved state-to-state three-dimensional angular-resolved scattering data.

## **Summary of research activities**

The control of photofragmentation and ionization in a polyatomic molecule has been studied by femtosecond chirped laser pulse excitation and velocity map photoelectron and ion imaging. The experiments aimed at controlling and investigating the photodynamics in  $\text{CH}_2\text{BrCl}$  using tunable chirped femtosecond pulses in the visible wavelength region 509–540 nm. We observed that the time-of-flight mass spectra as well as the photoelectron images can be strongly modified by manipulating the chirp parameter of ultrashort laser pulses. Specifically, a strong enhancement of the  $\text{CH}_2\text{Cl}^+/\text{CH}_2\text{BrCl}^+$  ion ratio by a factor of five and changes in the photoelectron spectra were observed for positively chirped pulses centered near 520 nm. These changes are only observed within a narrow window of wavelengths around 520 nm and only for positively chirped pulses. From the combination of the photoelectron spectra and the ion recoil energy of the  $\text{CH}_2\text{Cl}^+$  fragment we can deduce that the parent ionization and fragmentation is induced by a multiphoton excitation with five photons. The photoelectron images and the fragment ion images also provide the anisotropy-parameter of the various electron bands and fragment ions. We conclude that multiphoton excitation of the highest occupied  $22a'$  and  $8a''$   $\text{CH}_2\text{BrCl}$  molecular orbitals of Br-character are both involved in the five-photon ionization, however, only excitation of the  $22a'$  orbital appears to be mostly involved in the chirped control dynamics leading to enhanced fragmentation to  $\text{CH}_2\text{Cl}^+ + \text{Br}$ . We propose that a wavepacket following on a time-delay resonance mechanism between the two-photon excited repulsive surface and the three-photon near-resonant Rydberg state of the neutral  $\text{CH}_2\text{BrCl}$  molecule is responsible for the enhanced excitation with up-chirped pulses.

Furthermore, the femtosecond multiphoton photoionization and dissociation dynamics of  $\text{NO}_2$  have been studied in a twocolor pump-probe experiment at 400 and 266 nm using velocity map ion imaging in conjunction with photoelectron imaging. We report here a series of experiments focusing on the oscillatory patterns in pump-probe transients of the photoelectron signal. By using the technique of spatially masked imaging detection, we can select different photoelectron channels enabling the rapid measurement of energy selected transients with good signal-to-noise ratio. Distinctive oscillatory patterns were

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found in the pump-probe transients of the photoelectron yield for both the slow and the fast photoelectron channels but with different periods of about 750 fs (slow) or 590 fs (fast). Extensive polarization experiments are reported for both linear and circular polarized pump and probe laser geometries. We discuss the oscillatory mechanism in relation to *ab initio* calculations of relevant Rydberg and valence type excited states of NO<sub>2</sub> near 9.3 eV. We propose that an oscillating wavepacket of mixed Rydberg and valence character that predissociates is responsible for the observed oscillations in the transients of the fast (0.88 eV) photoelectron channel.

### Key publications 2007-2010

- Vredenburg, W.G. Roeterdink and M.H.M. Janssen  
A photoelectron-photoion coincidence imaging apparatus for femtosecond time-resolved molecular dynamics with electron TOF resolution of  $\sigma=18$  ps and energy resolution  $\Delta E/E=3.5\%$ , *Rev. Sci. Instrum.* **79** (2008), 063108 (9 pages) Selected for Virtual Journal of Ultrafast Science 7, Issue July (2008)
- D. Irimia, R. Kortekaas and M.H.M. Janssen  
In situ characterization of a cold and short pulsed molecular beam by femtosecond ion imaging *Phys. Chem. Chem. Phys.* **11** (2009), 3958 (9 pages)
- D. Irimia, and M. H. M. Janssen, Toward elucidating the mechanism of femtosecond pulse shaping control in photodynamics of molecules by velocity map photoelectron and ion imaging, *J. Chem. Phys.* **132** (2010), 234302 (9 pages) Selected for Virtual Journal of Ultrafast Science 9, Issue July (2010)

### Future developments

At present a strong effort is developed (supported by NWO/CW en EU) in the direction of coherent control using pulse shaping and advanced imaging techniques. In addition, we see good opportunities for a novel research direction in the field of Cold Molecules and Chemistry. This new direction (supported by NWO/CW) will have strong synergy with research lines within the Physics-group of Prof. Ubachs on spectroscopy/metrology in cold molecules (also with ERC/VIDI- Dr. Bethlem and VICI-Prof. Eikema). Furthermore, we will pursue (supported by NWO/CW) the 'complete experiment', providing key benchmark data for testing and fostering *ab initio* quantum chemical dynamics theory. Additional ideas exist to capitalize on recent technological innovations developed in our group regarding high-repetition rate pulsed molecular beams, both in fundamental research as well as in mass spectrometric applications. We collaborate with ERC/VIDI fellow Dr. Iannuzzi within LaserLaB Amsterdam applying laser machining for specially designed nozzle structures for sophisticated high-performance and compact molecular beam experiments. Various groups are very interested in our pulsed valve innovations or have purchased our piezo valve recently (Leeds, Oxford, Nijmegen, Daresbury, Fritz-Haber-Institute Berlin, Beijing, Shanghai, Vancouver, Hamburg XFEL/CFEL).

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## Surface chemistry and Catalysis

*Prof. dr. M. Koper, Dr. L.B.F. Juurlink, Dr. A.I. Yanson (UL)*

### **Research topics**

The research aim of the Surface Chemistry and Catalysis group is to probe and understand chemical reactions on well-defined, mostly single crystalline, surfaces at the molecular level. The group combines state-of-the-art experimental setups to study surface catalytic reactions using a variety of spectroscopic techniques, both at the metal-uvh and metal-liquid interface, with computational techniques based on density functional theory and dynamic Monte Carlo simulations.

Our aim is to unravel mechanistic and kinetic aspects of important catalytic reactions that feature in industrial processes, fuel reforming, fuel cells, the hydrogen economy, and environmental catalysis. Equipped with this fundamental insight, we aim to contribute to the rational design of catalysts. An important area of inspiration is biocatalysis and enzymes, and the comparison of reactions at different catalysts (metal surfaces, enzymes) at different interfaces (metal-gas, metal-liquid, enzyme-liquid).

The group currently has three main research themes: electrocatalysis (Koper), ultra-high vacuum surface science (Juurlink), and scanning probe microscopy of catalytic surfaces (Yanson). Funding for our research comes from Leiden University, the Netherlands Organization for Scientific Research NWO (VICI, VIDI, ECHO, ASPECT), Catchbio, the European Union (various projects), the European Science Foundation, and the National Research School Catalysis (NRSC).

### **Summary of research activities**

- Structure sensitivity of catalytic reactions at stepped platinum
- surfaces, both in UHV and electrochemical environments
- Carbon dioxide reduction
- Nitrogen cycle electrocatalysis
- Gold (electro)catalysis
- Electrochemistry of and at nanoparticles

### **Key publications 2007-2010**

- P.Rodríguez, A.A.Koverga, M.T.M.Koper, Carbon monoxide as a promotor for its own oxidation on a gold electrode, *Ang. Chem. Int. Ed.* **49** (2010) 1241-1243.
- S.C.S.Lai, S.E.F.Kleijn, V.Rosca, M.T.M.Koper, Mechanism of the dissociation and electrooxidation of ethanol and acetaldehyde on platinum as studied by SERS, *J. Phys. Chem. C* **112** (2008) 19080-19087.
- M.J.T.C. van der Niet, A.den Dunnen, L.B.F.Juurlink, M.T.M.Koper, Co-adsorption of O and H<sub>2</sub>O on nano-structured platinum surfaces: does OH form at steps?, *Ang. Chem. Int. Ed.* **49** (2010) 6572-6575.

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- M.Duca, M.Oroval Cucurella, P.Rodriguez, M.T.M.Koper, Direct reduction of nitrite to N<sub>2</sub> on a Pt(100) electrode in alkaline media, *J. Am. Chem. Soc.* **132** (2010) 18042-18044.
  - V.Rosca, M.Duca, M.T.de Groot, M.T.M.Koper, Nitrogen cycle electrocatalysis, *Chem. Rev.* **109** (2009) 2209-2244

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# Raymond and Beverly Sackler Laboratory for Astrophysics

*Prof. dr. H. Linnartz (UL)*

## **Research topics**

- Solid state astrochemistry
- Gas phase spectroscopy of molecular transients of astrophysical interest
- Astrochemical modeling

## **Summary of research activities**

Our Galaxy is largely empty. By terrestrial standards the space between stars can be considered as a near-perfect vacuum: the average particle density in the solar neighbourhood is roughly a factor of  $10^{19}$  less than in the terrestrial atmosphere at sea level. Nevertheless, the highly diluted material present between the stars, the InterStellar Medium (ISM), plays a central role in the chemical evolution of the Galaxy. More than 150 different molecular species have been identified meanwhile in star-forming regions, following detailed high resolution spectroscopic laboratory studies. The presence of these species in space is explained as the cumulative outcome of gas, grain and gas-grain interactions, i.e. a complex interplay between the gas phase and the solid state.

In the Sackler Laboratory for Astrophysics (SLA) the research is focused on identifying spectral fingerprints of molecular transients of astrophysical interest and to study the solid state processes that provide pathways towards molecular complexity in space. For this special plasma expansions and cryogenic ultra-high vacuum setups are used to simulate the conditions in the ISM.

A new setup has been constructed, based upon continuous infrared cavity ring down spectroscopy of expanding supersonic plasma. The experiment aims at recording fully resolved rovibrational transitions of molecular ions and radicals, providing fingerprint spectra for astronomical searches.

On October 14<sup>th</sup>, Jordy Bouwman defended his thesis on the 'Spectroscopy and Chemistry of Interstellar ice analogues'. The research was performed in collaboration with NASA AMES using a state-of-the-art setup to study in real time and in situ chemical reactions in ices upon VUV excitation. A special focus has been on the spectroscopy and chemistry of PAH containing water ices. The outcome makes it possible to search for the presence of PAHs in space in a different way than done so far. It furthermore shows that PAH chemistry in the solid state is rich and should not be neglected a priori in astrochemical models. Dr. Bouwman has continued his scientific career with a postdoc at the University of Berkeley.

On December 9<sup>th</sup>, Sergio Ioppolo defended his thesis on 'Surface Formation Routes of Interstellar Molecules'. His work focussed on H<sub>2</sub>O formation upon H-atom addition reactions of O<sub>2</sub> and O<sub>3</sub> containing ices and CH<sub>3</sub>OH formation upon hydrogenation of CO-

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ice. A study of mixed O<sub>2</sub>/CO ices shows the formation of CO<sub>2</sub> through OH reactions and makes it likely that H<sub>2</sub>O and CO<sub>2</sub> are chemically linked in interstellar formation routes as confirmed by astronomical observations.

UV irradiation of ices is an important chemical trigger that was shown to play an important role in the formation of more complex 'prebiotic' species on grains. In space this radiation is mainly dominated by Ly alpha radiation. We have investigated in addition the frequency dependent photoprocessing behavior of ice by using tunable synchrotron radiation (SOLEIL). This provides information on the impact of different UV radiation fields on ice at different astronomical settings, and in addition provides direct insight in the actual physical-chemical processes at work.

### **Key publications 2007-2010**

- K.I. Öberg, R.T. Garrod, E.F. van Dishoeck, H. Linnartz, Formation rates of complex organics in UV irradiated CH<sub>3</sub>OH-rich ices I: *Experiments; Astron. Astrophys.* **504** (2009) 891.
- Water formation at low temperatures by surface O<sub>2</sub> hydrogenation II; the reaction network, H.M. Cuppen, S. Ioppolo, H. Linnartz, *Phys. Chem. Chem. Phys.* **12** (2010) 12077.
- A coincidence between a hydrocarbon plasma absorption spectrum and the lambda 5450 DIB, H. Linnartz, N. Wehres, H. van Winkel, G.A.H. Walker, D.A. Bohlander, A.G.G.M. Tielens *A&A* **511** (2010) L3.

### **Future developments**

The influence of the simultaneous UV irradiation and atom bombardment of inter- and circumstellar ice analogue will be tested in a new ultrasensitive setup, MATRI2CES that recently yielded its first signals. The setup combines laser desorption and time-of-flight detection and is expected to visualize solid state chemical pathways towards molecular complexity in much more detail than possible with the regular UHV techniques.

In 2010 the Dutch Astrochemistry Network started. The SLA is part of this NWO funded program and participates with a research project 'Shining light on ices', focussing on the characterization of ice photoprocessing at astronomically relevant temperatures. The SLA furthermore participates in an FP7 interdisciplinary research and training network - LASSIE (Laboratory Astrophysical Surface Science in Europe) - comprising 12 research groups in Europe that started in 2010 as well.

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## 2.3 Theme 3 - Theoretical Chemistry

Understanding the structure of molecules and their chemistry from first principles represents the holy grail of theoretical chemistry. Many molecular properties can be understood directly from the electronic structure. When considering reactivity, it is usually necessary to consider the dynamics of the nuclei taking part in the reaction as well. The three theoretical chemistry groups of HRSMC work in both areas of research.

The groups of **Baerends**, **Bickelhaupt** and **Visscher** concentrate their efforts in the electronic structure research on the further development and application of both density (matrix) functional (D(M)FT) and wave function (WFT) based methods. This ties in very well with the group's research in the field of time-dependent DFT, and time-dependent DMFT, where applications are being made to excitation energies and to many other response properties. The group is also active in structure and reactivity, molecular recognition and nanostructures, (bio)catalysis, scattering and dissociation of small molecules at metallic surfaces, accurate calculation of properties (NMR, electric field gradients) where relativistic effects are important, and biochemistry. The group participates in the NRSC-Catalysis and in the IRTG.

The research in the Computational Physics and Chemistry groups of **Bolhuis and Meijer** focuses on the study of materials, biological systems, and solution chemistry. Development and application of novel computational techniques are an essential part of the research. With many of the studied structures and processes intrinsically multiscale their computational approach focuses strongly on multiscale techniques. International collaboration with experimental and computational groups plays an important role.

The main research activities of the **Neugebauer** group deal with the development of subsystem-based methods within time-dependent density functional theory for the investigation of excited states and response properties of complex molecular systems like photosynthetic light-harvesting complexes and solute-solvent systems. In addition, selective techniques for theoretical vibrational and electronic spectroscopy based on subspace iteration methods are developed, which are employed in studies on active parts of biomolecules and adsorbates on surface models.

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## Theoretical Chemistry

*Prof. dr. E.J. Baerends, Prof. dr. F.M. Bickelhaupt, Prof. dr. L. Visscher (VU)*

### Research topics

- Theoretical Chemistry / Density Functional Theory (Baerends)
- Theoretical Organic Chemistry and Biocatalysis (Bickelhaupt)
- Quantum Chemistry and Multiscale Modeling (Visscher)

### Summary of research activities

The TC group develops molecular electronic structure theory and devises quantum chemical methods for the calculation of the electronic structure and the properties following from it. Research focuses on physical models, numerical methods and computer implementations. Density functional theory and methods are a central theme, as well as WFT and DFT methods for the simultaneous treatment of relativistic effects and electron correlation. A third point of focus is the conceptual development of chemistry in particular the development of models that enable a qualitative understanding, based on accurate calculations, of chemical reactivity and, thus, a more rational tuning of elementary chemical processes.

Actual electronic structure investigations ("applications") are carried out to understand and predict phenomena in a variety of chemical subdisciplines. Issues in chemical bonding, structure, bonding and reactivity are addressed: metal-ligand and metal-metal bonding in organometallic chemistry including studies in photochemistry; complexation and solvation of (actinide) metal complexes; elementary chemical reactions; rational, fragment-oriented design of catalysts; hydrogen bonding in DNA, molecular recognition in general and nanoswitches; *ab initio* molecular dynamics (Car-Parrinello) for solvent effects in reactions. Methods are developed and applied for relativistic effects, which are needed in the study of heavy element chemistry and spectroscopy. Reactivity at and scattering from crystal surfaces is studied with a combination of electronic structure calculations (for the potential energy surfaces) and (quantum) dynamics for the nuclear motions (heterogeneous catalysis). Time-dependent DFT calculations of response properties afford detailed study of electronic absorption spectra and nonlinear optical properties of large molecules such as substituted and dimeric porphyrines and phthalocyanines. A new research line deals with astrochemistry.

### Key publications 2007-2010

- K. J. H. Giesbertz, O. V. Gritsenko and E. J. Baerends; Response calculations with an independent particle system with an exact one-particle density matrix. *Phys. Rev. Lett.* **105** (2010) 013002/1-4.
- L. Bernasconi, E. J. Baerends; Generation of ferryl species through dioxygen activation in iron/EDTA systems: a computational study. *Inorg. Chem.* **48** (2009) 527-540.
- V. P. Nicu, E. J. Baerends; Robust normal modes in vibrational circular dichroism spectra. *Phys. Chem. Chem. Phys.* **11** (2009) 6107-6118.

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- W.-J. van Zeist, F. M. Bickelhaupt; The Activation Strain Model of Chemical Reactivity. *Org. Biomol. Chem.* **2010**, *8*, 3118-3127.
  - S. C. A. H. Pierrefixe, S. J. M. van Stralen, J. N. P. van Stralen, C. Fonseca Guerra, F. M. Bickelhaupt; Hypervalent Carbon. "Freezing" the S<sub>N</sub>2 Transition State. *Angew. Chem.* **2009**, *121*, 6591-6593; *Angew. Chem. Int. Ed.* **2009**, *48*, 6469-6471.
  - T. van der Wijst, C. Fonseca Guerra, M. Swart, F. M. Bickelhaupt, B. Lippert; A Ditopic Ion-Pair Receptor Based on Stacked Nucleobase Quartets. *Angew. Chem.* **2009**, *121*, 3335-3337; *Angew. Chem. Int. Ed.* **2009**, *48*, 3285-3287.
  - U. Ekstrom, L. Visscher, R. Bast, A. J. Thorvaldsen, K. Ruud, Arbitrary-Order Density Functional Response Theory from Automatic Differentiation, *J. Chem. Theory Comput.* **2010**, *6*, 1971.
  - R. Bulo, B. Ensing, J. Sikkema, L. Visscher, Toward a Practical Method for Adaptive QM/MM Simulations, *J. Chem. Theory Comput.* **2009**, *5*, 2212.
  - C.R. Jacob, L. Visscher, A subsystem density-functional theory approach for the quantum chemical treatment of proteins, *J. Chem. Phys.* **2008**, *128*, 155102

### Future developments

In the project dealing with the development of theory, methods and applications of density (matrix) functional theory we envisage;

1) Further development of density *matrix* functional theory (DMFT). We will investigate the extension of DMFT to time-dependent fields, and in particular develop the formalism for response properties (excitation energies). Orbital dependent functionals will be further developed and their potential to describe in particular weak bonding situations (dissociation) will be investigated.

2) In the field of homogeneous catalysis the special status of the ferryl ion (oxidoiron(IV)) will continue to be the main focus, but also a range of other metal-oxo compounds will be investigated. Use of O<sub>2</sub> as stoichiometric oxidation reactant will be explored.

3) The calculation of chiral properties of molecules has become an important research field. The development of techniques for vibrational circular dichroism (VCD) will be continued, and work on vibrational Raman optical activity (ROA) has been started. The concept of "robustness" of VCD peaks, which we have introduced, greatly aids in the use of VCD for the determination of the absolute configuration of a molecule. It will be investigated for ROA as well. The next important problem for VCD is the sensitivity of the spectra to the conformation of a molecule. A long term goal is the theoretical understanding of the conformational effects, and to find on that basis a way to deal with this problem in absolute configuration determination.

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In the project dealing with the conceptual development of chemistry we envisage:

1) Further extension of the activation strain model of chemical reactivity and its application to (bio)catalysis and archetypal organic reactions. The classes of organic reactions are extended from  $S_N2$ , E2 and proton transfer to pericyclic reactions. Also, we will more and more go from analyzing and understanding catalytic reactions toward rationally designing tailor-made catalysts.

2) In the fields of computational biochemistry and nanostructures, we will develop three lines of research: a) DNA structure and stability will be further developed towards DNA replication; and b) towards telomer structure, stability and function; c) molecular recognition will be extended towards supramolecular catalysts.

3) In the subproject on structure and bonding, the development is towards new structural motifs (e.g., stable 5-coordinate carbon).

In the project dealing with development of relativistic quantum chemical methods we plan further development of general-order coupled cluster methods for benchmark applications on heavy-element compounds. This type of methods is e.g. used to calibrate applications of TD-DFT to the spectroscopy of actinide complexes.

Development of subsystem DFT methods based on the frozen density ansatz is continued with an emphasis towards treatment of biological systems by extending the 3-FDE scheme for proteins to a more general treatment of the individual subsystems and better efficiency in the capping procedure. In this project we will also consider further development of the WFT-in-DFT scheme in which one or more subsystems can be treated by the accurate (relativistic) wave function based methods.

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# Computational Chemistry

*Prof. P.G. Bolhuis, Dr. E.J. Meijer, Dr. B. Ensing, and Dr. D. Dubbeldam (UvA)*

## Research topics

- Development of computational techniques to model properties of many-particle systems
- Nanoporous materials
- Micellar structures
- Reactivity in complex environment
- Polymers in flow
- Stability and structure of carbon materials
- Biological membranes
- Protein folding
- Photoactive proteins
- Signalling proteins
- Protein fiber formation

## Summary of research activities

The group has kept a strong record in modelling complex phenomena in chemical, physical, and biological systems.

*Materials* The design and development of novel nanoporous materials is of paramount importance in the areas as storage, separation, and catalysis. A targeted approach requires a proper quantitative description of the materials. We have focussed on zeolites, metal organic frameworks (MOFs) and carbon. In the area of zeolites we elucidated the how Al-substituted MFI zeolites containing nonframework cations can be used for enantioseparation. If one enantiomer is present in excess it will organize the nearby cations such that all adsorption sites become effectively chiral (van Erp, Caremans, Dubbeldam, Martin-Calvo, Calero, *Angew. Chem. Int. Ed.* **49**, 3010). Carbon may adopt a large variety of structures. Using a state-of-the-art approach we have obtained an accurate picture of the thermal stability of carbon over a large range of pressures (Ghiringhelli and Meijer, *Springer Series on Carbon Materials*, **3**, 1).

### *Biomaterials*

Self-assembly of polypeptides into fibrils promises the development of new functional supra-molecular biomaterials. Here, prediction of structure and kinetics is crucial to control the design of such novel biomaterials. We studied the self-assembling fiber formation of a triblock copolymer consisting of a middle silk-like block flanked by two hydrophilic end blocks. By extensive replica exchange molecular dynamics simulation we predicted the thermodynamically stable conformation of the middle block to be a  $\beta$ -roll. This all-atom approach was at the limit of what is feasible, and therefore we developed a coarse-grained force field to describe the assembled polypeptide including the hydrophilic flanks (Schor, Ensing, Bolhuis, *Faraday Discuss.* **2010**, 144, 127-141). Using this force field we predicted e.g. the fiber persistence length. These predictions are corroborated by experiments in Wageningen UR and facilitate the design of new self-assembling silk-like materials with novel functionality.

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Whey proteins such as  $\beta$ -lactoglobulin are often used as thickening agents in the food industry. Cold-set gelation of whey proteins proceeds via heat-induced formation of small aggregates, followed by pH-induced gel-formation. In both steps thiol exchanges plays a crucial role.  $\beta$ -lactoglobulin contains buried two disulfide bridges, that need to be exposed during heating Using replica exchange molecular dynamics we found subtle exposure mechanism, in which the alpha-helical structure is not lost.

#### *Protein conformational changes*

Using a combination of four advanced rare event molecular simulation techniques we conducted a numerical study of the folding routes of the truncated FBP28 WW domain at ambient conditions (Juraszek, Bolhuis, *Biophysical Journal* **2010**, 98, 646-656.) We explored the free energy landscape as well as the dynamical folding pathways with replica exchange molecular dynamics, bias-exchange metadynamics, transition path sampling and metadynamics. We find two major folding routes, differing in the formation order of the two main hairpins, and in hydrophobic side-chain interactions. The computed barriers are in agreement with experiments. Combining several powerful simulation techniques thus provides a more complete understanding of the kinetic mechanism of protein folding.

Understanding the dynamics of large-scale conformational changes in proteins still poses a challenge for molecular simulations. We employed transition path sampling of explicit solvent molecular dynamics trajectories to obtain atomistic insight in the reaction network of the millisecond timescale partial unfolding transition in the photo cycle of the bacterial sensor photoactive yellow protein. Likelihood maximization analysis predicts the best model for the reaction coordinates of each substep as well as tentative transition states, without further simulation. Our results open the way for studying millisecond conformational changes in other medium-sized (signaling) proteins (Vreede, Juraszek, Bolhuis, *Proceedings of the National Academy of Sciences of the United States of America* **2010**, 107 (6), 2397-2402.)

#### *Soft matter systems*

The stability of colloidal dispersions can be severely affected by the presence of surfactants. Because surfactants can adsorb at colloidal surfaces as well as form micelles, one can expect interplay between both phenomena. Using grand-canonical coarse-grained Monte Carlo simulations on surfactant solutions confined between two surfaces, we investigate how adsorption and micelle formation affects the effective interaction between two colloidal particles, and hence, the stability of the colloidal dispersion. We find that the formation of micelles at concentrations above the CMC causes an additional depletion effect, resulting in an effective attraction, which in turn can destabilize a colloidal dispersion. (Pool, Bolhuis, *Physical Chemistry Chemical Physics* **2010**, 12 (44), 14789-14797.)

#### *Chemical reactivity in complex environment*

Most (bio-)chemical processes occur in complex fluctuating environment, such as solvent, protein, or nanostructured cavities. We apply advanced ab initio molecular simulation techniques to address the role of the fluctuating environment. Silicic acid and the hexa-aqua of  $Al^{3+}$  are fundamental model aqueous species of chemical importance in nature.

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Combining ab initio MD with rare events methods we elucidated the hydroxyl dissociation mechanism of these compounds in aqueous solution. This provided a quantitative estimate for the pKa of these compounds that were in good agreement with experimental values. This study provides an encouraging basis for applying the present methodology to predict acidity constants of those groups that are difficult to measure experimentally. Acid dissociation mechanism of SiOH<sub>4</sub> and Al(H<sub>2</sub>O)<sub>6</sub><sup>3+</sup> in aqueous solution (Liu, Meijer, et al., *Geochimica et Cosmochimica Acta* 74, 510).

Cisplatin (cis-[Pt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>]) is an important compound in cancer treatment. The mode of action of cisplatin starts inside the cell with the hydrolysis of Pt-Cl bonds to form a Pt-aqua complex. Our metadynamics ab initio simulations show that hydrogen bonding between solvent water molecules and metal complexes in the hydrolyzed product systems is stronger than that in the reactant cisplatin system, and that the second hydrolysis of cisplatin is thermodynamically favourable than the first, which is in good agreement with experimental results. (Kai-Chi and Ensing, *PCCP* **12**, 10348)

#### *Methods for Simulation Complex Systems*

The multiple state transition path sampling aims to sample from an extended path ensemble including all possible trajectories between any pair of metastable states. We introduced a Wang-Landau based biasing approach to improve the sampling. We found that the biasing of the multiple state path ensemble does not influence the switching behavior, but does improve the sampling and thus the quality of the individual path ensembles (Rogal, Bolhuis, *Journal of Chemical Physics* **2010**, 133, 174109.)

We also introduced a new reweighting scheme for the path ensembles in the transition interface sampling framework. The reweighting allows for the analysis of free energy landscapes and committor projections in any collective variable space (Rogal, Lechner, Juraszek, Ensing, Bolhuis, *Journal of Chemical Physics* **2010**, 133, 174110). The reweighted path ensemble can be used to optimize possible nonlinear reaction coordinates based on a likelihood maximization approach in combination with a string projection method. While developed for use with path sampling, this analysis method can also be applied to regular molecular dynamics trajectories. (Lechner, Rogal, Juraszek, Ensing, B.; Bolhuis, P. G., Nonlinear reaction coordinate analysis in the reweighted path ensemble. *Journal of Chemical Physics* **2010**, 133 (17).

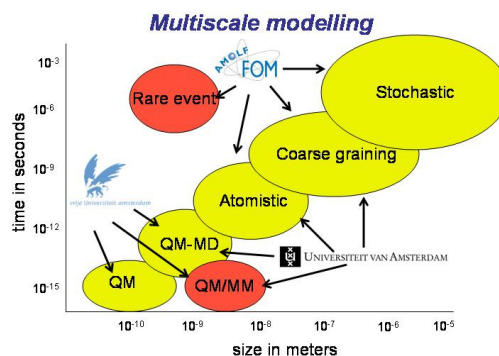
Until now, adaptive atomistic-coarse-grain (A/CG) molecular dynamics simulations have had very limited applicability because the on-the-fly CG→A transformation is problematic for all but those molecules whose CG representation consists of a single particle. We have solve this problem by combining a transitional healing region with a rotational dynamics of rigid atomistic fragments in the CG region. The applicability of method is demonstrated with adaptive multiscale simulations of liquid hexane and of a dilute polymer solution (Nielsen, Moore, and Ensing, *Phys. Rev. Lett.* 105, 237802).

## Key publications 2007-2010

- J. Juraszek, P.G. Bolhuis, Sampling the multiple folding mechanisms of Trp-cage in explicit solvent. *Proc. Natl. Acad. Sci. USA* **103** (2006) 15859.
- J.-W. Handgraaf and E.J. Meijer, E.J., Realistic Modeling of Ruthenium-Catalyzed Transfer Hydrogenation, *J. Am. Chem. Soc.* **129** (2007) 3099.
- S.O. Nielsen, P.B. Moore, and B. Ensing, *Phys. Rev. Lett.* **105** (2010), 237802.

## Future developments

Over the past years the research environment has been strengthened by establishing the Amsterdam Center for Multiscale Modeling (ACMM). The ACMM combines the groups of Baerends/Bickelhaupt/Visscher (VU) and Bolhuis/Krishna/Meijer at (UvA) together with other groups active in computational science in the Amsterdam area. The ACMM has become the basis for the development and application of



computational methods for research in the fields under 2). It also serves as a partner in external collaborations both nationally and internationally and will be a national and international training center. We have extended our staff by attracting David Dubbeldam. We aim to broaden our activities by converting the present ATOSIM MSc program into an international graduate school that combines a MSc and PhD training program in computational science. Specific research topics will be in the field of complex (bio)molecular systems where we focus on the role of macromolecules in the cell (e.g. photoactive protein complexes, protein aggregation and protein folding, and cytoskeleton filaments), and on catalysis in solution and (semi-)structured environment. In the field of materials and engineering we will focus on carbon materials, nanoporous materials (focusing on metal-organic frameworks) and reactor intensification and -miniaturization, nanofluidic reactors, respectively.

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## Theoretical Chemistry

*Dr. J. Neugebauer, Prof. dr. M.C. van Hemert (UL)*

### **Research topics**

- Quantum Chemical Methods for Photosynthetic Systems
- Subsystem-Based Density Functional Theory
- Excited States of Adsorbed Molecules
- Theoretical Resonance Raman Spectroscopy

### **Summary of research activities**

The research of the Neugebauer group is directed towards the development of quantum chemical methods which facilitate investigations on properties of functional molecular aggregates. Typical examples are protein-pigment complexes as occurring in photosynthetic light-harvesting systems, which consist of many dye molecules embedded in a protein matrix. The efficiency of these complexes depends not only on the properties of the individual pigments, but also on their mutual arrangement and their interaction with the surrounding protein. We are developing subsystem-based methods within density-functional theory which allow to study excited electronic states and response properties of such functional aggregates. We are currently employing these methods to investigate the role of individual pigment molecules on the spectra of light-harvesting complexes of green plants as well as the color-tuning mechanisms in chromophore-carrying proteins.

Besides such subsystem-based methods, we also develop efficient techniques for conventional time-dependent density-functional theory that is particularly suited for local excitations in extended systems. The idea here is to start from the properties of isolated molecules or idealized electronic transitions and iteratively determine how these properties *change*, e.g., if the molecule is adsorbed on a surface. Conventional methods can be problematic in such investigations if the sought-after excitation has a rather high energy or appears within a dense region of substrate excitations.

Another field of research is vibrational spectroscopy and in particular resonance Raman spectroscopy for investigations on photophysical and photochemical processes. This includes studies on models for artificial and natural photosynthetic systems, the photochemistry of nitro-arenes, and methodological developments concerning, e.g., vibrational resonance Raman optical activity (VRROA). Furthermore, we are developing so-called purpose-driven methods for theoretical spectroscopy, in which the property to be determined is used to steer the calculation. E.g., if the resonance Raman spectrum of a complex molecular system shall be calculated, it is possible to determine the intense vibrations selectively in an iterative process. This considerably reduces the computational effort for the calculation, since resonance Raman spectroscopy often leads to an enhancement of a small subset of vibrations.

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### Key publications 2007-2010

- J. Neugebauer; Couplings between electronic transitions in a subsystem formulation of time-dependent density functional theory. *J. Chem. Phys.* **126** (2007), 134116.
- J. Neugebauer; Subsystem-Based Theoretical Spectroscopy of Biomolecules and Biomolecular Assemblies. *ChemPhysChem* **10** (2009), 3148.
- A. Kovyrshin, J. Neugebauer, State-Selective Optimization of Local Excited Electronic States in Extended Systems. *J. Chem. Phys.* **133** (2010), 174114.

### Future developments

In our future research, we are going to investigate energy-transfer and energy-dissipation pathways in natural and biomimetic photosynthetic systems. This requires further methodological developments for subsystem-based response techniques. But it will also be important to establish connections between these *first-principle* methods and highly reduced physical model theories that are usually employed to study such phenomena.

Furthermore, we plan to work on purpose-driven methods for the vibronic structure of absorption spectra, and to apply these techniques in the analysis of energy dissipation pathways in photosynthetic pigments. These analyses shall be augmented with resonance Raman studies on typical chromophores in light-harvesting systems.

The work on local excited states for adsorbate molecules shall be extended, so that quasi-diabatization schemes can be defined. The background here is that adsorbate excited states are often extremely difficult to identify in a calculation, since they can couple to a multitude of substrate excitations and are then spread out over a rather broad region in the spectrum.



## 2.4 HRSMC Co-operations

<b>Research topic</b>	<b>Co-operating groups</b>	<b>Theme</b>	<b>University</b>
2-D IR spectroelectrochemistry	Buma – Hartl	1,2	UvA
2DIR of Protein folding	Woutersen – Bolhuis	2,3	UvA
Adaptive QMMM methods	Ensing-Bulo	3	UvA,VU
Aromaticity in inter/circumstellar ice analogues a combined experimental and theoretical approach	Linnartz - Bickelhaupt	2,3	UL, VU
Artizymes	Lammertsma-Overhand	1	VU, UL
Calculations of solvent effects on the fluorescence of isoflavones	Visscher - Gooijer	2,3	VU
Calculations on homogeneous catalytic mechanisms	Ehlers - Bouwman	1	UvA, UL
Calculations on Multicomponent Syntheses	Bickelhaupt - Orru	1,3	VU
Calculations on Resonance Raman spectra	Baerends - Gooijer	2,3	VU
Chiral anion-mediated catalysis	Orru - Lammertsma	1	VU
Conformational Analysis RGD-peptides	Orru – Overhand	1	VU, UL
Development of device compatible charge separators	Orru - Lammertsma	1	VU
Dutch Compound Library	Orru – Overkleeft – van Maarseveen	1	VU, UL, UvA
Early stage dynamics of protein folding	Woutersen - Bolhuis	2,3	UvA
Electronic structure calculations on organometallic complexes	Baerends - Lammertsma	1,3	VU
Electronic structure of phosphinidene complexes	Baerends - Lammertsma	1,3	VU
Enzyme cascade reactions	Wever	1	UvA
Exact embedding potentials in QM/QM methods	Neugebauer - Visscher	3	UL, VU
Fenton oxidation reaction	Baerends - de Groot	2,3	VU, UL
Fluorescent organocatalysts	Brouwer - Hiemstra	1,2	UvA
Fragment-oriented rational design of catalysis	Bickelhaupt/Reek	1,3	VU, UvA
Glass transition	Orrit - Brouwer	2	VU, UvA
Homogeneous catalysis by metal	Baerends -	1,3	UL, VU

centers on organometallic complexes	Reedijk		
Homogeneous vs. heterogeneous electrocatalysis	Koper - Bouwman	1,3	UL
Homogenous Catalysis in transition metal complexes	Meijer-Reek-de Bruin	1,3	UvA
Infrared studies of (di)manganese carbonyl ions	Buma - Ingemann	1,2	UvA
Ionic complexes: towards molecular complexity in space	Bickelhaupt - Linnartz	1,2	VU, UL
Isotope-labeled peptides	Woutersen - v. Maarseveen	1,2	UvA
Light harvesting dyes	Brouwer - Orru - Lammertsma 1,2 UvA/VU	1,2	UvA,VU
Modelling of conformation of peptidomimetics	Orru - Ehlers	1	VU
Optimalisation of NHC-ligands	Orru - Rothenberg	1,3	VU, UvA
PAHs in the laboratory and in space	Buma-Ubachs - Linnartz	2	UVA, VU, UL
Palladium catalysis, click chemistry involving NHC-triazole compounds	Elsevier - Hiemstra - van Maarseveen	1	UvA
Photocatalysis	Brouwer - Reek - Hartl -van der Vlugt	1,2	UvA
Photocatalysis	Reek - van der Vlugt- de Groot	1,2	UvA, UL
Photodissociation dynamics of iron complexes	van Hemert - Kroes - Lammertsma - Ehlers	1,3	UL, VU
Photo-organic dynamics resolved in real time by ultrafast femtosec laser spectroscopy	Lammertsma - Janssen	1,2	VU
Photophysics/chemistry of flavonoids	Ariese - Gooijer - Visscher	2,3	VU
Photophysics/chemistry of pyridine N-oxides	Ariese - Gooijer - vd Zwan - Buma - Zhang	2	VU, UvA
Photosynthesis	de Groot - Koper	2,3	UL
Resonance Raman spectroscopy of spheroidene	v. Hemert - Neugebauer	3	UL
Selective enzymatic phosphorylation	Hiemstra - Wever	1	UvA
Single-molecule probing of glass	Orrit-Brouwer	2	UL, UvA

transition			
Solvation effects in protonated water clusters	Bickelhaupt - Linnartz	3,2	VU, UL
Spectro-electrochemistry (VCD) and TRIR of organic and organometallic compounds	Woutersen - Hartl	2,1	UvA
Spectro-electrochemistry of complexes with heterocyclic phosphorus ligands	Lammertsma - Hartl	1,3	VU, UvA
Spectro-electrochemistry of rotaxanes	Hartl - Brouwer - Buma	1,2	UvA
Spectro-electrochemistry on biomimetic homogeneous catalyst systems	Hartl - Buda - Reedijk	1,3	UvA, UL
Supramolecular coordination complexes: XRD and DFT	Buda - Reedijk - Bouwman	1,3	UL
Spectroscopy (2D-IR)	Reek - van der Vlugt - Woutersen	1.2	UvA
Subsystem DFT methods	Visscher - Neugebauer	3	VU, UL
Theoretical Spectroscopy of Protein-Pigment Complexes	Neugebauer - Buda	3	UL
TR spectroscopy applied to supramolecular catalysis	Reek - Hartl - Brouwer	1,2	UvA
Transition-metal NMR	Elsevier - Reedijk - Bouwman	1	UvA, UL
Use of phosphatases and sulfatases in enantioselective reactions	Wever	1	UvA
Various Synthetic products	Hiemstra - Orru - van Maarseveen	1	UvA, UL
Vibrational circular dichroism	Woutersen - De Bruin	1,2	UvA

**Cooperations HRSMC-Cooperating groups Westfälische Wilhelms Universität Münster**

<b>Research topic</b>	<b>Cooperating groups HRSMC (UvA, VU, UL)</b>	<b>Theme</b>	<b>Cooperating groups WWU Münster</b>
Building blocks for Container Molecules	Orru	1	Uhl
Carbene chemistry	Bouwman	1	Hahn
Container molecules	Lammertsma	1	Mitzel, Uhl, Grimme
Container molecules	Orru	1	Uhl
Macrocyclic NHCs	Orru	1	Hahn
Macrocyclic NHCs	Lammertsma	1	Hahn
Metallo-radical reactivity; EPR spectroscopy	Bruin, de	1	Wolf
Supramolecular Interactions	Lammertsma	1	Wuerthwein
Metal-mediated base pairs containing artificial nucleobases	Bickelhaupt	3	Müller
Multidentate NHCs	Elsevier	1	Hahn
NHCs	Orru	1	Hahn
Organophosphor	Lammertsma	1	Weigand
Organophosphor	Lammertsma	1	Uhl
Organophosphor	Lammertsma	1	Wolf
Photophysics of coordination compounds: energy and electron transfer in supramolecular systems	Hartl en Reek	1	De Cola
Quantum chemical investigation of inclusion and cage compounds	Bickelhaupt	3	Grimme
Spectroelectrochemistry of unusual organometallic compounds	Hartl -Reek	1	Wolf
Synthesis/Theory	Lammertsma	1	Hahn
Synthesis/Theory	Lammertsma	1	Würthwein
Template chemistry	Reedijk	1	Hahn
Theory	Lammertsma	3	Grimme
Tripod molecules	Williams	3	De Cola
Triazapentadienes	Bouwman - Bonnet	1	Wuerthwein
Photochemistry	Bouwman - Bonnet	1	De Cola

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## Memberships international editorial boards 2010

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<b>Name of Staffmember</b>	<b>Member of:</b>
Ariese	Polycyclic Aromatic Compounds
Baerends	Chemical Physics Letters
Baerends	Journal of Computational Chemistry
Baerends	Theoretical Chemistry Accounts
Bickelhaupt	Journal of Computational Chemistry
Bickelhaupt	Physical Chemistry Chemical Physics
Bouwman	Applied Organometallic Chemistry (advisory board)
Bouwman	European Journal of Inorganic Chemistry (advisory board)
Brouwer	International Journal of Spectroscopy
Buma	Research Letters in Physical Chemistry
Elsevier	Collection Czechoslovak Chemical Communications (advisory board)
Elsevier	Editor-in-Chief of Applied Organometallic Chemistry (Wiley)
Elsevier	Magnetic Resonance in Chemistry (advisory board)
Gooijer	Analytica Chimica Acta
Gooijer	Current Analytical Chemistry
Hartl	Collection Czechoslovak Chemical Communications (editorial board)
Hiemstra	European Journal of Organic Chemistry (Editorial Board)
Hiemstra	Progress in Heterocyclic Chemistry (Editorial Advisory Board)
Hiemstra	Science of Synthesis (Editor Vol 48)
Koomen	European Journal of Inorganic Chemistry and Organic Chemistry
Koomen	Heterocycles
Koper	Advances in Physical Chemistry
Koper	Catalysis Today
Koper	Electrochimica Acta
Koper	Journal of Electroanalytical Chemistry
Lammertsma	Beilstein Journal of Organic Chemistry (advisory board member)
Lammertsma	Heteroatom Chemistry (editorial board member)
Lammertsma	Organometallics (editorial board member)
Linnartz	Editor CAMOP -Phys. Scripta
Orrit	Angewandte Chemie
Orrit	Chemical Physics
Orrit	ChemPhysChem
Orrit	Molecular Physics
Orrit	PCCP
Orru	Current Organic Chemistry (Advisory Board Member)
Orru	Topics in heterocyclic chemistry (volume ditor)
Overkleeft	European Journal of Organic Chemistry (international advisory board member)
Reedijk	Advances in Inorganic Chemistry
Reedijk	Comments on Inorganic Chemistry
Reedijk	European Journal of Inorganic Chemistry (editor)
Reedijk	Journal of Biological Inorganic Chemistry

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Reedijk	Journal of Inorganic Biochemistry
Reedijk	Polyhedron
Stolte	Laser Chemistry (editorial advisor)
Völker	Journal of Luminescence
Verhoeven	ChemPhysChem
Verhoeven	European Journal of Organic Chemistry
Verhoeven	International Journal of Photoenergy
Williams	The Open Inorganic Chemistry Journal
Zhang	Guest editor Journal of Luminescence

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## 2.5 Memberships and awards

### Memberships organising committees international meetings 2010

<b>Name of Staff member</b>	<b>Activity</b>
Baerends	Member Scientific Committee 8th Girona Seminar of the Chemical Bond, Girona, Spain, July 2010
Bickelhaupt	Member Scientific Committee 8th Girona Seminar of the Chemical Bond, Girona, Spain, July 2010
Bickelhaupt	Member Scientific Committee 9th Girona Seminar of the Chemical Bond, Girona, Spain, July 2012
Bonnet	Member of HRSMC Autumn School "Advanced course in Metal-Organic Chemistry", September 2010, Doorn, The Netherlands
Bouwman	Member of HRSMC Autumn School "Advanced course in Metal-Organic Chemistry", September 2010, Doorn, The Netherlands
Bruin, de	Member of HRSMC Autumn School "Advanced course in Metal-Organic Chemistry", September 2010, Doorn, The Netherlands
Ehlers	Member of HRSMC Autumn School "Advanced course in Metal-Organic Chemistry", September 2010, Doorn, The Netherlands
Elsevier	Member of HRSMC Autumn School "Advanced course in Metal-Organic Chemistry", September 2010, Doorn, The Netherlands
Elsevier	Board EUCHEMS conferences Organometallic Chemistry since 2007Member
Gooijer	Scientific Committee XIV Int. Symp. on Luminescence Spectrometry. Prague (Cz) July 2010
Groot	Member of Organising Committee, 3rd International Training School on Solid State NMR, June 2010, Leiden, The Netherlands
Hiemstra	Member International Scientific Committee European Symposia on Organic Chemistry (ESOC)
Koomen	Organising committee FECHEM: Heterocycles in Bio-organic Chemistry
Koomen	Titular member IUPAC Organic Division
Koper	Chair 2012 Spring Meeting of the International Society of Electrochemistry, Washington DC
Koper	Advisory board member International Conference on Electrified Interfaces, Geneva New York, June 2010
Koper	Organizer CECAM Workshop on Ab Initio Electrochemistry, Lausanne, July 2010
Lammertsma	Member Organizing Committee of the International Conference on Phosphorus Chemistry
Linnartz	Member international committee of the biannual workshop on infrared plasma spectroscopy
Maarseveen, van	Treasurer of the Organic Section of the Royal Netherlands Chemical Society ,

Meijer	Coordinating organizer international school 'Understanding Molecular Simulation' 2010
Orru	Scientific Committee, 4th international Conference on MCRs and Related Chemistry, Jekatarinaburg, 2009
Orru	Chairman of the 3rd International HRSMC-school on bioorganic synthesis, Maastricht, 2009
Orru	Chairman of 3rd International Conference on Multicomponent Reactions and Related Chemistry, MCR2006, Amsterdam, 2006
Orru	Organizing & scientific committee of BIOTRANS '05, Delft, 2005
Reedijk	Executive Secretary International Coordination Chemistry Conferences (ICCC)
Reedijk	Member International Committee EURASIA Conferences of Chemistry
Reedijk	Member International Conferences on Bioinorganic Chemistry
Reedijk	Member International organizing committee of the International Symposium on Macromolecule Metal Complexes
Reedijk	Chair European Research Conferences Inorganic Chemistry
Reedijk	Vice-chair (chair 2010), Gordon Research Conference metals in Medicin
Stolte	Member of International committee MOLEC, European Conference on Dynamics of Molecular Collisions
Stolte	of the international Advisory Committee Internatiponal Symposium on Molecular Beams ember
Stolte	Member of the Graduate College of the conference on Molecular Energy Transfer COMETMember
Stolte	Member International Scientific Committee Conference on Stereodynamics of Chemical Reactions
Visscher	Member Scientific Committee Relativistic Effects in Heavy Elements, (REHE2010), Beijing September 2010

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## Board memberships scientific organisations/academies/awards

<b>Naam</b>	<b>Activiteit</b>
Ariese	Board Member International Society on Polycyclic Aromatic Compounds
Baerends	Chairman Board HRSMC (1994-2009)
Baerends	Member Gebiedsbestuur Chemische Wetenschappen (NWO) (2004-2010); Chairman 2008-2010.
Baerends	Member Koninklijke Nederlandse Academie van Wetenschappen
Baerends	Member of International Academy of Quantum Molecular Science
Baerends	Member Raad van Bestuur FOM 2001-2010
Baerends	Member Raad van Toezicht Leids Institute for Chemistry (2004-)
Baerends	Member WGS, NCF (-2009)
Baerends	World Class University Distinguished Professorship South-Korea, 2009-2014.
Bickelhaupt	Chairman Board HRSMC
Bickelhaupt	Secretary Board NWO-CW studiegroep Spectroscopie en Theorie
Bickelhaupt	Visiting professorship at the University of Girona, Spain
Bickelhaupt	Member VENI GO committee NOW
Bickelhaupt	NWO Astrochemistry program committee
Bouwman	Member, VIDI jury CW
Brouwer	Co-chair IUPAC project Photoluminescence Standards
Brouwer	Guest Professor École Normale Supérieure Cachan (France) 2008-2009
Brouwer	Member of the sub-committee on Photochemistry IUPAC Division III
Brouwer	Project leader ERA NanoSciences program MOLIMEN (2007-2011)
Buma	Member American Chemical Society
Buma	Chairman board CW/NWO study group "Spectroscopy and Theory"
Buma	Member Senate UvA
Buma	Scientific Director HRSMC
Elsevier	Member Board HRSMC (2008- )
Elsevier	Member Board NIOK
Elsevier	Member panel TOP-ECHO subsidies NWO-CW since 2006
Elsevier	Member Scientific Council NRSC-Catalysis
Elsevier	Scientific Director HRSMC 2002-2007
Elsevier	Visiting professorship at the Weizman Institute of Science (Israel)
Elsevier	Visiting professorship at ULP Strasbourg and at ENSIACET Toulouse
Gooijer	Chairman Kamer Scheikunde, VSNU
Gooijer	Member NWO-CW Comm TOP/Echo proposals
Gooijer	Member of Panel Chemistry/Academy of Finland
Gooijer	Member Scientific Committee Int. Symposia on Luminescence Spectrometry
Groenen	Chairman of the "Syllabuscommissie Nieuwe Natuurkunde"
Groenen	Member of the International Scientific Advisory Board of the Max Planck Institute for Bioinorganic Chemistry (Mülheim, Germany)
Groot, de	Scientific director Researchprogram TBSC (Towards BioSolar Cells)
Groot, de	Member of Koninklijke Hollandsche Maatschappij der Wetenschappen

Groot, de	Member of curriculum committee for the Leiden University College
Groot, de	Member of the Honours Council
Groot, de	Member of the Int.Eva.Panel (IEP) evaluation of projects in the area of Integrated Infrastructure Initiative on Bio-NMR
Groot, de	Member of Raad van Toezicht (Leids Instituut voor onderzoek in Natuurkunde)
Groot, de	Member of Raad voor Aard en Levenswetenschappen KNAW
Hartl	Visiting professorship at the Chuo University, Tokio (Japan)
Hartl	Visiting professorship at the Joseph Fourier University, Grenoble (France)
Hiemstra	Member CW/NWO VIDI proposal committee
Hiemstra	Director of the Master School of Sciences, University of Amsterdam
Hiemstra	Member of the management committee of EU-COST action CM0905 ORCA "Organocatalysis"
Janssen	Management Board Laser Centre Vrije Universiteit
Koomen	Chairman Managementcommittee COST D13 "New Molecules towards Human Health Care"
Koomen	Royal Holland Society of Arts and Sciences Society for the Advancement of Natural Sciences, Medicine and Surgery
Koomen	Titular member IUPAC Division III Organic Chemistry
Koper	Chair of Physical Electrochemistry Division of the International Society of Electrochemistry
Lammertsma	Chairman Organic Chemistry Section of the Royal Dutch Chemical Society (KNCV)
Lammertsma	Co-chair COST Action CM0802, the European Phosphorus Science Network
Lammertsma	Member of the Board NWO/CW study group "Coordination Chemistry and Homogeneous Catalysis"
Lammertsma	Member of the Board of NWO Chemical Sciences
Lammertsma	Member of the Netherlands Initiative on Material Scarcity (NIMS)
Lammertsma	Member of the Dutch Nutrient Platform (NP)
Lammertsma	Chairman of the Dutch "Kamer Scheikunde" (the Chemistry Deans in the Netherlands)
Lammertsma	Member of the KNCV thinktank "Chemistry & Society"
Linnartz	Research coordinator FP7 ITN 'Laboratory Astrochemistry in the Solid State in Europe'
Linnartz	VICI 2009
Linnartz	NWO Astrochemistry program committee
Maarseveen, van	Treasurer of the Organic Section of the Royal Netherlands Chemical Society
Marel, van der	Educational Director of MSc Chemistry
Meijer	Member, Scientific Council CECAM
Meijer	Workgroup chair ESF-COST program MOLSIMU
Neugebauer	Member Management Committee COST Action CODECS "CONvergent Distributed Environment for Computational Spectroscopy"

Orrit	Member Academia Europaea
Orrit	Member VICI panel NWO 2010
Orru	Member of the management committee of EU-COST action D32 "Chemistry in high-energy micro environments"
Orru	Member Organic Chemistry Section of the Royal Dutch Chemical Society (KNCV)
Orru	Chairman Organic Chemistry Section of the Royal Dutch Chemical Society (KNCV)
Reedijk	Fellow of the Royal Society of Chemistry
Reedijk	Fellow of the Royal Society of Chemistry
Reedijk	Member Academia Europaea
Reedijk	Member Academia Europaea
Reedijk	Member board HRSMC
Reedijk	Member board HRSMC
Reedijk	Member National Finnish Academy of Sciences
Reedijk	Member National Finnish Academy of Sciences
Reedijk	Member Royal Netherlands Academy of Arts and Sciences (KNAW)
Reedijk	Member Royal Netherlands Academy of Arts and Sciences (KNAW)
Stolte	Member Astrophysical Chemistry Group of the Royal Society of Chemistry
Verhoeven	Member of the Royal Netherlands Academy of Sciences and Arts (KNAW)
Verhoeven	Ridder in de Orde van de Nederlandse Leeuw (royal honour)
Visscher	Member Management Committee COST Action D37 'GRIDCHEM: Grid Computing in Chemistry' (EU)
Völker	Member FOM Advisory Committee FOM/v
Völker	Member of the "TOP/ ECHO Beoordelingscommissie" of NWO-CW.
Völker	Member of the Peer Review Committee of the Dutch Graduate School "Experimental Plant Sciences (EPS)".
Wever	Member board Dutch Society for Biochemistry and Molecular Biology
Williams	Auditor to the International Treasurer of the European Photochemistry Association
Williams	Local Treasurer of the European Photochemistry Association

## Research Cooperations outside the HRSMC

<b>Research Topic</b>	<b>Staff Member</b>	<b>Working together with</b>	<b>Title</b>	<b>From University or Organization</b>	<b>The me</b>
Cavity ring down spectroscopy coupled to fibers	Ariese	Loock	Dr.	Univ. of Kingston, Ontario, Canada	2
Depth Raman spectroscopy	Ariese	Matousek	Prof. dr.	Rutherford Appleton Lab, UK	2
High-resolution cryogenic luminescence spectroscopy	Ariese	Kumke	Dr.	Univ. of Potsdam, Germany	2
Phosphorescence of drug-proteins	Ariese	Miranda	Prof. dr.	Univ. of Valencia, Spain	2
Raman spectroscopy at the nanoscale	Ariese	Mank	Dr.	Philips, Eindhoven	2
Raman spectroscopy of coatings	Ariese	Maanen van / Brink v.d.	Dr. / Dr.	AKZO-Nobel Arnhem/ Deventer	2
Chiral Separations and Detection	Ariese	Garcia-Ruiz	Dr.	Univ. of Alcala de Henares, Spain	2
1) Chemistry and spectroscopy of metal-macrocyle systems. 2) Oxidation catalysis	Baerends	Rosa	Prof. dr.	Universita della Basilicata, Potenza, Italy	3
Oxidation catalysis	Baerends	Belanzoni	Prof. dr.	Univ. Perugia, Italy	3
Oxidation catalysis	Baerends	Bernasconi	Dr.	Rutherford-Appleton Lab, Oxford, UK	3
Density MATRIX functional theory	Baerends	Pernal	Prof. dr.	Dep. of Physics, Univ. Lodz, Poland	3
Real space representations (Coulomb holes) of electron correlation	Baerends	Kim		Pohang Univ. of Science and Technology, South-Korea	3
Real space representations (Coulomb holes) of electron correlation	Baerends	Wang	Prof. dr.	Dep. of Chemistry, Huzhou Univ., China	3
Theoretical treatment of photoelectron spectroscopy	Baerends	Chong	Prof. dr.	Univ. of British Columbia, Vancouver, Canada	3

Theory of chiral spectroscopies.	Baerends	Ding/ Tian	Drs./ Prof. dr.	Dep. of Chemistry and State Key Lab of Phys. Chem. of Solid Surfaces, Xiamen Univ. , China	3
Fundamentals of density functional theory.	Baerends	Gál	Dr.	Univ. of Debrecen, Hungary	
Aromaticity, polar bonds, reactivity	Bickelhaupt	Solà	Prof. dr.	University of Girona, Spain	3
Benzoquinone structures, Li-ion batteries, bond theory	Bickelhaupt	Galembeck	Prof. dr.	University of Sao Paulo, Ribeirao Preto, Brazil	3
Cationic versus anionic E2 and SN2 reactions	Bickelhaupt	Ren	Prof. dr.	Sichuan University, Chendu, China	3
Dihydrogen bonds and hydrogen storage	Bickelhaupt	Simon	Dr.	University of Girona, Spain	3
Dihydrogen bonds and hydrogen storage	Bickelhaupt	Duran	Prof. dr.	University of Girona, Spain	3
DNA base quartets and metal complexes	Bickelhaupt	Lippert	Prof. dr.	TU Dortmund, Germany	1,3
DNA intercalation	Bickelhaupt	Barone	Prof. dr.	University of Palermo, Italy	3
DNA quartets	Bickelhaupt	Paragi	Dr.	University of Szeged, Hungary	3
Functionalized allyl and pentadienyl carbanions	Bickelhaupt	Layfield	Dr.	University of Manchester, UK	1,3
Mass spectrometry of silver-adducted ferrocenyl catalyst complexes	Bickelhaupt	Niessen	Prof. dr.	VU University Amsterdam, Netherlands	1,3
Metathesis reactions	Bickelhaupt	Orian	Dr.	University of Padova, Italy	3
Multilevel methods, NMR of DNA structures, reactivity	Bickelhaupt	Swart	Dr.	University of Girona, Spain	3
N-heterocyclic ligands and complexes thereof	Bickelhaupt	Radius	Prof. dr.	University of Würzburg, Germany	1,3
NMR of DNA structures	Bickelhaupt	Sychrovsky	Dr.	Academy of Sciences of the Czech Republic, Prague, Czech Republic	2,3

NMR of DNA structures	Bickelhaupt	Sponer	Prof. dr.	Academy of Sciences of the Czech Republic, Brno, Czech Republic	2,3
NMR of DNA structures and metal complexes thereof	Bickelhaupt	Wijmenga	Prof. dr.	University of Nijmegen, Netherlands	2,3
Noblegas compounds, helicene complexes, H---H interactions in annulenes	Bickelhaupt	Merino	Prof. dr.	University of Guanajuato, Mexico	3
Pericylci reactions	Bickelhaupt	Cossio	Prof. dr.	University of San Sebastian, Spain	3
Pericylci reactions	Bickelhaupt	Fernandez	Dr.	University Complutense, Madrid, Spain	3
Reductive elimination from Ag(I) complexes	Bickelhaupt	Sijbesma	Prof. dr.	TU Eindhoven, Netherlands	1,3
SEAr reactivity	Bickelhaupt	DeProft	Prof. dr.	Vrije Universiteit Brussel, Belgium	3
SN2 reactions and ab initio benchmarks	Bickelhaupt	Allen	Prof. dr.	University of Georgia, Athens, USA	3
Structure and bonding in palladium phosphine complexes	Bickelhaupt	Leitner	Prof. dr.	RWTH Achen, Germany	1,3
Collodial self-assembly	Bolhuis	Kegel	Prof. dr	Utrecht University	3
Critical casimir interaction in colloids	Bolhuis	Schall	Dr.	University of Amsterdam	3
Denaturation and aggregation of whey proteins	Bolhuis	Floris	Dr.	NIZO	3
Effect of small co-solvents on biomolecules	Bolhuis	Bakker	Prof. dr.	FOM-AMOLF	3
Methods for protein folding	Bolhuis	Codera	Dr.	University of California, Berkeley	3
Photoactive proteins	Bolhuis	Hellingwerf	Prof. dr	Universiteit van Amsterdam	3
Polypeptide self-assembly	Bolhuis	Cohen-Stuart	Prof. dr	Wageningen University	3
Protein conformational transitions	Bolhuis	Huber	Dr.	University of Leiden	3
Protein folding in optical tweezers	Bolhuis	Tans	Prof. dr.	FOM-AMOLF	3

Rare event methods	Bolhuis	Peters	Prof. dr.	University of California, Santa Barbara	3
Transmembrane receptors	Bolhuis	Frenkel	Prof. dr.	University of Cambridge	3
Rare event methods	Bolhuis	Dellago	Prof. dr.	University of Vienna	3
THIS IS JUST AN EXAMPLE: Computational Chemistry	Bolhuis - Meijer	Smit	Prof. dr.	University of Berkeley, California	3
biological studies	Bonnet	Kilian	Prof. dr.	Utrecht University	1
Biological testing	Bonnet	Heger	Dr.	Amsterdam Medical Center	
Catalysis	Bonnet	Klein Gebbink	Prof. dr.	Utrecht University	1
DFT calculations	Bonnet	Van Lenthe	Dr.	Utrecht University	1
DFT calculations	Bonnet	Robert	Prof. dr.	University of Strasbourg, France	1
DFT calculations	Bonnet	Van Dam	Dr.	Pacific Northwestern Laboratory, Richland, USA	1
DFT calculations	Bonnet	Van Lenthe	Dr.	Utrecht University	1
DSC	Bonnet	Roubeau	Dr.	University of Zaragoza, Spain	1
Spectroscopy	Bonnet	Bousseksou & Molnar	Prof. dr.	LCC Toulouse, France	1
STM	Bonnet	Aarts	Prof. dr.	Leiden University	1
X-ray	Bonnet	Siegler	Dr.	Univ. John Hopkins, Baltimore, USA	1
Electrocatalysis	Bouwman	DuBois	Prof. dr.	Pacific Northwestern National Laboratory, Richland, USA	1
Molecular sensing	Bouwman	Woltering	Prof. dr.	Wageningen University	1
Photocatalysis	Bouwman	Mul	Prof. dr.	Twente University	1
X-ray crystallography	Bouwman	Lutz	Dr.	Utrecht University	1

X-ray crystallography	Bouwman	Mutikainen	Prof. dr.	University of Helsinki, Helsinki, Finland	1
Confocal microscopy	Brouwer	de Groot	Dr.	VU	2
Confocal microscopy	Brouwer	de Boer	Prof. dr.	VU	2
Imaging of film formation Cohen Stuart Prof. dr. M. WUR	Brouwer	Cohen Stuart	Prof. dr.	WUR	2
Imaging of force networks	Brouwer	Bonn	Prof. dr.	IoP/UvA	2
Imaging of force networks	Brouwer	Schall	Dr.	IoP/UvA	2
Tetrazines	Brouwer	Audebert	Prof. dr.	ENS Cachan, France	2
Photoactive azo compounds	Brouwer	Ishow	Prof. dr.	Nantes, France	2
Metal enhanced fluorescence	Brouwer	Gacoin	Prof. dr.	Ecole Polytechnique, Palaiseau, France	2
Metal enhanced fluorescence Peretti dr. J. Ecole Polytechnique, Palaiseau, France	Brouwer	Peretti	Dr.	Ecole Polytechnique, Palaiseau, France	2
Molecules in metal nanostructures	Brouwer	Mennucci	Prof. dr.	Pisa, Italy	2
Molecules in metal nanostructures	Brouwer	Débarre	Dr.	Orsay, France	2
Molecules in metal nanostructures	Brouwer	Werts	Dr.	Bruz, France	2
Fluorescent rotaxanes	Brouwer	Smith	Prof. dr.	Notre Dame, USA	2
Electrochemical shuttling in rotaxanes	Brouwer	Paolucci	Prof. dr.	Bologna, Italy	2
Topic: Metallo-radical reactivity	Bruin, de	Wayland	Prof. dr.	University of Pennsylvania (USA)	1
Olefin Polymerisation.	Bruin, de	Busico	Prof. dr.	University of Naples (Italy)	1
Metallo-radical reactivity	Bruin, de	Grützmacher	Prof. dr.	ETH Zürich (Switzerland)	1
Computational catalysis	Bruin, de	Budzelaar	Prof. dr.	University of Manitoba (Canada)	1

Olefin Polymerisation	Bruin, de	Macchioni	Prof. dr.	University of Perugia, (Italy)	1
Metallo-radical reactivity	Bruin, de	Gambarotta	Prof. dr.	University of Ottawa (Canada)	1
Computational catalysis	Bruin, de	Cole-Hamilton	Prof. dr.	University of St Andrews (UK)	1
Metallo-radical reactivity; EPR spectroscopy	Bruin, de	Reijerse	Dr.	MPI für Bioanorganische Chemie, Mülheim a/d Ruhr (Germany)	1
Metallo-radical reactivity	Bruin, de	Plattner	Prof. dr.	Albert Ludwigs University Freiburg (Germany)	1
Metallo-radical reactivity	Bruin, de	Chan	Prof. dr.	Chinese University of Hong Kong	1
Catalysis with cooperative ligands	Bruin, de	Ciriano/Dr. C. Tejel	Prof. dr.	University of Zaragoza (Spain)	1
Metallo-radical reactivity	Bruin, de	Zhang	Prof. dr.	University of South California (USA)	1
Metallo-radical reactivity	Bruin, de	Fu	Prof. dr.	University of Peking (China)	1
Excited-state proton transfer	Buma	Waluk	Prof. dr.	Polish Academy of Sciences, Poland	2
Fe and FeS nanoparticles	Buma	Waters	Prof. dr.	SRON	2
Helium nanodroplet spectroscopy	Buma	Drabbels	Dr.	EPFL, Switzerland	2
High-resolution spectroscopy GFP	Buma	Pratt	Prof. dr.	University of Pittsburgh, USA	2
Laser desorption spectroscopy	Buma	de Vries	Prof. dr.	UCSB, USA	2
PAHs	Buma	Oomens	Prof. dr.	FOM Rijnhuizen	2
Rotaxane spectroscopy	Buma	Rijs	Dr.	FOM Rijnhuizen	2
Rotaxanes	Buma	Leigh	Prof. dr.	University of Edinburgh	2
Silicon nanoparticles	Buma	Gregorkiewicz	Prof. dr.	Van der Waals-Zeeman	2

				Institute, UvA	
VCD	Buma	Nafie	Prof. dr.	Syracuse University, USA	2
	Buma	Zerbetto	Prof. dr.	University of Bologna, Italy	2,3
	Buma	Biscarini	Dr.	CNR Bologna, Italy	2
Chiral zeolites/MOFs	David Dubbeldam	Vlugt	Prof.	TU Delft	3
Adsorption nanoporous materials	David Dubbeldam	Calero	Prof.	University Pablo de Olavide, Seville, Spain	3
Simulation software	David Dubbeldam	Snurr	Prof.	Northwestern University, Evanston, USA	3
Diffusion in nanoporous materials	David Dubbeldam	Stallmach	Prof.	University of Leipzig	3
Adsorption in zeolites	David Dubbeldam	Kapteijn	Prof.	TU Delft	3
Method development	David Dubbeldam	Van Erp	Dr.	Catholic University of Leuven, Belgium	3
Adsorption and diffusion in MOFs, catalysis in MOFs, and synthesis of nanomaterials	David Dubbeldam	Walton	Prof.	Georgia Tech, Atlanta, USA	3
Properties and reactivity of transition-metal-carbene compounds	Elsevier	Cavell	Prof.	University of Cardiff, Wales. UK	1
Hydrogenation reactions	Elsevier	Catellani	Prof.	University of Parma	1
Luminescence, ceramic scintillators	Fu	Ronda	Prof. dr.	Philips Technologie GmbH Forschungslaboratorien, Germany	1
Luminescence, ceramic scintillators	Fu	Barbieri	Prof. dr.	ISOF-CNR, Bologna, Italy	1
Luminescence, ceramic scintillators	Fu	Meijerink	Prof. dr.	Utrecht University	1
Nano oxides, transparent ceramics	Fu	Bettinelli	Prof. dr.	University of Verona, Italy	1
Nano oxides, transparent ceramics	Fu	Tietz	Dr.	Institut für Energie-	1

				forschung (IEF-1, Jülich, Germany)	
Nanomaterials, transparent ceramics	Fu	Kelder	Dr.	Delft University of Technology	1
Time-dependent density matrix functional theory	Gritsenko	van Leeuwen	Prof.	University of Jyvaskyla, Finland	3
Copper proteins and enzymes by EPR/ENDOR	Groenen	Canthers	Prof. dr.	Leiden University	2
High-frequency EPR	Groenen	Moebius	Prof. dr.	Max-Planck Institute for Bio-inorganic Chemistry, Muelheim	2
Multi-frequency EPR studies of bio-mimetic cobalt and iron coordination compounds	Groenen	Kyritsis	Prof. dr.	University of Athens	2
Polarity and proticity probing through spin-labeled proteins	Groenen	Steinhoff	Prof. dr.	University of Osnabrueck	2
Resonance Raman spectroscopy of carotenoids	Groenen	Lugtenburg, Frank	Prof. dr.	Leiden University, University of Connecticut	2
X-ray crystallography	Hiemstra	De Gelder	Dr.	Radboud University Nijmegen	1
Insect repellents	Hiemstra	Schuurink	Dr.	Biology, UvA	1
An alternative mechanism for methane conversion	Juurlink	Santen	Prof. dr. ir.	TU Eindhoven	2
Electrochemistry	Koper	Markovic	Dr.	Argonne National Lab	1,2
Theory of electrochemistry	Koper	Schmickler	Prof. dr.	Ulm University	3
Electrochemistry	Koper	Feliu	Prof. dr.	Univ. Alicante	1,2
Artizymes	Lammertsma	van Raaij	Prof. dr.	Crt Nac.Biotec. Madrid	1
Artizymes	Lammertsma	Kamer	Prof. dr.	Univ. St. Andrews	1
X-ray crystallography	Lammertsma	Lutz	Dr.	University Utrecht	1
Metalloenzymes	Lammertsma	Vermeulen	Prof. dr.	VU	1

Organophosphor	Lammertsma	Grützmaacher	Prof. dr.	ETH, Zürich	1
Organophosphor	Lammertsma	Gudat	Prof. dr.	Univ. Stuttgart	1
Physical Organic	Lammertsma	Chen	Prof. dr.	ETH, Zürich	1
Physical Organic	Lammertsma	Manners	Prof. dr.	Univ. Bristol	1
Polymers	Lammertsma	Sareav	Prof. dr.	Irkutsk State Univ.	1
Silicates	Lammertsma	Wagler	Prof. dr.	Tech. Univ. Freiberg	1
Solid state astrochemistry	Linnartz	McCoustra (Lassie consortium)	Prof. dr.	Heriot Watt University, Edingburg	2
Astrochemistry	Linnartz	Tielens (Dutch Astrochemistry Network)	Prof. dr.	Leiden University	2
Solid state astrochemistry	Linnartz	Fillion	Prof. dr.	SOLEIL, Paris	2
Solid state astrochemistry	Linnartz	Cuppen	Dr.	Radboud Universiteit Nijmegen	2
Gas phase astrochemistry	Linnartz	van Winckel	Prof. dr.	Universiteit van Leuven	2
PAH in space	Linnartz	Allamandola	Dr.	NASA Ames	2
UV Photolysis of ice	Linnartz	Oberg	Dr.	Smithsonian Harvard	2
Exciton Coupling	Neugebauer	Mennucci	Prof. dr.	University of Pisa	3
Exciton Coupling	Neugebauer	Curutchet	Dr.	University of Girona	3
Vibrational Spectroscopy	Neugebauer	Reiher	Prof. dr.	ETH Zurich	3
Vibrational Spectroscopy	Neugebauer	Gilch	Prof. dr.	University of Duesseldorf	3
Biocatalysis and MCRs	Orru	Turner	Prof. dr.	Univ Manchester	1
Biorenewables	Orru	Stevens	Prof. dr.	Ghent University	1
IBOS; Biocatalysis and MCRs	Orru	Hanefeld	Dr.	TUD	1

Insertion reactions of Isonitriles	Orru	Maes	Prof. dr.	University of Antwerp	1
Isonitriles	Orru	Nenaidenko	Prof. dr.	Moscow State Univ	1
MCRs	Orru	Zhu	Prof. dr.	CNRS(F)/univ Lausanne (SUI)	1
MCRs in medchem	Orru	Gijssen	Dr.	Johnson & Johnson	1
Microreactors	Orru	Irth	Prof. dr.	VU-FEW	1
Microwave chemistry	Orru	Kappe	Prof. dr.	Karl Franszens University Austria	1
Microwave chemistry and MCRS in Med Chem	Orru	Leurs	Prof. dr.	VU-FEW	1
Microwaves	Orru	Bogdal	Prof. dr.	Krakov Univ of Technology	1
Molecular Biology Probes	Orru	Luirink	Dr.	VU-FALW	1
NHC-Ru Catalysts/Predictive Modelling	Orru	Rothenberg	Prof. dr.	UvA	1
Plant biochemistry & MCRs	Orru	Wessjohann	Prof. dr.	Leibniz institute, Halle, Germany	1
reactive building blocks	Orru	Elkaim	Prof. dr.	ENSTA, Paris	1
Ugi reactions	Orru	vd Eycken	Prof. dr.	Leuven University	1
ZONMW Programme: Antimicrobial Resistance	Orru	van Belkum	Prof. dr.	Microbiology, Erasmus Medical Center	1
ZONMW-programme:Antimicrobial Resistance	Orru	Breukink	Dr.	Biochemistry, Utrecht University	1
Glycolipid Metabolism	Overkleeft	Aerts	Prof. dr.	AMC	1
Proteasome Enzymology	Overkleeft	Kisselev	Dr.	Dartmouth Medical Centre, New Hampshire, USA,	1
Proteasome Tumour Biology	Overkleeft	Driessen	Dr.	St. Gallen Medical Centre, Switzerland	1
Matrix Metalloproteases	Overkleeft	Bischoff	Prof. dr.	RUG	1

Kinase Inhibitors	Overkleeft	Neefjes	Prof. dr.	NKI	1
Vaccine Development	Overkleeft	Ossendorp	Prof. dr.	LUMC	1
Synthesis	Reek	Gryko	Dr.	Polish Academy of Sciences, Poland	1
Catalysis	Reek	Berkessel	Prof. dr.	University of Bonn	1
Catalysis	Reek	Schmalz	Prof. dr.	University of Bonn	1
X-ray crystallography	Reek - de Bruin - van der Vlugt	Lutz	Dr.	Utrecht University	1
Microfluidics	Reek - van der Vlugt	Gardeniers	Prof. dr.	Twente University	1
Photocatalysis	Reek - van der Vlugt	Holzwarth	Prof. dr.	MPI Mulheim	1
Photocatalysis	Reek - van der Vlugt	Barber	Prof. dr.	Imperial College London	1
Catalysis	van der Vlugt	Schneider	Prof. dr.	TU Munich	1
Catalysis	van der Vlugt	Meyer	Prof. dr.	University of Goettingen	1
Catalysis	van der Vlugt	Perruzzini	Prof. dr.	ICCOM - CNR Florence	1
DFT calculations	van der Vlugt	Pidko	Dr.	Eindhoven University of Technology	1
DIRAC program package	Visscher	Saue	Dr.	Univ. Paul Sabatier Toulouse	3
DIRAC program package	Visscher	Ruud	Prof. dr.	Univ Tromsø	3
DIRAC program package	Visscher	Jensen	Prof. dr.	Univ of Southern Denmark	3
Relativistic Coupled Cluster	Visscher	Kallay	Prof. dr.	Univ of Budapest	3
Subsystem DFT methods	Visscher	Jacob	Dr.	Karlsruhe Institute of Technology	3
Actinide Chemistry	Visscher	Vallet	Prof. dr.	Univ. of Lille	3
WFT in DFT embedding	Visscher	de Jong	Dr.	Pacific Northwest National Laboratory	3

Artizymen	Wever	Kamer	Prof. dr.	Univ. St. Andrews	1
Biofilm prevention	Wever	Crielaard	Prof. dr.	ACTA, University of Amsterdam	1
Enzymatic cascade reactions	Wever	Rutjes	Prof. dr.	Radboud University Nijmegen	1
Enzymatic cascade reactions	Wever	Van der Oost	Prof. dr.	University Wageningen	1
V2O5 nanowires	Wever	Tremel	Prof. dr.	Johannes Gutenberg University, Mainz, Germany	1
Photodegradation of pigments	Williams	Neevel	Dr.	Netherlands Institute for Cultural Heritage (ICN)	2
Spectroscopy of salen complexes	Williams	Reek	Prof. dr.	UvA-HIMS	2
Analysis of femtosecond transient absorption data	Williams	van Stokkum	Dr.	VU	2
Fast spectroscopy of solar cell materials and model systems	Williams	Janssen	Prof. dr.	TU-Eindhoven	2
Fast spectroscopy of solar cell materials and model systems	Williams	Hummelen	Prof. dr.	Groningen	2
Photoinduced hydrogen evolution	Williams	Feiters	Dr.	Nijmegen	2
Fast spectroscopy of thin films of organic n-type semiconductors	Williams	Loi	Prof. dr.	Groningen	2
Fast spectroscopy of porphyrine-quinone systems	Williams	Galloni	Dr.	Rome	2
Spectroscopy of covalently linked catechol-quinones systems	Williams	Aviram	Dr.	Qutronics (USA)	2
Fast spectroscopy of homoconjugated energy transfer systems	Williams	Barcina	Prof. dr.	Madrid	2
Fast spectroscopy of functionalized and organized dye systems	Williams	Würthner	Prof. dr.	Wurzburg	2
Fast spectroscopy of organic n-type semiconductors	Williams	Hudhomme	Prof. dr.	Angers	2

Photoinduced processes in functionalized and organized dye systems	Williams	Le Cong	Prof. dr.	Hanoi	2
2DIR of Protein folding	Woutersen	Peter Hamm	Prof.	Univ. of Zurich	2
Proton transport in nanoconfinement	Woutersen	Sager	Dr.	FZ Jülich	2
Proton transport in nanoconfinement	Woutersen	Bakker	Prof.	AMOLF	2
Electrochemistry of heme proteins	Zwan	Borsari	Prof. dr.	Univ. of Modena, Italy	2
Raman and fluorescence spectroscopy on resveratrol-tyrosinase	Zwan	Gonzalez	Dr.	Univ. of Madrid, Spain	2
Resonance Raman on P450-BM3 mutants	Zwan	Vermeulen	Prof. dr.	Molecular Toxicology, VU, Amsterdam	2
Stark spectroscopy and nanoparticles	Zwan	Mourik van	Dr.	Univ. of Lausanne, Switzerland	2
Vibrational spectroscopy of heme-proteins	Zwan	Hildebrandt	Prof. dr.	TU Berlin, Germany	2
Spectroscopy of ATP and derivatives	Zwan	Heger	Dr.	UvA/AMC, Amsterdam	2



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### 3. Education and Research Training

The main mission of the HRSMC is to provide its PhD students with high-level education training. Apart from completing a research project, the PhD students of the HRSMC follow an individual education and training programme. For this purpose the education committee supplies them with a selection of courses, which are announced annually in the study guide on the HRSMC website. The management of the school administers the credit points obtained by the PhD students and presents HRSMC certificates to those students who have fulfilled their education programme. The requirements of the education program with a minimum of 18 ECTS can be found in Annex 4.5.

#### 3.1 HRSMC Education Programme

The HRSMC offers PhD students a broad programme of inter-university courses and schools.

##### HRSMC Courses (3 or 4 ECTS)

- Molecular Modelling (every two or three years, HRSMC theme 2 and 3)
- Physical Methods in Inorganic Chemistry (biannually, HRSMC theme 1)
- Photophysics, Photochemistry, and Photobiology (every three years, HRSMC theme 2)
- Molecular Simulation (yearly, HRSMC theme 3)
- Synthetic Chemistry problem sessions (+ three times a year, HRSMC theme 1)

All courses are 3 ECTS. Except for Molecular Simulation, which is 4 ECTS.

Character:

- Courses are given at UvA, UL or VU (or in combinations).
- Participants are mostly from HRSMC. A few from other Dutch universities, from the Westfälische Wilhelms Universität Münster or from Dutch chemical companies. The Molecular Simulation course has a lot of participants from abroad.
- Lecturers are mainly from Holland or from Münster.

##### HRSMC schools (3 ECTS)

- Summer School on Photochemistry (every 4 years, HRSMC theme 2)
- Tulip School 'Modern Developments in Spectroscopy' (every 3 years, HRSMC theme 2)
- Summer School 'Synthetic Bio-organic Chemistry' (every 4 years, HRSMC theme 1)
- Autumn School on Metal-organic Chemistry (every 4 years, HRSMC theme 1)

Character:

- More like a conference with lectures, discussion sessions and poster sessions.
- The schools are given at an external location.
- Participants come partly from the HRSMC. Many participants come from other Dutch universities and from abroad.
- Lecturers come mostly from abroad.

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### Activities of 2010

The HRSMC educational activities of 2010 consisted of:

- the two weeks Course 'Molecular Simulation', organised under the auspices of CECAM (January 4-15, 2010, UvA)
- the Course Photophysics, Photochemistry & Photobiology, (May 31 - June 11 2010, UvA/VU)
- the Autumn School 'Advanced Metal-Organic Chemistry', (September 26 - 29, hotel Zonheuvel, Doorn)

In addition to these Schools and Courses, the research groups of Prof. dr. H. Hiemstra (UvA), Prof. dr. R.V.A. Orru (VU) and Prof. dr. H.S. Overkleeft/Prof. dr. G. van der Marel organized two 'Synthetic Chemistry problem solving sessions'.

In 2010, a new activity was organized together on May 25 with the KNCV (Royal Dutch Chemistry Association): the KNCV/HRSMC Career Advice Event for PhD students and postdocs.

Details of the courses that were specifically developed for the HRSMC by its members were:

#### **HRSMC Course Understanding Molecular Simulation, Molsim 2010 (January 4-15, 2010, UvA)**

Coordinators: Dr. B. Ensing (UvA), Dr. E.J. Meijer (UvA) and I. Weijer (HRSMC)  
Lecturers: Dr. B. Ensing (UvA), Dr. E.J. Meijer (UvA)  
Guest Lecturers: Prof. dr. Charbonneau, Prof. dr. Daan Frenkel, Dr. Christopher Lowe, Prof. dr. Berend Smit, and Dr. Thijs Vlugt  
Participants: 61 (6 Master students, 55 PhD students and Postdocs: 6 from the HRSMC, 5 from other Dutch Universities and 44 from abroad varying from Norway to Spain, from Israel to Iran)

#### **KNCV/HRSMC Career Advice Event for PhD students and postdocs (May 25 2010, UvA)**

With various lectures regarding career possibilities and job-application. In addition, each participant got 30 min. quality time with a career consultant.

Coordinators: Drs. J. van der Zwan (KNCV), R. Weijer (HRSMC) en Drs. H.E. Zwaan (HRSMC)  
Participants: 24 (11 HRSMC PhD students, 13 other Dutch Universities)

#### **HRSMC Course Photophysics, Photochemistry & Photobiology, (May 31 - June 11 2010, UvA/VU)**

Coordinators: Prof. dr. W.J. Buma (UvA), Dr. F. Buda (UL), Dr. R. Williams (UvA), Dr. G. van der Zwan (VU), Drs. H.E. Zwaan-v.d. Plas (HRSMC) and I. Weijer (HRSMC)  
Lecturers: Prof. dr. W.J. Buma (UvA), Dr. F. Buda (UL), Prof. dr. C. Gooijer (VU) Dr. R. Williams (UvA) and Dr. G. van der Zwan (VU),  
Guest lecturers: Dr. Maurice Aalders (AMC, NL)  
Participants: 15 (12 HRSMC members, 3 other Dutch Univerisites)

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**HRSMC Autumn School 'Advanced Metal-Organic Chemistry  
(September 26-29, 2010, hotel Zonheuvel, Doorn)**

This school was organized with dr Robert Wolf (WWU Münster) from outside the HRSMC as a part of the cooperation between the HRSMC and the WWU Münster

Coordinators: Prof. dr. E. Bouwman (UL), Dr. S. Bonnet (UL), Dr. B. de Bruin (UvA), Dr. A. Ehlers (VU), Prof. dr. C.J. Elsevier (UvA), Drs. H.E. Zwaan-v.d. Plas (HRSMC) and I. Weijer (HRSMC)

Guest Lecturers: Prof. dr. R. Alberto (Universität Zürich), Prof. dr. M. Albrecht (University College Dublin), Prof. dr. N. Champness, (University of Nottingham), Prof. dr. B. Chaudret (Laboratoire de Chimie de Coordination du CNRS, Toulouse) and Prof. dr. P. Norrby (University of Gothenburg)

Participants: 32 (18 HRSMC PhD students, 7 WWU Münster, 7 other Dutch Universities)

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## 3.2 Symposium

The symposium, which was attended by ca. 140 scientists, also included poster sessions with 46 posters, mainly presented by PhD students. Contrary to previous symposia, this symposium had a different set-up: less posters and less posters per session, and more and shorter lectures.

The following lectures were given:

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

- Prof. dr. Henk Hiemstra (UvA)  
*Chiral Brønsted Acid Base Organocatalysis*
- PhD lecture Henrik Gold (UL)  
*Synthesis and applications of  $^{13}\text{C}$ -labeled lysoCTH, a biomarker for Fabry's disease*

Theme 2 'Photochemistry and (Laser) Spectroscopy'

- Dr. Alex Yanson (UL)  
*Cathodic corrosion? A quick, clean and versatile method for the synthesis of metallic nanoparticles*
- PhD lecture Stefan Lehmann (VU)  
*Femtosecond pulse shaping and quantum control in multichannel molecular dynamics studied by photoelectron-photoion coincidence imaging*
- PhD lecture Matthijs Panman (UvA)  
*Operation Mechanism of a Molecular Machine Revealed Using Time-Resolved Vibrational Spectroscopy*

Theme 3 'Theoretical Chemistry'

- Dr. Rosa Buló (VU)  
*Chemistry in Water with Adaptive QM/MM Simulations*
- Dr. Jocelyne Vreede (UvA)  
*What is the conformation of the H-NS dimerization domain? The effect of ionic strength and temperature on coiled coil structure*

Guest lectures

- Prof. dr. Rutger van Santen (TUE)  
*Catalysis, playing dice with molecules*
- IRTG lecture: Dr. Dominik Megger (WWU Münster)  
*Metal-mediated Hoogsteen-type base pairs: A promising approach for the site-specific functionalization of DNA with metal ions*
- Dr. Niels Elders (Akzo Nobel) winner Dick Stufkens Prize for the most outstanding PhD thesis

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### 3.3 Seminars

The list of seminars given below is not complete, but it gives a good impression of the extent and quality of these education activities:

**January 15, Leiden University**

*'Vanadium oxide films on Au(111): model catalysts for methanol oxidation'*

Dr.ir. Marko Sturm

FOM Institute for Plasma Physics Rijnhuizen

The Netherlands

**February 12, Leiden University**

*'Iron-based Fischer-Tropsch Synthesis: A Density Functional Study'*

Dr. Jose M. Gracia Budria

University of Technology Eindhoven

The Netherlands

**February 16, VU University**

*'Recent experiences in enzyme inhibitor development: selected cases with an emphasis on protease targets'*

Prof. dr. Pieter Van der Veken

Universiteit Antwerpen

Belgium

**March 1, VU University**

*'Elucidation of the Mechanism of Asparagine Deamidation in Peptides'*

Saron Catak

**March 3, University of Amsterdam**

*'Path-integral rate-theory in the deep-tunnelling regime'*

Dr. Stuart C. Althorpe

Department of Chemistry

University of Cambridge

United Kingdom

**March 8, Leiden University**

*'Detection of Nitric Oxide: Combining EPR and NMR'*

Prof. Dr. Lawrence J. Berliner

Department of Chemistry and Biochemistry

University of Denver

U.S.A.

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**March 22, Leiden University**

*'Hydrogen siting and dynamics in hydrogen-storage materials with 1H and 2H NMR'*

Dr. Pieter C.M.M. Magusin  
Chemical Engineering and Chemistry  
Eindhoven University of Technology  
The Netherlands

**March 23, VU University**

*'E pluribus unum: a pluripotent multicomponent approach to DOS libraries'*

Dr. Andrea Basso  
Bioorganic Chemistry Group  
University of Genova  
Italy

**March 24, University of Amsterdam**

*'Multiscale Modelling of Photoactive Materials'*

Dr. Nikos L. Doltsinis  
Department of Physics King's College London  
United Kingdom

**March 31, VU University**

*'1,3-Dicarbonyls : Old Substrates for the Development of New Synthetic Methodologies'*

Prof. dr. Jean Rodriguez  
Université Paul Cézanne (Aix-Marseille III)  
Institut des Sciences Moléculaires de Marseille  
France

**April 8, Leiden University**

*'Some Challenges of Proton NMR on Solids'*

Van Arkel Chairholder Prof. dr. Shimon Vega  
Chemical Physics Department Weizmann Institute of Science  
Rehovot  
Israel

**April 24, VU University**

*'Optical dichroism and electronic structure of stratified media'*

Lorenzo Sponza

**April 28, University of Amsterdam**

*'Cucurbiturils: Macrocycles with New Opportunities'*

Prof. Dr. Werner Nau  
Jacobs University Bremen  
Germany

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**May 20, VU University**

*'Explicitly correlated MP2 theory'*

Sebastian Hoefener

**May 25, VU University**

*'Modeling Charge Resonance in PAH clusters - the DFTB+CI Method'*

Andre Mirtschink

**May 31, Leiden University**

*'Nonlinear coherent microscopy of tissues nanostructures and single molecules'*

Eric Potma

Department of Chemistry

University of California Irvine

U.S.A.

**May 28, Leiden University**

*'Farewell Symposium Prof. dr. Ben Nieuwenhuys: 'Catalytic Surface Science'*

In Honour of Prof. dr. Ben Nieuwenhuys

Leiden University

The Netherlands

**June 14, Leiden University**

*'The intermolecular hydroamination of non activated olefins: challenges and progress using Pt catalysis';*

Prof. dr. R. Poli

CNRS; Université de Toulouse

France

**June 16, Leiden University**

*'In situ characterisation of electrocatalyst structure'*

Professor Andrea E. Russell

University of Southampton

United Kingdom

**June 24, VU University**

*'Catalytic Enantioselective Henry Reaction. Development and Applications'*

Prof. dr. Gonzalo Blay

Departament de Química Orgànica

Facultat de Química-Universitat de València

Spain

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**June 29, Leiden University**

*'Role of Composition and Distribution on Platinum Alloys with Late Transition Metals'*

Dr. Federico Calle Vallejo

Center for Atomic-scale Materials Design

Dept of Physics. Technical University of Denmark,

Denmark

**July 1, University of Amsterdam**

*'Practical asymmetric hydrogenation and hydroformylation reactions'*

Prof. Xumu Zhang

Rutgers The State University of New Jersey

**July 7, University of Amsterdam**

*'Thermodynamic Forces in Adaptive Resolution Simulations'*.

Simon Poblete

Max-Planck

Institut fuer Polymerforschung

Mainz

**July 8, VU University**

*'Multiplication and Hydride Reduction of P-Heterocyclic Biradicals'*

Shigekazu ITO DSc.

Department of Applied Chemistry

Graduate School of Science and Engineering

Tokyo Institute of Technology

Japan

**July 14, VU University**

*'An ensemble DFT method and its applications in photochemistry'*

Andranik Kazaryan

**August 23, Leiden University**

*'Multiple spin echoes and instabilities in dissolved hyperpolarized  $^3\text{He}$  or  $^{129}\text{Xe}$ '*

Dr. Steven W. Morgan

Laboratoire Kastler Brossel & CEA Saclay

**August 23, Leiden University**

*'Spins as Probes for Charge Transport in Solar Cells'*

Dr. Jan Behrends

Helmholtz-Zentrum Berlin für Materialien und Energie

Germany

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**August 26, VU University**

*'Chirogenesis and Catalysis with Metallosalen Architectures'*

Dr. Arjan Kleij

Catalan Institution for Research and Advanced Studies (ICREA) & Institute of Chemical Research of Catalonia (ICIQ)

Spain

**September 3, Leiden University**

*'Magnetoresistance caused by molecular hyperfine fields and ferromagnetic stray fields'*

Prof. dr. Markus Wohlgenannt

department of Physics and Astronomy

University of Iowa

U.S.A.

**September 3, Leiden University**

*'Initial Sticking Coefficients of O<sub>2</sub> and H<sub>2</sub> on Ultrathin Cu Layers on Ru(0001)'*

Dr. Marina Minniti

Universidad Autónoma de Madrid

Spain

**September 10. Leiden University**

*'The Role of Non-adiabatic Electronic Effects in Molecular Processes on Metal Surfaces'*

Prof. dr. Dan Auerbach

GRT Inc. and the University of California.

Santa Barbara

U.S.A.

**September 14, Leiden University**

*MCBIM-minisymposium 'Catalytic allylation'*

*'Playing with anions: 1) Fast, environmentally friendly ruthenium-allylation catalysts and 2) Understanding and predicting ion pairing'*

Prof. dr. P.S. Pregosin (ETH Hönggerberg Zürich Switzerland);

*'Transformation of olefins with ruthenium catalysts: olefin metathesis and allylic substitution'*

Dr. C. Bruneau (Université de Rennes1 Rennes France);

*'Catalytic allylation of phenols: chloride-free route to epoxy resins'*

J.A. van Rijn (Leiden University Leiden NL);

**September 22. Leiden University**

*'Understanding the complexity of electrochemical interfaces'*

Dr. Nenad Markovic

Materials Sciences Division Argonne National Laboratory

USA

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**October 8, Leiden University**

*'The use of Nickel-NHC compounds in C-H activation'*

Prof. dr. M. Chetcuti  
Université de Strasbourg  
France

**October 11, Leiden University**

*'Nickel – N-heterocyclic carbene chemistry: synthesis catalysis and C–H activation reactions'*

Michael J. Chetcuti  
Laboratoire de Chimie Organométallique Appliquée Ecole Européenne de Chimie  
Polymères et Matériaux (EPCM)  
Université de Strasbourg  
France

**October 13, Leiden University**

*'Alloying Particle Size and Support Effects in Electrocatalysis'*

Prof. dr. Brian E. Hayden  
School of Chemistry  
University of Southampton  
United Kingdom

**October 13, University of Amsterdam**

*'Polyethylene the Hard Way One Carbon at a Time. The Living Polymerization of Ylides and Diazoalkanes'*

Prof. Kenneth J. Shea  
The University of California at Irvine  
U.S.A.

**October 15, University of Amsterdam**

*'Quantum Chemical Perspectives on Structure-Property Relationships in Environmentally Sensitive Methine Dyes'*

Dr. Seth Olsen  
The University of Queensland Brisbane  
Australia

**October 15, Leiden University**

*'Water Dissociation on Modified Transition Metal Surfaces'*

Prof. dr. Georg Held  
University of Reading  
United Kingdom

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**October 27, Leiden University**

*'Electrostatics and Protein Function: From Molecular Structures to Thermodynamics and Kinetics'*

Prof. Matthias Ullmann  
University of Bayreuth  
Germany

**October 29, Leiden University**

*"Reedijk Symposium"*

*"Borderline specificity: Transient interactions between promiscuous proteins"*

Prof. dr. M. Ubbink  
(Leiden University Leiden NL)

*"Streptomyces: the beauty of the beast"*

Prof. dr. G.P. van Wezel  
(Leiden University Leiden NL)

*"Development of transition-metal catalysts for new atom-efficient reactions"*

Prof. dr. E. Bouwman  
(Leiden University Leiden NL)

*"Electrocatalysis: potential-dependent coordination chemistry at surfaces"*

Prof. dr. M.T.M. Koper  
(Leiden University Leiden NL)

*"Chemical biology of human glucosylceramide metabolism"*

Prof. dr. H.S. Overkleeft  
(Leiden University Leiden NL)

*"Hydrogen generation and storage"*

Prof. dr. M. Schröder  
(University of Nottingham UK)

**November 2, University of Amsterdam**

*"NMR Spectroscopy of Protein Assemblies Vanadium-Containing Haloperoxidases and Bioinorganic Material"*

Dr. Tatyana Polenova  
Department of Chemistry and Biochemistry  
University of Delaware  
U.S.A.

**November 2, Leiden University**

*"Stereoselective Reactions of Oxocarbenium Ions"*

Prof. dr. Keith Woerpel  
Department of Chemistry  
New York University  
U.S.A.

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**November 10, University of Amsterdam**

*"Reaction coordinates for complex chemical transformations – how enzymes really work"*

Prof. dr. Steven D. Schwartz

Depts. of Biophysics and Biochemistry Albert Einstein College of Medicine New York and  
L'Institut des hautes études scientifiques Bures-sur-Yvette  
France.

**November 2, VU University**

*"Theoretical Investigations of the Acetylene Analogues of Group 14 Elements E2X2 (E=Si-Pb X=F-I)"*

Dr. Takayasu Shimuzu

**November 23, Leiden University**

*"Photoactivation of the Blue Light Sensor Cryptochrome"*

Dr. Tilman Kottke

Department of Biophysical Chemistry  
Bielefeld University  
Germany

**November 16, Leiden University**

*"Diboron porphyrins and corroles: unexpected chemistry for both boron and the ligands"*

Prof. dr. P.J. Brothers

The University of Auckland  
New Zealand

**December 9, Leiden University**

*"Insight from scanning tunneling microscopy and photoemission experiments for surface-supported (supra)molecular assemblies"*

Dr. Meike A. Stöhr

Surfaces and Thin Films  
Zernike Institute for Advanced Materials  
University of Groningen

**December 21, University of Amsterdam**

*"Mechanochemical Processes in Biology"*

Dr. Sean Sun

Johns Hopkins University Baltimore, U.S.A

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### 3.4 PhD Graduations (in alphabetical order) & first job after PhD Graduation

**Bodis, P.**

*'Structure and dynamics of complex hydrogen-bonded systems'*

Prof. dr. W.J. Buma (promotor) and Dr. S. Woutersen (co-promotor)

June 8, 2010

Employed by TNO

**Bouwman, J.**

*'Spectroscopy and Chemistry of Interstellar Ice Analogues'*

promotor Prof. dr. H.V.J. Linnartz (promotor)

October 12, 2010

Post-doctoral Fellow University of California, Berkeley

**Elders, N.**

*'Multicomponent Approaches to Molecular Diversity & Complexity'*

Prof. dr. ir. R.V.A. Orru (promotor), Prof. dr. M.B. Groen (promotor)

and Dr. E. Ruijter (co-promotor)

April 1, 2010

Researcher at Akzo Nobel

**Geurink, P.P.**

*'Synthetic tools to illuminate matrix metalloproteinase and proteasome activities'*

Prof. dr. H.S. Overkleeft (promotor) en Prof.dr. G.A. van der Marel (promotor)

October 6, 2010

Post-doctoral Fellow Dutch Cancer Institute (NKI)

**Giesbertz, K.J.H.**

*'Time-Dependent One-Body Reduced Density Matrix Functional Theory'*

Prof. dr. E.J. Baerends (promotor) and Dr. O.V. Gritsenko (co-promotor)

November 5, 2010

Post-doctoral Fellow with the group of Prof. Robert van Leeuwen,  
University of Jyväskylä, Finland

**Gunbas, D.D.**

*'Hydrogen-Bonded Rotaxanes. Structure and Dynamics of Mechanically Interlocked Molecular Shuttles'*

Prof. dr. A.M. Brouwer (promotor)

October 12, 2010

Post-doctoral Fellow with the group of Dr. F. Grozema, Delft Technical University

**Ioppolo, S.**

*'Surface formation routes of interstellar molecules'*

Prof. dr. H.V.J. Linnartz (promotor), Prof. dr. E.F. van Dishoeck (promotor)

December 9, 2010

Post-doctoral Fellow NOVA, Leiden University

**Irimia, D.**

*'Femtosecond imaging and control of molecular photodynamics'*

Prof. dr. M.H.M. Janssen (promotor)

September 30, 2010

Applying for jobs

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**Jagesar, D.C.**

*'Intercomponent interactions and mobility in hydrogen-bonded rotaxanes'*  
Prof. dr. A.M. Brouwer (promotor) and Prof. dr. W.J. Buma (co-promotor)  
November 26, 2010  
Employed by DSM

**Jansen, H.**

*'Electrophilic Phosphinidenes: Science or Fiction?'*  
Prof. dr. K. Lammertsma (promotor) and Dr. A.W. Ehlers (co-promotor)  
October 29, 2010  
Teacher Hogeschool Leiden

**Jellema, E.**

*'Rhodium mediated stereoselective polymerization of carbenes'*  
Prof. dr. J.N.H. Reek (promotor) and Dr. B. de Bruin (co-promotor).  
October 14, 2010  
'Kraton Polymers Research', Amsterdam

**Lai, S.**

*'The electrocatalytic oxidation of ethanol studied on a molecular scale'*  
Prof. M. Koper (promotor)  
June 16, 2010  
Post-doctoral Fellow Chemistry Department, Warwick University, United Kingdom

**Megger, D.A.**

*'DFT Calculations on Metal-Nucleobase Complexes'*  
Prof. Dr. J. Muller (promotor) and Prof. dr. F.M. Bickelhaupt (promotor)  
August 26, 2010, **Westfälische Wilhelms-Universität Münster**  
postdoc bij:  
Post-doctoral Fellow Medizinisches Proteom-Center, Ruhr-Universität Bochum

**Nessen, M.**

*'Development of an enrichment method for azide-containing peptides to study proteome dynamics by mass spectrometry'*  
Prof. dr. C.G. de Koster (promotor), Prof. dr. H. Hiemstra (promotor) Dr. L. de Jong (co-promotor) and Dr. J.H. van Maarseveen (co-promotor)  
December 10, 2010

**Niet van der, M.J.T.C**

*'Water on well-defined platinum surfaces: an ultra high vacuum and electrochemical study'*  
Prof. dr. M.T.M. Koper (promotor)  
October 14, 2010  
Collis, Technical consultant

**Rijn van, J.A.**

*'Catalytic allylation of phenols: chloride-free route towards epoxy resins'*  
Prof. dr. E. Drent (promotor) en Prof. dr. E. Bouwman (promotor)  
September 14, 2010  
Researcher with Momentive, Vlaardingen

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**Scheffelaar, R.**

*'Isonitrile-Functionalized 3,4-Dihydropyridin-2-ones. Multicomponent Synthesis and Synthetic Potential'*

Prof. dr. ir. R.V.A. Orru (promotor)

October 13, 2010

Applying for jobs

**Siekierzycka, J.**

*'Applications of microspectroscope'*

Prof. dr. A.M. Brouwer (promotor)

November 2, 2010

Post-doctoral Fellow with the group of Prof. M. Orrit, Leiden University

**Van der Vliet, D.**

*'Fuel Cell Electrocatalysis: Oxygen reduction on Pt-based nanoparticle catalysts.'*

Prof. dr. Marc Koper (promotor)

September 21, 2010

Postdoc Materials Science Division, Argonne National Laboratory, USA

**Wassenaar, J.**

*'Indole-based phosphorus ligands in asymmetric catalysis'*

Prof. dr. J.N.H. Reek (promotor)

June 30, 2010

Total Petrochemicals, Brussel, Belgium

**Xia, T.**

*'Probing spatial heterogeneity in supercooled glycerol and temporal heterogeneity with single-molecule FRET in polyprolines'*

Prof. dr. M. Orrit (promotor)

March 25, 2010

Post-doctoral Fellow with the group of prof Fang Xiaohong at the Institute of Chemistry of the Chinese Academy of Sciences



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## 4. Annexes

### 4.1 Annex 1 - HRSMC Organisation

#### **Organisation Structure**

The interuniversity research school HRSMC is a cooperation between the University of Amsterdam (UvA), the Vrije Universiteit Amsterdam (VU) and Leiden University (UL), UvA being the university in charge of the HRSMC ('penvoerder'). The HRSMC organisation structure consists of:

#### **Scientific Director and Managing Staff**

- Prof. dr. W.J. Buma (UvA), Scientific Director
- Drs. H.E. Zwaan – van der Plas, Executive Secretary
- Mrs I. Weijer, Administration Officer

#### **Board**

- Prof. dr. F.M. Bickelhaupt (VU, chairman)
- Prof. dr. C.J. Elsevier (UvA)
- Prof. dr. M. Koper (UL)

The scientific director and executive secretary of the HRSMC prepare and attend the meetings of the Board.

#### **Research Committee (OZC)**

- Dr. F. Buda (UL, research theme 2/3)
- Prof. dr. H. Hiemstra (chairman, UvA, research theme 1)
- Prof. dr. S. Stolte (VU, research theme 2)

#### **Education Committee (OWC)**

- Dr. B. Ensing (UvA, research theme 3)
- Prof. dr. ir. R.V.A. Orru (VU, chairman, research theme 1)
- Dr. L. Juurlink (UL, research theme 2)
- MSc L. Smeenk (UvA, research theme 1, PhD student)

#### **External Advisory Committee (WAR)**

- Prof. dr. W.J. Briels (TU-Twente)
- Prof. dr. E. Drent (SRTCA, UL)
- Prof. dr. R. Hage (Rahu Catalytics)
- Prof. dr. J.W. Verhoeven (emeritus UvA)
- Prof. dr. J.G. de Vries (DSM/RUG)

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### **PhD Platform**

- MSc F. Bertini, PhD student in the Organic and Organometallic Chemistry Group of Prof. dr. K. Lammertsma at the VU
- MSc S. Hoogendoorn and/or MSc M. Walvoort, PhD students in the Bio-organic Synthesis Group of Prof. dr. H.S. Overkleeft and Prof. dr. G.A. van der Marel at the UL
- MSc M. Panman, PhD student in the Molecular Photonics Group of Prof. dr. W.J. Buma and Prof. dr. A.M. Brouwer, at the UvA
- MSc L. Smeenk, PhD student in the Synthetic Organic Chemistry Group of Prof. dr. H. Hiemstra and Prof. dr. P. Timmerman at the UvA
- MSc L. Wolters, PhD student in the Theoretical Chemistry Group of Prof. dr. E.J. Baerends, Prof. dr. Matthias Bickelhaupt and Prof. dr. L. Visscher at the VU

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## 4.2 Annex 2 - Financial Account

<b>Income</b>		<b>Expenses</b>	
Contribution UvA 2010	50.000	Personnel Costs	64.862
Contribution UL 2010	6.806	Bureau Costs	2.570
Contribution VU 2010	6.806	Board	1.155
	960		
Symposium		Symposium	6.783
KNCV/HRSMC Career Advice	311	KNCV/HRSMC Career Advice	
Event		Event	381
Autumn School Advanced Metal- Organic Chemistry	29.115	Autumn School Advanced Metal- Organic Chemistry	29.718
Interest	1.282	Annual Report 2009	1.238
IRTG Contribution to Personnel Costs	11.022	HRSMC website	1.244
		Courses	1.519
		Dick Stufkens PhD prize	1.000
		Other	876
	<b>€ 106.302</b>		<b>€ 111.345</b>
Income minus Expenses	<b>-€ 5.043</b>		
Reservation from 2007	<b>€ 5.043</b>		
Result 2010	<b>0</b>		

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#### 4.3 – Annex 3 Staff and Temporary Personnel 2010

<b>Elsevier</b>	<i>HGL</i>	Elsevier	C.J.	
	<i>Emeritus</i>	Oskam	A.	
		Vrieze	K.	
	<i>UHD-Guest</i>	Frühauf	H.-W.	
	<i>OBP</i>	Collignon	P.F.	
		Ernsting	J.M.	
		Mittelmeijer-Hazeleger	M.	
		Tromp	D.S.	
		<i>PhD</i>	Drost	R.M.
	<b>Hiemstra/Timmerman</b>	<i>HGL</i>	Hauwert	P.
			Jansen	E.
		<i>HGL-BZ</i>	Warsink	S
			Hiemstra	H.
<i>Emeritus</i>		Timmerman	P.	
<i>UHD</i>		Koomen	G.-J.	
<i>UD</i>		Maarseveen, van	J.H.	
<i>PD</i>		Ingemann Jorgensen	S.	
		Kinderman	S.S.	
<i>OBP</i>		Bieraugel	H.	
		Dijkink	J.	
		Geenevasen	J.A.J.	
		Klein Nijenhuis	R.	
	Steeneken	J.C.M.		
	Wanner	M.J.		
	<i>PhD</i>	Breman	A.C.	
		Lutteke	G.	
		Nessen	M.	
		Rutters	J.P.A.	
	Smeenk	L.		

<b>Lammertsma</b>	<i>HGL</i>	Lammertsma	K.
	<i>UD</i>	Ehlers	A.W.
		Slootweg	C.
	<i>PD</i>	Lyaskovskyy	V.
	<i>OBP</i>	Jong	B.
	<i>PhD</i>	Bertini	F.
		Dijk, van	T.
	<i>PhD/PD</i>	Jansen	H.
		Lami	C.F.
		Rong	M.
		Tazelaar	N.
		<i>SECR</i>	Smits-Weijers
	<b>Orru</b>	<i>HGL</i>	Orru
<i>UD</i>		Kanter	F. de
		Ruijter	E.
<i>PD</i>		Baelen, van	G. van
		Heeten, den	R. den
<i>OBP</i>		Janssen	E.
<i>PhD</i>		Born	D.
		Bouwman	S.
		Elders	N.
		Kruithof	A.
		Magnee	L.
		Scheffelaar	R.
		Vlaar	T.
	Znabet	A.	
<b>Lammertsma/Orru</b>	Janssen	G.	
<b>Overkleeft</b>	<i>HGL</i>	Marel, van der	G.A.
		Overkleeft	H.S.
	<i>HGL-BZ</i>	Boeckel, van	C.A.A.
<i>Emeritus</i>	Lugtenburg	J.	

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<i>DU</i>	Filippov	D.V.
	Overhand	M.
<i>WP-Gast</i>	Lodder	G.
<i>PD</i>	Berg, van den	R.J.B.H.N.
	Codée	J.D.C.
	Castelli	
	Florea	B.
	Li	J.
<i>OBP</i>	Elst, van der	H.
	Meeuwenoord	N.J.
	Nieuwendijk, van den	A.M.C.H.
	Ruben	M.
<i>PhD</i>	Asghar	A.
	Christina	A.
	Delft, van	P.
	Dinkelaar	J.
	Duivenvoorden	B.A.
	Geurink	P.P.
	Ghisaidoobe	A.
	Gold	K.H.
	Heden, van der	G.
	Hogendorf	W.F.J.
	Hoogendoorn	S..
	Jong, de	N.R.
	Knaap, van der	M.
	Knijnenburg	A.D.
	Li	N.
	Li	K-J.
	Linden, van der	W.
	Liu	L.
	Walvoort	M.T.C.
	Willems	L.

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		Willems	M.
	<i>PhD-Gast</i>		
		Tuin	A.W.
	<i>SECR</i>		
		Bruin, de	C.
<b>Bouwman</b>	<i>HGL</i>	Bouwman	E.
	<i>HGL-BZ</i>	Drent	E.
	<i>Emeritus</i>	Maaskant	W.J.A.
	<i>Emeritus</i>	Reedijk	J.
	<i>Tenure Tracker</i>	Bonnet	S.
	<i>WP-Gast</i>	Hage	R.
		IJdo	D.J.W.
	<i>PD</i>	Gouré	E.
	<i>OBP</i>	Brussel, van	J.J.M.
		Dijk	J.
		Erkelens-Duijndam	J.O.
	<i>PhD</i>	Akerboom	S.
		Bahreman	A.
		Marquès	P.
		Mooibroek	T.
		Raoufmoghaddam	S.
		Rijn	J. van
		Viciano-Chumillas	M.
		Wenker	E.
		Zheng	S.
	<i>PhD-Gast</i>	Gamba	I.
	<i>SECR</i>	Snellenberg	Y.
<b>Reek/Hartl</b>	<i>HGL</i>	Reek	J.N.H.
	<i>UD</i>	Bruin, de	B.
		Hartl	F.
		Vlugt, van der	J.I.
	<i>OBP</i>	Mahabiersing	Ch.

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	<i>PhD</i>	Dydio	P.
		Dzik	R.
		Franssen	N.M.G.
		Gumrukcu	Y.
		Jellema	E.
		Olivos Suarez	A.I.
		Terrade	F.G.
		Walters	A.J.C.
		Wassenaar	J.
<b>Wever</b>	<i>HGL</i>	Wever	R.
	<i>PD</i>	Horst, van der	M.A.
	<i>PD-Guest</i>	Herk, van	T.
	<i>OBP</i>	Bury	A.
		Hartog	A.F.
	<i>PhD</i>	Babich	L.
<b>Buma/Brouwer</b>	<i>HGL</i>	Buma	W.J.
	<i>HGL-BZ</i>	Brouwer	A.M.
	<i>HGL-BZ</i>	Oomens	J.
	<i>Emeritus</i>	Verhoeven	J.W.
	<i>UD</i>	Williams	R.M.
		Woutersen	S.
		Zhang	H.
	<i>Pd</i>	Vdovin	O.
	<i>PD-Gast</i>	Rijs	A.M.
		Zeng	Q.
	<i>OBP</i>	Bebelaar	D.
		Groeneveld	M.M.
		Hilbers	M.
		Kettelarij	A.J.
		Reinders	P.P.
	<i>PhD</i>	Bodis	P.
		Carpentier	C.E.

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		Colonna	F.
		Grzetic	J.
		Gunbas	D.D.
		Huerta Viga	A.
		Kumpulainen	T.
		Liu	K.
		Loop van der	T.
		Meuzelaar	H.
		Nguyen	V.A.
		Panman	M.
		Plugge	M.
		Raja	T.N.
		Rosa Domingos	S.M.
		Siekierzycka	J.R.
		Smolarek	S.
		Tan	E.M.M.
		Zhang	C.
	<i>PhD-Gast</i>	Jagesar	D.C.
		Mes	E.M.
		Raja	T.N.
		Wang	Y.
<b>Gooijer/Ariese</b>	<i>HGL</i>	Gooijer	C.
	<i>UHD</i>	Ariese	F.
		Zwan, van der	G.
	<i>PD</i>	Castro-Puyana	M.
	<i>OBP</i>	Buijs	J.
		Wiskerke	A.
	<i>PhD</i>	Hooijschuur	J.H.
		Lammers	I.
		Petterson	I.
		Tardioli	S.
		Vidami - Negoescu	E.C.

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**Groenen/Orrit/Völker**

<i>HGL</i>	Groenen	E.J.J.
<i>HGL</i>	Orrit	M.
<i>HGL</i>	Völker	S.
<i>UD</i>	Gast	P.
	Huber	M.
<i>PD</i>	Gaiduk	A.
	Sottini	S.
	Zijlstra	P.
<i>PhD</i>	Hashemi Shabestari	M.
	Mathies	J.
	Navarro Perez	P.
	Ruijgrok	P.
	Son van	M. van
	Yorulmaz	M.
	Yuan	H.

**De Groot/Buda**

<i>SECR</i>	Leeuwen van	H. van
<i>HGL</i>	Groot	H. de
<i>HGL-BZ</i>	Grip	W.
<i>UD</i>	Alia	
	Buda	F.
	Matysik	J.
<i>PD</i>	Anger	B.C.
	Bode	B.
	Chen	F.C.
	Song	C.
<i>PhD</i>	Eisenmayer	T.J.
	Janssen	G.
	Joya	K.S.
	Kara	F.
	Saisankar Gupta	K.B.
	Sunku	K.
	Thamarath Surendran	S.

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		Vallés Pardo	J.L.
<b>Janssen</b>	<i>SECR</i>	Velden, van der	L.
	<i>HGL</i>	Janssen	M.
	<i>PD</i>	Niraghatam	B.R.
		Sofikitis	D.
	<i>OBP</i>	Tuinder	V.
		Wiskerke	A.E.
	<i>PhD</i>	Irimia	D.
		Ityaksov	D.
		Meng	C.
		Rafiee Fanood	M.
<b>Koper</b>		Lehmann	C.S.
	<i>HGL</i>	Koper	M.
	<i>Ass. Prof.</i>	Juurlink	L.
		Yanson	A.
	<i>HGL-Guest</i>	Kleijn	A.F.
	<i>PhD</i>	Dunnen, den	A.
		Hahn	C.
		Bashlakov	D.
		Kleijn	S.
		Kwon	Y.
		Lai	S.
		Niet	M.J.T.C
		Schouten	K.J.
<b>Linnartz</b>	<i>SECR</i>	Dijkzeul	J.
	<i>HGL-BZ</i>	Linnartz	H.
	<i>PhD</i>	Fedoseev	G.
		Ioppolo	S.
<b>Baerends/Bickelhaupt/ Visscher</b>		Isokoski	K.
	<i>HGL</i>	Baerends	E.J.
		Bickelhaupt	M.
		Visscher	L.

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	<i>UD</i>	Gori-Giorgi	P.
		Gritsenko	O.
	<i>PD</i>	Bulo	R.
		Ekström	U.
		Faassen, van	M.
		Fonseca Guerra	C.
		Gopinadhanpillai	G.
		Heshmat	M.
		Höfener	S.
		Kazaryan	A.
		Kiewisch	K.
	<i>PhD</i>	Beyhan	M.
		Giesbertz	K.
		Mentel	M.
		Mirtschink	A.
		Nicu	P.
		Ruiz Soares	J.M.
		Tecmer	P.
		Meer, van	R.
		Wolters	L.
		Zeist, van	W.J.
	<i>SECR</i>	Jaddoe	S.
<b>Bolhuis/Meijer</b>	<i>HGL</i>	Bolhuis, P.G.	PG.
	<i>HGL</i>	Frenkel	D.
	<i>UHD</i>	Meijer	E.J.
	<i>UD</i>	Ensing	B.
		Dubbeldam	D.
	<i>PD</i>	Marino	K.A.
		Vreede	J.
	<i>PhD</i>	Diaz Leines	G.
		Du	W.
		Kilic	M.

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		Pavlova	A.
		Singhal, K.	K.
		Zeiler	R.N.W.
		Zhu	L.
<b>Neugebauer</b>	<i>PhD-Guest</i>	Colonna	F.
	<i>UHD</i>	Neugebauer	J.
	<i>PD</i>	Pavanello	M.
		König	C.
		Kovyrshin	A.
		Solovyeva	A.
<b>HRSMC</b>	<i>OBP</i>	Zwaan-van der Plas	H.
	<i>SECR</i>	Weijer	R.

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## 4.4 Annex 4 – Publications

Publications theme 1

**Metals in Catalysis, Biomimetics & Inorganic Materials** (Bouwman/Reedijk/  
/Bonnet/Fu/Haasnoot)

Aliaga-Alcalde, N.; Marques-Gallego, P.; Kraaijkamp, M.; Herranz-Lancho, C.; den Dulk, H.; Gorner, H.; Roubeau, O.; Teat, S. J.; Weyhermuller, T.; Reedijk, J., Copper Curcuminoids Containing Anthracene Groups: Fluorescent Molecules with Cytotoxic Activity. *Inorganic Chemistry* **2010**, 49, (20), 9655-9663.

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Bouwman, E., CARBON DIOXIDE FIXATION WITH COPPER Response. *Chemical & Engineering News* **2010**, 88, (18), 5-5.

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Fu, W. T.; Gotz, R. J.; Ijdo, D. J. W., On the symmetry and crystal structures of Ba<sub>2</sub>LaIrO<sub>6</sub>. *Journal of Solid State Chemistry* **2010**, 183, (2), 419-424.

Ghazzali, M.; Al-Farhan, K.; El-Faham, A.; Reedijk, J., Coordination chemistry of the ligand 7-aza-1-hydroxy-benzotriazole. Crystal structures and antimicrobial activity of the

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catena-poly-  $\mu$ -chlorido( $\mu$ -7-aza-1-oxy-  $\kappa$  N-2:O-benzotriazolyl- $\kappa$  N) cobalt(II)methanol coordination polymer and of a new polymorph of the free ligand 3H-1,2,3 triazolo 4,5-b pyridin-3-ol. *Polyhedron* **2010**, 29, (14), 2829-2832.

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Mohamadou, A.; van Albada, G. A.; Mutikainen, I.; Turpeinen, U.; Reedijk, J., A novel hexagonal honeycomb K-Cr-oxalate anionic network with layers separated by a five-coordinated Cu(II)-pypn complex (pypn = N,N'-bis(2-pyridylmethyl)-1,3-propanediamine). Synthesis, characterisation, spectroscopy and crystal structure of {KCr(C<sub>2</sub>O<sub>4</sub>)(3) Cu(pypn)(H<sub>2</sub>O) (H<sub>2</sub>O)(4)}. *Inorganic Chemistry Communications* **2010**, 13, (10), 1221-1224.

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## 4.5 Annex 5 – The HRSMC Education Programme

The management of the school administers the credit points obtained by the PhD students and presents HRSMC certificates to those students who have fulfilled their education programme with a minimum of 18 ECTS.

	ECTS system 1 ECTS = 28 h
Literature research	3
Colloquium (see remarks for explanation)	1
Paper (see remarks for explanation)	3
HRSMC school	3
HRSMC course	3
External course of + 1 week	3
Course on didactics	1-2
Presenting a poster at an (inter)national conference	1
Giving a lecture at an (inter)national conference	2
2x attendance of a guest lecture and a scientific discussion	1
Research in another laboratory (preferably outside Holland)	max. 6
<b>Minimum</b>	<b>18</b>

### Remarks:

- Every PhD needs to follow at least one HRSMC course and one HRSMC school for the HRSMC certificate. If there is no HRSMC school or course available supporting the aspects of the PhD research, an external course can be chosen instead (but for 95% of the PhD student this is not necessary). The other items are optional: for the certificate it is not 'a must' to do a course on didactics or a research in another laboratory, but when this is done a maximum of 6 ECTS can be given for this activity.
- The Han-sur-Lesse Winter school 'Theoretical Chemistry & Spectroscopy' is not organized by the HRSMC, but many HRSMC staff members are involved. Therefore, this course is considered as a HRSMC school for the HRSMC certificate.
- An external course of one week is 3 ECTS, a course of two weeks 6 ECTS. However, if the organisation of this course has chosen for a different (higher or lower) validation, this validation is applicable for the HRSMC credit point administration as well.
- A colloquium is a presentation, which a PhD gives at the beginning (normally after 3-6 months). A PhD researcher presents his/her research plans and gives a general background of the project. This colloquium can be based on the paper.
- A paper should not be confused with a scientific article. A paper is a document, which a PhD researcher normally makes at the beginning of his/her research. This paper includes items like:
  - The general background of the research project
  - The plans a PhD researcher has for the first years of his/her research project.
- 18 points is a minimum and can, of course, be exceeded.

#### 4.6 Annex 6 - Major specialised equipment/ expertise

<b>Group</b>	<b>Equipment</b>
Baerends/Bickelhaupt/Visscher	Equipment: Compute servers consisting of Clusters of Linux Workstations / Pentium PCs. Three clusters: A) 16 nodes PIII 450Mhz, B) 20 nodes AMD Athlon 650+, C) 40 nodes AMD Athlon 1700+
Bolhuis/Meijer	Compute facility consisting of Clusters of Linux PCs with in total ca 500 cores; performance ca. 2TFLOP. Four clusters: A) 32 nodes dual processor dual core Xeon 3GHz with Infiniband interconnect B) 48 nodes AMD Athlon 2700/3200 C) 30 nodes AMD Athlon 54 3200+ D) 32 nodes Intel dual processor quad cores with Infiniband interconnect
Bouwman	EPR equipment at X band; down to 4.2 K
	Diffuse reflectance spectrometer (300 - 2000 nm)
	Far-IR spectrometer
	Electrochemistry: computer-aided Autolab PGstat 10 potentiostat controlled by GPES4 software
	Magnetic Susceptibility Equipment down to 2 K
	XRD powder diffractometer, X'celerator detector; variable T 80 - 723 K
Buma/ Brouwer	3 UV/VIS/NIR Absorption spectrometers (Cary and HP)
	Bruker FTIR and VCD
	2 Fluorescence spectrometers (SPEX)
	1 Excimer laser with dye laser (Lumonics)
	2 Excimer laser (Lambda Physik) with dye laser (Lumonics)
	1 Nd:YAG laser (Quanta-Ray) with dye laser (Sirah)
	1 Excimer laser (Lumonics)
	1 Nd-YAG laser with 2nd,3rd,4th harmonic generation (Spectra Physics)
	1 Nd-YAG laser with 2nd and 3rd harmonic generation and XPO+2nd harmonic generation (Coherent)
	2 Nitrogen lasers (LTB)
	1 Nanosecond gated CCD camera detection system (Princeton Instr.)
	1 Streak camera picosecond detection system (Hamamatsu)
	2 x femtosecond pulsed Ti:Sapphire laser system including OMAs; UV to IR detection
	Femtosecond transient absorption setup
	Fluorescence upconversion setup
	1 HPLC system with absorption diode array and fluorescence detectors (Shimadzu)
	Confocal microscope, equipped with femtosecond excitation sources covering the whole UV-Vis-NIR range, xyz-scanning stage; detectors for time-resolved imaging and lifetime measurement (two SPADs), for recording emission spectra, and for wide field imaging, all with single-molecule detection capabilities.
	Molecular beam spectrometer with mass-resolved ion and electron detection; laser desorption module
	Molecular beam spectrometer with dispersed emission detection

DeGroot/Buda/ Matysik	High and Ultra High Field Magic Angle Spinning NMR Spectrometer 400MHz
	600 MHz, 759 MHz
	Magnetic Resonance Microscopy at 750 MHz, 400 MHz
	The group owns a Beowulfcluster with 11 dual-core Intel Xeon nodes
de Koster	Mass spectrometry instrumentation
	Highly specialized mass spectrometry expertise
Elsevier	NMR narrow bore spectrometers frequency range (1H) 200 - 500 MHz
	Broad band NMR probeheads for heteronuclear double and triple resonance applications (H,X, H,X,Y and X,Y)
	High pressure equipment (tubes) for semi-routine NMR under pressure
	Experience with numerous NMR techniques and applications, almost all NMR active nuclei.
	Equipment for synthesis, catalysis and NMR in supercritical fluids and liquefied gases
Gooijer/Ariese	Picosecond pulsed Ti:Sapphire laser system (Verdi+Mira). Detection: TCSPC, Multiphoton counting arrays, pulsepicker.
	Nanosecond Nd:YAG laser driving a T-Jump set-up (based on Raman shifter)
	CW Argon-ion lasers, including FRED (UV); excimer laser.
	Cryogenic setups for high resolution luminescence, Shpol'ski, Fluorescence line narrowing spectroscopy, low-temperature absorption.
	Liquid Core Waveguide based Raman detection. Raman microscope with Ar and Kr lasers.
	Equipment for liquid chromatography and capillary electrophoresis, degassing and time-resolved detection for phosphorescence detection.
	Pico second laser system (Verdi+Mira), frequency doubling/tripling equipment, high- resolution spectrograph and 250 ps intensified gated CCD camera.
	Small volume flow cell for combining electrochemistry and Raman Spectroscopy.
Groenen/Orrit/Völker	cw/pulsed EPR/ENDOR spectrometers at 9, 95, and 275 GHz for experiments on solutions, powders and crystals in the temperature range of 2 to 300 K.
	Single-molecule microscopes equipped with: liquid-helium cryostats, single-frequency lasers (dye and titanium-sapphire), tunable pulsed (200 fs) laser with high repetition rate (70 MHz) and OPO with intracavity doubling, sensitive photon detectors, CCD. Optical trap with fiber laser, 5 W 1064 nm for single gold nanoparticles.
	Absorption, fluorescence and fluorescence excitation spectrometers for experiments from 0.3 to 300 K
	Confocal microscope for simultaneous photothermal and fluorescence imaging.
Hartl/Reek	Thermonicolet NXR 9650 FT-Raman spectrometer and Renishaw inVia dispersive Raman microscope equipped with several UV and visible laser sources.

	<p>Varian Cary Eclipse spectrofluorimeter with a multi-cell temperature control unit, a stopped-flow module with rapid mixing (8 ms) and fibre optics dip probe for in situ measurements.</p> <p>Optically transparent and reflection spectro-electrochemical cells (UV-VIS-NIR-MIR-FIR, Raman, ECL, VCD, 2D-IR (no laser light scattering) and (bi)potentiostats-galvanostats (EG&amp;G PAR, Ametek, Eco-Chemie, EKOM). RRDE.</p> <p>Vacuum-tight three-electrode tubular EPR spectroelectrochemical cell.</p> <p>UV-Vis-NIR-IR-FIR spectro(photo)meters (Bruker Vertex 70v, Nicolet, Varian, Perkin Elmer).</p> <p>Perkin Elmer 100 FTIR spectrometer interfaced to a Spotlight 400 imaging system (special resolution down to 10 microns); an ATR attachment and Atmospheric Vapour Compensation (AVC).</p> <p>Diode-array UV-Vis spectrophotometers (HP and Scinco S3100)</p>
	<p>EPR spectrometer (Varian) at X-band, suited for LT spectro-electrochemistry</p> <p>Circular-dichroism spectrometer.</p> <p>X-ray diffraction facilities including NanoStar SAXS.</p>
Hiemstra/Timmerman	<p>LC-MS instrument</p>
	<p>Several analytical HPLC instruments and one preparative HPLC instrument</p> <p>Polarimeter</p> <p>Usual equipment for synthetic (organic) research, including ozonolysis apparatus and photochemical equipment</p> <p>NMR narrow bore spectrometers frequency range (1H) 400 - 500 MHz</p> <p>FT IR instrument</p> <p>Peptide synthesizer</p> <p>Freeze dryer</p>
Janssen	<p>Various nanosecond and femtosecond laser systems, hexapole state selectors, molecular beam machines, CCD and delay-line based ion imaging detection systems.</p>
Koper	<p>Various UHV setups equipped with TPD, STM, LEED, EELS, IR, MS</p>
	<p>Electrochemical workstations</p> <p>Electrochemical cells combined with FTIR, SERS, STM, MS, HPLC</p>
Lammertsma / Orru	<p>32-node Linux cluster</p>
	<p>250, 400 and 500 MHz NMR equipped with cryoprobes</p> <p>Advanced LC and LC-MS machines including preparative LC-MS</p> <p>Bruker Daltonics MicroQTOF MS</p> <p>FT-IR</p> <p>Parallel synthesis equipment, microwave synthesizer, ozonolysis, gloveboxes and other standard synthesis equipment</p>

Linnartz	UHV equipment for solid state astrochemistry / FTIR-RAIRS and TPD-QMS detection / Atom sources / Supersonic plasma facilities / Cavity enhanced, DAS en LIF and spectrometric detection techniques
Neugebauer	Beowulfcluster with 272 cores in total: 28 dual-quadcore Intel Nehalem nodes (24 GB memory each) plus a head node and 5 dual-quadcore Intel Harpertown nodes (16 GB memory each).
Overkleeft / van der Marel	LTQ OrbiTrap
	LC-MSMS equipment
	PNA synthesizer
	DNA/RNA synthesizer
	Peptide synthesizer
	HPLC equipment
Wever	2. UV/VIS/NIR absorption spectrophotometers (Cary and HP)
	2. Medium speed centrifuges for isolation of enzymes
	2 HPLC systems (one with diode array)
	1 FPLC
Wever	1 High- throughput screening robotics
	1 Laminar Flow cabinet
	1 medium speed centrifuge for centrifugation of microtiterplates